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Michael Demuth
Bert-Wolfgang Schulze
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Editors

Partial Differential Equations and Spectral Theory

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Preface

Nowadays mathematical analysis progresses very rapidly and in many different directions. This development is carried by a lot of research groups worldwide that then constantly leads to a great number of new results and achievements. For the individual, active researcher it is difficult to keep track of this development in its full breadth. Thus it has become an imperative to review this rapid development from time to time.

The present volume contributes in this direction. It collects six articles on selected topics in the interface between partial differential equations and spectral theory, written by leading specialists in their respective fields. Apart from the main bodies on attractive fields of current research, with original contributions from the authors, the articles are written in an expository style that makes them accessible to a broader audience. They contain a detailed introduction along with surveys on recent developments, motivations, and necessary tools. Moreover, the authors share their views on future developments, hypotheses, and unsolved problems.

These six articles reflect to some extend the thematic diversity of current research in the area of mathematical analysis:

The first article, by Chen and Dreher, discusses macroscopic models of quantum semiconductor theory, in particular, quantum drift diffusion models and quantum hydrodynamic models. The authors present both the modeling and an rigorous analytic treatment of these models. They formulate the models as nonlinear mixed-order parameter-elliptic systems which then makes semigroup techniques applicable.

The following article, by BelHadjAli, Ben Amor, and Brasche, treats various asymptotic problems related to large coupling convergence of non-negative quadratic forms. This treatment is accompanied by a collection of well-chosen, also higher-dimensional, model problems which are carefully analyzed, where the authors place much emphasis on the interplay between abstract results and concrete applications.

Ben-Artzi presents in his contribution a smooth spectral calculus for a self-adjoint operator in an abstract Hilbert space setting. The author derives a limiting absorption principle under the assumption that the density of states is Hölder continuous and provides as an application a general eigenfunction expansion theorem as well as global space-time estimates for associated inhomogeneous wave equations.

The article by Bauer, Furutani, and Iwasaki studies subelliptic operators in the framework of sub-Riemannian geometry. It gives explicit representations for sub-Riemannian geodesics, heat kernels, and sub-Riemannian structures. Specifically, the authors determine geodesics of the Grushin plane and Grushin sphere and provide the heat kernel for the sub-Laplacian on the six-dimensional free nilpotent Lie group, among others. They also analyze the spectra on certain compact nilmanifolds.

Mendoza discusses in his contribution the singularities of the zeta function for elliptic cone differential operators. The author first recalls the framework of cone-differential calculus and discusses the existence of rays of minimal growth, before he deals with the short-term asymptotics of the heat trace. The constructions rely on a symbolic handling of the resolvent.

The final article, by McKeag and Safarov, is concerned with a coordinate-free approach to pseudodifferential operators. The introduction of the class of pseudodifferential operators is facilitated by choosing a linear connection on the base manifold. The authors discuss elements of a calculus under such an approach and describe an application to approximate spectral projections of the Laplace operator.

The volume addresses people generally interested in an overview of current developments in partial differential equations and spectral theory. It is mainly intended for specialists in partial differential equations, spectral theory, stochastic analysis, and mathematical physics, but it is also suitable for doctoral students who wish to gather first-hand information from leading scientists on these topics.

The idea for this volume originated from an "International Conference on Partial Differential Equations and Spectral Theory" held in Goslar, Germany, August 31 to September, 2008, which was jointly co-organized by the three editors. We would like to express our thanks to the authors for their contributions, to the participants in the conference who made it a very successful event, and to the Birkhäuser publisher for the constant support.

The editors

M. Demuth
B.-W. Schulze
I. Witt

Quantum Semiconductor Models

Li Chen and Michael Dreher

Abstract. We give an overview of analytic investigations of quantum semiconductor models, where we focus our attention on two classes of models: quantum drift diffusion models, and quantum hydrodynamic models. The key feature of those models is a quantum interaction term which introduces a perturbation term with higher-order derivatives into a system which otherwise might be seen as a fluid dynamic system. After a discussion of the modeling, we present the *quantum drift diffusion model* in detail, discuss various versions of this model, list typical questions and the tools how to answer them, and we give an account of the state-of-the-art of concerning this model. Then we discuss the *quantum hydrodynamic model*, which figures as an application of the theory of mixed-order parameter-elliptic systems in the sense of Douglis, Nirenberg, and Volevich. For various versions of this model, we give a unified proof of the local existence of classical solutions. Furthermore, we present new results on the existence as well as the exponential stability of steady states, with explicit description of the decay rate.

Mathematics Subject Classification (2000). Primary: 35J45, 35K35; Secondary: 76Y05, 35B40, 65M20.

Keywords. quantum drift diffusion model; quantum hydrodynamic model; entropy based methods; parameter-elliptic systems; Douglis–Nirenberg systems; analytic semigroups; stationary states; exponential stability; decay rates.

1. Introduction

1.1. A first example

We start with a simple Schrödinger equation, describing one single particle (without spin) of mass m and charge q, in a potential V:

$$\begin{cases} \mathrm{i}\hbar\partial_t\psi(t,x) = -\dfrac{\hbar^2}{2m} \triangle \psi(t,x) - qV(x)\psi(t,x), & (t,x) \in \mathbb{R}\times\mathbb{R}^d, \\ \quad \psi(0,x) = \psi_0(x). \end{cases}$$

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We take the freedom to change the units of time and space variables (t, x) as well as of the potential V, ending up with the scaled equation

$$\mathrm{i}\varepsilon\partial_t\psi(t,x) = -\frac{\varepsilon^2}{2}\triangle\psi(t,x) - V(x)\psi(t,x). \tag{1.1}$$

The positive constant ε describes the quantum effects and is typically small.

The squared modulus of the complex-valued function $\psi(t,\cdot)$ is the probability density to find the particle at a certain location, and therefore

$$\int_{\mathbb{R}^d} |\psi(t,x)|^2 \,\mathrm{d}x = 1.$$

We may introduce polar coordinates for $\psi \in \mathbb{C}$:

$$\psi(t,x) = \sqrt{n(t,x)}\exp\left(\frac{\mathrm{i}}{\varepsilon}S(t,x)\right), \qquad \psi_0(x) = \sqrt{n_0(x)}\exp\left(\frac{\mathrm{i}}{\varepsilon}S_0(x)\right),$$

where n and S are real-valued functions, and $n \geq 0$. Define the *probability current density* J,

$$J(t,x) = -\varepsilon\Im\left(\overline{\psi(t,x)}\nabla\psi(t,x)\right) = -n(t,x)\nabla S(t,x), \qquad \nabla = \nabla_x.$$

Keeping in mind that the potential V is real-valued, we can then derive the *Madelung equations* [93]:

$$\begin{cases} \partial_t n - \operatorname{div} J = 0, \\ \partial_t J - \operatorname{div}\left(\dfrac{J\otimes J}{n}\right) + n\nabla V + \dfrac{\varepsilon^2}{2}n\nabla\left(\dfrac{\triangle\sqrt{n}}{\sqrt{n}}\right) = 0, \end{cases} \tag{1.2}$$

with the natural initial conditions

$$(n, J)(0,x) = (n_0, J_0)(x).$$

Here $J\otimes J$ is a $d\times d$ symmetric matrix with entries $J_k J_l$, and the divergence operator is to be applied to each row separately.

This system is also called the *quantum hydrodynamic system at zero temperature*. This relates to the fact that temperature is a statistical effect which will only be observable when we consider an ensemble of a large number of particles.

Looking back, we find that we started our considerations with the linear problem (1.1), for which the global in time existence of weak solutions $\psi \in C(\mathbb{R}; L^2(\mathbb{R}^d))$ is a well-established fact; we refer to [103] or any text book on mathematical physics. Then we have transformed (1.1) into the coupled system (1.2), which is nonlinear, contains third-order derivatives, and whose meaning is at least unspecified for those points where $n = 0$. So the question arises of the advantage of (1.2) in comparison to (1.1).

The answer is: from (1.2) we learn that quantum mechanical systems may be amenable to a hydrodynamical description. Indeed, putting $J = -nu$ we find

$$\begin{cases} \partial_t n + \operatorname{div}(nu) = 0, \\ \partial_t(nu) + \operatorname{div}(nu \otimes u) = n\nabla\left(V + \frac{\varepsilon^2}{2}B(n)\right), \qquad B(n) = \frac{\triangle\sqrt{n}}{\sqrt{n}}, \end{cases} \tag{1.3}$$

which are the Euler equations for a fluid without pressure and viscous stress. The scalar function n can be understood as density of the fluid, and the vector-valued function u as velocity. Then the first equation corresponds to the conservation of mass, and the second to the conservation of momentum. On the right-hand side of the second equation, we can see a force term which has a potential $V + \frac{\varepsilon^2}{2}B$. The quantum correction term B is also called *Bohm potential term*, and it can also be written as a non-diagonal pressure tensor like this:

$$P = \frac{\varepsilon^2}{2}n(\nabla \otimes \nabla)\ln n, \qquad \operatorname{div} P = \frac{\varepsilon^2}{2}n\nabla B(n).$$

These observations nourish the hope that the analytical methods of fluid dynamics might prove useful when investigating semiconductor systems. Indeed, the quantum hydrodynamic model (2.13) describing the flow of a particle ensemble through an electronic device will look very similar to (1.2), although the functions n and J will later have a quite different meaning.

1.2. Structure of the paper

First we sketch how to derive several macroscopic semiconductor models from basic principles of physics, and we will concentrate our attention on two classes of models: *quantum drift diffusion models*, and *quantum hydrodynamic models*. In both cases, the quantum influence will be visible in terms with third-order spatial derivatives, similar to the Bohm potential term $B(n)$ in (1.2) and (1.3). These higher-order terms make standard methods like maximum principles unavailable, and many analytical questions are still open.

In Section 3, we discuss the quantum drift diffusion model in detail and give an overview on analytical results of the last 10 years, where we concentrate on the transient case. Results will be presented in Sections 3.2 till 3.4, and Section 3.5 will give an outline of the methods. Then the quantum hydrodynamic model will be discussed in Section 4. We will concentrate on a special kind of this model, namely the viscous version. The viscosity effect comes into the system via a description of collisions between the electrons and thermic oscillations of the crystal, so-called phonons. In the time-independent case, we then end up with a nonlinear mixed-order parameter-elliptic system in the sense of Douglis–Nirenberg–Volevich. We will prove new results on analyticity of the associated semigroup and asymptotic behaviour of the solutions.

Our notations are standard: the L^p based Sobolev spaces over the domain Ω are denoted by $W_p^k(\Omega)$, and $H^k(\Omega) = W_2^k(\Omega)$. The constant C is allowed to change its value from one occurrence to the next, but is independent of the solutions we are looking for.

2. Derivation of the models

2.1. Quantum Vlasov and quantum Boltzmann equations

We consider the Schrödinger equation for a large number of identical particles in a potential V:

$$\begin{cases} i\hbar\partial_t\psi(t,x) = -\dfrac{\hbar^2}{2m}\displaystyle\sum_{j=1}^{M}\triangle_{x_j}\psi(t,x) - qV(t,x)\psi(t,x), \\ \qquad \psi(0,x) = \psi_0(x), \end{cases} \tag{2.1}$$

where $(t,x) \in \mathbb{R}\times\mathbb{R}^{dM}$ or $(t,x)\in\mathbb{R}\times\Omega^M$ with $\Omega\subset\mathbb{R}^d$ being a domain. This equation is not usable for numerical simulations, for several reasons: first, the number of particles M is in general quite large ($M > 10^4$); and second, we do not know physically reasonable boundary conditions for the wave function ψ.

To overcome these obstacles, so-called macroscopic equations for physical quantities like particle density or current density can be derived. For details of these macroscopic models, we refer the reader to [67] or [96].

Suppose that ψ is a solution to (2.1) of sufficiently high regularity. First, we scale the variables as for (1.1), i.e., replace $\hbar\to\varepsilon$, $m\to 1$, $q\to 1$, and introduce the *density matrix*

$$\varrho(t,r,s) = \overline{\psi(t,r)}\psi(t,s), \qquad (r,s)\in\mathbb{R}^{dM}, \tag{2.2}$$

which then has the initial values $\varrho_0(r,s) = \overline{\psi_0(r)}\psi_0(s)$, and ϱ is a solution to the *Heisenberg equation*

$$i\varepsilon\partial_t\varrho(t,r,s) = (H_s - H_r)\varrho(t,r,s),$$

with H being the *Hamiltonian*,

$$H_x = -\frac{\varepsilon^2}{2}\sum_{j=1}^{M}\triangle_{x_j} - V(t,x).$$

Next, we define the *Wigner function* as a kind of inverse Fourier transform of the density matrix:

$$w(t,x,v) = \frac{1}{(2\pi)^{dM}}\int_{\mathbb{R}^{dM}_\eta} e^{i\eta v}\varrho\left(t, x+\frac{\varepsilon}{2}\eta, x-\frac{\varepsilon}{2}\eta\right)\,d\eta, \tag{2.3}$$

with initial values $w(0,x,v) = w_0(x,v)$ for $t=0$. This function was introduced by Wigner [121] in 1932. We will come back to the Wigner transform in Section 2.2. Then it is easy to check that this function w solves, at least formally, the so-called *quantum Liouville equation*:

$$\partial_t w + v\cdot\nabla_x w + \theta[V]w = 0, \qquad (t,x,v)\in\mathbb{R}_+\times\mathbb{R}^{dM}\times\mathbb{R}^{dM}, \tag{2.4}$$

where $\theta[V]$ is a pseudodifferential operator acting on the v-variables with symbol

$$\delta V(t,x,\eta) = \frac{\mathrm{i}}{\varepsilon}\left(V\left(t,x+\frac{\varepsilon}{2}\eta\right) - V\left(t,x-\frac{\varepsilon}{2}\eta\right)\right),$$

and the action of $\theta[V]$ on w is defined as

$$(\theta[V]w)(t,x,v) = \frac{1}{(2\pi)^{dM}}\int_{\mathbb{R}^{dM}_\eta}\int_{\mathbb{R}^{dM}_{v'}} e^{\mathrm{i}\eta(v-v')}\delta V(t,x,\eta)w(t,x,v')\,\mathrm{d}v'\,\mathrm{d}\eta. \quad (2.5)$$

To reduce the dimension of the variables (x,v) in the Liouville equation (2.4), we derive an equation of Boltzmann type for a function W defined on $\mathbb{R}_+ \times \mathbb{R}^d_x \times \mathbb{R}^d_v$, after having made some physical symmetry assumptions:

- the potential V can be split into an external potential V_{ext} and a sum of potentials describing the interaction of particle pairs,

$$V(t,x_1,\ldots,x_M) = \sum_{j=1}^M V_{\mathrm{ext}}(t,x_j) + \frac{1}{2}\sum_{i,j=1}^M V_{\mathrm{inter}}(x_i,x_j);$$

- each contribution V_{inter} is symmetric and of order $\mathcal{O}(1/M)$;
- the electrons are indistinguishable, and they are Fermions (which means that the probability of finding two electrons in the same state is zero),

$$\psi(t,x_1,\ldots,x_M) = \mathrm{sign}(\pi)\psi(t,x_{\pi(1)},\ldots,x_{\pi(M)}),$$

  for all permutations π;
- the density matrix $\varrho^{(m)}$ of a sub-ensemble of m electrons, defined as

$$\varrho^{(m)}(t,r_1,\ldots,r_m,s_1,\ldots,s_m)$$
$$= \int_{\mathbb{R}^{d(M-m)}} \varrho(t,r^{(m)},z_{m+1},\ldots,z_M,s^{(m)},z_{m+1},\ldots,z_M)\,\mathrm{d}(z_{m+1}\ldots z_M),$$

  where $r^{(m)} = (r_1,\ldots,r_m)$ and $s^{(m)} = (s_1,\ldots,s_m)$ for brevity, can be factorized at $t=0$:

$$\varrho^{(m)}(0,r_1,\ldots,r_m,s_1,\ldots,s_m) = \prod_{j=1}^m R_0(r_j,s_j), \qquad m = 1,\ldots,M-1.$$

The last assumption is known as the so-called *Hartree* ansatz. It turns out that, for fixed m and choosing M very large, the Hartree ansatz can be justified for $t>0$ as well,

$$\varrho^{(m)}(t,r_1,\ldots,r_m,s_1,\ldots,s_m) = \prod_{j=1}^m R(t,r_j,s_j),$$

where the function R solves a certain differential equation. Put, similar to (2.3),

$$W(t,x,v) = \frac{M}{(2\pi)^d}\int_{\mathbb{R}^d_\eta} e^{\mathrm{i}\eta v} R\left(t,x+\frac{\varepsilon}{2}\eta, x-\frac{\varepsilon}{2}\eta\right)\mathrm{d}\eta, \qquad (t,x,v)\in\mathbb{R}_+\times\mathbb{R}^d\times\mathbb{R}^d.$$

Then it can be shown that W solves the equation

$$\partial_t W + v\cdot\nabla_x W + \theta[V_{\mathrm{eff}}]W = 0, \qquad (t,x,v)\in\mathbb{R}_+\times\mathbb{R}^d\times\mathbb{R}^d, \quad (2.6)$$

where the pseudodifferential operator θ is specified as in (2.5) (with obvious replacements $dM \to d$), and the effective potential V_{eff} is defined as

$$V_{\text{eff}}(t,x) = V_{\text{ext}}(x) + \int_{\mathbb{R}^d_z} n(t,z) V_{\text{inter}}(x,z)\,\mathrm{d}z, \qquad (t,x) \in \mathbb{R}_+ \times \mathbb{R}^d,$$

and where the quantum electron density $n = n(t,x)$ is given by

$$n(t,x) = \int_{\mathbb{R}^d_v} W(t,x,v)\,\mathrm{d}v = MR(t,x,x). \tag{2.7}$$

In general, the interaction potential V_{inter} is related to the *Coulomb* potential,

$$V_{\text{Coul}}(x,y) = -\frac{1}{4\pi\varepsilon_s}\frac{1}{|x-y|}, \qquad x,y \in \mathbb{R}^3,$$

with ε_s being the electric permittivity of the semiconductor material, and we have scaled the charge q to one, as always. Then the effective potential solves the *Poisson* equation

$$\varepsilon_s \triangle V_{\text{eff}}(t,x) = n(t,x) - C(x), \tag{2.8}$$

where $C(x) = -\varepsilon_s \triangle V_{\text{ext}}(x)$ is known as the *doping profile* if the external potential is generated by ions with positive charge.

The system (2.6)–(2.8) is called the *quantum Vlasov–Poisson system.* Details of the derivation of this system can be found in [96].

The system derived so far gives a macroscopic description of the flow of electrons in a semiconductor (under several simplifying assumptions which we have not mentioned), incorporating quantum effects and long range electrostatic interactions as given by the Coulomb potential. However, a realistic model should include also short range interactions like collisions, or scattering events between particles. A heuristic approach is to add an interaction term to the right-hand side of (2.6), giving us the *quantum Boltzmann equation*

$$\partial_t W + v \cdot \nabla_x W + \theta[V_{\text{eff}}]W = Q(W), \qquad (t,x,v) \in \mathbb{R}_+ \times \mathbb{R}^d \times \mathbb{R}^d. \tag{2.9}$$

In numerical studies, the following collision operators Q are traditionally used:

- the *relaxation time model* or *BGK* model [104], [15]

  $$Q(W) = \frac{1}{\tau}\left(\frac{n}{n_0}W_0 - W\right),$$

  where τ is the relaxation time, W_0 is the Wigner function to the quantum mechanical thermal equilibrium, and the particles densities n and n_0 are related to W and W_0 via

  $$n(t,x) = \int_{\mathbb{R}^d} W(t,x,v)\,\mathrm{d}v, \qquad n_0(t,x) = \int_{\mathbb{R}^d} W_0(t,x,v)\,\mathrm{d}v.$$

- the *Caldeira–Leggett* operator [18]

  $$Q(W) = \frac{1}{\tau_0}\operatorname{div}_v\left(c_1\nabla_v W + vW\right),$$

  where c_1 is a certain physical constant, and τ_0 figures as relaxation time.

- the *Fokker–Planck* operator [21]

$$Q(W) = \frac{1}{\tau_0} \operatorname{div}_v \left(c_1 \nabla_v W + vW \right) + \frac{1}{\tau_0} \operatorname{div}_x \left(c_2 \nabla_v W + c_3 \nabla_x W \right), \tag{2.10}$$

  where c_1 has the same value as in the case of the Caldeira–Leggett operator, and c_2, c_3 are certain other positive constants.

The quantum Boltzmann equation (2.9), with a suitably chosen collision operator, will be the starting point for deriving the quantum drift diffusion equations as well as the quantum hydrodynamic equations.

2.2. Quantum drift diffusion equations

The quantum drift diffusion model (also called the *density gradient model*) can be obtained from the quantum Boltzmann equation

$$\begin{cases} \partial_t w + v \cdot \nabla_x w + \theta[V]w = Q(w), & (t,x,v) \in \mathbb{R}_+ \times \mathbb{R}^d \times \mathbb{R}^d, \\ \lambda^2 \triangle V(t,x) = n(t,x) - C(x), & (t,x) \in \mathbb{R}_+ \times \mathbb{R}^d, \\ n(t,x) = \displaystyle\int_{\mathbb{R}^d} w(t,x,v)\,\mathrm{d}v, & (t,x) \in \mathbb{R}_+ \times \mathbb{R}^d, \end{cases}$$

in a way we will sketch soon, after having chosen a special collision operator Q. This operator Q has the form

$$Q(w) = M[w] - w,$$

where M is the *quantum Maxwellian*, for whose definition we need some preparations.

We begin with recalling the *Wigner transform* of a function ϱ, evaluated at a point $(x,v) \in \mathbb{R}^d \times \mathbb{R}^d$:

$$(\mathcal{W}(\varrho))(x,v) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d_\eta} e^{\mathrm{i}\eta v} \varrho\left(x + \frac{\varepsilon}{2}\eta, x - \frac{\varepsilon}{2}\eta\right) \mathrm{d}\eta,$$

whose inverse map is

$$(\mathcal{W}^{-1}(w))(x,y) = \int_{\mathbb{R}^d_v} e^{\mathrm{i}v(x-y)/\varepsilon} w\left(\frac{x+y}{2}, v\right) \mathrm{d}v,$$

which is related to the *Weyl quantization* $\mathrm{Op}_W(w)$ of a pseudodifferential symbol w via the Schwartz kernel theorem and

$$(\mathrm{Op}_W(w)\varphi)(x) = \int_{\mathbb{R}^d_y} \left(\mathcal{W}^{-1}(w)\right)(x,y)\varphi(y)\,\mathrm{d}y, \qquad \varphi \in \mathcal{S}(\mathbb{R}^d).$$

Write $\mathrm{Op}_{\mathrm{Schw}}$ for the isomorphism which maps a Schwartz kernel to the associated operator. We take a function $w = w(x,v)$, for which $\mathrm{Op}_{\mathrm{Schw}}(\mathcal{W}^{-1}(w))$ is a self-adjoint positive definite operator. The physical idea behind this restriction on w is that the function ψ (if it exists) which is connected to $\varrho := \mathcal{W}^{-1}(w)$ via (2.2) shall describe a quantum mechanical system in which, for each quantum state, the probability of being occupied is non-zero. For such a function w, we then define a *quantum logarithm* and a *quantum exponential* as

$$\operatorname{Ln} w := \mathcal{W}(\operatorname{Op}_{\text{Schw}}^{-1} \ln \operatorname{Op}_{\text{Schw}} \mathcal{W}^{-1}(w)),$$
$$\operatorname{Exp} w := \mathcal{W}(\operatorname{Op}_{\text{Schw}}^{-1} \exp \operatorname{Op}_{\text{Schw}} \mathcal{W}^{-1}(w)),$$

with ln and exp to be understood via the spectral theorem. These mappings are inverses to each other, and their Fréchet derivatives behave as expected. To simplify the notation, it is common practice to identify each operator with its kernel.

Next we define the *quantum entropy* of the Wigner function w,

$$H(w) := \iint_{\mathbb{R}^d \times \mathbb{R}^d} w \left(\operatorname{Ln} w - 1 + \frac{1}{2}|v|^2 - V(x) \right) \mathrm{d}x \, \mathrm{d}v.$$

For a given function $n = n(x)$, we consider the constrained minimization problem

$$H(w^*) = \min \left\{ H(w) \colon \int_{\mathbb{R}^d} w(x, v) \, \mathrm{d}v = n(x), \qquad \forall x \in \mathbb{R}^d \right\}.$$

It can be shown that the solution w^* (if it exists) has the form

$$w^*(x, v) = \operatorname{Exp} \left(A(x) - \frac{1}{2}|v|^2 \right),$$

and the function A is selected by the condition $\int_{\mathbb{R}^d} w^*(x, v) \, \mathrm{d}v = n(x)$. We suppose that this condition determines A uniquely, and, finally, we define the quantum Maxwellian as

$$M[w] := \operatorname{Exp} \left(A(x) - \frac{1}{2}|v|^2 \right), \qquad \int_{\mathbb{R}^d} M[w](x, v) \, \mathrm{d}v = \int_{\mathbb{R}^d} w(x, v) \, \mathrm{d}v.$$

In this sense, the quantum Maxwellian minimizes the quantum entropy functional under the constraint of given particle density.

Now a physical assumption comes in: we suppose that the collisions have dominating influence and that the relevant time interval is long. Therefore we replace t by t/δ and $Q(w)$ by $Q(w)/\delta$, and we consider small values of δ:

$$\begin{cases} \delta \partial_t w^{(\delta)} + v \cdot \nabla_x w^{(\delta)} + \theta[V] w^{(\delta)} = \dfrac{1}{\delta}(M[w^{(\delta)}] - w^{(\delta)}), \\ \qquad\qquad w^{(\delta)}(0, x, v) = w_0(x, v). \end{cases}$$

On a formal level, we have a limit $w^{(0)} = \lim_{\delta \to 0} w^{(\delta)}$ of the form $w^{(0)}(t, x, v) = \operatorname{Exp}(A(t, x) - |v|^2/2)$, and it holds

$$\begin{cases} \partial_t n - \operatorname{div} J = 0, \\ J = \operatorname{div} P - n \nabla V, \\ n(t, x) = \displaystyle\int_{\mathbb{R}^d} w^{(0)}(t, x, v) \, \mathrm{d}v, \\ P(t, x) = \displaystyle\int_{\mathbb{R}^d} v \otimes v w^{(0)}(t, x, v) \, \mathrm{d}v. \end{cases} \tag{2.11}$$

To get rid of the functional Exp (which is numerically hard to evaluate), one then shows the asymptotic expansions

$$\begin{aligned}&\operatorname{Exp}\left(A-\frac{1}{2}|v|^2\right)\\&\quad=\exp\left(A-\frac{1}{2}|v|^2\right)\left(1+\frac{\varepsilon^2}{8}\left(\Delta A+\frac{1}{3}|\nabla A|^2-\frac{1}{3}v^\top D^2Av\right)\right)+\mathcal{O}(\varepsilon^4),\end{aligned}$$

for $\varepsilon \to 0$, and a proof can be found in [37]. Then it follows that

$$\begin{aligned}n&=(2\pi)^{d/2}e^A+\mathcal{O}(\varepsilon^2),\\ \operatorname{div}P&=\nabla n-\frac{\varepsilon^2}{12}n\nabla\left(\triangle A+\frac{1}{2}|\nabla A|^2\right)+\mathcal{O}(\varepsilon^4),\\ \nabla A&=\frac{\nabla n}{n}+\mathcal{O}(\varepsilon^2),\end{aligned}$$

and our final step then is: if (n, J) is a solution to (2.11), then $J = J_0 + \mathcal{O}(\varepsilon^4)$, where the pair (n, J_0) solves

$$\begin{cases}\partial_t n-\operatorname{div}J_0=0,\\ \qquad J_0=\nabla n-n\nabla V-\dfrac{\varepsilon^2}{6}n\nabla\left(\dfrac{\triangle\sqrt{n}}{\sqrt{n}}\right),\\ \lambda^2\triangle V=n-C(x),\end{cases}\tag{2.12}$$

at least in a formal sense. In the remainder of the paper, we will write again J instead of J_0.

Compared to other macroscopic quantum models, the main advantage of the quantum drift diffusion model comes from its parabolic structure, which gives us boundary conditions in a natural way and makes numerical simulation relatively easier. However, quantum drift diffusion systems only give us information about the electron density. To study more phenomena in semiconductor devices such as heat conduction, one should use more elaborate models like the full hydrodynamic model or the energy transport model.

2.3. Viscous quantum hydrodynamics

In this part, we start from the quantum Boltzmann equation (2.9) with the Fokker–Planck collision operator (2.10) and sketch how to derive then a system of equations for macroscopic quantities like the particle density $n = n(t, x)$, the current density $J = J(t, x)$ or the energy density $ne = (ne)(t, x)$. There are several ways of deriving such systems; and detailed representations can be found in, for instance, [53] or [96].

Here, we use a moment method, following an approach of Gardner [51]. First we define for $(t, x) \in \mathbb{R}_+ \times \mathbb{R}^d$ the functions

$$n(t,x) = \int_{\mathbb{R}^d} w(t,x,v)\,\mathrm{d}v,$$
$$J(t,x) = -\int_{\mathbb{R}^d} vw(t,x,v)\,\mathrm{d}v,$$
$$(ne)(t,x) = \frac{1}{2}\int_{\mathbb{R}^d} |v|^2 w(t,x,v)\,\mathrm{d}v,$$

and the motivation for the minus sign in the definition of J is the negative charge of the electron. We also introduce the notation

$$\langle f(v)\rangle = \int_{\mathbb{R}^d_v} f(v)w(t,x,v)\,\mathrm{d}v$$

for a general function $f = f(v)$.

Integrating (2.9) (with $W \equiv w$) over $\mathbb{R}^d_v$ and assuming tacitly that the function w and all its relevant derivatives have fast decay for $v \to \infty$, we then obtain

$$\partial_t n(t,x) - \operatorname{div}_x J(t,x) + \int_{\mathbb{R}^d_v} (\theta[V]w)(t,x,v)\,\mathrm{d}v = \nu_0 \triangle_x n(t,x),$$

with $\nu_0 = \frac{c_3}{\tau_0}$, compare (2.10). To compute the integral on the left-hand side, we note that the pseudodifferential operator $\theta[V]$ acts on the “velocity” variables v, and it has a pseudodifferential symbol $\delta V = \delta V(t,x,\eta)$, where η is the cotangent variable associated to v. Therefore, this operator behaves like a Fourier multiplier, and we have (writing $\mathcal{F}$ for the Fourier transform)

$$\begin{aligned}\int_{\mathbb{R}^d_v} (\theta[V]w)(t,x,v)\,\mathrm{d}v &= (2\pi)^{d/2} \left(\mathcal{F}_{v\to\eta}\theta[V]w\right)(t,x,\eta)\big|_{\eta=0} \\ &= (2\pi)^{d/2} \left((\delta V)(t,x,\eta)\hat{w}(t,x,\eta)\right)\big|_{\eta=0} = 0.\end{aligned}$$

This gives us the first equation of the viscous model of quantum hydrodynamics:

$$\partial_t n - \operatorname{div} J = \nu_0 \triangle n.$$

In a similar fashion, we multiply the quantum Boltzmann equation (2.9) with v and integrate over $\mathbb{R}^d_v$:

$$-\partial_t J + \operatorname{div}_x\langle v \otimes v\rangle - n\nabla_x V = -\nu_0 \triangle_x J - \nu_2 \nabla_x n + \frac{1}{\tau_0} J,$$

with $\nu_2 = \frac{c_2}{\tau_0}$. Likewise, we multiply (2.9) with $|v|^2/2$, integrate over $\mathbb{R}^d_v$ and find

$$\partial_t(ne) + \operatorname{div}_x \left\langle \frac{1}{2} v|v|^2 \right\rangle + \nabla V \cdot J = -\frac{2}{\tau_0} ne + \frac{dc_1}{\tau_0} n + \frac{c_2}{\tau_0} \operatorname{div} J + \nu_0 \triangle (ne),$$

with d being the spatial dimension. We wish to express the terms $\langle v \otimes v\rangle$ and $\langle v|v|^2/2\rangle$ on the left-hand sides in terms of n, J, and e, but this seems impossible. To overcome this difficulty, we bring assumptions from physics into play, so-called *closure conditions*, of which there are several to be found in the literature. One such approach exploits the entropy minimization principle [38], see also [87].

Here, we suppose that w is in a neighborhood of the thermal equilibrium density (up to some shift u in the velocity variables),

$$w(t, x, v) = w_{\mathrm{eq}}(t, x, v - u(t, x)),$$

where u is some unknown group velocity of the electrons, and w_{eq} is given by

$$\begin{aligned} w_{\mathrm{eq}}(t, x, v) &= A(t, x) \exp\left(-\frac{|v|^2}{2T} + \frac{V}{T}\right) \\ &\quad \times \left(1 + \frac{\varepsilon^2}{8T} \triangle_x V + \frac{\varepsilon^2}{24T^3}|\nabla_x V|^2 - \frac{\varepsilon^2}{24T^3} \sum_{i,j=1}^{d} v_i v_j \frac{\partial^2 V}{\partial_{x_i} \partial_{x_j}} + \mathcal{O}(\varepsilon^4)\right), \end{aligned}$$

where $T = T(t, x)$ is the scalar temperature of the electrons. We suppose that T is always positive and that the function A varies only slowly. Then one can show, after quite long calculations, that

$$\begin{aligned} n &= A(t, x)(2\pi T)^{d/2} e^{V/T} \left(1 + \frac{\varepsilon^2}{12T^2} \triangle V + \frac{\varepsilon^2}{24T^3}|\nabla V|^2\right) + \mathcal{O}(\varepsilon^4), \\ J &= -nu, \\ \langle v \otimes v \rangle &= nu \otimes u + nT\mathbf{1}_d - \frac{\varepsilon^2}{12T} n(\nabla \otimes \nabla)V + \mathcal{O}(\varepsilon^4), \\ \langle v|v|^2 \rangle &= nu|u|^2 + \left(dT - \frac{\varepsilon^2}{12T} \triangle V\right) + 2\left(T\mathbf{1}_d - \frac{\varepsilon^2}{12T}(\nabla \otimes \nabla)V\right) nu + \mathcal{O}(\varepsilon^4), \end{aligned}$$

with $\mathbf{1}_d$ being the $d \times d$ identity matrix. In the last two formulas, we prefer to eliminate the derivatives of V (a discussion of this preference can be found in [51]). To this end, we note that (at least formally)

$$\begin{aligned} \ln n &= \ln\left(A(2\pi T)^{d/2}\right) + \frac{V}{T} + \mathcal{O}(\varepsilon^2), \\ \partial_j \partial_k \ln n &= \partial_j \partial_k \left(AT^{d/2} + \frac{V}{T}\right) + \mathcal{O}(\varepsilon^2). \end{aligned}$$

Now the physical assumption is that A and T vary much slower than V, and then it follows that

$$\partial_j \partial_k \ln n = \frac{1}{T} \partial_j \partial_k V + \mathcal{O}(\varepsilon^2).$$

This way we can express second-order derivatives of V by means of n.

Combining the equations obtained so far and taking the freedom to scale the dependent and independent variables once more, we can arrive at the *full viscous* *quantum hydrodynamic system*

$$\begin{cases} \partial_t n - \operatorname{div} J = \nu \triangle n, \\ \partial_t J - \operatorname{div}\left(\dfrac{J\otimes J}{n}\right) - \nabla(Tn) \\ \qquad + n\nabla V + \dfrac{\varepsilon^2}{6} n \nabla\left(\dfrac{\triangle\sqrt{n}}{\sqrt{n}}\right) = \nu \triangle J - \dfrac{1}{\tau}J + \mu\nabla n, \\ \partial_t(ne) - \operatorname{div}\left(\dfrac{J}{n}(ne+P)\right) + J\cdot\nabla V = -\dfrac{2}{\tau}\left(ne - \dfrac{d}{2}n\right) + \nu\triangle(ne) \\ \qquad + \mu \operatorname{div} J, \\ \lambda^2 \triangle V = n - C(x), \end{cases} \tag{2.13}$$

where the scalar temperature $T = T(t,x)$ and the pressure tensor $P = P(t,x)$ are related to the other unknown functions by

$$P = Tn\mathbf{1}_d - \frac{\varepsilon^2}{12} n(\nabla\otimes\nabla)\ln n,$$
$$ne = \frac{|J|^2}{2n} + \frac{d}{2}Tn - \frac{\varepsilon^2}{24} n \triangle \ln n.$$

For details on this scaling, we refer to [75].

Remark 2.1. If the temperature T is constant, then the first two differential equations in (2.13) are decoupled from the third, which then can be omitted. If we furthermore assume $\nu = 0$ and neglect the acceleration term $\partial_t J - \operatorname{div}(J\otimes J/n)$, the constant temperature (also called *isothermal*) quantum hydrodynamic model turns into the quantum drift diffusion model.

More precisely, the following can be shown in the isothermal case $T \equiv \text{const.}$: choose a new time variable $s = t\tau$, and set $n^{(\tau)}(s,x) = n(s/\tau,x)$, $J^{(\tau)}(s,x) = J(s/\tau,x)/\tau$, $V^{(\tau)}(s,x) = V(s,\tau,x)$. Then as $\tau \to 0$, the functions $(n^{(\tau)}, J^{(\tau)}, V^{(\tau)})$ converge (if $\nu = 0$) to a limit (n^*, J^*, V^*) which solves the quantum drift diffusion model (2.12), but with time variable s instead of t. We refer to [71], and [94], [5], and also [123] for a bipolar model.

Another choice is to assume $T = cn^{\gamma-1}$ for some constants c and $\gamma \geq 1$. This is the *isentropic* case, and again the differential equation for ne can be omitted.

2.4. Historical background and further models

The *drift diffusion equations* (without quantum terms) were first developed by van Roosbroeck 1950 [116]. The underlying physical assumptions are valid for certain devices with diameters down to 10^{-6}m, and for smaller devices, numerical simulations fail because the quantum effects are no longer negligible.

Then the *quantum drift diffusion* (or *density gradient*) model was first introduced in 1987 by M.G. Ancona [11, 7] in order to find a macroscopic description of the behavior of smaller devices, where the classical description gives the wrong predictions. Further physical results are to be found in, e.g., [12, 8, 9, 10]. Concerning fast numerical schemes for the quantum drift diffusion model, we refer to [20, 35, 118, 97, 99]. By using simulations of single barriers (MOS diodes, MOSFETs) and double barriers (resonant tunnel diodes), Höher et al. in [59] showed the limitations of the quantum drift diffusion model, see also [119]. Suggestions for new models were given in [36] and [37].

In the 1990s, macroscopic quantum models have been formally obtained from the Schrödinger–Poisson or Wigner–Poisson systems by asymptotic analysis, see the books [96, 51, 52]. The family of fluid dynamic models contains also *quantum energy transport* models, additionally to the quantum drift diffusion and quantum hydrodynamic models. All these models can be arranged into the form of a model hierarchy, and for details we refer the reader to [96] and [67], [69]. Compare also the review article [100].

Two of the first analytical results on the quantum drift diffusion model were the steady state solution and its semiclassical limit by Ben Abdallah and Unterreiter in 1998 [13], and a positivity preserving scheme and the existence of a weak solution in the one-dimensional transient case by Jüngel and Pinnau [77, 78].

Then the quantum drift diffusion model was extensively studied analytically and numerically. By numerical simulation, it was shown that this model, relatively simple compared to other quantum models, works quite well in describing tunneling effect for several devices, while the approach via mathematical analysis helps in understanding this model more clearly. We will give a review of those results in Section 3.

Concerning the quantum hydrodynamic model (2.13), let us first recall some basic facts from fluid dynamics. If we assume the positive temperature T as constant and write $Tn = p(n)$ as pressure, and $J = -nu$, neglect the collision terms $(\nu = 0, \tau = \infty)$, the quantum effects $(\varepsilon = 0)$ as well as the electrostatic potential $(V \equiv 0)$, then we end up with the classical Euler equations

$$\begin{cases} \partial_t n + \operatorname{div}(nu) = 0, \\ \partial_t(nu) + \operatorname{div}(nu \otimes u) + \nabla p(n) = 0. \end{cases} \tag{2.14}$$

By thermodynamical reasons, we may assume $p'(n) > 0$ for all $n > 0$, which makes this system symmetrizably hyperbolic, and the local in time existence of classical solutions is a well-established result, and it is known that jump-type discontinuities (shocks) typically appear after finite time. Solutions which are global in time can only exist as weak solutions. For details, we recommend the text books [34], [112] and the overview article [86]. The number $c = \sqrt{p'(n)}$ is called *sound speed*, and the flow is called *subsonic* wherever $|u| < c$, otherwise *supersonic*. If a Bohm potential term $(\varepsilon^2/2)n\nabla B(n)$ (compare (1.3)) is added to (2.14), solutions still become irregular in finite time, see [50].

If we put the electrostatic potential V back into the Euler equations, we obtain the Euler–Poisson system, for which the global existence of weak solutions was shown in [102] and [33] by an approach similar to the celebrated Glimm scheme [55], for the isothermal case. We mention also [95], [122], [65].

Incorporating the electrostatic potential V as well as the quantum Bohm potential B into (2.14) leads to the inviscid quantum hydrodynamic model, which was first studied by Gardner [51]. A quantum derivation of this model from physical principles, in particular the entropy minimization principle, was given by Degond and Ringhofer [38]. For a nice review, see [62]. The full viscous model (2.13) was established in [21], and it was treated as a parameter-elliptic system of Douglis–Nirenberg type for the first time in [23].

3. The quantum drift diffusion model

3.1. Introduction

3.1.1. Full models and simplified models. If we refine a bit the calculations which have led us to (2.12), the following scaled transient quantum drift diffusion model can be derived:

$$\begin{cases} n_t = \operatorname{div}\left(-\varepsilon^2 n \nabla \left(\frac{\triangle\sqrt{n}}{\sqrt{n}}\right) + \nabla P(n) - n\nabla V\right), \\ \lambda^2 \triangle V = n - C(x). \end{cases} \tag{3.1}$$

Here $P = P(n)$ is the pressure, a known function of n. Typically we have either $P(n) = \theta n$, the so-called *isothermal* case with θ being a (positive) constant temperature, or $P(n) = T_0 n^\gamma$, the *isentropic* case with T_0 as the (positive) lattice temperature and $\gamma > 1$. The scaled Planck constant ε and the scaled Debye length λ are positive, as always.

An equivalent way of writing (3.1) is

$$\begin{cases} n_t = \operatorname{div}(n\nabla F), \\ F = -\varepsilon^2 \frac{\triangle\sqrt{n}}{\sqrt{n}} + h(n) - V, \\ \lambda^2 \triangle V = n - C(x), \end{cases} \tag{3.2}$$

with F being the *quasi Fermi potential* and $h = h(n)$ the *enthalpy* defined by $h'(n) = P'(n)/n$.

Greater generality is obtained when we consider the *bipolar quantum drift diffusion system.* In this model, also the *holes*'s contribution to the electric current in the device is included. Holes are artificially introduced particles of positive charge describing the vacations in the valence band, and they follow the same physical principles as the electrons, except their positive charge and a (possibly) different effective mass.

Then the *bipolar quantum drift diffusion system* reads

$$\begin{cases} \quad n_t = \operatorname{div}\left(-\varepsilon^2 n\nabla\left(\frac{\triangle\sqrt{n}}{\sqrt{n}}\right) + \nabla(P_n(n)) - n\nabla V\right), \\ \quad p_t = \operatorname{div}\left(-\xi\varepsilon^2 p\nabla\left(\frac{\triangle\sqrt{p}}{\sqrt{p}}\right) + \nabla(P_p(p)) + p\nabla V\right), \\ \lambda^2 \triangle V = n - p - C(x), \end{cases} \tag{3.3}$$

with n being the electron density, p the hole density, $P_n(n) = n^\alpha$ and $P_p(p) = p^\beta$ are pressures with $\alpha, \beta \geq 1$, and ξ is the (positive) ratio of the effective masses of electrons and holes.

We impose the initial conditions

$$\begin{cases} n(0,x) = n_0(x) \geq 0, & \\ n(0,x) = n_0(x) \geq 0, & p(0,x) = p_0(x) \geq 0, \end{cases} \tag{3.4}$$

in the unipolar and the bipolar cases, respectively.

Sometimes we require the crystal at initial time to be electrically neutral:

$$\int_\Omega n_0(x) - C(x)\,\mathrm{d}x = 0. \tag{3.5}$$

It is reasonable to pose the problem in a bounded domain $\Omega \subset \mathbb{R}^d$ and let $\partial\Omega$ be comprised of two disjoint parts: Γ_D (the Ohmic contacts, also called source and drain in semiconductor devices), and Γ_N (the insulating part).

Physical considerations make the following assumptions natural:

- at the Ohmic contacts, the charge should be locally neutral,
- the potential is a superposition of its equilibrium value V_{eq} and the applied voltage U at the Ohmic contacts,
- the normal components of the current and quantum current are vanishing along the insulating part of the boundary;
- no quantum effects occur at the contacts.

These motivations correspond to the following Dirichlet-Neumann conditions:

$$\left.\begin{aligned} n &= C(x), \\ V &= V_{\mathrm{eq}} + U, \\ \triangle\sqrt{n} &= 0, \end{aligned}\right\} \text{ on } \Gamma_D$$
$$\left.\begin{aligned} \nabla V\cdot\nu &= 0, \\ n\nabla F\cdot\nu &= 0, \\ \nabla\left(\frac{\triangle\sqrt{n}}{\sqrt{n}}\right)\cdot\nu &= 0. \end{aligned}\right\} \text{ on } \Gamma_N \tag{3.6}$$

As far as we know, a mathematical theory on this full multi-dimensional problem (3.2) or (3.3) with initial data (3.4) and boundary conditions (3.6) has not been given in the literature so far.

However, the following simplifications of this problem are custom:

A special fourth-order parabolic equation. Neglecting certain terms in (3.2), we obtain a problem for only one unknown function. This model corresponds to the zero temperature and zero electronic potential case in the quantum drift diffusion model. This sounds on the one hand like a severe restriction, but on the other hand this system also appears in the studies of interface fluctuations in a two-dimensional spin system. It is also called the Derrida–Lebowitz–Speer–Spohn equation, which was first derived by Derrida et al. in [40]. In the one-dimensional case, it is also related to the so-called Fisher information. Results obtained for this model will be reported in Section 3.2.

One space dimension. In the one space dimension case, the fourth-order term can be recast as

$$\operatorname{div}\left(n\nabla\left(\frac{\triangle\sqrt{n}}{\sqrt{n}}\right)\right)=\frac{1}{2}\left(n(\ln x)_{xx}\right)_{xx},$$

which makes getting *a priori* estimates much easier. A series of results has been obtained including the existence of weak solutions, their long time behavior, quasineutral limit and semiclassical limit with many kinds of boundary conditions. We will show them in Section 3.3.

Simplified boundary conditions. In Section 3.4, two-dimensional and three-dimensional results are shown, with a focus on the periodic case.

3.1.2. Questions and problems. The Bohm potential terms appearing in (3.1) and (3.3) can be split into a linear third-order part and a lower-order nonlinear part, or rewritten in various other ways,

$$n\nabla\left(\frac{\triangle\sqrt{n}}{\sqrt{n}}\right)=\frac{1}{2}\nabla\triangle n-\frac{1}{2}\operatorname{div}\left(\frac{\nabla n\otimes\nabla n}{n}\right), \tag{3.7}$$

$$\operatorname{div}\left(n\nabla\left(\frac{\triangle\sqrt{n}}{\sqrt{n}}\right)\right)=\frac{1}{2}\sum_{i,j=1}^{d}\partial_i\partial_j\Big(n\partial_i\partial_j\ln n\Big),$$

and hence the unipolar and bipolar quantum drift diffusion models are nonlinear parabolic systems, to which the methods of the theory of analytic semigroups (as presented in [6] or [92], for instance) can be applied, giving us the uniqueness and the local in time existence of strong solutions.

As usual, a blow-up of the solution in finite time or the occurrence of vacuum ($n(t_*,x_*)=0$ for some (t_*,x_*)), which make global in time smooth solutions impossible, are hard to exclude using semigroup arguments alone.

Typical questions and problems to be solved are:

Global in time existence of weak solutions. We wish to solve (3.1) or (3.3) on any time interval $(0,T)$, independent of the size of the initial data. The solutions n shall be nonnegative everywhere.

Long time asymptotics of solutions. In particular, the exponential stability of stationary states is of interest.

The semiclassical limit $\varepsilon \to 0$. Then the fourth-order parabolic problems (3.1) and (3.3) formally turn into second-order parabolic problems, and the question is whether the sequence $(n_\varepsilon)_{\varepsilon\to 0}$ has the expected limit for $\varepsilon \to 0$, and in which topologies this limit is valid. Physically, this limit means that quantum effects are getting neglected.

The quasineutral limit $\lambda \to 0$. This limit is relevant mainly in the case of the bipolar model (3.3). The physical meaning of this limit is that the crystal is locally of neutral charge.

Each of these questions will be answered in this paper.

3.1.3. Methods. The key to proving global existence of solutions and studying their behavior is finding appropriate quantities for which powerful *a priori* estimates can be derived. Such quantities are called entropies (in other schools the expression *Lyapunov functional* is common), and the following entropies have proved useful in the past:

$$\begin{aligned}
E_1(n) &= \int_\Omega (n(\ln n - 1) + 3)\,\mathrm{d}x,\\
E_2(n) &= \int_\Omega (n - \ln n)\,\mathrm{d}x,\\
E_3(n) &= \int_\Omega |\nabla\sqrt{n}|^2\,\mathrm{d}x,\\
\tilde{E}_1(n) &= \int_\Omega n \ln\left(\frac{n}{\bar{n}}\right)\mathrm{d}x, \qquad \text{with} \quad \bar{n} = \frac{1}{|\Omega|}\int_\Omega n\,\mathrm{d}x,\\
\tilde{E}_\gamma(n) &= \frac{1}{\gamma(\gamma-1)}\int_\Omega (n^\gamma - \bar{n}^\gamma)\,\mathrm{d}x.
\end{aligned}$$

These terms are adapted to the nonlinearities appearing in the differential equations; and which entropy is available in a concrete situation depends also on the boundary condition, since estimating entropies requires certain partial integrations. Examples of the obtained identities are (3.13), (3.14), and (3.15); see also (3.19), (3.20), (3.33).

In deriving *a priori* estimates, one often finds an inequality which contains such an entropy, and additionally a positive term which "produces" this (or another) entropy. Such inequalities will be called *entropy entropy-production inequalities*. The connection between this positive term and the above entropies is typically provided by *logarithmic Sobolev inequalities*, see the discussion around (3.16).

If enough *a priori* estimates are derived which are independent of ε, then the semiclassical limit $\varepsilon \to 0$ can be performed, by weak compactness of bounded subsets in reflexive spaces and related arguments. Similarly for the quasineutral limit $\lambda \to 0$.

In case the global existence of weak solutions has not been established yet, *Rothe's method* [83] may be employed. In this method, the time interval is discretized, the time derivatives are replaced by the difference quotients, leading to a nonlinear elliptic problem at each time step. This is solved using fixed point theorems of Schauder type, and an exponential transform of the unknown function makes sure that the solution to the elliptic problem takes only positive values. Then the limit of vanishing time step size has to be performed. A detailed presentation of Rothe's method will be given in Section 3.5.

This approach has the key advantage that the existence of a weak solution can be shown on any time interval $(0, T)$, without any restrictions on the size of the physical constants or the size of the initial data (except positivity of $n(0, \cdot)$, of course). As one can expect from fixed point theorems of Schauder type, the uniqueness of such solutions is unknown in many situations. And also the regularity of the solutions obtained by this approach is lower in comparison to the method of analytic semigroups combined with the concept of maximal regularity ([6], [39], [92]), but our approach can handle the vacuum effect, making global in time solutions possible.

3.2. A special fourth-order parabolic equation

As it was mentioned in the introduction, there are at least two motivations to study the fourth-order parabolic equation

$$\begin{cases} n_t = -\operatorname{div}\left(n\nabla\left(\frac{\triangle\sqrt{n}}{\sqrt{n}}\right)\right), \quad \Big(n_t + (n(\ln n)_{xx})_{xx} = 0 \quad \text{if } d = 1\Big), \\ n(0, x) = n_0(x). \end{cases} \tag{3.8}$$

One motivation is that it shows the main structure of quantum drift diffusion. A good understanding of this fourth-order term might help a lot to study the full system (3.1). The other motivation is that (3.8) itself is a complete model which arises in the context of fluctuations of a stationary nonequilibrium interface in a two-dimensional spin system.

The following boundary conditions are common in the literature:

$$\text{periodic boundary conditions,} \tag{3.9}$$

$$\nabla n \cdot \gamma = 0, \qquad n\nabla\left(\frac{\triangle\sqrt{n}}{\sqrt{n}}\right) \cdot \gamma = 0 \text{ on } \partial\Omega, \tag{3.10}$$

$$n = 1, \quad n_x = 0 \text{ on } \partial\Omega \quad \text{if} \quad \Omega = (0, 1) \subset \mathbb{R}^1, \tag{3.11}$$

$$\begin{cases} n(0, t) = n_0, \quad n(1, t) = n_1, \\ n_x(0, t) = w_0, \quad n_x(1, t) = w_1, \end{cases} \quad \text{if} \quad \Omega = (0, 1). \tag{3.12}$$

Here γ denotes the outer unit normal on $\partial\Omega$.

The first analytical result was given by Bleher et al. in [16], where the local existence of positive solutions with periodic boundary conditions was proved. Later on, within the last ten years, it was observed that this model has the following entropies:

- the physical entropy $\int_\Omega n \ln\left(\frac{n}{\int n\,\mathrm{d}x}\right)\mathrm{d}x$;
- the Lyapunov functional $\int_\Omega (n - \ln n)\,\mathrm{d}x$ if $\Omega \subset \mathbb{R}^1$;
- the Fisher information $\int_\Omega \left((\sqrt{n})_x\right)^2 \mathrm{d}x$ if $\Omega \subset \mathbb{R}^1$;

and subsequently this nonlinear fourth-order equation has been extensively studied. The equation (3.8) with periodic boundary conditions or the boundary conditions (3.10) or (3.11) with $\Omega \subset \mathbb{R}^1$ has been investigated in [17, 19, 41, 80], including the global existence of a nonnegative weak solution and its exponential decay to a steady state. Similar results can be found in [58]. First-order entropies of this fourth-order equation have been studied in [81]. Due to the importance of the entropy in higher-order PDEs, Jüngel and Matthes derived a new approach to the construction of entropies and entropy productions for a large class of nonlinear evolutionary PDEs of even order in the case of one spatial dimension in [73], by means of a reformulation as a decision problem from real algebraic geometry.

Concerning the existence of a global weak solution and the long time behavior in the multi-dimensional case, we are aware of only two works: Gianazza et al. [54] and Jüngel et al. [74]. The results in [54] are more general. With the boundary condition (3.10), by using the special structure of the equation, i.e., the equation is the gradient flow of the Fisher information function $\frac{1}{2}\int |\nabla \ln n|^2 n\,\mathrm{d}x$ with respect to the Kantorovich–Rubinstein–Wasserstein distance between probability measures, the nonnegative weak solution was obtained as the limit of a variational approximation scheme. The existence results in [74] concern bounded domains in two and three dimensions, and the method used there is more direct. A better convergence rate on the long time behavior of the weak solution is also given.

Now we come to a presentation of recent results on global existence and exponential decay, with various boundary conditions and in one or more spatial dimensions.

3.2.1. The one-dimensional case.

Periodic or homogeneous Dirichlet-Neumann boundary conditions (3.11)

In the one-dimensional case, there are some nice entropy equations with periodic boundary conditions or homogeneous Neumann boundary conditions (3.10):

$$\frac{\mathrm{d}}{\mathrm{d}t}E_1(n) + \int_\Omega n|(\ln n)_{xx}|^2\,\mathrm{d}x = 0, \tag{3.13}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}E_2(n) + \int_\Omega |(\ln n)_{xx}|^2\,\mathrm{d}x = 0, \tag{3.14}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}E_3(n) + 2\int_\Omega \left|\sqrt{n}\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_x\right|^2 \mathrm{d}x = 0, \tag{3.15}$$

valid for positive-valued functions n of sufficient regularity. It seems that the entropy $E_3(n)$ has been used for the first time in [24], in order to show the semi-classical limit $\varepsilon \to 0$. We will introduce this result in Section 3.3.2. The first two entropies $E_1(n)$ and $E_2(n)$ were extensively used in the study of (3.8), and we quote some of the results in the following.

In [41], the following logarithmic Sobolev inequality for functions of period length L has been derived (see also [120])

$$\int_\Omega u^2 \ln\left(\frac{u^2}{\int u^2\,\mathrm{d}x/L}\right)\mathrm{d}x \le 2\left(\frac{L}{2\pi}\right)^j \int_\Omega \left|\partial_x^j u\right|^2 \mathrm{d}x, \tag{3.16}$$

where $\Omega = (0, L)$ and $j \in \mathbb{N}_+$. This inequality with $u = \sqrt{n}$ and $j = 2$, together with the identity

$$\int_\Omega n\left|(\ln n)_{xx}\right|^2 \mathrm{d}x = 4\int_\Omega \left|(\sqrt{n})_{xx}\right|^2 \mathrm{d}x + \frac{1}{12}\int_\Omega \frac{(n_x)^4}{n^3}\,\mathrm{d}x$$

enables us to connect the entropy production term in (3.13) back to E_1, which then turns out to decay exponentially.

The precise results are as follows:

Theorem 3.1 ([76] and [41]). *Let $E_2(n_0)$ be finite. Then the following results hold:*

Global weak solution. *There exists a global weak solution $n \ge 0$ of* (3.8), (3.9) (*or* (3.11)) *satisfying*

$$n \in L^{5/2}_{\mathrm{loc}}((0,\infty); W^1_1(0,L)) \cap W^1_{1,\mathrm{loc}}((0,\infty); H^{-2}(0,L)),$$
$$\ln n \in L^2_{\mathrm{loc}}((0,\infty); H^2(0,L)),$$

and for all positive T and all smooth test functions ϕ,

$$\int_0^T \langle \partial_t n, \phi\rangle_{H^{-2},H^2}\,\mathrm{d}t + \int_0^T\int_0^L n(\ln n)_{xx}\phi_{xx}\,\mathrm{d}x\,\mathrm{d}t = 0.$$

Uniqueness. *Let n_1, n_2 be two weak solutions of* (3.8) *with periodic boundary conditions and with the regularity $n_1, n_2 \in C^0([0,T]; L^1(0,L))$, and suppose that $\sqrt{n_1/n_2}, \sqrt{n_2/n_1} \in L^2((0,T); H^2((0,L)^2))$ for some $T > 0$. Then $n_1 = n_2$ in $(0,T)\times(0,L)$.*

Decay. *If $E_1(n_0) < \infty$, then*

$$E_1(n) \le e^{-Mt}E_1(n_0), \quad M = \frac{32\pi^4}{L^4},$$

and the weak solution has higher regularity: $n \in L^{16/15}_{\mathrm{loc}}((0,\infty); H^2(0,L))$.

Nonhomogeneous Dirichlet Neumann boundary condition (3.12)

Gualdani et al. considered the problem (3.8) with the boundary condition (3.12), where n_0, n_1 are positive, and w_0, $w_1 \in \mathbb{R}$. Then (see [58]) there is a positive constant m depending only on the boundary data, and a unique classical solution n_∞ to

$$(n(\ln n)_{xx})_{xx} = 0, \text{ in } (0,1),$$

with $n_\infty \ge m$ everywhere. Using the entropy

$$E_{1/2}(n) = \int_0^1 \left(\sqrt{n} - \sqrt{n_\infty}\right)^2 \mathrm{d}x,$$

the entropy identity

$$\frac{\mathrm{d}}{\mathrm{d}t}E_{1/2}(n) + 2\int_0^1 \left(\sqrt[4]{\frac{n_\infty}{n}}(\sqrt{n})_{xx} - \sqrt[4]{\frac{n}{n_\infty}}(\sqrt{n_\infty})_{xx}\right)^2 \mathrm{d}x = 0$$

was derived in [58]. Further, it was shown that a nonnegative weak global in time solution n to (3.8), (3.4), (3.12) exists with regularity as described in Theorem 3.1 provided that $E_2(n_0) < \infty$. And if additionally $E_1(n_0)$ is finite and $\ln n_\infty$ is a concave function, then $n(t,\cdot)$ approaches n_∞ exponentially:

$$\|n(t,\cdot) - n_\infty\|_{L^1(0,1)} \le ce^{-\lambda t}, \qquad 0 < t < \infty.$$

3.2.2. The two- and three-dimensional cases. The differential equation (3.8) can now be rewritten as

$$\partial_t n + \frac{1}{2}\sum_{i,j=1}^{d} \partial_i\partial_j(n\partial_i\partial_j \ln n) = 0, \tag{3.17}$$

$$\partial_t n + \sum_{i,j=1}^{d} \partial_i\partial_j\Big(\sqrt{n}\partial_i\partial_j\sqrt{n} - (\partial_i\sqrt{n})(\partial_j\sqrt{n})\Big) = 0. \tag{3.18}$$

We may write $\rho = \sqrt{n}$, multiply (3.17) and (3.18) by $\ln\rho^2$ and $\rho^{2(\gamma-1)}/(\gamma-1)$, integrate over $\Omega = \mathbb{T}^d = (\mathbb{R}/\mathbb{Z})^d$ and find formally

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{E}_1 + \frac{1}{2}\int_{\mathbb{T}^d} n\sum_{i,j}\Big(\partial_i\partial_j \ln n\Big)^2 \mathrm{d}x = 0, \tag{3.19}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{E}_\gamma + \frac{1}{\gamma-1}\int_{\mathbb{T}^d} \rho^2\sum_{i,j}(\partial_i\partial_j\ln\rho)\Big(\partial_i\partial_j\rho^{2(\gamma-1)}\Big)\,\mathrm{d}x = 0, \qquad \gamma \neq 1. \tag{3.20}$$

Note that the number $\overline{n}$ appearing in the definition of $\tilde{E}_1$ and $\tilde{E}_\gamma$ is a conserved quantity, by the periodic boundary conditions. And the above two integrals over $\mathbb{T}^d$ can be connected to $\tilde{E}_1$ and $\tilde{E}_\gamma$ via the inequalities

$$\frac{1}{4}\int_{\mathbb{T}^d} n\sum_{i,j}\Big(\partial_i\partial_j\ln n\Big)^2 \mathrm{d}x \ge \kappa_1\int_{\mathbb{T}^d}\sum_{i,j}\left(\partial_i\partial_j\sqrt{n}\right)^2\,\mathrm{d}x, \tag{3.21}$$

$$\int_{\mathbb{T}^d}\rho^2\sum_{i,j}(\partial_i\partial_j\ln\rho)\Big(\partial_i\partial_j\rho^{2(\gamma-1)}\Big)\,\mathrm{d}x \ge 2(\gamma-1)\kappa_\gamma\int_{\mathbb{T}^d}(\triangle\rho^\gamma)^2\,\mathrm{d}x, \tag{3.22}$$

with $\kappa_1 = (4d-1)/(d(d+2))$, and with a certain constant κ_γ (depending only on γ and d) explicitly given in [74], see also [54]. This constant κ_γ is positive if and only if $(\sqrt{d}-1)^2/(d+2) < \gamma < (\sqrt{d}+1)^2/(d+2)$. Proving (3.22) is equivalent to solving a decision problem from real algebraic geometry, compare the methods of [73]. Then the following result can be obtained:

Theorem 3.2 ([74]). *If $d \le 3$ and $E_1(n_0) < \infty$, then* (3.8), (3.9), (3.4) *has a nonnegative weak solution of the regularity*

$$n \in W_1^1((0,T); H^{-2}(\mathbb{T}^d)), \quad \sqrt{n} \in L^2((0,T); H^2(\mathbb{T}^d)),$$

and n is a weak solution to (3.18) *in the sense that for all $z \in L^\infty((0,T); H^2(\mathbb{T}^d))$, we have*

$$\int_0^T \langle \partial_t n, z \rangle_{H^{-2},H^2} \, \mathrm{d}t + \iint_{Q_T} \sum_{i,j=1}^d \left(\sqrt{n} \partial_i \partial_j \sqrt{n} - (\partial_i \sqrt{n})(\partial_j \sqrt{n}) \right) \partial_i \partial_j z \, \mathrm{d}x \, \mathrm{d}t = 0.$$

The entropies decay exponentially fast,

$$\tilde{E}_\gamma(n(t,\cdot)) \le \tilde{E}_\gamma(n_0) \exp\left(-16\pi^4 \gamma^2 \kappa_\gamma t\right), \quad \text{for} \quad 1 \le \gamma < \frac{(\sqrt{d}+1)^2}{d+2},$$

and the solution itself decays exponentially in the L^1 norm,

$$\left\| n(t,\cdot) - \frac{\int_{\mathbb{T}^d} n_0 \, \mathrm{d}x}{|\mathbb{T}^d|} \right\|_{L^1(\mathbb{T}^d)} \le \sqrt{2\tilde{E}_2(n_0)} \exp\left(-8\pi^4 \kappa_1 t\right).$$

3.3. Quantum drift diffusion equations in one dimension

In the one-dimensional case, the quantum drift diffusion model is written in the following form (compare (3.2))

$$\begin{cases} n_t = J_x, \quad J = nF_x, \\ F = -\varepsilon^2 \dfrac{(\sqrt{n})_{xx}}{\sqrt{n}} + h(n) - V, \\ \lambda^2 V_{xx} = n - C(x), \end{cases} \tag{3.23}$$

where $(t,x) \in (0,T) \times (0,1)$ and the enthalpy $h(n)$ is a function of n with $h'(n) = P'(n)/n$.

The system is complemented with the usual initial data condition (3.4). The boundary conditions studied so far are

$$\text{periodic boundary conditions}, \tag{3.24}$$
$$n_x = 0, \quad n_{xxx} = 0, \quad V_x = 0, \tag{3.25}$$
$$n = n_D, \quad V = V_D, \quad F = F_D, \tag{3.26}$$
$$n = n_D, \quad n_x = 0, \quad V = V_D. \tag{3.27}$$

Here the subscript D recalls that these values refer to Dirichlet data. In fact, the following non-homogenous conditions look more physical, but solving system (3.23) with this condition seems an open problem:

$$n(t,0) = n_0, \quad n(t,1) = n_1, \quad n_x(t,0) = w_0, \quad n_x(t,1) = w_1, \quad V = V_\Omega. \tag{3.28}$$

3.3.1. Global weak solution.

Isothermal case $P(n) = \theta n$

Jüngel and Pinnau [77, 78] gave a positivity preserving numerical scheme for (3.2) with boundary conditions (3.26) and (3.27), where they used a certain exponential transformation and a backward Euler scheme. We will sketch this method in Section 3.5. They showed that in each time step, the problem admits a strictly positive solution. But due to the lack of enough *a priori* estimates, only the convergence of the scheme in the one-dimensional case could be proved, or in the multi-dimensional case with temperature θ large enough, and certain other restrictions on the solution. Furthermore, also a numerical simulation on the switching behavior of a resonant tunnel diode was given.

In these two papers, the function F was used as test function, and the following entropy was obtained there:

$$E(n) = \varepsilon^2 \int_\Omega \left|\nabla\sqrt{n}\right|^2 \mathrm{d}x + \theta \int_\Omega (n(\ln n - 1) + 3)\,\mathrm{d}x + \frac{\lambda^2}{2}\int_\Omega |\nabla V|^2\,\mathrm{d}x, \tag{3.29}$$

which is formally nonincreasing in time as long as the Dirichlet data F_D are nonpositive.

For completeness, recall that the enthalpy is $h(n) = \theta \ln n$ in case of $P(n) = \theta n$, and we mention also that it is custom to write $\rho = \sqrt{n}$ as unknown variable.

Theorem 3.3 ([77]). *Let the Dirichlet data n_D be positive, and let F_D be negative, and suppose $C(x) \in C^{0,\gamma}(\overline{\Omega})$ with $0 < \gamma < 1$, and also $\ln\rho_0 \in L^1(\Omega)$, $\rho_0 \in H^2(\Omega)$. Then there exist functions $\rho \in L^2((0,T); H^2(\Omega)) \cap C^0([0,T]; C^{0,\gamma}(\overline{\Omega}))$ and $J \in L^2((0,T); L^2(\Omega))$ as well as $V \in C^0([0,T]; C^{2,\gamma}(\overline{\Omega}))$, such that for all $\phi \in C_0^\infty((0,T)\times\Omega)$ the following identities hold:*

$$\int_0^T\int_\Omega \rho^2 \partial_t\phi\,\mathrm{d}x\,\mathrm{d}t - \int_0^T\int_\Omega J\phi_x\,\mathrm{d}x\,\mathrm{d}t = 0,$$

$$\int_0^T\int_\Omega [\varepsilon^2\rho_{xx}(2\rho_x\phi + \rho\phi_x) - \theta\rho^2\phi_x + V(\rho^2\phi)_x]\,\mathrm{d}x\,\mathrm{d}t = \int_0^T\int_\Omega J\phi\,\mathrm{d}x\,\mathrm{d}t,$$

$$-\lambda^2\int_0^T\int_\Omega V_x\phi_x\,\mathrm{d}x\,\mathrm{d}t = \int_0^T\int_\Omega (\rho^2 - C)\phi\,\mathrm{d}x\,\mathrm{d}t.$$

These equations are to be understood in the sense that (ρ, V) is a distributional solution to

$$\begin{cases} \partial_t(\rho^2) = \left(-\varepsilon^2\rho^2\left(\dfrac{\rho_{xx}}{\rho}\right)_x + \theta(\rho^2)_x - \rho^2 V_x\right)_x, \\ \lambda^2 V_{xx} = \rho^2 - C, \end{cases}$$

with boundary conditions $\rho = \rho_D$, $\rho_x = 0$, $V = V_D$.

For related results on time global existence of weak solutions, we refer to [30] and also [32]. The boundary conditions (3.25) and (3.24) are comparably easier to handle than (3.26) because of the boundary values being zero. In contrast to this, the boundary condition (3.27) makes it harder to find an estimate for the quantum entropy $E_3(n)$. For details, see [32].

Isentropic pressure $P(n) = T_0 n^\gamma$

In comparison to the isothermal case where $P(n) = \theta n$, the isentropic term brings additional difficulties in getting the *a priori* estimates due to its nonlinearity. By careful use of Sobolev's embedding theorem and Aubin's lemma ([111]), the global existence of weak solution with various boundary conditions can be obtained. We list here a result from [31] on boundary conditions (3.24) and (3.25). Here we have set $E = -V_x$ as new unknown function, and the function G mentioned below will become equal to $\rho^2 \left(\frac{\rho_{xx}}{\rho}\right)_x$ if ρ has the necessary regularity.

Theorem 3.4 ([31]). *Let $C(x) \in L^\infty(\Omega)$ and suppose $0 \le \rho_0 \in H^1(\Omega)$, $\ln \rho_0 \in L^1(\Omega)$ and (3.5) with $n_0 = \rho_0^2$. Put $\mathcal{H} = \{u \in H^2(\Omega) \colon u_x \in H_0^1(\Omega)\}$.*

Then for any fixed positive ε, there exists (ρ, E) with ρ being nonnegative such that

$$\begin{aligned}
\rho &\in L^\infty((0,T); H^1(\Omega)) \cap L^2((0,T); \mathcal{H}) \cap L^{6/5}((0,T); W^3_{6/5}(\Omega)),\\
E &\in L^\infty((0,T); L^2(\Omega)),\\
\rho^2 &\in C([0,T]; C^{0,\alpha}(\overline{\Omega})) \cap L^2((0,T); C^{1,\alpha}(\overline{\Omega})) \cap L^{6/5}((0,T); C^{2,\beta}(\overline{\Omega})),\\
\partial_t \rho^2 &\in L^2((0,T); (H^1(\Omega))'),
\end{aligned}$$

where $0 < \alpha < 1/2$, $0 < \beta < 1/6$. And for all $\varphi \in L^6((0,T); \mathcal{H})$,

$$\begin{aligned}
\int_0^T \left\langle \partial_t \rho^2, \varphi \right\rangle_{(H^1)' \times H^1} \mathrm{d}t &= \varepsilon^2 \int_0^T \int_\Omega (2\rho\rho_{xxx}\varphi_x + \rho\rho_{xx}\varphi_{xx})\,\mathrm{d}x\,\mathrm{d}t \\
&\quad - \int_0^T \int_\Omega [P'(\rho^2)(\rho^2)_x + \rho^2 E]\varphi_x \,\mathrm{d}x\,\mathrm{d}t,
\end{aligned} \tag{3.30}$$

and for a.e. $t \in (0,T)$, we have the following identity for all $\eta \in H^1(\Omega)$:

$$\lambda^2 \int_\Omega E(t,x)\eta_x(x)\,\mathrm{d}x = \int_\Omega [\rho^2(t,x) - C(x)]\eta(x)\,\mathrm{d}x. \tag{3.31}$$

Moreover, there exists $G \in L^2(Q_T)$ such that for all $\psi \in L^2((0,T); H^1(\Omega))$,

$$\begin{aligned}
&\int_0^T \left\langle \partial_t \rho^2, \psi \right\rangle_{(H^1)' \times H^1} \mathrm{d}t \\
&\quad = \varepsilon^2 \int_0^T \int_\Omega G\psi_x \,\mathrm{d}x\,\mathrm{d}t - \int_0^T \int_\Omega [P'(\rho^2)(\rho^2)_x + \rho^2 E]\psi_x \,\mathrm{d}x\,\mathrm{d}t.
\end{aligned} \tag{3.32}$$

In particular, if $1 < \gamma \le 3/2$, we have the following estimate uniformly in ε

$$\|\rho\|_{L^\infty((0,T);H^1(\Omega))} + \|E\|_{L^\infty((0,T);L^2(\Omega))} + \left\|(\rho^2)_x\right\|_{L^2(Q_T)} + \|\varepsilon G\|_{L^2(Q_T)} \le C,$$

where C is a constant independent of ε.

The last uniform in ε estimates will be used in the discussion of the semiclassical limit $\varepsilon \to 0$ in the next section.

3.3.2. Semiclassical limit $\varepsilon \to 0$. The main difference between the quantum and classical drift diffusion models is the quantum correction term $\varepsilon^2 n \nabla \left(\frac{\triangle\sqrt{n}}{\sqrt{n}}\right)$. To discuss the relation between these two models, i.e., to send ε to zero, is interesting both mathematically and physically. Mathematically, it is the process of going from a fourth-order PDE to a second-order PDE, which is usually quite hard. Physically, this relation describes the connection between classical models and quantum models, i.e., one attempts to treat a classical model as the classical limit of its corresponding quantum model. For the stationary quantum drift diffusion model, Ben Abdallah and Unterreiter [13] proved the semiclassical limit. For the transient case, the first result was by Chen and Ju in [24] with periodic boundary conditions (3.24) or homogeneous Neumann boundary condition (3.25) in the one-dimensional case. Later on, a series of works has appeared with other boundary conditions, and also the isentropic case has been studied. The key point to get the semiclassical limit is to have uniform in ε estimates, which is harder with mixed boundary conditions and in the isentropic case. We will present them step by step in this section.

Homogeneous Neumann boundary conditions (3.25)
The entropy inequality introduced by [77] reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\varepsilon^2 E_3(\rho^2)+\theta E_1(\rho^2)+\frac{\lambda^2}{2}\int_\Omega |V_x|^2\,\mathrm{d}x\right)+\int_\Omega \rho^2|F_x|^2\,\mathrm{d}x\le C, \tag{3.33}$$

and can be formally obtained by using $F=-\varepsilon^2\frac{\rho_{xx}}{\rho}+\theta\ln\rho^2-V$ as test function. Unfortunately, the entropy production term $\int_\Omega \rho^2|F_x|^2\,\mathrm{d}x$ does not give us more detailed information on the solution ρ, and then it seems hard to find the semiclassical limit using only this inequality. The key point in [24] is to separate the quasi Fermi level $F=-\varepsilon^2\frac{\rho_{xx}}{\rho}+\theta\ln\rho^2-V$ into the classical part $\theta\ln\rho^2-V$ and the quantum part $-\varepsilon^2\frac{\rho_{xx}}{\rho}$. Formally by using $\theta\ln\rho^2-V$ and $-\rho_{xx}/\rho$ as test function separately, the following inequalities can be obtained:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\theta E_1(\rho^2)+\frac{\lambda^2}{2}\int_\Omega |V_x|^2\,\mathrm{d}x\right)+\frac{\theta\varepsilon^2}{4}\int_\Omega \rho^2|(\ln\rho^2)_{xx}|^2\,\mathrm{d}x\\ +\frac{\varepsilon^2}{\lambda^2}\int_\Omega |(\rho^2)_x|^2\,\mathrm{d}x+\int_\Omega \frac{|\theta(\rho^2)_x-\rho^2V_x|^2}{\rho^2}\,\mathrm{d}x\le C\int_\Omega \varrho^2\,\mathrm{d}x,\end{aligned} \tag{3.34}$$

and

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}E_3(\rho^2)+\varepsilon^2\int_\Omega\left|\rho\left(\frac{\rho_{xx}}{\rho}\right)_x\right|^2\mathrm{d}x+\theta\int_\Omega|\rho_{xx}|^2\,\mathrm{d}x+\frac{32}{3}\theta\int_\Omega|(\sqrt{\rho})_x|^4\,\mathrm{d}x\\ +\frac{1}{\lambda^2}\int_\Omega|(\rho^2)_x|^2\,\mathrm{d}x\le C\int_\Omega\left(|\rho_x|^2+\rho^2\right)\mathrm{d}x.\end{aligned} \tag{3.35}$$

This estimate will enable us to justify the semiclassical limit. One can even show the existence of a global nonnegative solution with regularity $\rho_{xxx}\in L^{6/5}(Q_T)$, see [24].

Moreover, following (3.14) we may use $1-1/\rho^2$ as test function and then derive the useful inequality

$$\frac{\mathrm{d}}{\mathrm{d}t}E_2(\rho^2)+2\varepsilon^2\int_\Omega|(\ln\rho)_{xx}|^2\,\mathrm{d}x+4\theta\int_\Omega|(\ln\rho)_x|^2\,\mathrm{d}x\le C\int_\Omega|\ln\rho^2|\,\mathrm{d}x. \tag{3.36}$$

Then the following result can be shown, where we study the problem (3.23) with boundary conditions (3.24) or (3.25):

Theorem 3.5 ([24]). *Assume that $E_1(\rho_0^2)$, $E_2(\rho_0^2)$, $E_3(\rho_0^2)$ are finite, $C(x) \in L^\infty(\Omega)$, and the initial state is electrically neutral in the sense of* (3.5). *Then there exists a pair of functions $(\rho_\varepsilon, E_\varepsilon)$ with*

$$\begin{aligned} \rho_\varepsilon^2 &\in L^\infty((0,T); L_\Psi(\Omega)) \cap L^2((0,T); H^1(\Omega)), \\ \rho_\varepsilon &\in L^\infty((0,T); H^1(\Omega)) \cap L^2((0,T); H^2(\Omega)), \\ (\rho_\varepsilon^2)_t &\in L^2((0,T); (H^1(\Omega))'), \\ E_\varepsilon &\in L^\infty((0,T); L^2(\Omega)), \end{aligned}$$

where $L_\Psi(\Omega)$ is the Orlicz space with the Young function $\Psi(s) = s(\ln s - 1) + 1$, such that for all $\varphi \in L^6((0,T); H^2(\Omega))$ with $\varphi_x \in L^6((0,T); H_0^1(\Omega))$, we have (3.30) *(with the canonical replacements of ρ and E by ρ_ε and E_ε). And for all $\eta \in H^1(\Omega)$, the variational identity* (3.31) *holds. Additionally, there is a function $\tilde{G}_\varepsilon \in L^2(Q_T)$ such that for all test functions $\psi \in L^2((0,T); H^1(\Omega))$,* (3.32) *holds with $G = \rho_\varepsilon \tilde{G}_\varepsilon$. Furthermore, as $\varepsilon \to 0$, we have the convergences*

$$\begin{aligned} \rho_\varepsilon^2 &\rightharpoonup n \quad \text{weakly-* in } L^\infty(\Omega); \\ E_\varepsilon &\rightharpoonup E \quad \text{weakly in } L^2(\Omega), \end{aligned}$$

for a.e. $t \in (0,T)$, and also

$$\begin{aligned} \rho_\varepsilon^2 &\to n \quad \text{strongly in } L^2(Q_T); \\ (\rho_\varepsilon^2)_t &\rightharpoonup n_t \quad \text{weakly in } L^2((0,T); (H^1(\Omega))'); \\ \varepsilon^2 \rho_\varepsilon \tilde{G}_\varepsilon &\to 0 \quad \text{strongly in } L^2(Q_T); \\ (\rho_\varepsilon^2)_x - \rho_\varepsilon^2 E_\varepsilon &\rightharpoonup n_x - nE \quad \text{weakly-* in } L^\infty((0,T); L^2(\Omega)). \end{aligned}$$

where (n, E) is a weak solution of the classical drift diffusion model.

Here $\varepsilon^2 \rho_\varepsilon \tilde{G}_\varepsilon$ equals the quantum term $\varepsilon^2 n \left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}} \right)_x$ for positive regular n.

Mixed Dirichlet-Neumann boundary condition (3.27)

If we exchange the boundary conditions (3.24) or (3.25) against the mixed Dirichlet–Neumann boundary condition (3.27), the entropy inequality (3.35) does not hold anymore, and other independent of ε estimates are to be found. In [32] it has been shown how inequalities similar to (3.34) and (3.36) provide enough information to send ε to zero. In particular, it was shown that $\left\| \varepsilon^{1/4} \rho \right\|_{L^8((0,T); L^\infty(\Omega))}$ can be bounded uniformly in ε, and then also $\varepsilon^{5/4} \rho^2 (\ln \rho)_{xx}$ has a uniform estimate in the space $L^{8/5}((0,T); L^2(\Omega))$. A sketch of this approach will be given in Section 3.5.

Isentropic case

In the semiclassical limit problem $\varepsilon \to 0$, we wish the fourth-order term $-\varepsilon^2 \mathrm{div}(n \nabla (n^{-1/2} \triangle n^{1/2}))$ to disappear, and therefore any estimates coming from this term alone are not enough in passing to the limit. The main estimates should come from the next lower-order term in the equation, which is the second-order diffusion term $\operatorname{div}(\nabla P(n))$. In the isothermal case, when $P(n) = \theta n$, this diffusion term gives automatically an estimate on ∇n, but in the isentropic case, $P(n) = T_0 n^\gamma$ being nonlinear, only an estimate on $\nabla(n^{\gamma/2})$ can be obtained. Due to some technical reasons, the first semiclassical limit for isentropic case was found only for $1 < \gamma \le 3/2$ with homogeneous Neumann boundary condition (3.25) in [31]. It was shown there that for $\varepsilon \to 0$, a subsequence of the solutions $(\rho_\varrho, E_\varepsilon, \varepsilon^2 G_\varepsilon)$ constructed in Theorem 3.4 converges in several weak and strong topologies to $(\sqrt{n}, B, 0)$, and n, B solve in a suitable weak sense the system

$$\begin{cases} \quad n_t = (P(n))_{xx} + (nB)_x, \\ -\lambda^2 B_x = n - C. \end{cases}$$

Later on, this result was extended to the case of $1 < \gamma \le 3$ utilizing some tools from the theory of Navier–Stokes equations, see [25]. For the bipolar case and mixed Dirichlet–Neumann boundary conditions (3.27), see [66, 29, 28].

The semiclassical limit of the isentropic quantum drift diffusion model seems to be an open problem for $\gamma > 3$.

3.3.3. Quasineutral limit $\boldsymbol{\lambda \to 0}$. Quasineutrality is widely used in charged particle transport as a means for finding simpler models, with many applications in semiconductor theory and plasma physics. Quasineutrality says that the densities of negative charges (electrons) and of positive charges (holes) are approximately equal over large volumes. Such quasineutral models are obtained in the limit of the (scaled) Debye length λ in (3.3) going to zero, see [63] for an example.

Consider as in [82] the bipolar model with mixed Dirichlet Neumann boundary conditions:

$$\begin{cases} n_t - J_{n,x} = 0, & J_n = -\dfrac{\varepsilon^2}{2}(n(\ln n)_{xx})_x + (P_n(n))_x - nV_x, \\ p_t + J_{p,x} = 0, & J_p = \dfrac{\varepsilon^2}{2}(p(\ln p)_{xx})_x - (P_p(p))_x - pV_x, \\ \quad \lambda^2 V_{xx} = n - p, & \end{cases} \tag{3.37}$$

for $(t, x) \in (0, T) \times (0, 1)$, with initial conditions (3.4) and boundary conditions

$$n = p = 1, \quad n_x = p_x = 0, \quad V = V_\Omega = xU, \quad U \in \mathbb{R}. \tag{3.38}$$

Formally, sending λ to zero in (3.37), we get $n = p$ (assuming the compatibility condition $n_0 = p_0$ for the initial data) and

$$n_t + \frac{\varepsilon^2}{2}(n(\ln n)_{xx})_{xx} = \frac{1}{2}(P_n(n) + P_p(n))_{xx}, \tag{3.39}$$

$$n = 1, \quad n_x = 0 \ \text{ for } x \in \{0, 1\}, \quad n(0, x) = n_0(x). \tag{3.40}$$

Assuming that n and p are positive, sufficiently regular solutions, we can show the identities

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(E_1(n)+E_1(p)\right)+\frac{\varepsilon^2}{2}\int_\Omega n\left((\ln n)_{xx}\right)^2+p\left((\ln p)_{xx}\right)^2\,\mathrm{d}x \tag{3.41}$$
$$+\int_\Omega P_n'(n)\frac{(n_x)^2}{n}+P_p'(p)\frac{(p_x)^2}{p}\,\mathrm{d}x+\frac{1}{\lambda^2}\int_\Omega (n-p)^2\,\mathrm{d}x=0,$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(E_2(n)+E_2(p)\right)+\frac{\varepsilon^2}{2}\int_\Omega \left((\ln n)_{xx}\right)^2+\left((\ln p)_{xx}\right)^2\,\mathrm{d}x \tag{3.42}$$
$$+\int_\Omega P_n'(n)((\ln n)_x)^2+P_p'(p)((\ln p)_x)^2\,\mathrm{d}x$$
$$+\frac{1}{\lambda^2}\int_\Omega (n-p)(\ln n-\ln p)\,\mathrm{d}x=0.$$

Then using several sophisticated estimates related to λ (compare Section 3.5), the quasineutral limit was shown in [82], and the result is the following:

Theorem 3.6. *Let n_0, p_0 be nonnegative initial data with finite entropies $E_1(n_0)$, $E_2(n_0)$, $E_1(p_0)$, $E_2(p_0)$. If the temperature terms are nondecreasing and satisfy the growth conditions $|P_n(s), P_p(s)| \le C(1+|s|^q)$ with $0<q<7/2$, then it holds:*

1. *There exists a pair of nonnegative weak solutions $n^{(\lambda)}, p^{(\lambda)} \in L^{7/2}(Q_T)$, $V^{(\lambda)} \in L^\infty((0,T);H^1(0,1))$ to* (3.37) *and* (3.4) *such that*
$$\ln n^{(\lambda)},\ \ln p^{(\lambda)} \in L^2((0,T);H_0^2(\Omega)),\quad n_t^{(\lambda)},\ p_t^{(\lambda)} \in L^1((0,T);H^{-3}(\Omega)).$$
2. *If in addition, $n_0=p_0$, $q\le 7/3$, then a subsequence of $(n^{(\lambda)}, p^{(\lambda)}, V^{(\lambda)})$ exists, which is not relabeled, such that, as $\lambda\to 0$,*
$$\begin{aligned}(n^{(\lambda)}, p^{(\lambda)}) &\to (n,n) && \text{strongly in } L^3(Q_T);\\ (n_t^{(\lambda)}, p_t^{(\lambda)}) &\rightharpoonup (n_t,n_t) && \text{weakly in } L^{42/41}((0,T);H^{-3}(\Omega));\\ (\ln n^{(\lambda)}, \ln p^{(\lambda)}) &\rightharpoonup (\ln n,\ln n) && \text{weakly in } L^2((0,T);H^2(\Omega));\end{aligned}$$
and the limit function n solves (3.39), (3.40).

Additionally, an idea is sketched in [82] how the critical exponent $q=7/3$ up to which the quasineutral limit can be shown may be raised to $q=5/2$. There seems to be no result on the quasineutral limit for $q>5/2$.

3.3.4. Long time behavior. For the periodic or insulating (homogeneous Neumann) boundary conditions (3.10), the quantum drift diffusion model has a conserved form, and we can expect to have similar long time behavior as in the case of the initial value problem (3.8), compare the results presented in Theorems 3.1 and 3.2. By the logarithmic Sobolev type inequality (3.16) derived in [41], the exponential decay then quickly follows from the entropy inequalities. For the isentropic case with periodic boundary conditions, we quote the following result:

Theorem 3.7 ([31]). *Let* $C(x) \equiv C$ *be a constant,* $\Omega = \mathbb{T}$, $\bar{\rho}_0^2 := \int_{\mathbb{T}} \rho_0^2 \, \mathrm{d}x/|\mathbb{T}|$ *and suppose* $0 \le \rho_0 \in H^1(\mathbb{T})$, $\ln \rho_0 \in L^1(\mathbb{T})$ *and* (3.5) *with* $n_0 = \rho_0^2$.

Then the weak solution ρ *to* (3.23) *obtained in Theorem* 3.4 *satisfies*

$$\left\| \rho(t,\cdot) - \sqrt{\bar{\rho}_0^2} \right\|_{L^2(\mathbb{T})}^2 \le C_0 e^{-Mt}, \ \ \forall\, t \in (0,T],$$

where $M = 16\pi^4\varepsilon^2/|\mathbb{T}|^4$ *and* $C_0^2 = \int_{\mathbb{T}} \rho_0^2 \ln(\rho_0^2/\bar{\rho}_0^2) \, \mathrm{d}x$.

For a decay result (with explicit description of decay rates) on an isentropic bipolar system with mixed Dirichlet–Neumann boundary conditions (3.27), we refer to [28].

3.4. Quantum drift diffusion equations in two and three dimensions

In the higher-dimensional case, the number of analytical results is considerably smaller. We mention some results of [26] on the system

$$\begin{cases} \partial_t \rho^2 = \operatorname{div}\left(-\varepsilon^2 \rho^2 \nabla \left(\dfrac{\triangle \rho}{\rho} \right) + \theta \nabla \rho^2 - \rho^2 \nabla V \right) \\ \lambda^2 \triangle V = \rho^2 - C(x), \end{cases} \tag{3.43}$$

where $x \in \Omega = \mathbb{T}^d$, with the nonnegative initial data ρ_0 and the usual condition (3.5) on the initial charge neutrality.

For such a periodic setting, an inequality for the entropy $E_1(n)$ can be obtained, and other boundary conditions are much harder to get under control. However, the inequality (3.21) brings us into a position to show enough *a priori* estimates only with information on $E_1(n)$. In [26], by careful use of interpolation and Sobolev inequalities, the global existence of weak solutions $(\rho_\varepsilon, V_\varepsilon)$ was shown, provided that $d = 2, 3$, $C \in L^\infty(\mathbb{T}^d)$ and $E_1(\rho_0) < \infty$. Furthermore, if $\int_{\mathbb{T}^d} V_\varepsilon \, \mathrm{d}x = 0$, then as $\varepsilon \to 0$, there is a subsequence which enjoys weak and strong convergences in several topologies to a limit $(\sqrt{n}, V)$ which is a weak solution to the classical drift diffusion equation.

The limit of vanishing scaled Debye length in the bipolar isentropic case was studied in [27] in two and three dimensions, with $1 \le \alpha, \beta < 9/2$ for $d = 2$ and $1 \le \alpha, \beta < 16/5$ in for $d = 3$, with α, β being the exponents of n and p in the pressures P_n and P_p.

3.5. Entropy based methods

In this section, we will give an outline on the entropy based methods to prove global existence, semiclassical limit and the long time behavior. Entropy based methods consist of several steps:

- Build an approximate problem, under the constraint that the entropy inequalities hold also for this problem. Prove that the approximate problem has a solution.
- Find a uniform estimate for the approximate solution, using entropy inequalities adapted to the problem, and Sobolev type inequalities.

- The global existence of the solution will follow from compactness arguments based on the *a priori* estimates obtained so far; and the semiclassical limit and the quasineutral limit can also be shown from *a priori* estimates uniform in the relevant parameters.
- The exponential decay of the solution will be a by-product of the entropy inequalities and special logarithmic Sobolev inequalities.

3.5.1. Approximate problems. As an example, we consider the unipolar case in conservative form, where $\Omega = (0,1) \subset \mathbb{R}^1$,

$$\begin{cases} (\rho^2)_t = J_x, \\ J = \rho^2 F_x, \\ F = -\varepsilon^2 \dfrac{\rho_{xx}}{\rho} + h(\rho^2) - V, \qquad h(\rho^2) = \dfrac{\gamma}{\gamma - 1}\rho^{2(\gamma-1)}, \\ V_{xx} = \rho^2 - C(x), \end{cases} \tag{3.44}$$

with one of the following boundary conditions,

$$\text{Periodic boundary condition} \tag{3.45}$$

$$\rho_x = 0, \quad \rho_{xxx} = 0, \quad V_x = 0, \tag{3.46}$$

$$\rho = 1, \quad V = V_D, \quad F = F_D, \tag{3.47}$$

$$\rho = 1, \quad \rho_x = 0, \quad V = V_D, \tag{3.48}$$

and the usual nonnegative initial values ρ_0 for $t = 0$. For simplicity of notation, we have put $T_0 = 1$ and $\lambda = 1$.

We will build the approximate problem by semidiscretization in time (Rothe's method) and use the implicit scheme, to solve a series of elliptic problems by suitable fixed point arguments.

Split the time interval $(0,T)$ into N parts of equal length τ, with $\tau = T/N$. For any $k = 1, 2, \ldots, N$, given ρ_{k-1}, we will solve the following problem

$$\begin{cases} \dfrac{\rho_k^2 - \rho_{k-1}^2}{\tau} = [\rho_k^2 (F_k)_x]_x & \text{in } \Omega, \\ -\varepsilon^2 \dfrac{(\rho_k)_{xx}}{\rho_k} + h(\rho_k^2) - V_k = F_k & \text{in } \Omega, \\ (V_k)_{xx} = \rho_k^2 - C(x) & \text{in } \Omega, \end{cases} \tag{3.49}$$

where (ρ_k, F_k, V_k) shall satisfy the selected boundary conditions.

We introduce the exponential transform $\rho = e^u$, rewrite (3.49) as elliptic problem for (u_k, F_k, V_k) and derive a first (rough) *a priori* estimate of u_k in $H^1(\Omega)$. By the embedding $H^1(\Omega) \hookrightarrow L^\infty(\Omega)$ we then find a positive constant c_k with $\rho_k(x) \geq c_k$ for all $x \in \Omega$, and it can be shown that (ρ_k, F_k, V_k) is a classical solution. The problem (3.49) can be solved for all k up to $k = N$, and the positive lower bounds c_k are allowed to become smaller and smaller with growing k and with decreasing time step size τ. Details of this positivity preserving scheme can be found in [77], and also [78], [29], [31]. Numerical results on semidiscretized schemes are in [48].

For completeness, we remark that in the higher-dimensional case, an additional term $\delta[\triangle^2(\ln \rho_k^2) + \ln \rho_k^2]$ is typically introduced to regularize the problem and ensure the existence of the approximate solutions, see [74], [26], [27].

3.5.2. Entropy inequalities. For the proof of the existence of (ρ_k, F_k, V_k), some *a priori* estimates coming from entropy inequalities have already been used, and now we list some of the ideas to get these entropy inequalities. A first estimate is immediately given as the conservation of the particle number,

$$\int_\Omega \rho_k^2(x)\,\mathrm{d}x = \int_\Omega \rho_0^2(x)\,\mathrm{d}x, \tag{3.50}$$

valid for periodic boundary conditions or whenever $F_x = 0$ on the boundary, see (3.46). In the case of the other boundary conditions, we need to invest more effort to get an estimate of $\|\rho_k\|_{L^2(\Omega)}$.

Formally, by using F_k as test function in the first equation of (3.49), we derive the inequality

$$\begin{aligned} &\varepsilon^2 \int_\Omega |(\rho_k)_x|^2\,\mathrm{d}x + \int_\Omega \frac{\rho_k^{2\gamma}}{\gamma-1}\,\mathrm{d}x + \frac{1}{2}\int_\Omega |(V_k)_x|^2\,\mathrm{d}x + \tau\int_\Omega \rho_k^2|(F_k)_x|^2\,\mathrm{d}x \\ &\quad\le \varepsilon^2 \int_\Omega |(\rho_{k-1})_x|^2\,\mathrm{d}x + \int_\Omega \frac{\rho_{k-1}^{2\gamma}}{\gamma-1}\,\mathrm{d}x + \frac{1}{2}\int_\Omega |(V_{k-1})_x|^2\,\mathrm{d}x, \end{aligned} \tag{3.51}$$

assuming (3.45) or (3.46). This inequality is a discretized isentropic version of the similar estimate (3.33). The fourth member on the left-hand side is called *entropy production term*. Note that it has no corresponding term on the right-hand side. Unfortunately, this entropy production terms gives us only a limited amount of information.

An idea is to separate the whole entropy into a classical part $\frac{1}{\gamma-1}\int_\Omega \rho_k^{2\gamma}\,\mathrm{d}x + \frac{1}{2}\int_\Omega |(V_k)_x|^2\,\mathrm{d}x$, and a quantum part $\varepsilon^2\int_\Omega |(\rho_k)_x|^2\,\mathrm{d}x$. Using $\ln\rho_k^2$ and $-\frac{(\rho_k)_{xx}}{\rho_k}$ as test functions separately, we find

$$\begin{aligned} &\int_\Omega \left[\rho_k^2(\ln\rho_k^2 - 1) + 3\right]\mathrm{d}x + 2\varepsilon^2\tau\int_\Omega |(\rho_k)_{xx}|^2\,\mathrm{d}x + \frac{32}{3}\varepsilon^2\tau\int_\Omega |(\sqrt{\rho_k})_x|^4\,\mathrm{d}x \\ &\qquad + 4\gamma\tau\int_\Omega \rho_k^{2(\gamma-1)}|(\rho_k)_x|^2\,\mathrm{d}x + \tau\int_\Omega \rho_k^4\,\mathrm{d}x \\ &\quad\le \int_\Omega \left[\rho_{k-1}^2(\ln\rho_{k-1}^2 - 1) + 3\right]\mathrm{d}x + C\tau\int_\Omega \rho_k^2\,\mathrm{d}x \end{aligned} \tag{3.52}$$

and also

$$\int_\Omega |(\rho_k)_x|^2 \,\mathrm{d}x + \frac{1}{2}\varepsilon^2\tau \int_\Omega \rho_k^2 \left|\left(\frac{(\rho_k)_{xx}}{\rho_k}\right)_x\right|^2 \mathrm{d}x + \tau \int_\Omega |(\rho_k^2)_x|^2 \,\mathrm{d}x$$
$$\leq \int_\Omega |(\rho_{k-1})_x|^2 \,\mathrm{d}x + C(\varepsilon)\tau \int_\Omega \rho_k^{4(\gamma-1)} |(\rho_k)_x|^2 \,\mathrm{d}x + C\tau \int_\Omega |(\rho_k)_{xx}|^2 \,\mathrm{d}x \quad (3.53)$$
$$+ C\tau \int_\Omega |(\rho_k)_x|^2 \,\mathrm{d}x + C\tau \int_\Omega \rho_k^2 \,\mathrm{d}x.$$

In the case of $1 < \gamma \leq 3/2$, this inequality can be refined, and in particular, the delicate second and third items of the right-hand side can be replaced by more harmless expressions, see [31].

By using $1 - 1/\rho_k^2$ as test function, we next deduce that

$$\int_\Omega (\rho_k^2 - \ln \rho_k^2) \,\mathrm{d}x + 2\varepsilon^2\tau \int_\Omega |(\ln \rho_k)_{xx}|^2 \,\mathrm{d}x + 4\gamma\tau \int_\Omega \rho_k^{2(\gamma-1)} |(\ln \rho_k)_x|^2 \,\mathrm{d}x$$
$$\leq \int_\Omega (\rho_{k-1}^2 - \ln \rho_{k-1}^2) \,\mathrm{d}x + C\tau \int_\Omega |\ln \rho_k^2| \,\mathrm{d}x + C\tau, \quad (3.54)$$

which corresponds to (3.36).

Remark 3.8. For other boundary conditions, partial integrations in the attempts to prove (3.51), (3.52), (3.53), (3.54) may produce additional terms. The precise situation is as follows:

- In case of the boundary conditions (3.45) and (3.46), the entropy estimates (3.51), (3.52), (3.53), (3.54) can be shown, [24, 31];
- In case of the boundary conditions (3.48), inequalities like (3.52) and (3.54) can be derived, [32];
- In case of (3.47), inequalities like (3.51) and (3.53) are valid, see [30].

Now we are in a position to build the approximate solution:

$$\rho_\tau(t,x) \triangleq \begin{cases} \rho_k(x) & : x \in \Omega,\ t \in ((k-1)\tau, k\tau] \\ \rho_0(x) & : x \in \Omega,\ t = 0 \end{cases}$$
$$V_\tau(t,x) \triangleq \begin{cases} V_k(x) & : x \in \Omega,\ t \in ((k-1)\tau, k\tau] \\ V_0(x) & : x \in \Omega,\ t = 0, \end{cases}$$
$$F_\tau(t,x) \triangleq F_k(x), \qquad \text{for} \quad x \in \Omega,\, t \in ((k-1)\tau, k\tau].$$

The *a priori* estimates obtained so far can be expressed in terms of these approximate solutions. If (3.51) holds, then we have

$$\varepsilon \|(\rho_\tau)_x\|_{L^\infty((0,T);L^2(\Omega))} + \|\rho_\tau\|_{L^\infty((0,T);L^{2\gamma}(\Omega))} \quad (3.55)$$
$$+ \|(V_\tau)_x\|_{L^\infty((0,T);L^2(\Omega))} + \|\rho_\tau (F_\tau)_x\|_{L^2(Q_T)} \leq C.$$

Now assume that only (3.52) and (3.54) are available. From $|\ln s| \leq s - \ln s$ for $s \in \mathbb{R}_+$, (3.54) and Gronwall's Lemma, we find

$$\|\rho_\tau\|_{L^\infty((0,T);L^2(\Omega))} + \varepsilon \|(\ln \rho_\tau)_{xx}\|_{L^2(Q_T)} + \left\|\rho_\tau^{\gamma-2}(\rho_\tau)_x\right\|_{L^2(Q_T)} \leq C. \tag{3.56}$$

Then (3.52) brings us

$$\sup_{[0,T]} E_1(\rho_\tau^2(t)) + \varepsilon^2 \|\rho_\tau\|^2_{L^2((0,T);H^2(\Omega))} + \varepsilon^2 \left\| \frac{((\rho_\tau)_x)^2}{\rho_\tau} \right\|^2_{L^2(Q_T)} \\ + \left\|\rho_\tau^{\gamma-1}(\rho_\tau)_x\right\|_{L^2(Q_T)} + \|\rho_\tau\|_{L^4(Q_T)} \leq C. \tag{3.57}$$

3.5.3. Compactness argument. Let $(\rho_\tau, V_\tau, F_\tau)$ be the approximate solution, obtained as above by piecewise constant interpolation. In general, to each entropy inequality for a smooth function, there is a corresponding discretized version for the approximate solution $(\rho_\tau, V_\tau, F_\tau)$.

The compactness argument will be used in getting both the existence of a global weak solution and the semiclassical limit. Since the problem is nonlinear in ρ_τ, we need strong convergence properties of the approximate solution ρ_τ, to prove a limit of the nonlinear terms, at least in a weak sense. Aubin's lemma ([111], see also the Appendix) will be used to get strong convergence. To apply Aubin's lemma, we need on the one hand some uniform bound for $(\rho_\tau^2)_x$, on the other hand some uniform bound for the discretized time derivative $\partial_t^\tau \rho_\tau^2$ (any Banach space containing functions of very weak regularity will do), which can be obtained from the differential equation if one can control each term of the right-hand side of that equation, including the quantum term. So in the compactness argument, the key steps are to show that

- $(\rho_\tau^2)_x$ is bounded in some sense (this is harder in the isentropic case in comparison to the isothermal case, which brings the restriction $1 < \gamma \leq 3$);
- $\varepsilon^2 \rho_\tau^2 \left(\frac{(\rho_\tau)_{xx}}{\rho_\tau}\right)_x$ is bounded in some sense;
- in the discussion of the semiclassical limit, we show that $\varepsilon^2 \rho_\tau^2 \left(\frac{(\rho_\tau)_{xx}}{\rho_\tau}\right)_x$ goes to zero in some sense.

Further convergences in weak topologies of reflexive spaces follow from the *a priori* estimates (3.55)–(3.57) in a standard way.

Global weak solution

In case of the homogeneous Neumann boundary condition (3.46) and the Dirichlet boundary condition (3.47), the estimate (3.55) holds, and then we find

$$\left\|\rho_\tau^2 (F_\tau)_x\right\|_{L^2(Q_T)} \leq \|\rho_\tau\|_{L^\infty(Q_T)} \|\rho_\tau (F_\tau)_x\|_{L^2(Q_T)} \leq C.$$

Since $H^1(\Omega)$ is an algebra, we also have $\rho_\tau^2 \in L^\infty((0,T); H^1(\Omega))$ with uniform in τ bound. The boundedness of the quantum term $\varepsilon^2 \rho_\tau \left(\frac{(\rho_\tau)_{xx}}{\rho_\tau}\right)_x$ comes from related entropy production terms, cf. [24, 30]. Then we can use the differential equation and obtain

$$\left\|\partial_t^\tau \rho_\tau^2\right\|_{L^2((0,T);(H^1(\Omega))')} \le C_\varepsilon,$$

and Aubin's Lemma can be applied, giving us the uniform convergence of a subsequence $(\rho_\tau)_{\tau\to 0}$ on the domain Q_T.

Next suppose that only the estimates (3.56) and (3.57) are available, but not (3.55). To obtain an estimate of the quantum interaction term $\varepsilon^2\rho_\tau^2\left(\frac{(\rho_\tau)_{xx}}{\rho_\tau}\right)_x = (\varepsilon^2/2)(\rho_\tau^2(\ln\rho_\tau)_{xx})_x$, we split $\varepsilon\rho_\tau(\ln\rho_\tau)_{xx}$ into $\varepsilon(\rho_\tau)_{xx}$ and $-\varepsilon((\rho_\tau)_x)^2/\rho_\tau$, which are both present in (3.57), and then it follows that

$$\|\varepsilon\rho_\tau(\ln\rho_\tau)_{xx}\|_{L^2(Q_T)} \le C.$$

Next we interpolate in Gagliardo–Nirenberg style (see [1], but also [14]),

$$\varepsilon^{1/4}\|\rho_\tau\|_{L^8((0,T);L^\infty(\Omega))} \le C\varepsilon^{1/4}\|\rho_\tau\|^{1/4}_{L^2((0,T);H^2(\Omega))}\|\rho_\tau\|^{3/4}_{L^\infty((0,T);L^2(\Omega))} \le C,$$

and therefore we can write

$$\begin{aligned}\left\|\varepsilon^2\rho_\tau^2(\ln\rho_\tau)_{xx}\right\|&_{L^{8/5}((0,T);L^2(\Omega))} \\ &\le \varepsilon^{3/4}\left\|\varepsilon^{1/4}\rho_\tau\right\|_{L^8((0,T);L^\infty(\Omega))}\|\varepsilon\rho_\tau(\ln\rho_\tau)_{xx}\|_{L^2(Q_T)} \\ &\le C\varepsilon^{3/4},\end{aligned} \tag{3.58}$$

hence we can give an estimate of $\partial_t^\tau\rho_\tau^2$ in the space $L^{8/5}((0,T);H^{-2}(\Omega))$, and Aubin's Lemma is applicable also here. The details can be found in [32].

Semiclassical limit

Now we wish to send ε to zero and consequently we need estimates independent of ε. Consider first the homogeneous Neumann boundary conditions (3.46). Then we can exploit a refined version of (3.53), and combining the estimates of the first two members of the left-hand side of (3.53) then implies

$$\left\|\varepsilon^2\rho_\tau^2\left(\frac{(\rho_\tau)_{xx}}{\rho_\tau}\right)_x\right\|_{L^2(Q_T)} \le \varepsilon\|\rho_\tau\|_{L^\infty(Q_T)}\left\|\varepsilon\rho_\tau\left(\frac{(\rho_\tau)_{xx}}{\rho_\tau}\right)_x\right\|_{L^2(Q_T)} \le C\varepsilon,$$

which vanishes for $\varepsilon\to 0$.

And in case of the mixed Dirichlet boundary condition (3.48), we have (3.56) and (3.57), and then (3.58) shows that the quantum interaction term vanishes weakly for $\varepsilon\to 0$.

Then it can be shown that a weak limit of $(\rho_\varepsilon^2)_{\varepsilon\to 0}$ exists in $L^2(Q_T)$ (at least for a subsequence), and this limit ρ^2 is a distributional solution to the classical drift diffusion equation. If we want to have ρ^2 as a weak solution however (and not just a distributional solution), we need an estimate of $(\rho_\varepsilon)_x$ or $(\rho_\varepsilon^2)_x$ uniform with respect to ε. This can be achieved as follows. If $1\le\gamma\le 2$, then (3.56) and (3.57) give

$$\begin{aligned}
&\|(\rho_\tau)_x\|^2_{L^2(Q_T)} \\
&\quad = \iint_{Q_T\cap\{\rho_\tau<1\}} |(\rho_\tau)_x|^2 \,\mathrm{d}x\,\mathrm{d}t + \iint_{Q_T\cap\{\rho_\tau\geq 1\}} |(\rho_\tau)_x|^2 \,\mathrm{d}x\,\mathrm{d}t \\
&\quad \leq \iint_{Q_T\cap\{\rho_\tau<1\}} \rho_\tau^{2(\gamma-2)}|(\rho_\tau)_x|^2 \,\mathrm{d}x\,\mathrm{d}t + \iint_{Q_T\cap\{\rho_\tau\geq 1\}} \rho_\tau^{2(\gamma-1)}|(\rho_\tau)_x|^2 \,\mathrm{d}x\,\mathrm{d}t \\
&\quad \leq \left\|\rho_\tau^{\gamma-2}(\rho_\tau)_x\right\|^2_{L^2(Q_T)} + \left\|\rho_\tau^{\gamma-1}(\rho_\tau)_x\right\|^2_{L^2(Q_T)} \\
&\quad \leq C.
\end{aligned}$$

And for $2 \leq \gamma \leq 3$ we similarly have

$$\begin{aligned}
&\left\|(\rho_\tau^2)_x\right\|^2_{L^2(Q_T)} \\
&\quad = 4\iint_{Q_T\cap\{\rho_\tau<1\}} \rho_\tau^2|(\rho_\tau)_x|^2 \,\mathrm{d}x\,\mathrm{d}t + 4\iint_{Q_T\cap\{\rho_\tau\geq 1\}} \rho_\tau^2|(\rho_\tau)_x|^2 \,\mathrm{d}x\,\mathrm{d}t \\
&\quad \leq 4\iint_{Q_T\cap\{\rho_\tau<1\}} \rho_\tau^{2(\gamma-2)}|(\rho_\tau)_x|^2 \,\mathrm{d}x\,\mathrm{d}t + 4\iint_{Q_T\cap\{\rho_\tau\geq 1\}} \rho_\tau^{2(\gamma-1)}|(\rho_\tau)_x|^2 \,\mathrm{d}x\,\mathrm{d}t \\
&\quad \leq 4\left\|\rho_\tau^{\gamma-2}(\rho_\tau)_x\right\|^2_{L^2(Q_T)} + 4\left\|\rho_\tau^{\gamma-1}(\rho_\tau)_x\right\|^2_{L^2(Q_T)} \\
&\quad \leq C.
\end{aligned}$$

Then we can send first τ to zero and second ε to zero, and the limit ρ^2 will have the regularity

$$\begin{aligned}
\rho^2 &\in L^4((0,T);L^2(\Omega)) \cap L^{4/3}((0,T);H^1(\Omega)), \\
\partial_t\rho^2 &\in L^{\min(6/(3+\gamma),4/3)}((0,T);H^{-2}(\Omega))
\end{aligned}$$

in case of $1 \leq \gamma \leq 2$, and

$$\begin{aligned}
\rho^2 &\in L^6((0,T);L^2(\Omega)) \cap L^2((0,T);H^1(\Omega)), \\
\partial_t\rho^2 &\in L^{8/(4+\gamma)}((0,T);H^{-2}(\Omega))
\end{aligned}$$

in case of $2 \leq \gamma \leq 3$, compare [28].

Quasineutral Limit

Obtaining the quasineutral limit, which is most meaningful in the bipolar case, is quite a challenge, so we sketch the philosophy of the approach first. From (3.41) and (3.42) we find

$$\begin{aligned}
\|(\ln n, \ln p)\|_{L^2((0,T);H^2(\Omega))} &\leq C, \\
\|n-p\|_{L^2(Q_T)} &\leq C\lambda,
\end{aligned}$$

and the elementary estimate $(x-y)(\ln x - \ln y) \geq 2(\sqrt{x}-\sqrt{y})^2$ implies then

$$\left\|\sqrt{n}-\sqrt{p}\right\|_{L^2(Q_T)} \leq C\lambda.$$

Multiplying (3.37) with a smooth test function ϕ and integrating over Q_T, an integral $\int_{Q_T}(n-p)V_x\phi_x \,\mathrm{d}x\,\mathrm{d}t$ appears which we would like to vanish for $\lambda \to 0$. However, our estimates obtained so far imply only $\|V_x\|_{L^2(Q_T)} \le C\lambda^{-1}$, which is not enough for performing the quasineutral limit.

In [82], a function W was constructed which has the same Dirichlet *and* Neumann boundary values as V, and then $V - W$ was taken as test function in (3.37), leading to an estimate

$$\left\|(\sqrt{n}+\sqrt{p})V_x\right\|_{L^2(Q_T)} \le C\lambda^{-8/9},$$

via several Nirenberg–Gagliardo interpolation steps. Then we quickly deduce the useful estimate

$$\|(n-p)V_x\|_{L^1(Q_T)} \le C\lambda^{1/9},$$

which makes the quasineutral limit possible.

However, some care is necessary here. First, the Neumann boundary values of V explode for $\lambda \to 0$, making the construction of W delicate. Second, the calculations which have led us to the identities (3.41) and (3.42) require a regularity of n and p which is however not available for the solutions $n^{(\lambda)}$ and $p^{(\lambda)}$ as provided by Theorem 3.6. Therefore all the calculations sketched above have been performed on the level of the more regular time-discretized solutions in [82].

3.5.4. Long time asymptotics. The key idea here is to combine an entropy inequality which contains a positive term producing that entropy (the so-called *entropy production term*) with a second inequality which connects this entropy production term back to the entropy under consideration.

A typical example is: in the case of constant doping $C(x)$, we have the entropy inequalities

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \left[\rho^2(\ln\rho^2 - 1) + 1\right]\mathrm{d}x + \frac{\varepsilon^2}{2}\int_\Omega \rho^2|(\ln\rho^2)_{xx}|^2\,\mathrm{d}x \le 0,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega (\rho^2 - \ln\rho^2)\,\mathrm{d}x + \frac{\varepsilon^2}{2}\int_\Omega |(\ln\rho^2)_{xx}|^2\,\mathrm{d}x \le 0.$$

With the help of one type of Logarithmic Sobolev inequality [41],

$$\int_\Omega \left[\rho^2(\ln\rho^2 - 1) + 1\right]\mathrm{d}x \le \frac{\left\|\rho_0^2 - \ln\rho_0^2\right\|_{L^1(\Omega)} + 1}{4}\int_\Omega \rho^2|(\ln\rho^2)_{xx}|^2\,\mathrm{d}x,$$

it is then easy to prove the exponential decay

$$\|\rho - 1\|^2_{L^2(\Omega)} \le \int_\Omega \left[\rho^2(\ln\rho^2 - 1) + 1\right]\mathrm{d}x \le \left\|\rho_0^2(\ln\rho_0^2 - 1) + 1\right\|_{L^1(\Omega)} e^{-2M_0 t},$$

where $M_0 = \varepsilon^2(\left\|\rho_0^2 - \ln\rho_0^2\right\|_{L^1(\Omega)} + 1)^{-1}$.

3.6. Open problems

Multi-dimensional case with physical boundary conditions. As mentioned before, most analytical results in the higher-dimensional case consider periodic boundary conditions only. It would be very interesting to study the whole problem (3.1) with the physically motivated boundary condition (3.6) in the general case.

Large time behavior for nonconstant doping. Here already the one-dimensional case is an open problem. From the view of applications, the stability of steady state solutions is of particular interest.

Internal layer problem (asymptotic analysis). In the generic case, the quantum effect plays its dominant role only in a very thin region. By formal asymptotic expansions, Uno et.al. [115] constructed so-called analytical solutions to the quantum drift diffusion model, with applications to MOS structures, and it was claimed that these analytical solutions reproduce major characteristics of a MOS structure. A rigorous approach could be to first study the limiting profile inside of the layer, then match it with the outer solution, and prove that the solution converges to the classical model. Of course, with different devices, the asymptotics of the layer could be quite complicated. Numerical investigations on boundary layers can be found in [101] and [106].

4. The viscous quantum hydrodynamic model

4.1. Known results

The systems we are studying in this section are first the isothermal viscous quantum hydrodynamic model,

$$\begin{cases} \partial_t n - \nu_0 \triangle n - \operatorname{div} J = 0, \\ \partial_t J + \dfrac{\varepsilon^2}{2} n \nabla \dfrac{\triangle \sqrt{n}}{\sqrt{n}} - \nu_0 \triangle J - T\nabla n + \dfrac{1}{\tau} J = \operatorname{div}\left(\dfrac{J \otimes J}{n}\right) - n\nabla V, \\ \lambda_D^2 \triangle V = n - C(x), \end{cases} \tag{4.1}$$

where the temperature T is a positive constant, and second the full viscous quantum hydrodynamic model, where T is an unknown function of (t, x), and an additional differential equation for the energy density ne is needed. Here $e = e(t, x)$ describes the energy density per mass of electrons, and ne then is the energy density per crystal volume, given by

$$ne = \frac{|J|^2}{2n} + \frac{d}{2} Tn - \frac{\varepsilon^2}{8} n \triangle \ln n = \frac{|J|^2 + \frac{\varepsilon^2}{4}|\nabla n|^2}{2n} + \frac{d}{2} Tn - \frac{\varepsilon^2}{8} \triangle n, \tag{4.2}$$

with d being the spatial dimension. The energy density comprises expressions related to the density of the kinetic energy of the moving particles, the thermic energy, and a quantum correction term. Then the full viscous quantum hydrodynamic system reads

$$\begin{cases} \partial_t n - \nu_0 \triangle n - \operatorname{div} J = 0, \\ \partial_t J + \dfrac{\varepsilon^2}{2} n \nabla \dfrac{\triangle\sqrt{n}}{\sqrt{n}} - \nabla(Tn) - \nu_0 \triangle J + \dfrac{1}{\tau} J = \operatorname{div}\left(\dfrac{J \otimes J}{n}\right) \\ \qquad + \mu \nabla n - n \nabla V, \\ \partial_t(ne) - \operatorname{div}\left(\dfrac{J}{n}(ne + P)\right) - \nu_0 \triangle (ne) + \dfrac{2}{\tau} ne = \mu \operatorname{div} J \\ \qquad - J \cdot \nabla V + \dfrac{d}{\tau} n, \\ \lambda_D^2 \triangle V = n - C(x), \end{cases} \tag{4.3}$$

where $P = Tn\mathbf{1}_d - \frac{\varepsilon^2}{4} n(\nabla \otimes \nabla) \ln n$ is the pressure tensor, $\mathbf{1}_d$ the identity matrix. The subscript at λ_D shall remember us that this parameter is related to the Debye length, in distinction to spectral parameters $\lambda \in \mathbb{C}$ as they appear in Section 4.3.

And the third system we are investigating here has been introduced in [49],

$$\begin{cases} \partial_t n - \nu_0 \triangle n - \operatorname{div} J = 0, \\ \partial_t J + \dfrac{\varepsilon^2}{2} n \nabla \dfrac{\triangle\sqrt{n}}{\sqrt{n}} - \nu_0 \triangle J - \delta \triangle \left(\dfrac{J}{n}\right) - \nabla p(n) + \dfrac{1}{\tau} J = \operatorname{div}\left(\dfrac{J \otimes J}{n}\right) \\ \qquad - n \nabla V, \\ \lambda_D^2 V = n - C(x), \end{cases} \tag{4.4}$$

with an additional term $\delta \triangle (J/n)$ for which also a physical motivation was given in [49]. The function p is a pressure term, typically of the form $p(n) = Tn^\gamma$ for some $\gamma \geq 1$.

Our boundary conditions are either *insulating boundary conditions*,

$$\partial_\nu n = 0, \qquad J = 0, \qquad \partial_\nu(ne) = 0, \qquad \partial_\nu V = 0 \tag{4.5}$$

with ∂_ν being the derivative in direction of the outward unit normal, or

$$n = n_D, \qquad \operatorname{div} J = 0, \qquad J_{\|} = 0, \qquad \partial_\nu(ne) = 0, \quad V = V_D, \tag{4.6}$$

where $J_{\|}$ denotes the tangential component of J at the boundary. This condition means that, at the contacts of the device, the current flows only perpendicular at the boundary, without resistance at the interface. Of course, the condition on ne has to be omitted in case of (4.1) or (4.4).

Or, following [49], we take periodic boundary conditions:

$$\Omega = \mathbb{T}^d. \tag{4.7}$$

Finally, we prescribe the usual initial conditions:

$$n(0, x) = n_0(x), \qquad J(0, x) = J_0(x), \qquad (ne)(0, x) = (ne)_0(x). \tag{4.8}$$

If we study systems with boundary conditions (4.5) or (4.7), we have to assume the initial charge neutrality:

$$\int_\Omega n_0(x) - C(x)\,\mathrm{d}x = 0, \tag{4.9}$$

because solving the Poisson equation for V would be impossible otherwise.

In presenting known results for quantum hydrodynamic systems, we start with an inviscid version ($\nu_0 = 0$) of (4.1), in the one-dimensional case. The existence of local in time solutions was shown in [72], and the stationary problem possesses solutions if we assume small currents [70], [89]. One of the key difficulties is to ensure that the particle density n remains nonnegative, and also the term $(J^2/n)_x$ is hard to get under control. If additionally the current is subsonic, then this stationary solution is exponentially stable. For small applied voltages, stationary solutions have been demonstrated also in [98]. Note that, by the discussion in Section 2.4, the subsonic condition becomes here $|J/n| < \sqrt{T}$.

There is a series of results concerning the Cauchy problem of an inviscid system (4.1), with the condition that the unknown functions approach constant values for $|x| \to \infty$. We mention the existence of a stationary state and its exponential stability in [64], and also results on semiclassical limits ($\varepsilon \to 0$) or relaxation time limits ($\tau \to 0$) of a bipolar quantum hydrodynamic system (for particles of two types) in [123]. Surprisingly, the stationary state to a *bi*polar system has been found to be stable, but only with algebraic decay like $(1+t)^{-k}$, and this is a sharp result [90]. Under some conditions, solutions approach a self-similar profile algebraically, as shown in [91]. The limit $\lambda \to 0$ for a unipolar system was studied in [88]. A further review can be found in [62].

Concerning the viscous version ($\nu_0 > 0$) of (4.1), the existence of classical solutions to the stationary one-dimensional problem for small currents was shown in [57], and this solution is unique in case of small values of ε, ν_0, $|J|$. Note that uniqueness for large current solutions can not be expected because there are electronic devices whose working principle relies on multiple solutions. The inviscid limit $\nu_0 \to 0$, the semiclassical limit $\varepsilon \to 0$, and the hybrid limit $\nu_0^2 + \varepsilon^2/4 \to 0$ were studied in [57], too. Later the existence of stationary solutions was shown for arbitrarily large values of $|J|$ in [75].

The exponential decay to zero of the physical energy (for $C(x) \equiv C_0$)

$$E(t) = \int_\Omega \frac{\varepsilon^2}{2}(\partial_x \sqrt{n})^2 + T\left(n\left(\ln\frac{n}{C_0} - 1\right) + C_0\right) + \frac{\lambda^2}{2}(\partial_x V)^2 + \frac{J^2}{2n}\,\mathrm{d}x$$

(compare also (3.29)) was proved in [56] for a one-dimensional system with a variant of insulating boundary conditions. This decay result was then extended to the higher-dimensional case in [22], where also the exponential stability (for $d = 1$) of a stationary state was shown. Results on the local existence of solutions to (4.1) with $d > 1$ are to be found in [43], as well as a proof of the inviscid limit $\nu_0 \to 0$. Semigroup properties and more stability results (even for the supersonic case, and with explicit description of decay rates) are in [23]. Extensions to general Douglis–Nirenberg systems were presented in [44].

Numerical simulations of the isothermal model (4.1) and the full model (4.3) can be found in [75] and [79]. The full model brings us the additional difficulty of how to ensure that also the temperature $T = T(t, x)$ stays positive everywhere. Combined with the quasilinear terms with third-order derivatives, this makes analytical results hard to reach.

It seems that (4.4) is the first system in quantum hydrodynamics for which the *global* existence of weak solutions could be shown, even for large initial data, see [49]. Then the global existence of weak solutions in the periodic case up to three spatial dimensions was shown in [68].

4.2. Main results

Theorem 4.1 (Local existence). *Let Ω be a bounded domain in $\mathbb{R}^d$ with boundary Γ of regularity $C^{2;1}$. For $p > 2d$ and $d \geq 2$, assume that*

$$n_0 \in W_p^3(\Omega), \qquad J_0 \in W_p^2(\Omega; \mathbb{R}^d), \qquad (ne)_0 \in W_p^2(\Omega),$$

and suppose that these initial data satisfy the chosen boundary condition (4.5) *or* (4.6)*. Moreover assume that $\triangle n_0$ has vanishing Dirichlet boundary values when we study* (4.6)*, and otherwise suppose* (4.9)*. Finally, let*

$$\inf_{x\in\Omega} n_0(x) > 0, \qquad C \in L^p(\Omega),$$
$$n_D \in W_p^{3-1/p}(\Gamma), \qquad V_D \in W_p^{2-1/p}(\Gamma) \qquad \text{(if applicable)}.$$

Then the problem (4.3), (4.8) *has a unique local in time solution satisfying the selected boundary condition, and it has the regularity*

$$\begin{cases} n \in C([0, t_0]; W_p^3(\Omega)) \cap C^1([0, t_0]; W_p^1(\Omega)), \\ J \in C([0, t_0]; W_p^2(\Omega)) \cap C^1([0, t_0]; L^p(\Omega)), \\ ne \in C([0, t_0]; W_p^2(\Omega)) \cap C^1([0, t_0]; L^p(\Omega)), \\ V \in C([0, t_0]; W_p^2(\Omega)) \cap C^1([0, t_0]; L^p(\Omega)). \end{cases}$$

The solution exists as long as n stays positive and n, J remain bounded in $C^{0;1}(\Omega)$ and $L^\infty(\Omega)$, respectively.

We remark that omitting all references to ne in this theorem gives local existence results for (4.1) and (4.4). For (4.1), $p > d$ is sufficient because the principal part of the system then is no longer quasilinear. And also the case $d = 1$ can be handled, after replacing the theory of elliptic systems presented in the next section by a theory of ordinary differential equations.

The proof of Theorem 4.1 will span the whole Section 4.3.

Our next result concerns stationary states of (4.1), which solve

$$\begin{cases} \nu_0 \triangle n + \operatorname{div} J = 0, \\ -\dfrac{\varepsilon^2}{2} n \nabla \dfrac{\triangle \sqrt{n}}{\sqrt{n}} + \nu_0 \triangle J + T \nabla n - \dfrac{1}{\tau} J = n \nabla V - \operatorname{div}\left(\dfrac{1}{n} J \otimes J\right), \\ \lambda_D^2 \triangle V = n - C(x), \end{cases} \tag{4.10}$$

with boundary conditions (4.6).

Theorem 4.2 (Stationary states with small currents). *Let Ω be a convex bounded domain in $\mathbb{R}^d$ with boundary Γ of regularity $C^{2;1}$. Define a function $\overline{V}$ by*

$$\lambda_D^2 \triangle \overline{V} = 0, \qquad \gamma_0 \overline{V} = V_D,$$

and suppose that, for some $p > d$, the data have the regularity

$$C \in W_p^1(\Omega), \qquad n_D \in W_p^{3-1/p}(\Gamma), \qquad V_D \in W_p^{2-1/p}(\Gamma),$$

and that

$$\begin{aligned} &\left\|\nabla \overline{V}\right\|_{L^p(\Omega)} \le \delta, \qquad \|\nabla C\|_{L^p(\Omega)} \le \delta, \\ &\overline{n} := \frac{1}{\operatorname{meas}(\Omega)} \int_\Omega C(x)\,\mathrm{d}x > 0, \\ &\lambda_D^{-2} \overline{n} > \frac{1}{2\tau^2}. \end{aligned} \tag{4.11}$$

Then, if δ is sufficiently small, the problem (4.10), (4.6) *possesses a solution $(n, J, V) \in W_p^3(\Omega) \times W_p^2(\Omega; \mathbb{R}^d) \times W_p^2(\Omega)$ with $\inf_\Omega n > 0$.*

Note that the condition (4.11) is fulfilled in realistic situations: if we follow the scaling from [75], then $\overline{n} \approx 1$, $\tau \approx 1$ and $\lambda_D^2 \approx 10^{-4}$.

Theorem 4.3 (Stability and decay rate). *Let Ω be as in Theorem* 4.2, *and write (n^*, J^*, V^*) for the stationary solution as constructed there, and suppose that*

$$\|n^* - \overline{n}\|_{W_p^2(\Omega)} \le \beta, \qquad \|J^*\|_{W_p^1(\Omega)} \le \beta,$$

for a sufficiently small number β. Let (n_0, J_0) be initial data satisfying the conditions of Theorem 4.1 *with $p > d$, and*

$$\|n_0 - n^*\|_{W_p^2(\Omega)} \le \beta_0, \qquad \|J^* - J_0\|_{W_p^1(\Omega)} \le \beta_0.$$

Then if β_0 is sufficiently small, the solution (n, J, V) provided by Theorem 4.1 *exists globally in time and approaches (n^*, J^*, V^*) exponentially:*

$$\|n(t,\cdot) - n^*(\cdot)\|_{W_p^2(\Omega)} + \|J(t,\cdot) - J^*(\cdot)\|_{W_p^1(\Omega)} \le C \exp\left(-\frac{t}{2\tau'}\right), \quad 0 < t < \infty,$$

for any $\tau' > \tau$, with $C = C(\tau')$.

Theorems 4.2 and 4.3 will be proved in Section 4.4.

Finally, we study the system (4.1) on a rectangular domain $\Omega = (0, L_1) \times (0, L_2) \subset \mathbb{R}^2$, and we restrict our attention to the case $d = 2$, for notational simplicity. The boundary $\Gamma = \partial\Omega$ is split into an insulating part Γ_N and a contacts part Γ_D,

$$\Gamma_N = \partial\Omega \cap (0, L_1) \times \{0, L_2\},$$
$$\Gamma_D = \partial\Omega \cap \{0, L_1\} \times (0, L_2)$$

and the boundary conditions are either

$$\begin{cases} n = n_D, & \partial_\nu J_1 = 0, \quad J_2 = 0, \quad V = V_D, \quad \text{on } \Gamma_D, \\ \partial_\nu n = 0, & \partial_\nu J_1 = 0, \quad J_2 = 0, \quad \partial_\nu V = 0, \quad \text{on } \Gamma_N, \end{cases} \tag{4.12}$$

with the natural compatibility conditions $\partial_2 n_D = \partial_2 V_D = 0$ in the four corners of Ω, or a variation of periodic boundary conditions

$$\begin{cases} (n, \partial_\nu n, J, \partial_\nu J, \partial_\nu V)(0, x_2) = (n, \partial_\nu n, J, \partial_\nu J, \partial_\nu V)(L_1, x_2), \quad x_2 \in (0, L_2), \\ \qquad \partial_\nu n = 0, \quad \partial_\nu J_1 = 0, \quad J_2 = 0, \quad \partial_\nu V = 0, \quad \text{on } \Gamma_N. \end{cases} \tag{4.13}$$

Note that V is allowed to jump when going from the right contact back to the left.

Theorem 4.4. *For $p > 2$, assume that the initial data have the regularity*

$$n_0 \in W_p^3(\Omega), \qquad J_0 \in W_p^2(\Omega), \qquad \inf_{x\in\Omega} n_0(x) > 0,$$

and satisfy the boundary conditions (4.12) *or* (4.13)*, respectively. In case of the latter we suppose* (4.9).

Then the problem (4.1), (4.12) *possesses a unique local in time solution with the regularity*

$$\begin{cases} n \in C([0, t_0]; W_p^3(\Omega)) \cap C^1([0, t_0]; W_p^1(\Omega)), \\ J \in C([0, t_0]; W_p^2(\Omega)) \cap C^1([0, t_0]; L^p(\Omega)), \\ V \in C([0, t_0]; W_p^2(\Omega)) \cap C^1([0, t_0]; L^p(\Omega)), \end{cases}$$

and so does the problem (4.1), (4.13).

Variants of the Theorems 4.2 and 4.3 also hold for the case of a rectangular Ω.

4.3. Elliptic systems of mixed order

In a first part, we recall known results about mixed-order elliptic systems, and in a second part, we apply these results to the quasilinear systems (4.1), (4.3), (4.4).

4.3.1. General results. Following the presentation in [3], we recall that a matrix differential operator of order m,

$$A(x, D_x) = \sum_{|\alpha|\le m} a_\alpha(x) D_x^\alpha, \qquad a_\alpha \in C_b^\infty(\mathbb{R}^n; \mathbb{C}^{N\times N}), \qquad D_x := \frac{1}{\mathrm{i}}\nabla_x, \tag{4.14}$$

is called *elliptic* if there are positive constants c_0 and C such that the *pseudodifferential symbol* $\sigma(A)$ of A,

$$\sigma(A)(x,\xi) := \sum_{|\alpha|\le m} a_\alpha(x)\xi^\alpha, \qquad (x,\xi)\in\mathbb{R}^n\times\mathbb{R}^n,$$

is an invertible matrix for $|\xi|\ge C$ and all $x\in\mathbb{R}^n$, with the estimate for the inverse matrix

$$\left|(\sigma(A)(x,\xi))^{-1}\right| \le c_0^{-1}\langle\xi\rangle^{-m}, \quad \forall\,(x,\xi)\in\mathbb{R}^n\times\{|\xi|\ge C\}, \quad \langle\xi\rangle := (1+|\xi|^2)^{1/2}.$$

This is equivalent to the condition on the *principal symbol* $\sigma_{\text{pr}}(A)$,

$$\sigma_{\text{pr}}(A)(x,\xi) := \sum_{|\alpha|=m} a_\alpha(x)\xi^\alpha, \qquad (x,\xi)\in\mathbb{R}^n\times\mathbb{R}^n,$$

to be uniformly invertible for $|\xi|=1$ (with possibly new constant c_0):

$$|\det(\sigma_{\text{pr}}(A)(x,\xi))| \ge c_0, \qquad \forall\,(x,\xi)\in\mathbb{R}^n\times\{|\xi|=1\}.$$

Then the next result is classical ([107], [60], and also [84]):

Theorem 4.5. *The following conditions are equivalent:*

- *the operator A from* (4.14) *is elliptic,*
- *there is a pseudodifferential operator $A^\sharp\in\Psi^{-m}(\mathbb{R}^n\times\mathbb{R}^n)$ (called a* parametrix) *such that the operators $A\circ A^\sharp-\text{id}$ and $A^\sharp\circ A-\text{id}$ are regularizing operators from $\mathcal{L}(H^t(\mathbb{R}^n;\mathbb{C}^N);H^r(\mathbb{R}^n;\mathbb{C}^N))$ for any $t,r\in\mathbb{R}$.*

Here $\mathcal{L}(X;Y)$ denotes the space of linear and continuous maps from the topological vector space X to the topological vector space Y.

An operator $B\in\mathcal{L}(C_0^\infty(\mathbb{R}^n);C^\infty(\mathbb{R}^n))$ is called a *pseudodifferential operator from the class* $\Psi^\mu(\mathbb{R}^n_x\times\mathbb{R}^n_\xi)$ if it has a representation

$$(Bu)(x) = \int_{\mathbb{R}^n_\xi} e^{\mathrm{i}x\xi} b(x,\xi)\hat{u}(\xi)\,đ\xi, \qquad u\in C_0^\infty(\mathbb{R}^n), \qquad đ\xi := \frac{\mathrm{d}\xi}{(2\pi)^n},$$

where $\hat{u}(\xi) = \{\mathcal{F}_{x\to\xi}u\}(\xi)$ is the Fourier transform of u, and the pseudodifferential symbol $b=\sigma(B)$ satisfies the estimates

$$\left|\partial_x^\alpha\partial_\xi^\beta b(x,\xi)\right| \le C_{\alpha\beta}\langle\xi\rangle^{\mu-|\beta|}, \qquad (x,\xi)\in\mathbb{R}^n\times\mathbb{R}^n.$$

For the theory of pseudodifferential operators, we refer to [46], [61, Vol.III], [85], or [113], [114]. Here we only mention that any operator from $\Psi^\mu(\mathbb{R}^n\times\mathbb{R}^n)$ can be extended to a continuous map from $H^{s+\mu}(\mathbb{R}^n)$ to $H^s(\mathbb{R}^n)$, for all $s\in\mathbb{R}$.

The concept of elliptic matrix differential operators of order m has been generalized by Douglis, Nirenberg [42], and Volevich [117] to matrix operators of *mixed order* as follows: consider the pseudodifferential symbol $\sigma(A)$ of A, where each entry of this matrix is a polynomial in the variable ξ. Define $L(x,\xi) := \det\sigma(A)(x,\xi)$, and this determinant comprises $N!$ summands. Call $r := \deg L(x,\xi)$ the degree of this determinant as a polynomial in ξ, and let R be the maximal degree of all the $N!$ summands. Clearly, $r \le R$. Then the (uniform) ellipticity in the sense of Douglis–Nirenberg and Volevich is defined as follows:

It holds $r = R$, and there are positive constants c_0 and C with the property that $|L(x,\xi)| \ge c_0 \langle \xi \rangle^r$ for all (x,ξ) with $x \in \mathbb{R}^n$ and $|\xi| \ge C$.

Volevich [117] has shown that then integers $s_1, \dots, s_N$ and $m_1, \dots, m_N$ exist such that $\deg a_{jk} \le s_j + m_k$ for all (j,k), and with $\sum_{j=1}^N (s_j + m_j) = r$. Here we follow the convention $a_{jk} \equiv 0$ for those (j,k) with $s_j + m_k < 0$. We write a^0_{jk} for that part of a_{jk} that has order exactly equal to $s_j + m_k$ (assuming that such a part of a_{jk} exists, otherwise $a^0_{jk} := 0$, of course). All those a^0_{jk} form the principal part A^0 of A, by definition. Write

$$a_{jk} = \sum_{|\beta| \le s_j + m_k} a_{jk\beta}(x) D_x^\beta, \qquad 1 \le j,k \le N. \tag{4.15}$$

We suppose *proper ellipticity*: the degree r of $\det \sigma(A^0)$ as a polynomial of ξ is even (say $2q$), and for all $x \in \overline{\Omega}$ and any pair ξ, η of linearly independent vectors from $\mathbb{R}^n$, the polynomial $z \mapsto \det \sigma(A^0)(x, \xi + z\eta)$ has exactly q roots $z = z(x,\xi,\eta)$ in the upper half-plane of $\mathbb{C}$. If the spatial dimension n is at least 3, then proper ellipticity follows from ellipticity; and for $n = 2$ it is an additional condition (compare the Cauchy–Riemann operator).

We need this number q to be an integer, because it is related to the number of boundary conditions if we wish to solve a system like $Au = f$ in an open bounded domain $\Omega \subset \mathbb{R}^n$, with smooth boundary $\Gamma = \partial\Omega$, as we do now.

Consider a matrix $B = (b_{jk})$ of differential operators at the boundary with entries

$$b_{jk} = \gamma_0 \sum_{|\beta| \le \deg b_{jk}} b_{jk\beta}(x) D_x^\beta, \qquad 1 \le j \le q, \qquad 1 \le k \le N, \tag{4.16}$$

where γ_0 is the usual trace operator at $\partial\Omega$, and we assume that there are integers $r_1, \dots, r_q$ such that $\deg b_{jk} \le r_j + m_k$, following again the convention $b_{jk} \equiv 0$ for those (j,k) with $r_j + m_k < 0$.

To formulate a condition which boundary differential operators B can lead to a well-posed boundary value problem to the interior differential operator A, we first construct the matrix B^0 of the principal parts b^0_{jk} of the scalar differential operators b_{jk}. Second, for any point $x^* \in \partial\Omega$, we shift and rotate the coordinate system in such a way that x^* becomes the origin, and the interior normal vector at x^* corresponds to the x_n-axis. In this new coordinate frame, the cotangent variable shall be written $\xi = (\xi_1, \dots, \xi_n) = (\xi', \xi_n)$.

Condition 4.1 (**Shapiro–Lopatinskii condition).** For each $\xi' \in \mathbb{R}^{n-1} \setminus \{0\}$, the system of ordinary differential equations on the half-line $\{0 < x_n < \infty\}$

$$A^0(0, \xi', D_{x_n}) v(x_n) = 0, \qquad 0 < x_n < \infty$$

with the initial condition

$$(B^0(0, \xi', D_{x_n}) v(x_n))_{|x_n = 0} = h$$

has exactly one solution in the space of functions $v \in C^\infty(\mathbb{R}_+; \mathbb{C}^N)$ that decay for $x_n \to \infty$, for each vector $h \in \mathbb{C}^q$.

Then the boundary value problem

$$\begin{cases} Au = f, & x \in \Omega, \\ Bu = g, & x \in \partial\Omega, \end{cases} \tag{4.17}$$

is called *elliptic* if A is a mixed-order elliptic operator of Douglis–Nirenberg type and Condition 4.1 is valid at each point $x^* \in \partial\Omega$.

To the fixed parameter sets $(s_1, \dots, s_N)$, $(m_1, \dots, m_N)$ and $(r_1, \dots, r_q)$, we define Sobolev spaces,

$$\begin{aligned} W_p^{\{\sigma+m_k\}}(\Omega) &= W_p^{\sigma+m_1}(\Omega) \times \cdots \times W_p^{\sigma+m_N}(\Omega), \\ W_p^{\{\sigma-s_j\}}(\Omega) &= W_p^{\sigma-s_1}(\Omega) \times \cdots \times W_p^{\sigma-s_N}(\Omega), \\ W_p^{\sigma}(\Omega, \Gamma) &= W_p^{\{\sigma-s_j\}}(\Omega) \times W_p^{\{\sigma-r_j-1/p\}}(\Gamma), \end{aligned}$$

where the Sobolev spaces on the boundary Γ are defined in a similar way as the Sobolev spaces in Ω.

A key result then is:

Theorem 4.6 ([3]). *Suppose that Ω is bounded and*

$$\sigma \geq -\min_k m_k, \qquad \sigma \geq \max_j s_j, \qquad \sigma \geq \max_j r_j + 1/2.$$

Then the following conditions are equivalent:

- *the problem* (4.17) *is elliptic,*
- *solutions u to* (4.17) *satisfy the* a priori *estimate*

$$\sum_{k=1}^{N} \|u_k\|_{W_2^{\sigma+m_k}(\Omega)} \leq C \left(\sum_{j=1}^{N} \|f_j\|_{W_2^{\sigma-s_j}(\Omega)} + \sum_{j=1}^{q} \|g_j\|_{W_2^{\sigma-r_j-1/2}(\Gamma)} + \sum_{k=1}^{N} \|u_k\|_{L^2(\Omega)} \right),$$

- *the operator*

$$\mathcal{A}_B := (A, B) \colon W_2^{\{\sigma+m_k\}}(\Omega) \to W_2^{\sigma}(\Omega, \Gamma)$$

is a Fredholm operator.

Remember that for Banach spaces X, Y, an operator $\mathcal{A} \in \mathcal{L}(X; Y)$ is called a *Fredholm operator* if the kernel of $\mathcal{A}$ is a finite-dimensional subspace of X, and the algebraically defined quotient space $Y/\operatorname{img}\mathcal{A}$ is also finite-dimensional. Then ([109]) the range space $\operatorname{img}\mathcal{A}$ is a closed subspace of Y, and the quotient space $Y/\operatorname{img}\mathcal{A}$ turns into a topological space in the usual way, called the *co-kernel of $\mathcal{A}$*.

Remark 4.7. The differing values of the order parameters may have surprising consequences. Suppose $s_j + m_k \geq 0$ for all (j,k). Then $W_2^{\{\sigma+m_k\}}(\Omega) \hookrightarrow W_2^{\{\sigma-s_j\}}(\Omega)$, and we can study the operator $\mathcal{A}$ in the ground space $W_2^{\{\sigma-s_j\}}(\Omega)$ with domain

$$D(\mathcal{A}) := \left\{ u \in W_2^{\{\sigma+m_k\}}(\Omega) \colon Bu = 0 \right\},$$

which is a closed operator by the *a priori* estimate from Theorem 4.6. But it is not densely defined if one of the boundary conditions expressed by the operator B is meaningful in the ground space $W_2^{\{\sigma-s_j\}}(\Omega)$. As a consequence, it is impossible to define the adjoint operator, at least without choosing another ground space.

And also the formally adjoint operator to (A, B) may not be elliptic because the number of boundary conditions differs from q. As an example, we choose a slightly modified principal part from (4.1),

$$A = \begin{pmatrix} \alpha\triangle & \operatorname{div} \\ -\nabla \operatorname{div} A'\nabla & \alpha \triangle \mathbf{1}_d \end{pmatrix}, \qquad B = \gamma_0 \mathbf{1}_{d+1}, \qquad x \in \Omega \subset \mathbb{R}^d,$$

with $\alpha > 0$ and $A' \in \mathbb{R}^{d\times d}$ being a symmetric positive definite matrix. By the methods from the proof of Proposition 4.11 one can show that (A, B) is an elliptic boundary value problem. For a function $U \in L^2(\Omega; \mathbb{C}^{d+1})$ we write $U = (u_1, \dots, u_{d+1})^\top = \binom{u_1}{u'}$, and set $(\varphi, \psi)_M := \int_M \varphi\psi \,\mathrm{d}x$ for scalar-valued or vector-valued φ, ψ and a manifold M. If $BU = 0$ and ν denotes the outer unit normal vector field, then we formally have

$$\begin{aligned} (AU, V)_\Omega = {} & \left(U, \begin{pmatrix} \alpha\triangle & \nabla A'\nabla \operatorname{div} \\ -\nabla & \alpha \triangle \mathbf{1}_d \end{pmatrix} V \right)_\Omega \\ & + (\nu\nabla u_1, \alpha v_1)_{\partial\Omega} + (\nu A'\nabla u_1, \operatorname{div} v')_{\partial\Omega} \\ & + (\nu\nabla u', \alpha v')_{\partial\Omega} - (\operatorname{div} A'\nabla u_1, \nu v')_{\partial\Omega}, \end{aligned}$$

giving us $q + 1$ boundary conditions in the adjoint operator B', namely $\gamma_0 v_1 = 0$, $\gamma_0 v' = 0$ and $\gamma_0 \operatorname{div} v' = 0$, assuming that A' is not a multiple of the identity matrix.

Now our goal shall be deriving estimates for the resolvent $(\mathcal{A} - \lambda)^{-1}$ in suitably chosen function spaces. To this end, we need the concept of *ellipticity with parameter* for the system

$$\begin{cases} (A - \lambda)u = f, & x \in \Omega, \\ Bu = g, & x \in \partial\Omega, \end{cases} \tag{4.18}$$

where λ is from a closed sector $\mathcal{L}$ of $\mathbb{C}$ with vertex at the origin. Here we restrict ourselves to the special case of

$$\begin{aligned} m_j + s_j &= m, \qquad \text{for all} \quad j = 1, \dots, N, \\ r_j &< m, \qquad \text{for all} \quad j = 1, \dots, mN/2 = q. \end{aligned}$$

Definition 4.8. The boundary value problem (4.18) is called *elliptic with parameter in the sector* $\mathcal{L}$ if the following conditions hold:

Interior ellipticity. $\det(A^0(x,\xi) - \lambda \mathbf{1}_N) \neq 0$ for all $(x,\xi,\lambda) \in \overline{\Omega} \times \mathbb{R}^n \times \mathcal{L}$ with $|\xi| + |\lambda| > 0$.

Shapiro–Lopatinskii condition. Let $x^0 \in \partial\Omega$ and the system (4.18) be rewritten in local coordinates near x^0 (using a translation and a rotation), in such a way that x^0 corresponds to $x = 0$, and the interior normal vector at x^0 corresponds to the coordinate half-axis with $x_n > 0$. Then the boundary value problem on the half-line

$$\begin{cases} A^0(0,\xi',D_{x_n})v(t) - \lambda v(t) = 0, & 0 < t = x_n < \infty, \\ B_j^0(0,\xi',D_{x_n})v(t) = 0, & t = 0, \qquad j = 1,\ldots,mN/2, \\ \lim\limits_{t\to+\infty} v(t) = 0 & \end{cases} \tag{4.19}$$

always has only the trivial solution $v \equiv 0$, for all $(\xi',\lambda) \in \mathbb{R}^{n-1} \times \mathcal{L}$ with $|\xi'| + |\lambda| > 0$.

For a parameter-elliptic system, it is no longer necessary to assume proper ellipticity, because in [4] it has been shown that the interior ellipticity condition has the consequence $mN \in 2\mathbb{N}$.

To prepare resolvent estimates, we define parameter-dependent norms,

$$\|v\|_{\sigma,p,\Omega;\lambda} = \|v\|_{W_p^\sigma(\Omega)} + |\lambda|^{\sigma/m} \|v\|_{L^p(\Omega)}, \qquad \sigma \in \mathbb{N}_0,$$

$$\|w\|_{\sigma-1/p,p,\Gamma;\lambda} = \|w\|_{W_p^{\sigma-1/p}(\Omega)} + |\lambda|^{(\sigma-1/p)/m} \|w\|_{L^p(\Gamma)}, \qquad \sigma \in \mathbb{N}_+,$$

where $1 < p < \infty$ and $\lambda \in \mathbb{C} \setminus \{0\}$.

Condition 4.2 (**Regularity of Ω and the coefficients**). We assume that Γ has the regularity $C^{\max_j m_j + m - 1;1}$, and the coefficients $a_{jk\beta}$ from (4.15) satisfy

$$a_{jk\beta} \in \begin{cases} C^{m_j-1;1}(\overline{\Omega}) & : |\beta| \le s_j + m_k, \quad m_j > 0, \\ C(\overline{\Omega}) & : |\beta| = s_j + m_k, \quad m_j = 0, \\ L^\infty(\Omega) & : |\beta| < s_j + m_k, \quad m_j = 0, \end{cases}$$

and furthermore $b_{jk\beta} \in C^{m-r_j-1;1}(\Gamma)$ for all j,k,β, cp. (4.16).

Then we have the following result on existence, uniqueness and estimates for solutions to (4.18) from [105], [47]. (See also [3, Theorem 6.4.1] for an L^2 based result for systems of much more general structure.)

Theorem 4.9. *Suppose that the boundary value problem* (4.18) *is parameter-elliptic in a sector* $\mathcal{L}_0$*, and assume Condition* 4.2.

Then there exists a $\lambda_0 = \lambda_0(p)$ *such that for* $\lambda \in \mathcal{L}_0$ *with* $|\lambda| \ge \lambda_0$*, problem* (4.18) *has a unique solution* $u \in W_p^{\{m+m_k\}}(\Omega)$ *for any* $f \in W_p^{\{m-s_j\}}(\Omega)$ *and* *boundary data* $g \in W_p^{\{m-r_j-1/p\}}(\Gamma)$*, and the* a priori *estimate*

$$\sum_{j=1}^{N} \|u_j\|_{m_j+m,p,\Omega;\lambda} \le C \left(\sum_{j=1}^{N} \|f_j\|_{m_j,p,\Omega;\lambda} + \sum_{j=1}^{mN/2} \|g_j\|_{m-r_j-1/p,p,\Gamma;\lambda} \right)$$

holds, where the constant C *does not depend upon* f, g *and* λ*.*

From this inequality in parameter-dependent norms, a resolvent estimate can be derived in a certain L^p based ground space which we construct now. By re-arranging, we may assume that the parameters m_k are ordered,

$$m_1 = \cdots = m_{p_1} > m_{p_1+1} = \cdots = m_{p_2} > m_{p_2+1} = \cdots > \cdots = m_{p_Q} = 0,$$
$$0 = p_0 < p_1 < \cdots < p_Q = N.$$

It is then natural to split the unknown functions,

$$u = (U_1, \dots, U_Q), \qquad U_k = (u_{p_{k-1}+1}, \dots, u_{p_k}), \qquad k = 1, \dots, Q,$$

and the right-hand side f is split in the same way.

By physical arguments, it seems reasonable to assume that components of u belonging to differing values of m_k do not appear in the same boundary condition, which leads us to the following two assumptions, which are valid for our boundary conditions (4.5) and (4.6).

Condition 4.3. The collection of boundary conditions $B_j u = g_j$ for $j = 1, \dots, q = mN/2$ can be expressed as

$$B^{(k)} U_k = G_k, \qquad k = 1, \dots, Q,$$

where $B^{(k)}$ is a matrix differential operator of size $m(p_k - p_{k-1})/2 \times (p_k - p_{k-1})$, of order less than m, and $m(p_k - p_{k-1}) \in 2\mathbb{N}_+$.

Condition 4.4. For $1 \le k \le Q - 1$, there is a $(p_k - p_{k-1}) \times (p_k - p_{k-1})$ matrix partial differential operator A_k on Ω of order m, such that

$$\mathcal{A}_k := (A_k, B^{(k)})$$

is a parameter-elliptic boundary value problem in a sector $\mathcal{L}_1$ of $\mathbb{C}$.

Then by elliptic regularity, we have

$$D(\mathcal{A}_k) = \left\{ v \in W_p^m(\Omega; \mathbb{C}^{p_k - p_{k-1}}) \colon B^{(k)} v = 0 \right\}.$$

Next we set, with $\lfloor x \rfloor$ as the largest integer not greater than x,

$$t_k = \lfloor \frac{m_{p_k}}{m} \rfloor, \qquad k = 1, \dots, Q,$$

and using the complex interpolation method (see [108]), we define

$$X_k = \begin{cases} \left[D(\mathcal{A}_k^{t_k}), D(\mathcal{A}_k^{t_k+1}) \right]_{(m_{p_k} - t_k m)/m} & : 1 \le k \le Q-1, \\ L^p(\Omega; \mathbb{C}^{p_Q - p_{Q-1}}) & : k = Q, \end{cases}$$
$$X = X_1 \times \cdots \times X_Q,$$

which shall be the base space for the operator $\mathcal{A}$. For related results on this idea of incorporating certain boundary conditions into the base space X, see [2].

Then the following key result was shown in [44]:

Theorem 4.10. *Suppose that* (4.18) *is a parameter-elliptic system in a sector* $\mathcal{L}_0$*, and assume the Conditions* 4.2, 4.3*,* 4.4*. Then the operator*

$$\begin{aligned}\mathcal{A} &:= \left(A, B_1, \dots, B_{mN/2}\right), \\ D(\mathcal{A}) &:= \{(U_1, \dots, U_Q) \in X\colon A_k U_k \in X_k, \quad (k = 1, \dots, Q-1) \\ &\qquad U_Q \in W_p^m(\Omega; \mathbb{C}^{p_Q - p_{Q-1}}), \quad B^{(Q)} U_Q = 0\Big\}\end{aligned}$$

enjoys the following resolvent estimate in the sector $\mathcal{L}_0 \cap \mathcal{L}_1$ *for large* $|\lambda|$*:*

$$|\lambda| \cdot \left\|(\mathcal{A} - \lambda)^{-1}\right\|_{\mathcal{L}(X;X)} + \left\|(\mathcal{A} - \lambda)^{-1}\right\|_{\mathcal{L}(X;D(\mathcal{A}))} \leq C.$$

And if $\mathcal{L}_0 \cap \mathcal{L}_1$ *is a sector of* $\mathbb{C}$ *that strictly contains the right half-plane, then* $\mathcal{A}$ *generates an analytic semigroup on the space* X*.*

A remark on the domain $D(\mathcal{A})$ is in order. First, the auxiliary operator A_k is not uniquely defined; for you can always modify its lower-order terms, at least. This will not affect $D(\mathcal{A}_k)$, but all the $D(\mathcal{A}_k^t)$ for $t \geq 2$ will be influenced by this choice, leading to variations in the definition of X and $D(\mathcal{A})$. The regularity of the elements of X and $D(\mathcal{A})$ will always be independent of the choice of A_k, only the asymptotic expansion at the boundary will change. One could use this variability in the definition of X and $D(\mathcal{A})$ for an additional fine-tuning. Note however that the variability of X will not become visible if all s_j are non-negative, because then m_{p_k} is at most m.

4.3.2. Mixed-order systems in quantum hydrodynamics. Now we discuss the ellipticity of the systems (4.1), (4.3) and (4.4) together with the boundary conditions (4.5) and (4.6). Concerning the periodic boundary condition (4.7), it only remains to mention that the general results from Section 4.3.1 can be directly transferred from $\mathbb{R}^n$ to the case of a closed smooth manifold.

Concerning (4.1), we have $N = d + 1$, $U = (n, J)^\top$, $(s_1, s_2, \dots, s_{d+1}) = (1, 2, \dots, 2)$ and $(m_1, m_2, \dots, m_{d+1}) = (1, 0, \dots, 0)$, and the system transfers into

$$\partial_t U - AU = \begin{pmatrix} 0 \\ \operatorname{div}\left(\frac{J \otimes J}{n} + \frac{\varepsilon^2}{4} \frac{(\nabla n) \otimes (\nabla n)}{n}\right) - n \nabla V \end{pmatrix},$$

$$A = \begin{pmatrix} \nu_0 \triangle & \operatorname{div} \\ -\frac{\varepsilon^2}{4} \nabla \triangle + T \nabla & \nu_0 \triangle \mathbf{1}_d - \frac{1}{\tau} \mathbf{1}_d \end{pmatrix}, \qquad A^0 = \begin{pmatrix} \nu_0 \triangle & \operatorname{div} \\ -\frac{\varepsilon^2}{4} \nabla \triangle & \nu_0 \triangle \mathbf{1}_d \end{pmatrix}, \quad (4.20)$$

compare (3.7).

With regard to the system (4.3), we note that, by (4.2),

$$\frac{d}{2}\nabla(Tn) = \frac{\varepsilon^2}{8}\nabla\triangle n + \nabla(ne) - \frac{1}{2}\nabla\left(\frac{|J|^2}{n} + \frac{\varepsilon^2}{4}\frac{|\nabla n|^2}{n}\right),$$

$$\begin{aligned}\operatorname{div}\left(\frac{J}{n}P\right) &= -\frac{\varepsilon^2}{4}\frac{d-1}{d}\frac{J}{n}\nabla\triangle n - \frac{\varepsilon^2}{4}\operatorname{tr}\left((\nabla\otimes\nabla n)\cdot\nabla\frac{J}{n}\right) + \frac{\varepsilon^2}{4d}\triangle n\cdot\operatorname{div}\frac{J}{n}\\ &\quad + \frac{\varepsilon^2}{4}\operatorname{div}\left(\frac{(\nabla n)\otimes(\nabla n)}{n}\cdot\frac{J}{n}\right) - \frac{1}{d}\operatorname{div}\left(\left(\frac{|J|^2}{n} + \frac{\varepsilon^2}{4}\frac{|\nabla n|^2}{n}\right)\frac{J}{n}\right)\\ &\quad + \frac{2}{d}\operatorname{div}\left(ne\cdot\frac{J}{n}\right),\end{aligned}$$

with tr being the trace of a matrix. Then the unknowns are $U = (n, J, ne)^\top$, the parameters are $(s_1, \ldots, s_{d+2}) = (1, 2, \ldots, 2)$ and $(m_1, \ldots, m_{d+2}) = (1, 0, \ldots, 0)$, and the system becomes

$$\partial_t U - A_{\text{full}}U = F\left(\{D_x^\alpha n\}_{|\alpha|\le 2}, \{D_x^\alpha J\}_{|\alpha|\le 1}, \{D_x^\alpha (ne)\}_{|\alpha|\le 1}, \nabla V\right),$$

now with a nonlinear matrix differential operator

$$A_{\text{full}} = \begin{pmatrix} \nu_0\triangle & \operatorname{div} & 0\\ -\frac{\varepsilon^2}{4}\frac{d-1}{d}\nabla\triangle + \mu\nabla & \nu_0\triangle\mathbf{1}_d - \frac{1}{\tau}\mathbf{1}_d & \frac{2}{d}\nabla\\ -\frac{\varepsilon^2}{4}\frac{d-1}{d}\frac{J}{n}\nabla\triangle + \frac{d}{\tau} & \mu\operatorname{div} & \nu_0\triangle \end{pmatrix}. \tag{4.21}$$

And (4.4) can be written as

$$\partial_t U - A_\delta U = \begin{pmatrix} 0\\ \operatorname{div}\left(\frac{J\otimes J}{n} + \frac{\varepsilon^2}{4}\frac{(\nabla n)\otimes(\nabla n)}{n}\right) - n\nabla V + 2\delta(\nabla J)\nabla n^{-1} + \delta J\triangle n^{-1}\end{pmatrix},$$

again with a nonlinear matrix differential operator

$$A_\delta = \begin{pmatrix} \nu_0\triangle & \operatorname{div}\\ -\frac{\varepsilon^2}{4}\nabla\triangle + p'(n)\nabla & \left(\nu_0 + \frac{\delta}{n}\right)\triangle\mathbf{1}_d - \frac{1}{\tau}\mathbf{1}_d \end{pmatrix}. \tag{4.22}$$

The insulating boundary conditions (4.5) are getting represented by the $(d+2)\times(d+2)$ matrix

$$B = \begin{pmatrix} \partial_\nu & 0 & 0\\ 0 & \mathbf{1}_d & 0\\ 0 & 0 & \partial_\nu \end{pmatrix}, \qquad (r_1, \ldots, r_{d+2}) = (0, 0, \ldots, 0, 1),$$

and, concerning the boundary condition (4.6), we have in local coordinates the principal part

$$B^0 = \begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & \mathbf{1}_{d-1} & 0 & 0\\ 0 & 0 & \partial_\nu & 0\\ 0 & 0 & 0 & \partial_\nu \end{pmatrix}, \qquad (r_1, \ldots, r_{d+2}) = (0, 0, \ldots, 0, 1, 1),$$

and we observe that Condition 4.3 holds in all cases. We follow the convention that the last row and column of B (taking care of ne) is tacitly omitted when we study A from (4.20) or A_δ from (4.22).

Proposition 4.11. *For frozen functions J and n, the latter taking only positive values, the linear matrix differential operators A, A_{full}, A_δ from* (4.20), (4.21), (4.22) *together with the boundary conditions* (4.5) *and* (4.6), *form boundary value problems which are elliptic with parameter in a sector $\mathcal{L}_0$ which is larger than the right half-plane of $\mathbb{C}$.*

Proof. The pseudodifferential symbol of A^0 from (4.20) is

$$\sigma(A^0)(x,\xi) = \begin{pmatrix} -\nu_0|\xi|^2 & \mathrm{i}(\xi_1,\dots,\xi_d) \\ \frac{\varepsilon^2}{4}\mathrm{i}\xi|\xi|^2 & -\nu_0|\xi|^2\mathbf{1}_d \end{pmatrix},$$

with eigenvalues in the left half-plane:

$$\lambda_{1,\dots,d-1}(x,\xi) = -\nu_0|\xi|^2, \qquad \lambda_{d,d+1}(x,\xi) = -\left(\nu_0 \pm \frac{\mathrm{i}\varepsilon}{2}\right)|\xi|^2.$$

Similarly for A^0_{full}:

$$\sigma(A^0_{\text{full}})(x,\xi) = \begin{pmatrix} -\nu_0|\xi|^2 & \mathrm{i}(\xi_1,\dots,\xi_d) & 0 \\ \frac{\varepsilon^2}{4}\frac{d-1}{d}\mathrm{i}\xi|\xi|^2 & -\nu_0|\xi|^2\mathbf{1}_d & 0 \\ \frac{\varepsilon^2}{4}\frac{d-1}{d}\mathrm{i}\frac{J(x)}{n(x)}\xi|\xi|^2 & 0 & -\nu_0|\xi|^2 \end{pmatrix},$$

$$\lambda_{1,\dots,d}(x,\xi) = -\nu_0|\xi|^2, \qquad \lambda_{d+1,d+2}(x,\xi) = -\left(\nu_0 \pm \frac{\mathrm{i}\varepsilon}{2}\sqrt{\frac{d-1}{d}}\right)|\xi|^2,$$

and for A^0_δ:

$$\sigma(A^0_\delta)(x,\xi) = \begin{pmatrix} -\nu_0|\xi|^2 & \mathrm{i}(\xi_1,\dots,\xi_d) \\ \frac{\varepsilon^2}{4}\mathrm{i}\xi|\xi|^2 & -\left(\nu_0 + \frac{\delta}{n(x)}\right)|\xi|^2\mathbf{1}_d \end{pmatrix},$$

$$\lambda_{1,\dots,d-1}(x,\xi) = -\nu_0|\xi|^2,$$

$$\lambda_{d,d+1}(x,\xi) = -\frac{1}{2}\left(2\nu_0 + \frac{\delta}{n(x)} \pm \sqrt{\left(\frac{\delta}{n(x)}\right)^2 - \varepsilon^2}\right)|\xi|^2,$$

all these roots having real part at most equal to $-\nu_0|\xi|^2$, for positive $n(x)$.

Concerning the Shapiro–Lopatinskii condition, we focus our attention to the combination of A_{full} with (4.6), the other combinations being easier. We let the boundary be located at $x_d = 0$, consider $\partial\Omega \ni x^0 = 0$, observe that the concept of parameter-ellipticity can be generalized in a canonical way to the case of sections through vector bundles, and then (4.19) with $v =: (m, K, g)^\top$ turns into

$$-\nu_0(|\xi'|^2 + D^2_{x_d})m + \mathrm{i}\xi_1 K_1 + \dots + \mathrm{i}\xi_{d-1}K_{d-1} + \mathrm{i}D_{x_d}K_d = \lambda m,$$

$$
\begin{aligned}
\frac{\varepsilon^2}{4}\frac{d-1}{d}\mathrm{i}\xi_k(|\xi'|^2+D_{x_d}^2)m-\nu_0(|\xi'|^2+D_{x_d}^2)K_k&=\lambda K_k, \quad 1\le k\le d-1,\\
\frac{\varepsilon^2}{4}\frac{d-1}{d}\mathrm{i}D_{x_d}(|\xi'|^2+D_{x_d}^2)m-\nu_0(|\xi'|^2+D_{x_d}^2)K_d&=\lambda K_d,\\
\frac{\varepsilon^2}{4}\frac{d-1}{d}\mathrm{i}\frac{J_d(0)}{n(0)}D_{x_d}(|\xi'|^2+D_{x_d}^2)m-\nu_0(|\xi'|^2+D_{x_d}^2)g&=\lambda g,\\
m(0)=K_1(0)=\dots=K_{d-1}(0)=(D_{x_d}K_d)(0)=(D_{x_d}g)(0)&=0,
\end{aligned}
$$

which is a system of ordinary differential equations with constant coefficients. Every solution which decays at infinity must decay exponentially, together with all its derivatives. Then we may plug each term of this system into the usual scalar product $\langle\cdot,\cdot\rangle$ and the associated norm $\|\cdot\|$ on $L^2(\mathbb{R}_+;\mathbb{C})$. First we note that $(D_{x_d}^2 m)(0)=0$, from the first equation. We select the equation for K_j, take the scalar product with K_j, and integrate by parts to obtain

$$
\begin{aligned}
-\frac{\varepsilon^2}{4}\frac{d-1}{d}\left\langle(|\xi'|^2+D_{x_d}^2)m,\mathrm{i}\xi_k K_k\right\rangle-\nu_0|\xi'|^2\|K_k\|^2-\nu_0\|D_{x_d}K_k\|^2&=\lambda\|K_k\|^2,\\
-\frac{\varepsilon^2}{4}\frac{d-1}{d}\left\langle(|\xi'|^2+D_{x_d}^2)m,\mathrm{i}D_{x_d} K_d\right\rangle-\nu_0|\xi'|^2\|K_d\|^2-\nu_0\|D_{x_d}K_d\|^2&=\lambda\|K_d\|^2.
\end{aligned}
$$

We sum up and insert the first differential equation, and it follows that

$$
\begin{aligned}
&-\frac{\varepsilon^2}{4}\frac{d-1}{d}\nu_0\left\|(|\xi'|^2+D_{x_d})^2m\right\|^2-\nu_0\sum_{j=1}^d\left(|\xi'|^2\|K_j\|^2+\|D_{x_d}K_d\|^2\right)\\
&\qquad=\lambda\sum_{j=1}^d\|K_j\|^2+\overline{\lambda}\frac{\varepsilon^2}{4}\frac{d-1}{d}\left(|\xi'|^2\|m\|^2+\|D_{x_d}m\|^2\right).
\end{aligned}
$$

The left-hand side is always nonpositive, and if $\Re\lambda\ge 0$, then the right-hand side has a nonnegative real part, which enforces $K\equiv 0$ and $m\equiv 0$, and from the differential equation for g, in this case also $g\equiv 0$ follows. Then the sector $\mathcal{L}_0$ in which the system is parameter-elliptic contains at least the right half-plane. And since the set of λ for which the Shapiro–Lopatinskii criterion is violated is a closed set of $\mathbb{C}$, the sector $\mathcal{L}_0$ is even strictly larger than the right half-plane of $\mathbb{C}$. □

In the sequel, we set $N=d+1$ in case of (4.20) or (4.22), but $N=d+2$ in case of (4.21).

Proposition 4.12. *Assume that the functions $J=J(x)$ and $n=n(x)$ have regularity $C^{0;1}(\overline{\Omega})$, and $n\ge$ const. >0. For $1<p<\infty$, define a function space*

$$
X=\left\{U\in W_p^1(\Omega)\times L^p(\Omega;\mathbb{C}^{N-1})\colon B_nU_1=0\right\} \tag{4.23}
$$

with B_n being the differential operator acting on n in the boundary conditions (4.5) *or* (4.6)*. Define $\mathcal{A}$ as A or A_{full} or A_δ from* (4.20) *and* (4.21) *and* (4.22)*, together* *with boundary operators $B_1, \ldots, B_N$ as expressed in* (4.5) *or* (4.6), *and domain*

$$D(\mathcal{A}) = \big\{(m,K,g) \in W_p^3(\Omega) \times W_p^2(\Omega;\mathbb{C}^{d+1})\colon B_n \triangle m = 0, \qquad B_n m = 0, \quad B_J K = 0, \quad B_{ne} g = 0\big\}, \tag{4.24}$$

$$D(\mathcal{A}) = \big\{(m,K) \in W_p^3(\Omega) \times W_p^2(\Omega;\mathbb{C}^{d})\colon B_n \triangle m = 0, \qquad B_n m = 0, \quad B_J K = 0\big\}, \tag{4.25}$$

(*depending on the height of* U), *where* B_J *and* B_{ne} *are the differential operators on* J *and* ne *in the chosen boundary condition.*

Then the operator $\mathcal{A}$ *generates an analytic semigroup on the space* X.

Proof. By our assumption on the regularity of n and J, Condition 4.2 holds, and also Condition 4.3 with $Q = 2$ and $p_1 = 1$. Finally, also Condition 4.4 is valid with $A_k = \triangle$ and $\mathcal{L}_1 = \Sigma_\theta := \{z \in \mathbb{C}\colon |\arg z| \le \theta + \pi/2\} \cup \{0\}$ for $\theta < \pi/2$. It remains to apply Theorem 4.10. □

Next we wish to solve the linear problem

$$\begin{cases} \partial_t U - \mathcal{A}U = F(t), & t \in (0,t_0], \\ U(0) = U_0, \end{cases} \tag{4.26}$$

with $U = (m,K,g)$ or $U = (m,K)$, for either $\mathcal{A} = (A_{\mathrm{full}}, B_n, B_J, B_{ne})$ or $\mathcal{A} = (A_\delta, B_n, B_J)$. Note that the case of $\mathcal{A} = (A, B_n, B_J)$ with A from (4.20) can be treated in a much easier way, because of the constant coefficients of the principal part. Concerning the functions n and J appearing in the coefficients of A_{full} and A_δ, we assume, for some $\rho \in (0,1)$, that

$$n, J \in C([0,t_0]; C^{0;1}(\overline{\Omega})) \cap C^\rho([0,t_0]; C(\overline{\Omega})),$$
$$n(t,x) \ge \text{const.} > 0, \qquad (t,x) \in [0,t_0] \times \overline{\Omega}.$$

Put $E_1 = D(\mathcal{A})$ and $E_0 = X$, Then (E_0, E_1) is a densely injected Banach space couple. For $\theta \in (0,1)$, set $E_\theta := [E_0, E_1]_\theta$, via the complex interpolation method. We write $\mathcal{H}(E_1; E_0)$ for the set of all $\mathcal{M} \in \mathcal{L}(E_1; E_0)$ such that $\mathcal{M}$, considered as a linear operator in E_0 with domain E_1, is the infinitesimal generator of a strongly continuous analytic semigroup in E_0 (compare [6], Section II.1.2). Then we have $\mathcal{A} \in C^\rho([0,t_0]; \mathcal{H}(E_1; E_0))$.

Theorem 4.13. *Suppose* $U_0 \in E_0$ *and assume*

$$F \in C^\epsilon([0,t_0]; E_\gamma) + C([0,t_0], E_{\gamma+\epsilon}),$$

where γ *and* ϵ *are numbers with* $0 < \gamma < \rho < 1$ *and* $0 < \epsilon < 1 - \gamma$. *Then the initial value problem* (4.26) *has a unique solution*

$$U \in C([0,t_0]; E_0) \cap C((0,t_0]; E_1) \cap C^1((0,t_0]; E_\gamma).$$

Write $\mathcal{A}_\gamma$ *for the* E_γ *realization of* $\mathcal{A}$. *Then* U *also solves* $\partial_t U - \mathcal{A}_\gamma U = F$ *in the interval* $(0,t_0]$. *If* $U_0 \in E_\gamma$, *then* $U \in C([0,t_0]; E_\gamma)$, *and if* $U_0 \in D(\mathcal{A}_\gamma(0))$, *then* $U \in C^1([0,t_0], E_\gamma)$.

On the other hand, if $F \in C^\rho([0,t_0];E_0)$ *and* $U_0 \in E_1$*, then*

$$U \in C^\rho((0,t_0];E_1) \cap C^{1+\rho}((0,t_0];E_0) \cap C^1([0,t_0];E_0).$$

Proof. This is Theorem 1.2.2 and Theorem 1.2.1 in [6], Chapter II. □

In [6], Chapter II, it has been shown that the solution U can be expressed as

$$U(t) = \mathcal{U}_{\mathcal{A}}(t,0)U_0 + \int_{\tau=0}^{t} \mathcal{U}_{\mathcal{A}}(t,\tau)F(\tau)\,\mathrm{d}\tau,$$

with $\mathcal{U}_{\mathcal{A}}$ being a parabolic evolution operator having E_1 as regularity subspace, which implies the following. Set $\mathcal{J} = [0,t_0]$ and

$$\begin{aligned} \mathcal{J}_\Delta &:= \{(t,s) \in \mathcal{J} \times \mathcal{J} \colon s \le t\}, \\ \mathcal{J}_\Delta^* &:= \{(t,s) \in \mathcal{J}_\Delta \colon s < t\}. \end{aligned}$$

Then $\mathcal{U}_{\mathcal{A}}$ has the properties

$$\begin{aligned} &\mathcal{U}_{\mathcal{A}} \in C(\mathcal{J}_\Delta; \mathcal{L}_s(E_0;E_0)) \cap C(\mathcal{J}_\Delta^*; \mathcal{L}(E_0;E_1)), \\ &\mathcal{U}_{\mathcal{A}}(t,t) = 1, \qquad t \in \mathcal{J}, \\ &\mathcal{U}_{\mathcal{A}}(t,s) = \mathcal{U}_{\mathcal{A}}(t,\tau)\mathcal{U}_{\mathcal{A}}(\tau,s), \qquad s \le \tau \le t, \quad (t,s) \in \mathcal{J}_\Delta, \end{aligned}$$

where $\mathcal{L}_s(E_0;E_0)$ is the space of linear maps from E_0 to E_0 equipped with the simple convergence topology (see [6] for details).

For Banach spaces E, F, and $\alpha \in \mathbb{R}$, call $\mathfrak{K}(E;F,\alpha)$ the Fréchet space of all $k \in C(\mathcal{J}_\Delta^*; \mathcal{L}(E;F))$ with the following finite seminorms:

$$\sup_{0 \le s < t \le T} (t-s)^\alpha \left\| k(t,s) \right\|_{\mathcal{L}(E;F)} < \infty, \qquad 0 < T \le t_0.$$

Next, we consider not only one operator $\mathcal{A}$ (with coefficients depending on t), but a whole family $\mathfrak{A} \subset C^\rho(\mathcal{J}; \mathcal{H}(E_1;E_0))$. We assume that there are constants $M, \eta \in \mathbb{R}_+$ and $\theta \in (0,\pi/2)$ such that Σ_θ is contained in the resolvent set $\varrho(\mathcal{A}(s))$ for all $\mathcal{A} \in \mathfrak{A}$ and all $s \in \mathcal{J}$, and the inequalities

$$\begin{aligned} \sup_{t,s \in \mathcal{J}, t \ne s} \frac{\left\| \mathcal{A}(t) - \mathcal{A}(s) \right\|_{\mathcal{L}(E_1;E_0)}}{|t-s|^\varrho} &\le \eta, \\ \left\| \mathcal{A}(s) \right\|_{\mathcal{L}(E_1;E_0)} + (1+|\lambda|)^{1-j} \left\| (\mathcal{A}(s)-\lambda)^{-1} \right\|_{\mathcal{L}(E_0;E_j)} &\le M \end{aligned}$$

hold for all $(s,\lambda,\mathcal{A}) \in \mathcal{J} \times \Sigma_\theta \times \mathfrak{A}$ and $j = 0,1$.

Then each operator $\mathcal{A}$ from this set $\mathfrak{A}$ possesses a unique parabolic evolution operator $\mathcal{U}_{\mathcal{A}}$, and this $\mathcal{U}_{\mathcal{A}}$ enjoys estimates as follows:

Theorem 4.14 ([6], Theorem II.4.4.1). *Suppose that the class* $\mathfrak{A}$ *is given as above. Then for each* $\mathcal{A} \in \mathfrak{A}$*, there is a unique parabolic evolution operator* $\mathcal{U}_{\mathcal{A}}$ *having* E_1 *as regularity subspace, such that*

$$\mathcal{U}_{\mathcal{A}} \in C(\mathcal{J}_\Delta; \mathcal{L}_s(E_1;E_1)) \cap \mathfrak{K}(E_0;E_0,0) \cap \mathfrak{K}(E_1;E_1,0) \cap \mathfrak{K}(E_0;E_1,1).$$

Further, there is a constant $C = C(\rho)$, independent of η, such that, with $\mu := C(\rho)\eta^{1/\rho}$, the estimates

$$\|\mathcal{U}_{\mathcal{A}}(t,s)\|_{\mathcal{L}(E_j;E_j)} + (t-s)\,\|\mathcal{U}_{\mathcal{A}}(t,s)\|_{\mathcal{L}(E_0;E_1)} \le C(\epsilon)\exp((\mu+\epsilon)(t-s))$$

hold for all positive ϵ, $(t,s) \in \mathcal{J}_\Delta^*$, $\mathcal{A} \in \mathfrak{A}$ and $j = 0, 1$.

In order to be able to apply this result to our situation, we only have to make sure that the functions (n, J) appearing in the coefficients of $\mathcal{A}$ are from the admissible class $\mathcal{Z}_{\rm ad}$, defined by the inequalities

$$\begin{aligned} n(t,x) &\ge c_0 > 0, \qquad (t,x) \in [0,t_0]\times\overline{\Omega}, \\ \|n\|_{C([0,t_0];C^{0;1}(\overline{\Omega}))} + \|J\|_{C([0,t_0];C^{0;1}(\overline{\Omega}))} &\le C_0, \\ \frac{\|n(t)-n(s)\|_{C(\overline{\Omega})}}{|t-s|^\rho} + \frac{\|J(t)-J(s)\|_{C(\overline{\Omega})}}{|t-s|^\rho} &\le C_1, \qquad 0 \le t \ne s \le t_0, \end{aligned}$$

with constants c_0 and C_0, C_1 fixed.

Interpolating between the estimates from Theorem 4.14, we then can conclude that

$$\begin{aligned} \|\mathcal{U}_{\mathcal{A}}(t,s)\|_{\mathcal{L}(E_\alpha;E_\beta)} &\le C(t-s)^{-(\beta-\alpha)}\exp((\mu+\epsilon)(t-s)), \qquad 0\le\alpha\le\beta\le 1, \\ \|\mathcal{A}(t)\mathcal{U}_{\mathcal{A}}(t,s)\|_{\mathcal{L}(E_\alpha;E_0)} &\le C(t-s)^{-(1-\alpha)}\exp((\mu+\epsilon)(t-s)), \qquad 0\le\alpha\le 1. \end{aligned}$$

Recall that for a closed linear operator $\mathcal{M}$ in a Banach space E, the spectral bound $s(\mathcal{M})$ is defined as

$$s(\mathcal{M}) := \sup\{\Re\lambda\colon \lambda \in \sigma(\mathcal{M})\},$$

with $\sigma(\mathcal{M})$ being the spectrum of $\mathcal{M}$. Note that the number $\lambda_0(p)$ appearing in Theorem 4.9 depends continuously on the coefficients of the operator, and therefore we can assume that there is a uniform number $\nu \in \mathbb{R}$ with the property that $\nu > s(\mathcal{A}(t))$, for all $t \in \mathcal{J} = [0,t_0]$ and all $\mathcal{A} \in \mathfrak{A}$.

Having secured this number ν, we now can compare the mild solutions $U^{(1)}$ and $U^{(2)}$ to the problems

$$\begin{cases} \partial_t U^{(1)} - \mathcal{A}^{(1)}U^{(1)} = F^{(1)}, \\ U^{(1)}(0) = U_0^{(1)}, \end{cases} \qquad \begin{cases} \partial_t U^{(2)} - \mathcal{A}^{(2)}U^{(2)} = F^{(2)}, \\ U^{(2)}(0) = U_0^{(2)}, \end{cases} \tag{4.27}$$

and their difference is estimated in the next theorem:

Theorem 4.15 ([6], Theorem II.5.2.1). *Suppose that $0 \le \beta \le \alpha \le 1$ with $\alpha > 0$ and $\beta < 1$, and $0 < \gamma \le 1$. For $(U_0^{(j)}, \mathcal{A}^{(j)}, F^{(j)}) \in E_\alpha \times \mathfrak{A} \times L^\infty_{\rm loc}(\mathcal{J}; E_\gamma)$, $j = 0, 1$,* *the mild solutions* $U^{(1)}$ *and* $U^{(2)}$ *to* (4.27) *exist, and the following estimate holds:*

$$\begin{aligned}&\left\|U^{(1)}(t)-U^{(2)}(t)\right\|_{E_\beta}\\ &\quad\le Ce^{\nu t}\Big(t^{\alpha-\beta}\left\|\mathcal{A}^{(1)}-\mathcal{A}^{(2)}\right\|_{C([0,t];\mathcal{L}(E_1;E_0))}\left\|U_0^{(1)}\right\|_{E_\alpha}\\ &\qquad+t^{1+\gamma-\beta}\left\|\mathcal{A}^{(1)}-\mathcal{A}^{(2)}\right\|_{C([0,t];\mathcal{L}(E_1;E_0))}\left\|F^{(1)}\right\|_{L^\infty((0,t);E_\gamma)}\\ &\qquad+\left\|U_0^{(1)}-U_0^{(2)}\right\|_{E_\beta}+t^{1-\beta}\left\|F^{(1)}-F^{(2)}\right\|_{L^\infty((0,t);E_0)}\Big).\end{aligned}$$

This will help us in solving the quasilinear problems (4.1), (4.3), (4.4) on a short time interval by a Picard style iteration procedure.

Our final tool is a Hölder type estimate for mild solutions.

Theorem 4.16 ([6], Theorem II.5.3.1). *Assume* $0 \le \beta \le \alpha < 1$ *and* $U_0 \in E_\alpha$, $F \in L^\infty_{\mathrm{loc}}(\mathcal{J}; E_0)$. *Then the estimate*

$$\|U(t)-U(s)\|_{E_\beta} \le C(t-s)^{\alpha-\beta}e^{\nu t}\left(\|U_0\|_{E_\alpha}+\|F\|_{L^\infty((0,t);E_0)}\right)$$

holds, uniformly in $(t,s) \in \mathcal{J}_\Delta$ *and* $(U_0,\mathcal{A},F) \in E_\alpha \times \mathfrak{A} \times L^\infty_{\mathrm{loc}}(\mathcal{J};E_0)$.

Proof of Theorem 4.1. Without loss of generality, we discuss only the boundary condition (4.6). For functions (n, J, ne) satisfying the initial and the boundary conditions, we set $W := (n - n_0, J, ne)$ which has homogeneous boundary values, and we consider then the problem

$$\begin{cases}\partial_t U - \mathcal{A}[W]U = F[W], & U = (m-n_0, K, g),\\ \qquad U(0) = U_0, & \end{cases}$$

with the intention to find a fixed point of the mapping $W \mapsto U$, locally in time. The numbers c_0, C_0, C_1 in the definition of $\mathcal{Z}_{\mathrm{ad}}$ shall be defined as

$$c_0 := \frac{1}{2}\inf_{x\in\Omega} n_0(x), \qquad C_0 := 2\left(\|n_0\|_{C^{0;1}(\overline{\Omega})}+\|J_0\|_{C^{0;1}(\overline{\Omega})}\right), \qquad C_1 := 1.$$

We suppose that $(n,J) \in \mathcal{Z}_{\mathrm{ad}}$, as a condition on W. Then we can apply Theorem 4.16 with $\beta = 3/4$, $\alpha = 7/8$ and $0 \le t \le t_0$,

$$\|U(t)-U_0\|_{E_{3/4}} \le Ct^{1/8}e^{\nu t}\left(\|U_0\|_{E_{7/8}}+\|F[W]\|_{L^\infty((0,t);X)}\right). \tag{4.28}$$

Note that $F[W]$ has the form

$$F[W] = \begin{pmatrix}\nu_0 \triangle n_0\\ B(\nabla J, \nabla^2 n)\Phi + (\nabla^2 n)\Psi_1 + (\nabla J)\Psi_2 + (\nabla(ne))\Psi_3 + \Psi_4 - n\nabla V\end{pmatrix},$$

with $B(\cdot,\cdot)$ being a certain bilinear form, Φ a smooth function of n, and Ψ_j being functions depending smoothly on n, ∇n, J, ne. By the definition of $\mathcal{Z}_{\mathrm{ad}}$, we have

$$\|(\Phi,\Psi_1,\Psi_2,\Psi_3,\Psi_4,\Psi_5,\nabla V,\nabla J)\|_{L^\infty(\Omega)} \le C(c_0,C_0).$$

Then we can conclude that

$$\begin{aligned}\|F[W]\|_{L^\infty((0,t);X)} &\le C\left(\left\|B(\nabla J,\nabla^2 n)\right\|_{L^\infty((0,t);L^p(\Omega))} + \|n\|_{L^\infty((0,t);W^2_p(\Omega))} + 1\right)\\ &\le C\left(\|W\|_{L^\infty((0,t);E_{1/2})} + 1\right).\end{aligned}$$

Now we define a set

$$\begin{aligned}Y := \Big\{&U = (m-n_0, K, g) \in L^\infty((0,t_0); E_{3/4}):\\ &\|U(t) - U(s)\|_{E_{3/4}} \le \delta_0 (t-s)^{1/16}, \qquad 0 \le s \le t \le t_0\Big\}.\end{aligned}$$

Since $E_{3/4}$ is a closed subspace of $W_p^{5/2}(\Omega)\times W_p^{3/2}(\Omega;\mathbb{C}^{d+1})$ which embeds continuously into $C^2(\overline{\Omega})\times C^1(\overline{\Omega};\mathbb{C}^{d+1})$ because of $p>2d$, the elements $U=(m-n_0,K,g)$ of Y satisfy

$$\begin{aligned}&m(t,x) \ge c_0, \qquad \|(m,K)\|_{C([0,t_0];C^{0,1}(\overline{\Omega}))} \le C_0,\\ &\frac{\|(m,K)(t) - (m,K)(s)\|_{C(\overline{\Omega})}}{|t-s|^{1/16}} \le C_1,\end{aligned}$$

for $0 \le s,t \le t_0$, if δ_0 and t_0 are chosen sufficiently small. Then the inequality $\|W - U_0\|_{L^\infty((0,t_0);E_{1/2})} \le \delta_0$ implies $\|U - U_0\|_{L^\infty((0,t_0);E_{3/4})} \le \delta_0$, by (4.28) and a small choice of t_0.

Again by using Theorem 4.16, we deduce that

$$\frac{\|U(t) - U(s)\|_{E_{3/4}}}{|t-s|^{1/16}} \le C(t-s)^{1/16} e^{\nu t}\left(\|U_0\|_{E_{7/8}} + \|F[W]\|_{L^\infty((0,t);X)}\right),$$

for $0 \le s < t \le t_0$. Then the map $W \mapsto U$ sends the set Y into itself, for small t_0, so that we only have to show the contraction, which follows from Theorem 4.15 with $\alpha = 1$, $\beta = 3/4$, $0 < \gamma \ll 1$ and Moser type inequalities for the term $\left\|F^{(1)}\right\|_{L^\infty((0,t);E_\gamma)}$. Then this map $W \mapsto U$ induces a sequence $(U^{(1)}, U^{(2)}, \dots)$ in Y with a limit U^* which is a mild solution to

$$\partial_t U^* - \mathcal{A}[U^*]U^* = F[U^*], \qquad U^*(0) = U_0.$$

Note that $U_0 \in E_1 = D(\mathcal{A}[U^*])$ and $F[U^*] \in C^{1/16}([0,t_0];E_0)$, and then $U^* \in C^1([0,t_0];E_0)$ by Theorem 4.13. Then Theorem 4.9 implies $U^* \in C([0,t_0];D(\mathcal{A}))$, which completes the proof of Theorem 4.1. □

4.4. Stationary states and their stability

In this part, we consider the isothermal system (4.1) and ask for the exponential stability of stationary states. The boundary condition will always be (4.6). We start with some geometric conclusions from the boundary condition (4.6), before we apply these results to the viscous quantum hydrodynamic system (4.1).

4.4.1. Geometric results. First we recall the orthogonal *Helmholtz decomposition* of second kind for an arbitrary bounded or unbounded domain $\Omega \subset \mathbb{R}^d$:

$$L^2(\Omega;\mathbb{C}^d) = L^2_{\mathrm{div}}(\Omega;\mathbb{C}^d) \oplus G^2_0(\Omega),$$

with $L^2_{\mathrm{div}}(\Omega;\mathbb{C}^d)$ being the space of vector fields v from $L^2(\Omega;\mathbb{C}^d)$ with $\operatorname{div} v = 0$ in the distributional sense, and $G^2_0(\Omega) = \nabla W^1_{2,0}(\Omega)$. To each $u \in L^2(\Omega;\mathbb{C}^d)$, the components u_{div} and $\nabla\varphi$ in $u = u_{\mathrm{div}} + \nabla\varphi$ can be found as follows: $\nabla\varphi \in G^2_0(\Omega)$ is the unique solution to the variational problem

$$\langle \nabla\varphi, \nabla\psi\rangle_{L^2(\Omega;\mathbb{C}^d)} = \langle u, \nabla\psi\rangle_{L^2(\Omega;\mathbb{C}^d)}, \qquad \forall \nabla\psi \in G^2_0(\Omega),$$

which can be solved using the Lax–Milgram theorem, and then $u_{\mathrm{div}} = u - \nabla\varphi$. The function φ also solves the elliptic boundary value problem

$$\triangle\varphi = \operatorname{div} u, \qquad \gamma_0\varphi = 0,$$

in the distributional sense.

The Helmholtz decomposition also holds for L^p spaces with $p \neq 2$, under slightly stronger assumptions on the domain Ω:

Lemma 4.17. *Let $1 < p < \infty$, Ω be a bounded open set in $\mathbb{R}^d$ with $\partial\Omega \in C^1$. Then each function $u \in L^p(\Omega;\mathbb{C}^d)$ can be uniquely decomposed as*

$$\begin{aligned} &u = u_{\mathrm{div}} + \nabla\varphi, \\ &u_{\mathrm{div}} \in L^p(\Omega;\mathbb{C}^d), \qquad \operatorname{div} u_{\mathrm{div}} = 0, \\ &\varphi \in W^1_{p,0}(\Omega), \end{aligned}$$

and $\nabla\varphi$ is the unique solution to the weak Dirichlet problem

$$\langle \nabla\varphi, \nabla\psi\rangle_{L^p(\Omega;\mathbb{C}^d)\times L^{p'}(\Omega;\mathbb{C}^d)} = \langle u, \nabla\psi\rangle_{L^p(\Omega;\mathbb{C}^d)\times L^{p'}(\Omega;\mathbb{C}^d)}, \qquad \forall \psi \in W^1_{p',0}(\Omega),$$

with $\frac{1}{p} + \frac{1}{p'} = 1$. The projections $u \mapsto u_{\mathrm{div}}$ and $u \mapsto \nabla\varphi$ are continuous in $L^p(\Omega;\mathbb{C}^d)$.

Proof. This is Theorem 10.7 in [110]. □

From now on, we write P_p for the projection map $u \mapsto u_{\mathrm{div}}$, defined on $L^p(\Omega;\mathbb{C}^d)$.

If a vector field $u \in W^2_p(\Omega;\mathbb{C}^d)$ satisfies the boundary conditions

$$\gamma_0 \operatorname{div} u = 0, \qquad \gamma_0 u_{\parallel} = 0,$$

with $u_{\parallel}$ being the tangential component of u, then we express this boundary condition as $B_J u = 0$.

Lemma 4.18. *If $1 < p < \infty$, Ω is a bounded domain with $\partial\Omega \in C^{2;1}$, then*

$$\mathsf{P}_p \in \mathcal{L}(W^2_p(\Omega;\mathbb{C}^d); W^2_p(\Omega;\mathbb{C}^d)),$$

and P_p *also maps*

$$W^2_{p;B}(\Omega;\mathbb{C}^d) := \big\{u \in W^2_p(\Omega;\mathbb{C}^d)\colon B_J u = 0\big\}$$

continuously into itself.

Proof. If $u \in W^2_{p,B}(\Omega;\mathbb{C}^d)$, then φ, defined via $\triangle\varphi = \operatorname{div} u$ and $\gamma_0\varphi = 0$, belongs to $W^3_p(\Omega)$. Then also $\gamma_0(\nabla\varphi)_{\|} = 0$ and $\gamma_0(\operatorname{div}\nabla\varphi) = \gamma_0(\operatorname{div} u) = 0$. □

Starting from now (except the proof of Theorem 4.4), Ω is always a bounded domain in $\mathbb{R}^d$ with $\partial\Omega \in C^{2;1}$.

Lemma 4.19. *If* $1 < p < \infty$, *then*

$$\mathsf{P}_p\triangle = \triangle\mathsf{P}_p \qquad \text{on } W^2_{p;B}(\Omega;\mathbb{C}^d).$$

Proof. If $u \in W^2_{p;B}(\Omega;\mathbb{C}^d)$, then $(\mathrm{id} - \mathsf{P}_p)u = \nabla\varphi$ with $B_J\nabla\varphi = 0$, in particular $\gamma_0 \triangle \varphi = 0$, hence $\triangle\varphi \in W^1_{p,0}(\Omega)$. Then

$$\mathsf{P}_p \triangle (\mathrm{id} - \mathsf{P}_p)u = \mathsf{P}_p\nabla\triangle\varphi = 0,$$

since $\nabla\triangle\varphi \in \nabla W^1_{p,0}(\Omega)$, and therefore

$$\mathsf{P}_p \triangle u = \mathsf{P}_p \triangle \mathsf{P}_p u, \qquad \forall u \in W^2_{p;B}(\Omega;\mathbb{C}^d).$$

Similarly,

$$(\mathrm{id} - \mathsf{P}_p) \triangle \mathsf{P}_p u = 0, \qquad \forall u \in W^2_{p;B}(\Omega;\mathbb{C}^d),$$

because $\operatorname{div}\triangle\mathsf{P}_p u = 0$ in distributional sense. Then we find, for such u, that

$$\mathsf{P}_p \triangle u = \mathsf{P}_p \triangle \mathsf{P}_p u = \triangle\mathsf{P}_p u.$$

□

Lemma 4.20. *Let N be a smooth real vector field defined in a tubular neighborhood of $\partial\Omega$ with $\|N(x)\| = 1$ for all x there, and N equals the unit outward normal vector field on $\partial\Omega$. Then it holds*

$$\begin{aligned}\int_\Omega (\triangle u)v\,\mathrm{d}x &= -\sum_{j=1}^d \int_\Omega (\nabla u_j)(\nabla v_j)\,\mathrm{d}x \\ &\quad - \int_{\partial\Omega} \langle u, N\rangle_{\mathbb{R}^d\times\mathbb{R}^d}\,\langle v, N\rangle_{\mathbb{R}^d\times\mathbb{R}^d}\,\operatorname{div} N\,\mathrm{d}\sigma, \\ &= \int_\Omega u \triangle v\,\mathrm{d}x,\end{aligned} \tag{4.29}$$

for all $u \in W^2_{p,B}(\Omega;\mathbb{C}^d)$ and all $v \in W^2_{p',B}(\Omega;\mathbb{C}^d)$, with $\frac{1}{p} + \frac{1}{p'} = 1$.

Moreover, if Ω is convex, then

$$-\int_\Omega (\triangle u)\overline{u}\,\mathrm{d}x \ge \sum_{j=1}^d \int_\Omega |\nabla u_j|^2\,\mathrm{d}x, \tag{4.30}$$

for all $u \in W^2_{2,B}(\Omega;\mathbb{C}^d)$.

Proof. From the Gauß Integral theorem and computing in local coordinates near the boundary, we obtain (4.29). And concerning (4.30), note that $\operatorname{div} N$ equals the mean curvature of the boundary $\partial\Omega$, which is nonnegative in case of Ω being convex. It remains to apply (4.29) with $v = \overline{u}$. □

4.4.2. Application to the viscous quantum hydrodynamic system. To investigate stationary states, we first consider a variation of the operator $\mathcal{A}$ from (4.20)

$$\mathcal{A} := \begin{pmatrix} \nu_0 \triangle & \operatorname{div} \\ -\frac{\varepsilon^2}{4}\nabla\triangle + T\nabla - \overline{n}\lambda_D^{-2}\nabla\triangle_D^{-1} & \nu_0 \triangle \mathbf{1}_d - \frac{1}{\tau}\mathbf{1}_d \end{pmatrix} \tag{4.31}$$

in the ground space X from (4.23), with domain $D(\mathcal{A})$ as in (4.25). Later we will see how the term $\overline{n}\lambda_D^{-2}\nabla\triangle_D^{-1}$ with $\overline{n}$ as a fixed positive constant and $\triangle_D$ as Dirichlet Laplacian on Ω originates from the item $n\nabla V$.

By the choice of $D(\mathcal{A})$, we have $\gamma_0 \triangle U_1 = 0$. With P_2 being the Helmholtz projector as given after Lemma 4.17, we introduce the notation

$$\begin{aligned} U = \begin{pmatrix} U_1 \\ \tilde{U} \end{pmatrix} &= \begin{pmatrix} 0 & 0 \\ 0 & \mathsf{P}_2 \end{pmatrix} U + \begin{pmatrix} \mathrm{id} & 0 \\ 0 & \mathrm{id} - \mathsf{P}_2 \end{pmatrix} U \\ &= \begin{pmatrix} 0 \\ \tilde{U}_{\mathrm{div}} \end{pmatrix} + \begin{pmatrix} U_1 \\ \nabla\varphi_U \end{pmatrix}, \end{aligned}$$

with $\gamma_0\varphi_U = 0$. This induces an orthogonal decomposition of the Hilbert space

$$\mathcal{H} := W^1_{2,0}(\Omega) \times L^2(\Omega; \mathbb{C}^d),$$

whose scalar product shall be defined as

$$\begin{aligned} \langle U, W\rangle_{\mathcal{H}} := &\left\langle -\triangle_D^{-1}\left(\frac{1}{2\tau}U_1 + \triangle\varphi_U\right), \frac{1}{2\tau}W_1 + \triangle\varphi_W \right\rangle_{L^2(\Omega)} \\ &+ \left\langle \left(-C_1\triangle + T - C_2\triangle_D^{-1}\right)U_1, W_1\right\rangle_{L^2(\Omega)} + \left\langle \tilde{U}_{\mathrm{div}}, \tilde{W}_{\mathrm{div}}\right\rangle_{L^2(\Omega)}, \end{aligned}$$

with positive constants

$$C_1 = \frac{\varepsilon^2}{4}, \qquad C_2 = \lambda_D^{-2}\overline{n} - \frac{1}{4\tau^2}.$$

Lemma 4.21. *Under the condition*

$$C_2 > \frac{1}{4\tau^2} \tag{4.32}$$

the above bilinear form $\langle\cdot,\cdot\rangle_{\mathcal{H}}$ is an admissible scalar product on $\mathcal{H}$.

Proof. We have

$$\begin{aligned} \langle U, W\rangle_{\mathcal{H}} = &C_1\langle \nabla U_1, \nabla W_1\rangle_{L^2(\Omega)} - \left(C_2 + \frac{1}{4\tau^2}\right)\langle \triangle_D^{-1}U_1, W_1\rangle_{L^2(\Omega)} \\ &+ T\langle U_1, W_1\rangle_{L^2(\Omega)} - \frac{1}{2\tau}\langle U_1, \varphi_W\rangle_{L^2(\Omega)} - \frac{1}{2\tau}\langle \varphi_U, W_1\rangle_{L^2(\Omega)} + \left\langle \tilde{U}, \tilde{W}\right\rangle_{L^2(\Omega)}, \end{aligned}$$

and in particular

$$\langle U, U\rangle_{\mathcal{H}} \geq C_1 \|\nabla U_1\|^2_{L^2(\Omega)} + \left(C_2 + \frac{1}{4\tau^2}\right) \left\|\nabla \triangle_D^{-1} U_1\right\|^2_{L^2(\Omega)}$$
$$+ T \|U_1\|^2_{L^2(\Omega)} - \frac{1}{\tau}\Re\left\langle \triangle \triangle_D^{-1} U_1, \varphi_U\right\rangle_{L^2(\Omega)} + \|\nabla\varphi_U\|^2_{L^2(\Omega)} + \left\|\tilde{U}_{\mathrm{div}}\right\|^2_{L^2(\Omega)},$$

and now it suffices to exploit Young's inequality via

$$-\frac{1}{\tau}\Re\left\langle \triangle \triangle_D^{-1} U_1, \varphi_U\right\rangle_{L^2(\Omega)} = \frac{1}{\tau}\Re\left\langle \nabla \triangle_D^{-1} U_1, \nabla\varphi_U\right\rangle_{L^2(\Omega)}$$
$$\geq -\frac{1}{2\tau^2}\left\|\nabla \triangle_D^{-1} U_1\right\|^2_{L^2(\Omega)} - \frac{1}{2}\|\nabla\varphi_U\|^2_{L^2(\Omega)}. \qquad \square$$

Lemma 4.22. *The spectral bound of the operator $\mathcal{A}$ from* (4.31) *acting on the space $X = W^1_{p,0}(\Omega) \times L^p(\Omega;\mathbb{C}^d)$ with $2 \leq p < \infty$, is at most $-1/(2\tau)$ if we assume* (4.32) *and Ω is convex.*

Proof. Since Ω is bounded, $\mathcal{A}$ extends canonically to an operator $\mathcal{A}_{\mathcal{H}}$ in $\mathcal{H}$. We wish to demonstrate that

$$\Re\langle(\mathcal{A}_{\mathcal{H}} + 1/2\tau)U, U\rangle_{\mathcal{H}} < 0$$

for all $U \neq 0$ from the set $U \in W^3_{2,0}(\Omega) \times W^2_{2;B}(\Omega;\mathbb{C}^d)$ which is a superset of $D(\mathcal{A})$. Remembering that

$$\gamma_0 \triangle_D^{-1} U_1 = \gamma_0 U_1 = \gamma_0 \triangle U_1 = \gamma_0\varphi_U = \gamma_0 \triangle \varphi_U = 0,$$

we first get

$$\left(\mathcal{A}_{\mathcal{H}} + \frac{1}{2\tau}\right) U = \begin{pmatrix} 0 \\ \nu_0 \triangle \tilde{U}_{\mathrm{div}} - \frac{1}{2\tau}\tilde{U}_{\mathrm{div}} \end{pmatrix}$$
$$+ \begin{pmatrix} \nu_0 \triangle U_1 + \triangle\varphi_U + \frac{1}{2\tau}U_1 \\ \nabla\left(-\frac{\varepsilon^2}{4} \triangle U_1 + TU_1 - \lambda_D^{-2}\overline{n} \triangle_D^{-1} U_1 + \nu_0 \triangle \varphi_U - \frac{1}{2\tau}\varphi_U\right) \end{pmatrix},$$

and consequently,

$$\left\langle \left(\mathcal{A}_{\mathcal{H}} + \frac{1}{2\tau}\right) U, U\right\rangle_{\mathcal{H}}$$
$$= \left\langle - \triangle_D^{-1}\left(\frac{1}{2\tau}\left(\nu_0 \triangle U_1 + \triangle\varphi_U + \frac{1}{2\tau}U_1\right)\right), \frac{1}{2\tau}U_1 + \triangle\varphi_U\right\rangle_{L^2(\Omega)}$$
$$+ \left\langle \frac{\varepsilon^2}{4} \triangle U_1 - TU_1 + \lambda_D^{-2}\overline{n} \triangle_D^{-1} U_1 - \nu_0 \triangle \varphi_U + \frac{1}{2\tau}\varphi_U, \frac{1}{2\tau}U_1 + \triangle\varphi_U\right\rangle_{L^2(\Omega)}$$
$$+ \left\langle (-C_1 \triangle + T - C_2\triangle_D^{-1})\left(\nu_0 \triangle U_1 + \triangle\varphi_U + \frac{1}{2\tau}U_1\right), U_1\right\rangle_{L^2(\Omega)}$$
$$+ \left\langle \nu_0 \triangle \tilde{U}_{\mathrm{div}} - \frac{1}{2\tau}\tilde{U}_{\mathrm{div}}, \tilde{U}_{\mathrm{div}}\right\rangle_{L^2(\Omega)}$$

$$
\begin{aligned}
&= \left\langle -\nu_0 \left(\frac{1}{2\tau} U_1 + \triangle \varphi_U \right) + C_1 \triangle U_1 - T U_1 + C_2 \triangle_D^{-1} U_1, \frac{1}{2\tau} U_1 + \triangle \varphi_U \right\rangle_{L^2(\Omega)} \\
&\quad - C_1 \left\langle \frac{1}{2\tau} U_1 + \triangle \varphi_U + \nu_0 \triangle U_1, \triangle U_1 \right\rangle_{L^2(\Omega)} + T \left\langle \frac{1}{2\tau} U_1 + \triangle \varphi_U, U_1 \right\rangle_{L^2(\Omega)} \\
&\quad - C_2 \left\langle \frac{1}{2\tau} \triangle_D^{-1} U_1 + \varphi_U + \nu_0 U_1, U_1 \right\rangle_{L^2(\Omega)} + T\nu_0 \langle \triangle U_1, U_1 \rangle_{L^2(\Omega)} \\
&\quad + \nu_0 \left\langle \triangle \tilde{U}_{\mathrm{div}}, \tilde{U}_{\mathrm{div}} \right\rangle_{L^2(\Omega)} - \frac{1}{2\tau} \left\| \tilde{U}_{\mathrm{div}} \right\|_{L^2(\Omega)}^2 \\
&= -\nu_0 \left\| \frac{1}{2\tau} U_1 + \triangle \varphi_U \right\|_{L^2(\Omega)}^2 - C_1 \nu_0 \| \triangle U_1 \|_{L^2(\Omega)}^2 - C_2 \nu_0 \| U_1 \|_{L^2(\Omega)}^2 \\
&\quad + 2\mathrm{i}\Im \left(\left\langle C_1 \triangle U_1 + C_2 \triangle_D^{-1} U_1, \frac{1}{2\tau} U_1 + \triangle \varphi_U \right\rangle_{L^2(\Omega)} + \langle T \triangle \varphi_U, U_1 \rangle_{L^2(\Omega)} \right) \\
&\quad + T\nu_0 \langle \triangle U_1, U_1 \rangle_{L^2(\Omega)} + \nu_0 \left\langle \triangle \tilde{U}_{\mathrm{div}}, \tilde{U}_{\mathrm{div}} \right\rangle_{L^2(\Omega)} - \frac{1}{2\tau} \left\| \tilde{U}_{\mathrm{div}} \right\|_{L^2(\Omega)}^2 .
\end{aligned}
$$

An application of (4.30) concludes the proof. □

After these preparations, we are now ready to show the existence of stationary states in the case of small currents.

Proof of Theorem 4.2. Write $V = \overline{V} + W$ with W solving $\lambda_D^2 \triangle W = n - C$, $\gamma_0 W = 0$. Put $n = \overline{n} + m$, and then we have

$$
\begin{aligned}
n \nabla V &= \overline{n} \nabla \left(\overline{V} + \lambda_D^{-2} \triangle_D^{-1} (\overline{n} - C) \right) + \overline{n} \lambda_D^{-2} \nabla \triangle_D^{-1} m \\
&\quad + m \nabla \overline{V} + m \lambda_D^{-2} \nabla \triangle_D^{-1} (m + \overline{n} - C).
\end{aligned}
$$

With $\mathcal{A}$ from (4.31) and $U = \binom{m}{J}$, we then have

$$
\begin{aligned}
\mathcal{A} U &= \begin{pmatrix} 0 \\ -\operatorname{div} \left(\frac{1}{\overline{n}+m} \left(J \otimes J + \frac{\varepsilon^2}{4} (\nabla m) \otimes (\nabla m) \right) \right) \end{pmatrix} \\
&\quad + \begin{pmatrix} 0 \\ \overline{n} \nabla \left(\overline{V} + \lambda_D^{-2} \triangle_D^{-1} (\overline{n} - C) \right) + m \nabla \overline{V} + m \lambda_D^{-2} \nabla \triangle_D^{-1} (m + \overline{n} - C) \end{pmatrix} \\
&=: R(U).
\end{aligned}
$$

In the Banach space

$$
Y = \left(W_p^2(\Omega) \cap W_{p,0}^1(\Omega) \right) \times W_{p,B}^1(\Omega; \mathbb{R}^d), \qquad p > d,
$$

we choose a closed set M,

$$
M = \left\{ (m, J) \colon \ \|m\|_{L^\infty(\Omega)} \leq \frac{1}{2} \overline{n}, \quad \|m\|_{W_p^2(\Omega)} \leq \beta_n, \quad \|J\|_{W_p^1(\Omega)} \leq \beta_J \right\},
$$

for some small constants β_n, β_J. Note that the embedding $W_p^1(\Omega) \hookrightarrow L^\infty(\Omega)$ yields

$$
\|R(U)\|_X \leq C_R \left((1 + \beta_n) \left(\|J\|_{W_p^1(\Omega)}^2 + \|m\|_{W_p^2(\Omega)}^2 \right) + \delta \right)
$$

if $U \in M$. By Lemma 4.22, there is a constant $C_{\mathcal{A},p}$ such that

$$\left\|\mathcal{A}^{-1}\right\|_{\mathcal{L}(X,Y)} \leq C_{\mathcal{A},p},$$

and now it remains to define a sequence

$$U^{(0)} = 0, \qquad U^{(k+1)} = \mathcal{A}^{-1} R(U^{(k)}),$$

which can be quickly verified to stay in M and to converge if β_n, β_J and δ are sufficiently small. □

Proof of Theorem 4.3. We connect with the notation and methods of the proof of Theorem 4.2, and write $U^* = \binom{n^*-\overline{n}}{J^*}$, $U = \binom{n-\overline{n}}{J}$, which gives us

$$\mathcal{A}U^* = R(U^*), \qquad \partial_t U - \mathcal{A}U = -R(U).$$

Now we apply Theorem 4.15 and Lemma 4.22, and the proof is complete. □

Proof of Theorem 4.4. We append a copy of Ω to it, obtaining $\tilde{\Omega} = (0, L_1) \times (-L_2, L_2)$, and define a reflection operator

$$\rho\colon \Omega \to \tilde{\Omega}, \qquad \rho(x_1, x_2) = (x_1, -x_2).$$

To a function triple (n, J, V) satisfying (4.12), we define an extension $(\tilde{n}, \tilde{J}, \tilde{V})$ to $\tilde{\Omega}$ by

$$(\tilde{n}, \tilde{J}_1, \tilde{J}_2, \tilde{V})(\rho(x)) := (n, J_1, -J_2, V)(x), \qquad x \in \Omega,$$

and similarly $\tilde{C}(\rho(x)) := C(x)$. Then if (n, J, V) solves (4.1) in Ω, then so does $(\tilde{n}, \tilde{J}, \tilde{V})$ on $\tilde{\Omega}$, and $\tilde{\Omega}$ can be construed as the lateral surface Ω_{cyl} of a cylinder after identification of $(0, L_1) \times \{-L_2\}$ with $(0, L_2) \times \{L_2\}$. Compare [45] for related results on treating fluid equations with the tools of global analysis. The boundary conditions on Γ_D of (4.12) turn into the boundary condition (4.6) on the manifold Ω_{cyl}, and then a generalization of Theorem 4.1 to the case of Ω being a manifold gives the first claim. The second claim is proved after identifying $\{0\} \times (-L_2, L_2)$ with $\{L_1\} \times (-L_2, L_2)$. The uniqueness of the solution $(\tilde{n}, \tilde{J}, \tilde{V})$ and the invariance of the system (4.1) under the reflection ρ guarantee that (n, J, V) satisfies the selected boundary condition. □

Appendix: A variant of Aubin's lemma

In [111, Theorem 5 and Corollary 4], we find the following result:

Lemma A.1 (Aubin's Lemma). *Let X, B, Y be Banach spaces with continuous embeddings $X \hookrightarrow B \hookrightarrow Y$, the left embedding being compact. Suppose that $\mathcal{F}$ is a bounded subset of $L^p((0,T); X)$ for a certain $p \in [1, \infty]$, and let $\partial\mathcal{F}/\partial t = \{f' \colon f \in \mathcal{F}\}$ be the set of distributional derivatives of elements of $\mathcal{F}$. For $f \in \mathcal{F}$ and $0 < h < T$, define a shifted copy $\sigma_h f$ of f as $(\sigma_h f)(t) := f(t+h)$, for $0 \leq t \leq T - h$.*

Then the following three criteria are valid:

- *If* $1 \le p \le \infty$ *and* $\lim_{h\to 0} \|\sigma_h f - f\|_{L^p((0,T-h);Y)} = 0$ *uniformly for* $f \in \mathcal{F}$, *then* $\mathcal{F}$ *is relatively compact in* $L^p((0,T);B)$.
- *If* $1 \le p < \infty$ *and* $\partial\mathcal{F}/\partial t$ *is bounded in* $L^1((0,T);Y)$, *then* $\mathcal{F}$ *is relatively compact in* $L^p((0,T);B)$.
- *If* $p = \infty$ *and* $\partial\mathcal{F}/\partial t$ *is bounded in* $L^r((0,T);Y)$ *for some* $r > 1$, *then* $\mathcal{F}$ *is relatively compact in* $C([0,T];B)$.

In the following, we wish to know when a family of piecewise constant functions forms a relatively compact subset of an evolution space. To this end, we split the time interval $(0,T)$ into N parts of equal length $\tau := T/N$, and for $k = 0, 1, \ldots, N$, let us be given elements $\rho_0, \ldots, \rho_N$ of B. Then we define a piecewise constant interpolation $\rho_\tau = \rho_\tau(t)$ as

$$\rho_\tau(t) := \begin{cases} \rho_k & : (k-1)\tau < t \le k\tau, \\ \rho_0 & : t = 0, \end{cases}$$

and a piecewise linear interpolation[1] $\hat{\rho}_\tau = \hat{\rho}_\tau(t)$ via

$$\hat{\rho}_\tau(t) := \frac{k\tau - t}{\tau}\rho_{k-1} + \frac{t - (k-1)\tau}{\tau}\rho_k, \qquad (k-1)\tau \le t \le k\tau.$$

For the piecewise constant function, we define a discretized derivative $\partial_t^\tau \rho_\tau(t) := \partial_t \hat{\rho}_\tau(t)$, for $t \notin \{k\tau \colon 0 \le k \le N\}$.

Now let $\mathcal{T}$ be a sequence of positive numbers τ approaching zero, and let us be given a set $\mathcal{F} := \{\rho_\tau \colon \tau \in \mathcal{T}\}$ of piecewise constant functions ρ_τ. We define a discretized L^p norm:

$$\|\rho_\tau\|_{L^p_\tau((0,T);X)} := \begin{cases} \left(\sum_{k=0}^N \tau \|\rho_k\|_B^p\right)^{1/p} & : 1 \le p < \infty, \\ \max_{k=0,\ldots,N} \|\rho_k\|_B & : p = \infty, \end{cases}$$

which is not the usual $L^p((0,T);B)$ norm of ρ_τ, since ρ_0 contributes to the sum. By the special choice of this norm, we can compare the linear against the constant interpolation function:

$$\|\hat{\rho}_\tau\|_{L^p((0,T);X)} \le 2^{1/p} \|\rho_\tau\|_{L^p_\tau((0,T);X)}, \qquad 1 \le p \le \infty.$$

Put $\partial\mathcal{F}/\partial t := \{\partial_t^\tau \rho_\tau \colon \tau \in \mathcal{T}\}$. Then we have the following result:

Lemma A.2. *Suppose that the above constructed set* $\mathcal{F}$ *is bounded in* $L^p_\tau((0,T);X)$, *and assume that* $\partial\mathcal{F}/\partial t$ *is bounded in* $L^r((0,T);Y)$ *with* $r = 1$ *for* $1 \le p < \infty$, *and* $r > 1$ *for* $p = \infty$. *Then the following holds:*

- *if* $1 \le p < \infty$, *then* $\mathcal{F}$ *is relatively compact in* $L^p((0,T);B)$;
- *if* $p = \infty$, *then* $\mathcal{F}$ *is relatively compact in* $C([0,T];B)$.

[1] Since ρ_τ and $\hat{\rho}_\tau$ are functions of t, but $\rho_0, \ldots, \rho_N$ are not, we do not consider this an abuse of notation.

Proof. The first part follows directly from Lemma A.1. However, for $p = \infty$, none of the three criteria is applicable. But we see that the set $\hat{\mathfrak{F}}$ of the piecewise linear interpolation functions $\hat{\rho}_\tau$ is relatively compact in $C([0,T];B)$, by the third criterion. Then there is a limit $\rho \in C([0,T];B)$ and a subsequence in $\hat{\mathfrak{F}}$ such that

$$\lim_{\tau\to 0} \|\rho - \hat{\rho}_\tau\|_{C([0,T];B)} = \lim_{\tau \to 0} \sup_{0\le t\le T} \|\rho(t) - \hat{\rho}_\tau(t)\|_B = 0.$$

Moreover, ρ is *uniformly* continuous, since $[0,T]$ is a compact interval. Then for any $\varepsilon > 0$ there is a $\delta = \delta(\varepsilon, \rho)$ such that $\|\rho(t) - \rho(t')\|_B < \varepsilon$ whenever $|t - t'| < \delta$. Now choose τ_0 so small that $\|\rho - \hat{\rho}_\tau\|_{C([0,T];B)} < \varepsilon/2$ for all $\tau \le \tau_0$, and additionally $\tau_0 \le \delta(\varepsilon/2, \rho)$. For fixed τ and $t \in ((k-1)\tau, k\tau]$ with $0 \le t \le T$ and $0 \le k \le N$, write $R(t,\tau) := k\tau$ for the right end-point of the sub-interval. Then we conclude as follows, if $\tau \le \tau_0$:

$$\begin{aligned}\|\rho(t) - \rho_\tau(t)\|_B &= \|\rho(t) - \rho_\tau(R(t,\tau))\|_B = \|\rho(t) - \hat{\rho}_\tau(R(t,\tau))\|_B \\ &\le \|\rho(t) - \rho(R(t,\tau))\|_B + \|\rho(R(t,\tau)) - \hat{\rho}_\tau(R(t,\tau))\|_B \\ &< \varepsilon,\end{aligned}$$

because of $|t - R(t,\tau)| \le \tau \le \delta(\varepsilon/2, \varrho)$ and the uniform continuity. □

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Large Coupling Convergence: Overview and New Results

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Abstract. In this paper we present a couple of old and new results related to the problem of large coupling convergence. Several aspects of convergence are discussed, namely norm resolvent convergence as well as convergence within Schatten-von Neumann classes. We also discuss the rate of convergence with a special emphasis on the optimal rate of convergence, for which we give necessary and sufficient conditions. The collected results are then used for the case of Dirichlet operators. Our method is purely analytical and is supported by a wide variety of examples.

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1. Introduction

For non-negative potentials V, convergence of Schrödinger operators $-\Delta + bV$ as the coupling constant b goes to infinity has been studied for a long time, cf. [9], [11], [12], and the references therein. Motivated by the fact that there has been created a rich theory of point interactions described in detail in the monograph [1], one has recently made an attempt to include singular, measure-valued potentials in these investigations. In addition, it turned out that perturbations by differential operators of the same order are important in a variety of applications in engineering, cf. [14], [15].

All the mentioned families $(H_b)_{b>0}$ of operators are of the following form: One is given a non-negative self-adjoint operator H in a Hilbert space $\mathcal{H}$. Set

$$D(\mathcal{E}) := D(\sqrt{H}),$$
$$\mathcal{E}(u,v) := (\sqrt{H}u, \sqrt{H}v) \quad \forall\, u, v \in D(\mathcal{E}).$$

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$\mathcal{E}$ is a form in $\mathcal{H}$, i.e., a semi-scalar product on a linear subspace of $\mathcal{H}$. Hence

$$\mathcal{E}_1(u,v) := \mathcal{E}(u,v) + (u,v) \quad \forall\, u,v \in D(\mathcal{E})$$

defines a scalar product on $D(\mathcal{E})$. The form $\mathcal{E}$ is closed, i.e., $(D(\mathcal{E}),\mathcal{E}_1)$ is a Hilbert space. Moreover, it is densely defined, i.e., $D(\mathcal{E})$ is dense in $\mathcal{H}$. In addition, one is given a form $\mathcal{P}$ in $\mathcal{H}$ such that for every $b>0$ the form $\mathcal{E}+b\mathcal{P}$, defined by

$$D(\mathcal{E}+b\mathcal{P}) := D(\mathcal{E}) \cap D(\mathcal{P}),$$
$$(\mathcal{E}+b\mathcal{P})(u,v) := \mathcal{E}(u,v) + b\,\mathcal{P}(u,v) \quad \forall\, u,v \in D(\mathcal{E}+b\mathcal{P}),$$

is densely defined and closed. Then, by Kato's representation theorem, for every $b>0$ there exists a unique non-negative self-adjoint operator H_b in $\mathcal{H}$ such that

$$D(\sqrt{H_b}) = D(\mathcal{E}+b\mathcal{P}),$$
$$\left\|\sqrt{H_b}u\right\|^2 = (\mathcal{E}+b\mathcal{P})(u,u) \quad \forall\, u \in D(\mathcal{E}+b\mathcal{P}).$$

H_b is called the self-adjoint operator associated with $\mathcal{E}+b\mathcal{P}$. By Kato's monotone convergence theorem, the operators $(H_b+1)^{-1}$ converge strongly as b goes to infinity. In a wide variety of applications it turns out that it is more easy to analyze the limit than the approximants $(H_b+1)^{-1}$. For this reason one might use the following strategy for the investigation of the operator H_b for large b: One studies the limit of the operators $(H_b+1)^{-1}$ and estimates the error one produces by replacing $(H_b+1)^{-1}$ by the limit. This leads to the question about how fast the operators $(H_b+1)^{-1}$ converge. It is also important to find out which kind of convergence takes place. For instance, convergence with respect to the operator norm admits much stronger conclusions about the spectral properties than strong convergence, cf., e.g., the discussion of this point in [22, Chap. VIII.7].

One has achieved a variety of results within the general framework described above. One has discovered that there exists a universal upper bound for the rate of convergence (Corollary 2.8), and one has derived a criterion for convergence with maximal rate (Theorem 2.7). In general, only strong convergence takes place. However, one has found a variety of conditions which are sufficient for locally uniform convergence (Theorem 2.6, Theorem 2.7, and Proposition 2.9), and in certain cases one has even arrived at estimates for the rate of convergence (Theorem 2.7 and Proposition 2.9).

One has even found conditions which are sufficient for convergence within a Schatten (-von Neumann) class of finite order, cf. Sections 2.5 and 2.6.2. This admits strong conclusions about the spectral properties. For instance, if H and H_0 are non-negative self-adjoint operators and $(H+1)^{-1}-(H_0+1)^{-1}$ belongs to the trace class, then, by the Birman-Kuroda theorem, the absolutely continuous spectral parts of H and H_0 are unitarily equivalent and, in particular, H and H_0 have the same absolutely continuous spectrum. Often, $(H+1)^{-1}-(H_0+1)^{-1}$ does not belong to the trace class, but $(H+1)^{-k}-(H_0+1)^{-k}$ for some sufficiently large k does and, again the Birman-Kuroda Theorem, this implies that the absolutely continuous parts of H and H_0 are unitarily equivalent. This note also contains some new results on the convergence of powers of resolvents, cf. Section 2.8. These results are based on a generalization of the celebrated Dynkin's formula in Section 2.7.

One has introduced the concept of the trace of a Dirichlet form in order to study time changed Markov processes. The generator of the time changed process plays also an important role in the investigation of large coupling convergence for the Dirichlet operators, cf. Section 3.2. If one perturbs a Dirichlet operator by an equilibrium measure times a coupling constant b and let b go to infinity, then one gets, at least in the conservative case, large coupling convergence with maximal rate, cf. Theorem 3.16. A simple domination principle described in Section 3.3 makes it possible to use results on the perturbation by one measure in order to derive results on perturbations by other measures.

In this note we concentrate on non-negative perturbations. If one studies large coupling convergence of magnetic Schrödinger operators, then one needs different techniques. We refer to [17] and the references therein for results in this direction.

In addition to new results we have collected material which can be found at the following places (we do not claim that these are the original sources in all cases):

[3]: Lemma 3.7
[4]: Lemmas 2.2 and 2.4, Theorems 2.6 and 2.7, Corollary 2.8, Proposition 2.9 a), Sections 2.5 and 3.4
[6]: Lemma 2.3, Lemma 2.15
[7]: Section 2.6.1, Examples 2.1 and 3.19, and Eqs. (3.20) and (3.22)
[8]: Section 2.7
[13]: Section 2.4 up to Lemma 2.15 and the examples, Section 3.1, and Theorem 3.5, cf. also [20]
[16]: Eq. (3.21)
[23]: Eq. (2.10)
[25]: Lemma 2.5

2. Non-negative form perturbations

2.1. Notation and general hypotheses

Let $\mathcal{E}$ denote a densely defined closed form in the Hilbert space $(\mathcal{H}, (\,\cdot, \cdot\,))$ and H be the self-adjoint operator associated with $\mathcal{E}$. Let $\mathcal{P}$ denote a form in $\mathcal{H}$ such that $\mathcal{E}+\mathcal{P}$ is a densely defined and closed form in $\mathcal{H}$. Note that we do not require $\mathcal{P}$ be closable, i.e., we do not only admit regular, but also singular form perturbations of H.

Example 2.1. Let J be a closed operator from the Hilbert space $(D(\mathcal{E}), \mathcal{E}_1)$ to an auxiliary Hilbert space $\mathcal{H}_{\text{aux}}$. Let

$$D(\mathcal{P}) := D(J),$$
$$\mathcal{P}(u,v) := (Ju, Jv)_{\text{aux}} \quad \forall\, u, v \in D(J).$$

Then $\mathcal{E} + b\mathcal{P}$ is a closed form in $\mathcal{H}$ for every $b > 0$. If $D(J)$ is dense in $(D(\mathcal{E}), \mathcal{E}_1)$ and, in addition, $\operatorname{ran}(J)$ is dense in $\mathcal{H}_{\text{aux}}$, then JJ^* is an invertible non-negative self-adjoint operator in $\mathcal{H}_{\text{aux}}$.

Proof. Let (u_n) be a sequence in $D(\mathcal{E} + b\mathcal{P}) = D(J)$ such that

$$\begin{aligned}(\mathcal{E} + b\mathcal{P})\,(u_n - u_m, u_n - u_m) &+ \|u_n - u_m\|^2 \\ &= \mathcal{E}_1(u_n - u_m, u_n - u_m) + b\|Ju_n - Ju_m\|^2_{\text{aux}} \to 0 \quad \text{as } n, m \to \infty. \quad (2.1)\end{aligned}$$

In order to prove that $\mathcal{E} + b\mathcal{P}$ is closed we only have to show that there exists a $u \in D(J)$ such that

$$\begin{aligned}(\mathcal{E} + b\mathcal{P})(u_n - u, u_n - u) &+ \|u_n - u\|^2 \\ &= \mathcal{E}_1(u_n - u, u_n - u) + b\,\|Ju_n - Ju\|^2_{\text{aux}} \to 0 \quad \text{as } n \to \infty.\end{aligned}$$

Since $\mathcal{E}_1$ is non-negative and $b > 0$, it follows from (2.1) that

$$\mathcal{E}_1(u_n - u_m, u_n - u_m) \to 0 \quad \text{as } n, m \to \infty.$$

Since $\mathcal{E}$ is closed, this implies that there exists a $u \in D(\mathcal{E})$ such that

$$\mathcal{E}_1(u_n - u, u_n - u) \to 0 \quad \text{as } n \to \infty. \tag{2.2}$$

Since $\mathcal{E}_1$ is non-negative and $b > 0$, it also follows from (2.1) that

$$\|Ju_n - Ju_m\|^2_{\text{aux}} \to 0 \quad \text{as } n, m \to \infty$$

and hence the sequence (Ju_n) in $\mathcal{H}_{\text{aux}}$ is convergent. Since J is a closed operator from the Hilbert space $(D(\mathcal{E}), \mathcal{E}_1)$ to the Hilbert space $\mathcal{H}_{\text{aux}}$ and (Ju_n) is convergent in $\mathcal{H}_{\text{aux}}$, (2.2) implies that $u \in D(J)$ and $\|Ju_n - Ju\|_{\text{aux}} \to 0$. Thus $\mathcal{E} + b\mathcal{P}$ is closed.

Suppose now, in addition, that $D(J)$ is dense in $(D(\mathcal{E}), \mathcal{E}_1)$ and $\operatorname{ran}(J)$ is dense in $\mathcal{H}_{\text{aux}}$. Since J is closed, the domain $D(J^*)$ of the adjoint J^* of J is dense in $\mathcal{H}_{\text{aux}}$ and $J = J^{**}$. Hence JJ^* is a non-negative self-adjoint operator in $\mathcal{H}_{\text{aux}}$. If $JJ^*u = 0$, then $\mathcal{E}_1(J^*u, J^*u) = (u, JJ^*u)_{\text{aux}} = 0$ and hence $u \in \ker(J^*) = \operatorname{ran}(J)^\perp$. $\operatorname{ran}(J)^\perp = \{0\}$, since $\operatorname{ran}(J)$ is dense in $\mathcal{H}_{\text{aux}}$. Thus all assertions in the example are proven. □

Indeed, Example 2.1 covers the most general non-negative form perturbation of H:

Lemma 2.2. *There exist an auxiliary Hilbert space $\mathcal{H}_{\text{aux}}$ and a closed operator J from the Hilbert space $(D(\mathcal{E}), \mathcal{E}_1)$ to $\mathcal{H}_{\text{aux}}$ such that*

$$\begin{aligned}D(J) &= D(\mathcal{E} + \mathcal{P}), \\ (Ju, Jv)_{\text{aux}} &= \mathcal{P}(u, v) \quad \forall\, u, v \in D(J),\end{aligned}$$

and $\operatorname{ran}(J)$ *is dense in $\mathcal{H}_{\text{aux}}$. Thus, in particular, $\mathcal{E} + b\mathcal{P}$ is closed for every $b > 0$.*

Proof. We define an equivalence relation $\sim$ on $D(\mathcal{E})\cap D(\mathcal{P})$ as follows: $f \sim g$ if and only if $\mathcal{P}(f-g, f-g) = 0$. For every $f \in D(\mathcal{E}) \cap D(\mathcal{P})$ let $[f]$ be the equivalence class with respect to this equivalence relation and denote by $\mathcal{H}_{\mathrm{aux}}$ the completion of the quotient space $(D(\mathcal{E}) \cap D(\mathcal{P}), \mathcal{P})/\sim$, with respect to the norm

$$|||[f]||| = \mathcal{P}(f, f), \ \forall\, [f] \in \big(D(\mathcal{E}) \cap D(\mathcal{P})\big)/\sim .$$

Then it easily follows from the hypothesis that $\mathcal{E} + \mathcal{P}$ is closed that

$$\begin{aligned} D(J) &:= D(\mathcal{E}) \cap D(\mathcal{P}), \\ Jf &:= [f] \quad \forall\, f \in D(J), \end{aligned}$$

defines a closed operator from $(D(\mathcal{E}), \mathcal{E}_1)$ to $\mathcal{H}_{\mathrm{aux}}$ with the required properties. □

In the following, we choose an auxiliary Hilbert space $\mathcal{H}_{\mathrm{aux}}$ and a closed operator J from $(D(\mathcal{E}), \mathcal{E}_1)$ to $\mathcal{H}_{\mathrm{aux}}$ as in the previous lemma, i.e., such that

$$\begin{aligned} D(J) &= D(\mathcal{E}) \cap D(\mathcal{P}), \\ (Ju, Jv)_{\mathrm{aux}} &= \mathcal{P}(u, v) \quad \forall\, u, v \in D(J), \end{aligned} \tag{2.3}$$

and set

$$\mathcal{E}^J := \mathcal{E} + \mathcal{P}. \tag{2.4}$$

For every $b > 0$, we denote by H_b^J (or simply by H_b if J is clear from the context) the self-adjoint operator in $\mathcal{H}$ associated with $\mathcal{E} + b\mathcal{P}$.

If not stated otherwise, we assume, in addition, that

$$D(J) \supset D(H). \tag{2.5}$$

This hypothesis is less restrictive than it might seem at a first glance. In fact, J may also be regarded as an operator from $\big(D(\mathcal{E}^J), \mathcal{E}_1^J\big)$ to $\mathcal{H}_{\mathrm{aux}}$ and then J is a bounded, everywhere defined operator and, in particular, it is closed. Thus, if necessary, we may replace $\mathcal{E}$ and H by $\mathcal{E}^J$ and H_1, respectively, and then the hypothesis (2.5) is satisfied (with H_1 in place of H). Moreover, we have

$$\begin{aligned} H_{b+1} &= (H_1)_b \quad \forall\, b > 0, \\ \lim_{b\to\infty} (H_b + 1)^{-1} &= \lim_{b\to\infty} ((H_1)_b + 1)^{-1}. \end{aligned} \tag{2.6}$$

Under the hypothesis (2.5), $D(J)$ is dense in $(D(\mathcal{E}), \mathcal{E}_1)$, and we set

$$\check{H} := (JJ^*)^{-1}. \tag{2.7}$$

Note that $\check{H}$ is an invertible non-negative self-adjoint operator in $\mathcal{H}_{\mathrm{aux}}$.

Let

$$\begin{aligned} D(\mathcal{E}_\infty^J) &:= \{u \in D(\mathcal{E} + \mathcal{P}) \colon \mathcal{P}(u, u) = 0\}, \\ \mathcal{E}_\infty^J(u, v) &:= \mathcal{E}(u, v) \quad \forall\, u, v \in D(\mathcal{E}_\infty), \end{aligned} \tag{2.8}$$

where J and $\mathcal{P}$ are related via (2.3) (often we shall omit J in the notation). Let

$$\mathcal{H}_\infty^J := \overline{\{u \in D(\mathcal{E} + \mathcal{P}) \colon \mathcal{P}(u, u) = 0\}}, \tag{2.9}$$

i.e., let $\mathcal{H}_\infty^J$ be the closure of the kernel of J in the Hilbert space $\mathcal{H}$. By Kato's monotone convergence theorem, $\mathcal{E}_\infty^J$ is a densely defined closed form in the Hilbert space $\mathcal{H}_\infty^J$ and

$$(H_b+1)^{-1} \to (H_\infty+1)^{-1} \oplus 0 \text{ strongly as } b \to \infty, \tag{2.10}$$

where H_∞ denotes the self-adjoint operator in $\mathcal{H}_\infty^J$ associated to $\mathcal{E}_\infty^J$. We shall abuse notation and write $(H_\infty+1)^{-1}$ instead of $(H_\infty+1)^{-1} \oplus 0$.

We set

$$L(H,P) := \liminf_{b\to\infty} b \, \|(H_b+1)^{-1} - (H_\infty+1)^{-1}\|.$$

We shall also use the following abbreviations:

$$D_b := (H+1)^{-1} - (H_b+1)^{-1}, \quad D_\infty := (H+1)^{-1} - (H_\infty+1)^{-1},$$
$$G := (H+1)^{-1}. \tag{2.11}$$

2.2. A resolvent formula

We have an explicit expression for the resolvents of the self-adjoint operators H_b. This fact will play a key role throughout this note.

Lemma 2.3. *Let J be a closed operator from $(D(\mathcal{E}), \mathcal{E}_1)$ to an auxiliary Hilbert space $\mathcal{H}_{\mathrm{aux}}$ such that*

$$D(J) \supset D(H).$$

Let $b > 0$ and let H_b be the self-adjoint operator in $\mathcal{H}$ associated with the closed form $\mathcal{E}^{bJ}$ in $\mathcal{H}$ defined as follows:

$$D(\mathcal{E}^{bJ}) := D(J),$$
$$\mathcal{E}^{bJ}(u,v) := \mathcal{E}(u,v) + b(Ju,Jv)_{\mathrm{aux}} \quad \forall\, u,v \in D(J).$$

Then, with $G := (H+1)^{-1}$, the following resolvent formula holds:

$$(H+1)^{-1} - (H_b+1)^{-1} = (JG)^* \left(\frac{1}{b} + JJ^*\right)^{-1} JG. \tag{2.12}$$

Proof. Replacing J by $\sqrt{b}J$, if necessary, we may assume that $b=1$. On the other hand the following identity holds true: for all $u \in \mathcal{H}$ and $v \in D(J^*)$

$$(J^*v,u) = \mathcal{E}_1(J^*v, Gu) = (v, JGu)_{\mathrm{aux}} = ((JG)^*v, u). \tag{2.13}$$

Let $u \in \mathcal{H}$. Since JJ^* is a non-negative self-adjoint operator in $\mathcal{H}_{\mathrm{aux}}$, the operator $1+JJ^*$ in $\mathcal{H}_{\mathrm{aux}}$ is bounded, self-adjoint, and invertible, and

$$D((1+JJ^*)^{-1}) = \mathcal{H}_{\mathrm{aux}}.$$

Since $\mathrm{ran}(1+JJ^*)^{-1} = D(JJ^*)$, we obtain that $u \in D(J^*(1+JJ^*)^{-1}JG)$ and $J^*(1+JJ^*)^{-1}JGu \in D(J) = D(\mathcal{E}^J)$.

By Kato's representation theorem,

$$\mathcal{E}_1^J((H_1+1)^{-1}u, v) = (u,v) \quad \forall\, u \in \mathcal{H}, v \in D(\mathcal{E}^J).$$

On the other hand,

$$\begin{aligned}\mathcal{E}_1^J&(Gu - J^*(1+JJ^*)^{-1}JGu, v)\\ &= \mathcal{E}_1(Gu, v) + (JGu, Jv)_{\text{aux}}\\ &\qquad - ((1+JJ^*)^{-1}JGu, Jv)_{\text{aux}} - (JJ^*(1+JJ^*)^{-1}JGu, Jv)_{\text{aux}}\\ &= (u, v) \quad \forall\, u \in \mathcal{H},\, v \in D(\mathcal{E}^J).\end{aligned}$$

Thus

$$(H_1+1)^{-1}u = Gu - J^*(1+JJ^*)^{-1}JGu \quad \forall\, u \in \mathcal{H},$$

and it only remains to show that

$$J^*v = (JG)^*v \quad \forall\, v \in D(J^*). \tag{2.14}$$

This is true by identity (2.13). □

2.3. Convergence with respect to the operator norm

If not otherwise stated, J is a closed operator from the Hilbert space $(D(\mathcal{E}), \mathcal{E}_1)$ to an auxiliary Hilbert space $\mathcal{H}_{\text{aux}}$ and, in addition, $D(J) \supset D(H)$. Let

$$\begin{aligned} D(\mathcal{P}) &:= D(J),\\ \mathcal{P}(u, v) &:= (Ju, Jv)_{\text{aux}} \quad \forall\, u, v \in D(J),\end{aligned}$$

and H_b be the self-adjoint operator in $\mathcal{H}$ associated to $\mathcal{E} + b\mathcal{P}$.

By Lemma 2.1, JJ^* is a non-negative invertible self-adjoint operator in $\mathcal{H}_{\text{aux}}$. For every $h \in \mathcal{H}_{\text{aux}}$ we denote by μ_h the spectral measure of h with respect to the self-adjoint operator $\check{H} := (JJ^*)^{-1}$ in $\mathcal{H}_{\text{aux}}$, i.e., the unique finite positive Radon measure on $\mathbb{R}$ such that, with $(E_{\check{H}}(\lambda))_{\lambda\in\mathbb{R}}$ being the spectral family of $\check{H}$,

$$\mu_h((-\infty, \lambda]) = \|E_{\check{H}}(\lambda)h\|_{\text{aux}}^2 \quad \forall \lambda \in \mathbb{R}. \tag{2.15}$$

Since $\check{H}$ is invertible and non-negative,

$$\mu_h((-\infty, 0]) = 0 \quad \forall\, h \in \mathcal{H}_{\text{aux}}. \tag{2.16}$$

By (2.12), for every $b > 0$

$$D_b := (H+1)^{-1} - (H_b+1)^{-1} = (JG)^*(\frac{1}{b} + JJ^*)^{-1}JG. \tag{2.17}$$

Hence D_b is a bounded non-negative self-adjoint operator in $\mathcal{H}$ and the spectral calculus yields that

$$\begin{aligned}(D_b f, f) &= ((JG)^*(\frac{1}{b} + JJ^*)^{-1}JGf, f)\\ &= ((\frac{1}{b} + JJ^*)^{-1}JGf, JGf)_{\text{aux}}\\ &= \int \frac{1}{\frac{1}{b} + \frac{1}{\lambda}}\, d\mu_h(\lambda) \quad \forall\, f \in \mathcal{H},\end{aligned} \tag{2.18}$$

where $h := JGf$. Thus $D_\infty := \lim_{b\to\infty} D_b = (H+1)^{-1} - (H_\infty + 1)^{-1}$ is also a bounded non-negative self-adjoint operator in $\mathcal{H}$ and it follows from (2.18) in conjunction with (2.16) and the monotone convergence theorem that

$$(D_\infty f, f) = \int \lambda \, d\mu_h(\lambda) \quad \forall f \in \mathcal{H}, \tag{2.19}$$

where $h := JGf$. By (2.18) and (2.19),

$$((D_\infty - D_b)f, f) = \int \frac{\lambda^2}{b+\lambda} \, d\mu_h(\lambda) \quad \forall f \in \mathcal{H}, \tag{2.20}$$

where $h := JGf$. Thus $D_\infty - D_b = (H_b + 1)^{-1} - (H_\infty + 1)^{-1}$ is a bounded non-negative self-adjoint operator in $\mathcal{H}$, too.

Lemma 2.4.

a) *We have*

$$\operatorname{ran}(JG) \subset D(\check{H}^{1/2}) \text{ and } D_\infty = (\check{H}^{1/2}JG)^* \check{H}^{1/2} JG. \tag{2.21}$$

In particular, D_∞ is compact if and only if $\check{H}^{1/2}JG$ is compact.

b) *If* $\operatorname{ran}(JG) \subset D(\check{H})$, *then*

$$D_\infty = (JG)^* \check{H} JG. \tag{2.22}$$

Proof. a) Let $f \in \mathcal{H}$ and $h := JGf$. By (2.19),

$$(D_\infty f, f) = \int \lambda \, d\mu_h(\lambda) < \infty,$$

and hence, by the spectral calculus, it follows that $h = JGf \in D(\check{H}^{1/2})$ and $\|\check{H}^{1/2}JGf\|^2_{\text{aux}} = (D_\infty f, f)$. Since D_∞ is a bounded non-negative self-adjoint operator, we have

$$\|D_\infty\| = \sup_{\|f\|=1} (D_\infty f, f).$$

Thus

$$\|\check{H}^{1/2}JG\|^2 = \|D_\infty\|. \tag{2.23}$$

Since $JGf \in D(\check{H}^{1/2})$ for every $f \in \mathcal{H}$, the spectral calculus yields

$$\left[\frac{1}{b} + \check{H}^{-1}\right]^{-1/2} JG \to \check{H}^{1/2}JG \text{ strongly as } b \to \infty,$$

and hence

$$\left(\left[\frac{1}{b} + \check{H}^{-1}\right]^{-1/2} JG\right)^* \left[\frac{1}{b} + \check{H}^{-1}\right]^{-1/2} JG \to (\check{H}^{1/2}JG)^* \check{H}^{1/2} JG \tag{2.24}$$

weakly as b goes to infinity. The operators on the left-hand side equal

$$(JG)^*(\frac{1}{b} + JJ^*)^{-1} JG = (H+1)^{-1} - (H_b + 1)^{-1} = D_b$$

and converge even strongly to D_∞ as $b \to \infty$. Thus (2.21) is proved.

b) (2.22) follows from (2.21) and the fact that $(JG)^* \check{H}^{1/2} \subset (\check{H}^{1/2}JG)^*$. □

By the preceding lemma, $\check{H}^{1/2}JG$ is a bounded everywhere defined operator from $\mathcal{H}$ to $\mathcal{H}_{\text{aux}}$. That does not guarantee that the resolvents $(H+b)^{-1}$ converge locally uniformly, cf. the examples 2.17 and 2.18. By Theorem 2.6 below, the stronger requirement that $\check{H}^{1/2}JG$ is compact implies convergence of the operators $(H_b+1)^{-1}$ with respect to the operator norm. We shall use the following result for the proof of Theorem 2.6.

Lemma 2.5. *Let (A_n) be a sequence of non-negative bounded self-adjoint operators converging strongly to the compact self-adjoint operator $C : \mathcal{H} \to \mathcal{H}$. Suppose that A_n is dominated by C, i.e.,*

$$(A_n f, f) \le (Cf, f) \quad \forall\, f \in \mathcal{H},$$

for every $n \in \mathbb{N}$. Then the operators A_n converge locally uniformly to C.

Proof. The operator $C - A_n$ is non-negative, bounded and self-adjoint and hence

$$\|C - A_n\| = \sup_{\|f\|=1} ((C - A_n)f, f)$$

for every n.

Let $\varepsilon > 0$. Since C is a non-negative compact self-adjoint operator and the A_n converge to C strongly, we can choose an orthonormal family $(e_j)_{j=1}^N$ and an n_0 such that

$$(Ch, h) \le \frac{\varepsilon}{2}\|h\|^2 \quad \forall\, h \in \operatorname{span}(e_1, \ldots, e_N)^\perp$$

and

$$\|(A_n - C)g\| \le \frac{\varepsilon}{6}\|g\| \quad \forall\, g \in \operatorname{span}(e_1, \ldots, e_N)\, \forall\, n \ge n_0,$$

respectively. Let $f \in \mathcal{H}$ and $\|f\| = 1$. Choose $g \in \operatorname{span}(e_1, \ldots, e_N)$ and $h \in \operatorname{span}(e_1, \ldots, e_N)^\perp$ such that $f = g + h$. For all $n \ge n_0$

$$\begin{aligned}((C - A_n)f, f) &= ((C - A_n)g, g) + 2\mathrm{Re}(((C - A_n)g, h)) + ((C - A_n)h, h) \\ &\le \|(C - A_n)g\|(\|g\| + 2\|h\|) + (Ch, h) \le \varepsilon.\end{aligned}$$

□

Theorem 2.6. *Suppose that $D(H) \subset D(J)$ and the operator $\check{H}^{1/2}JG$ from $\mathcal{H}$ to $\mathcal{H}_{\text{aux}}$ is compact. Then*

$$\|(H_b + 1)^{-1} - (H_\infty + 1)^{-1}\| \to 0, \quad b \to \infty.$$

Proof. We only need to show that $D_\infty - D_b = (H_b + 1)^{-1} - (H_\infty + 1)^{-1}$ converge to zero with respect to the operator norm as b goes to infinity. By (2.17), D_b is a non-negative bounded self-adjoint operator in $\mathcal{H}$ for every $b > 0$. By (2.16) in conjunction with (2.20), $D_\infty - D_b$ is a non-negative bounded self-adjoint operator in $\mathcal{H}$, too. By definition, $D_\infty - D_b$ converge to zero strongly as b goes to infinity. By (2.21), along with $\check{H}^{1/2}JG$ also D_∞ is a compact operator.

The remaining part of the proof follows now from the preceding lemma: The operators D_b are non-negative self-adjoint operators and, by (2.16) in conjunction with (2.20), are dominated by the compact self-adjoint operator D_∞, and they converge to D_∞ strongly as b goes to infinity. Hence $\lim_{b\to\infty} \|D_\infty - D_b\| = 0$. □

Of course, one is not only interested in the question whether norm convergence takes place but one also wants to derive estimates for the rate of convergence. We shall show that convergence faster than $O(1/b)$ is not possible for the operators $(H_b+1)^{-1}$, cf. Corollary 2.8 below. Under the additional assumption that the domain $D(H)$ of H is contained in the domain $D(J)$ of J we can even provide a criterion for convergence with maximal rate $O(1/b)$:

Theorem 2.7. *Suppose that*

$$D(H) \subset D(J)$$

and $Ju \neq 0$ for at least one $u \in D(J)$. Then the following holds:

a) *The mapping $b \mapsto b\,\|(H_b+1)^{-1} - (H_\infty+1)^{-1}\|$ is nondecreasing and*

$$\begin{aligned} L(H,P) &:= \liminf_{b\to\infty} b\,\|(H_b+1)^{-1} - (H_\infty+1)^{-1}\| \\ &= \limsup_{b\to\infty} b\,\|(H_b+1)^{-1} - (H_\infty+1)^{-1}\| > 0 \end{aligned}$$

b) *$L(H,P) < \infty \iff J(D(H)) \subset D(\check{H})$.*

c) *If $J(D(H)) \subset D(\check{H})$, then*

$$L(H,P) = \|\check{H}JG\|^2 < \infty. \tag{2.25}$$

Proof. Let $f \in \mathcal{H}$, $h = JGf$, and μ_h be the spectral measure of h with respect to $\check{H}$. By (2.20),

$$b((D_\infty - D_b)f, f) = \int \frac{b\lambda^2}{b+\lambda}\, d\mu_h(\lambda).$$

This implies in conjunction with (2.16) and the monotone convergence theorem (from measure theory), that the mapping $b \mapsto b((D_\infty - D_b)f, f)$ is nondecreasing and

$$\lim_{b\to\infty} b((D_\infty - D_b)f, f) = \int \lambda^2\, d\mu_h(\lambda).$$

Since μ_h is the spectral measure of h with respect to the self-adjoint operator $\check{H}$, it follows that

$$\lim_{b\to\infty} b((D_\infty - D_b)f, f) = \|\check{H}JGf\|^2_{\text{aux}} \quad \text{if } JGf \in D(\check{H}), \tag{2.26}$$

$$\lim_{b\to\infty} b((D_\infty - D_b)f, f) = \infty \quad \text{if } JGf \notin D(\check{H}). \tag{2.27}$$

By (2.27),

$$\liminf_{b\to\infty} b\|D_\infty - D_b\| = \infty, \tag{2.28}$$

if there exists an $f \in \mathcal{H}$ such that $JGf \notin D(\check{H})$.

Suppose now that $\operatorname{ran}(JG) \subset D(\check{H}) = \operatorname{ran}(JJ^*)$. JG is closed, since J is closed and G is bounded and closed. Since $D(JG) = \mathcal{H}$, it follows from the closed graph theorem that JG is bounded. Since $\check{H}$ is closed, this implies that $\check{H}JG$ is closed. Since $D(\check{H}JG) = \mathcal{H}$, it follows from the closed graph theorem that $\check{H}JG$ is bounded. Moreover, by (2.26),

$$\liminf_{b\to\infty} b\|D_\infty - D_b\| \geq \|\check{H}JGf\|^2_{\mathrm{aux}},$$

if $\|f\| = 1$, and hence

$$\liminf_{b\to\infty} b\|D_\infty - D_b\| \geq \|\check{H}JG\|^2. \tag{2.29}$$

By (2.20) in conjunction with (2.16), $D_\infty - D_b$ is a non-negative self-adjoint operator in $\mathcal{H}$. Thus

$$\|D_\infty - D_b\| = \sup_{\|f\|=1} ((D_\infty - D_b)f, f). \tag{2.30}$$

(2.20) in conjunction with (2.16) also implies that for every normalized $f \in \mathcal{H}$ and $h = JGf$

$$b((D_\infty - D_b)f, f) \leq \int \lambda^2 \, d\mu_h(\lambda) \leq \|\check{H}JG\|^2.$$

In conjunction with (2.30), this implies that

$$b\|D_\infty - D_b\| \leq \|\check{H}JG\|^2 \quad \forall b > 0. \tag{2.31}$$

By (2.28), (2.29), (2.31), part b) and c) of the theorem are proved. In addition, we have shown that the mapping

$$b \mapsto b\,\|D_b - D_\infty\| = b\,\|(H_b + 1)^{-1} - (H_\infty + 1)^{-1}\|$$

is nondecreasing and hence

$$\begin{aligned} L(H, P) &:= \liminf_{b\to\infty} b\,\|(H_b + 1)^{-1} - (H_\infty + 1)^{-1}\| \\ &= \limsup_{b\to\infty} b\,\|(H_b + 1)^{-1} - (H_\infty + 1)^{-1}\|. \end{aligned} \tag{2.32}$$

It remains to prove that $L(H, P) > 0$. We conduct the proof by contradiction. If $L(H, P)$ were equal to zero, then, by c), we would have $JG = 0$. Thus the kernel of J would contain $\mathrm{ran}(G) = D(H)$ and hence it would be dense in $(D(\mathcal{E}), \mathcal{E}_1)$. Since the kernel of a closed operator is closed it would follow that $J = 0$, which contradicts the fact that the range of J is dense in $\mathcal{H}_{\mathrm{aux}}$. Thus $L(H, P) > 0$. □

Part a) of the preceding theorem in conjunction with formula (2.6) yields the following corollary where we do not require that $D(J) \supset D(H)$.

Corollary 2.8. *Let $\mathcal{P}$ be a form in $\mathcal{H}$ such that $\mathcal{E} + \mathcal{P}$ is a densely defined closed form in $\mathcal{H}$. Let $\mathcal{P}(u, u) \neq 0$ for at least one $u \in D(\mathcal{E} + \mathcal{P})$. For every $b > 0$ let H_b be the self-adjoint operator in $\mathcal{H}$ associated to $\mathcal{E} + b\mathcal{P}$. Then*

$$\begin{aligned} L(H, P) &:= \liminf_{b\to\infty} b\,\|(H_b + 1)^{-1} - (H_\infty + 1)^{-1}\| \\ &= \limsup_{b\to\infty} b\,\|(H_b + 1)^{-1} - (H_\infty + 1)^{-1}\| \, > 0. \end{aligned}$$

Trivially, we get large coupling convergence with maximal rate, i.e., as fast as $O(1/b)$, if the auxiliary Hilbert space $\mathcal{H}_{\text{aux}}$ is finite-dimensional. We shall also give a variety of nontrivial examples. On the other hand, there are other examples, where $\|(H_b+1)^{-1}-(H_\infty+1)^{-1}\|$ converge to zero as c/b^r for some strictly positive finite constant c and some $r \in (0,1)$. Let $0<r<1$. It is an open problem to find a criterion for convergence with rate $O(1/b^r)$ to take place. In part a) of the following proposition we give a sufficient condition and in part b) we show that this condition is "almost necessary".

Proposition 2.9. *Let $0<r<1$ and $s_0 = \frac{1}{2}+\frac{r}{2}$. Suppose that $D(H) \subset D(J)$.*

a) *If $J(D(H)) \subset D(\check{H}^{s_0})$, then*

$$\|(H_b+1)^{-1}-(H_\infty+1)^{-1}\| \le (1-r)^{1-r} r^r \|\check{H}^{1/2+r/2} JG\|^2 \frac{1}{b^r} \quad \forall\, b>0.$$

b) *Let $u \in \mathcal{H}$. If*

$$\|(H_b+1)^{-1}u-(H_\infty+1)^{-1}u\| \le \frac{c}{b^r} \quad \forall\, b>0,$$

for some finite constant c, then $JGu \in D(\check{H}^s)$ for every $s<s_0$.

Proof. a) By (2.16) in conjunction with (2.20), $(H_b+1)^{-1}-(H_\infty+1)^{-1}$ is a non-negative bounded self-adjoint operator in $\mathcal{H}$ and hence

$$\|(H_b+1)^{-1}-(H_\infty+1)^{-1}\| = \sup_{\|f\|=1} ((D_\infty - D_b)f, f).$$

By (2.20), this implies that

$$\|(H_b+1)^{-1}-(H_\infty+1)^{-1}\| = \sup_{\|f\|=1} \int \frac{\lambda^2}{\lambda+b}\, d\mu_h(\lambda),$$

where f and h are related via $h=JGf$ and μ_h denotes the spectral measure of h with respect to $\check{H}$. Moreover,

$$\int \frac{\lambda^2}{\lambda+b}\, d\mu_h(\lambda) \le \max_{\lambda\in(0,\infty)} \frac{\lambda^{1-r}}{\lambda+b} \int |\lambda^{1/2+r/2}|^2\, d\mu_h(\lambda).$$

By elementary calculus,

$$\max_{\lambda\in(0,\infty)} \frac{\lambda^{1-r}}{\lambda+b} = \frac{(1-r)^{1-r}\, r^r}{b^r}.$$

By the spectral calculus,

$$\int |\lambda^{1/2+r/2}|^2\, d\mu_h(\lambda) = \|\check{H}^{1/2+r/2} h\|^2_{\text{aux}}.$$

If $h=JGf$ and $\|f\|=1$, then

$$\|\check{H}^{1/2+r/2} h\|_{\text{aux}} \le \|\check{H}^{1/2+r/2} JG\|,$$

and part a) of the Proposition is proved.

b) Conversely let $f \in \mathcal{H}$ and assume that

$$\|(H_b+1)^{-1} - (H_\infty+1)^{-1}\| \le \frac{c}{b^r} \quad \forall\, b>0,$$

for some finite constant c. Let $h = JGf$. We may assume that $\|f\| = 1$. Let $1/2 < s < s_1 < s_0 := r/2 + 1/2$. Then

$$\begin{aligned} c &\ge b^r \|D_\infty f - D_b f\| \ge b^r \,(D_\infty f - D_b f, f) \\ &= b^r \int \frac{\lambda^2}{\lambda+b}\mu_h(d\lambda) = \int \lambda^{2s_1}\frac{b^r\,\lambda^{2-2s_1}}{\lambda+b}\, d\mu_h(\lambda) \quad \forall\, b>0. \end{aligned} \tag{2.33}$$

In the second step we have used (2.20). Since $2s_0 - 1 = r$, we have

$$t := \frac{r}{2s_1-1} > \frac{r}{2s_0-1} = 1.$$

For all $b \ge 1$ and $\lambda \in [b, b^t]$, we have

$$\frac{b^r\,\lambda^{2-2s_1}}{\lambda+b} \ge \frac{1}{2}\,\lambda^{1-2s_1} b^r \ge \frac{1}{2}\,(b^t)^{1-2s_1} b^r = \frac{1}{2}.$$

By (2.33), this implies

$$\int_{[b,b^t]} \lambda^{2s_1}\,\frac{1}{2}\, d\mu_h(\lambda) \le c \quad \forall\, b\ge 1.$$

Thus

$$\begin{aligned} \int_{[2,\infty)} \lambda^{2s}\, d\mu_h(\lambda) &\le \sum_{n=0}^{\infty} \int_{[2^{t^n}, 2^{t^{n+1}})} \lambda^{2s_1}\, \frac{1}{(2^{t^n})^{2s_1-2s}}\, d\mu_h(\lambda) \\ &\le 2c \sum_{n=0}^{\infty} \left(\frac{1}{2^{2s_1-2s}}\right)^{t^n} < \infty \end{aligned}$$

and hence $h = JGf \in D(\check{H}^s)$. Thus the assertion b) of Proposition 2.9 is also proved. □

2.4. Schrödinger operators

In this section we illustrate above general definitions and results with the aid of Schrödinger operators with regular and singular potentials.

We denote by $\mathbb{D}$ the classical Dirichlet form, i.e., the form in $L^2(\mathbb{R}^d) := L^2(\mathbb{R}^d, dx)$ defined as follows:

$$\begin{aligned} D(\mathbb{D}) &:= H^1(\mathbb{R}^d), \\ \mathbb{D}(u,v) &:= \int \nabla\bar{u}\cdot\nabla v dx \quad \forall\, u,v \in H^1(\mathbb{R}^d). \end{aligned} \tag{2.34}$$

Here dx denotes the Lebesgue measure and $H^1(\mathbb{R}^d)$ the Sobolev space of order one. $\mathbb{D}$ is a densely defined closed form in $L^2(\mathbb{R}^d)$. We shall denote by $-\Delta$ the self-adjoint operator in $L^2(\mathbb{R}^d)$ associated to $\mathbb{D}$.

The capacity of a compact subset K of $\mathbb{R}^d$ and an arbitrary subset B of $\mathbb{R}^d$ is defined as follows:

$$\begin{aligned} \operatorname{cap}(K) &:= \inf\{\mathbb{D}_1(u,u)\colon u \in C_0^\infty(\mathbb{R}^d),\, u \geq 1 \text{ on } K\}, \\ \operatorname{cap}(B) &:= \sup\{\operatorname{cap}(K)\colon K \subset B,\, K \text{ is compact}\}, \end{aligned} \tag{2.35}$$

respectively. A function $u : \mathbb{R}^d \to \mathbb{C}$ is quasi-continuous if and only if for every $\varepsilon > 0$ there exists an open set G_ε such that

$$\operatorname{cap}(G_\varepsilon) < \varepsilon \tag{2.36}$$

and the restriction $u \restriction \mathbb{R}^d \setminus G_\varepsilon$ of u to $\mathbb{R}^d \setminus G_\varepsilon$ is continuous. We shall use the following elementary results:

Lemma 2.10.

a) *Every $u \in H^1(\mathbb{R}^d)$ has a quasi-continuous representative.*
b) *If $\tilde{u}$ and u° are quasi-continuous and $\tilde{u} = u^\circ$ dx-a.e., then $\tilde{u} = u^\circ$ q.e. (quasi-everywhere), i.e.,*

$$\operatorname{cap}(\{x \in \mathbb{R}^d\colon \tilde{u}(x) \neq u^\circ(x)\}) = 0. \tag{2.37}$$

c) *If (u_n) is a sequence in $H^1(\mathbb{R}^d)$, $u \in H^1(\mathbb{R}^d)$ and $\mathbb{D}_1(u_n - u, u_n - u) \to 0$ as $n \to \infty$, then there exists a subsequence (u_{n_j}) of (u_n) such that*

$$\tilde{u}_{n_j} \to \tilde{u} \text{ q.e.,} \tag{2.38}$$

i.e., $\operatorname{cap}(\{x \in \mathbb{R}^d\colon \tilde{u}_{n_j}(x) \not\to \tilde{u}(x)\}) = 0$*. Here $\tilde{u}_{n_j}$ and $\tilde{u}$ denote any quasi-continuous representative of u_{n_j} and u, respectively.*

The proof of the latter lemma can be found in [13].

In the following we shall denote by u both an element of $H^1(\mathbb{R}^d)$ and any quasi-continuous representative of u. It will not matter which quasi-continuous representative is chosen and it will always be clear from the context what is meant.

Remark 2.11. In the one-dimensional case $\operatorname{cap}(\{a\}) = 2$ for every $a \in \mathbb{R}$ and hence a function is quasi-continuous if and only if it is continuous. Thus, in the one-dimensional case, it makes sense to write $u(a)$ if $u \in H^1(\mathbb{R})$ and $a \in \mathbb{R}$. Here $u(a)$ is just the value of the unique continuous representative of u at the point a.

Definition 2.12. Let μ be a positive Radon measure on $\mathbb{R}^d$ charging no set with capacity zero.

a) We define the form $\mathcal{P}_\mu$ in $L^2(\mathbb{R}^d)$ as follows:

$$\begin{aligned} D(\mathcal{P}_\mu) &:= \{u \in H^1(\mathbb{R}^d) : \int |u|^2\, d\mu < \infty\}, \\ \mathcal{P}_\mu(u,v) &:= \int \bar{u}\, v\, d\mu \quad \forall\, u, v \in D(\mathcal{P}_\mu). \end{aligned} \tag{2.39}$$

b) We define the operator J^μ from $H^1(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d,\mu)$ as follows:

$$\begin{aligned} D(J^\mu) &:= \{u \in H^1(\mathbb{R}^d) : \int |u|^2\, d\mu < \infty\}, \\ J^\mu u &:= u \quad \mu\text{-a.e. } \forall\, u \in D(J^\mu). \end{aligned} \tag{2.40}$$

Lemma 2.13. *Let μ be a positive Radon measure on $\mathbb{R}^d$ charging no set with capacity zero. Then the operator J^μ is closed and $\mathbb{D} + b\mathcal{P}_\mu$ is a non-negative densely defined closed form in $L^2(\mathbb{R}^d)$ for any $b > 0$.*

Proof. Let (u_n) be a sequence in $D(J^\mu)$, $u \in H^1(\mathbb{R}^d)$ and $v \in L^2(\mathbb{R}^d,\mu)$ satisfying $\mathbb{D}_1(u_n - u, u_n - u) \to 0$ as $n \to \infty$, and $J^\mu u_n \to v$ as $n \to \infty$. By Lemma 2.10 c), a suitably chosen subsequence of (u_n) converges to u q.e. and hence μ-a.e. Thus $u = v$ μ-a.e. and hence $u \in D(J^\mu)$ and $J^\mu u_n \to u$ as $n \to \infty$. Thus the operator J^μ is closed, and, by Lemma 2.1, it follows that $\mathbb{D} + b\mathcal{P}_\mu$ is also closed. □

Definition 2.14. Let μ be a positive Radon measure on $\mathbb{R}^d$ charging no set with capacity zero. We denote by $-\Delta + \mu$ the non-negative self-adjoint operator in $L^2(\mathbb{R}^d)$ associated to $\mathbb{D} + \mathcal{P}_\mu$ and put

$$(-\Delta + \infty\mu + 1)^{-1} := \lim_{b\to\infty} (-\Delta + b\mu + 1)^{-1}.$$

In the absolutely continuous case, i.e., if $d\mu = V dx$ for some function V, we also write V instead of $V dx$.

In a wide variety of applications one is interested in the question whether the operator J^μ is compact. There exists a rich literature on this topic. Here we shall only need the following result.

Lemma 2.15. *Suppose that $D(J^\mu) = H^1(\mathbb{R})$ and*

$$\mu(\{y \in \mathbb{R} : |x - y| < 1\}) \to 0, \quad |x| \to \infty. \tag{2.41}$$

Then the operator J^μ from $H^1(\mathbb{R})$ to $L^2(\mathbb{R},\mu)$ is compact.

The proof of this lemma can be found in [6].

Example 2.16. Let $(x_n)_{\in\mathbb{Z}}$ and $(a_n)_{\in\mathbb{Z}}$ be families of real numbers satisfying

$$d := \inf_{n\in\mathbb{Z}} (x_{n+1} - x_n) > 0 \text{ and } a_n > 0 \quad \forall\, n \in \mathbb{Z}. \tag{2.42}$$

Let $\Gamma := \{x_n : n \in \mathbb{Z}\}$ and $-\Delta_D^\Gamma$ the Laplacian in $L^2(\mathbb{R})$ with Dirichlet boundary conditions at every point of Γ, i.e., let $-\Delta_D^\Gamma$ be the non-negative self-adjoint operator in $L^2(\mathbb{R})$ associated to the form $\mathbb{D}_\infty$ in $L^2(\mathbb{R})$ defined as follows:

$$\begin{aligned} D(\mathbb{D}_\infty) &:= \{u \in H^1(\mathbb{R}) \colon u = 0 \text{ on } \Gamma\}, \\ \mathbb{D}_\infty(u,v) &:= \mathbb{D}(u,v) \quad \forall\, u,v \in D(\mathbb{D}_\infty). \end{aligned} \tag{2.43}$$

Then the operators $-\Delta + b\sum_{n\in\mathbb{Z}} a_n\delta_{x_n}$ converge in the strong resolvent sense to $-\Delta_D^\Gamma$. Here δ_x denotes the Dirac measure with unit mass at x.

Proof. $-\Delta + b\sum_{n\in\mathbb{Z}} a_n\delta_{x_n}$ is the self-adjoint operator associated to $\mathbb{D} + b\mathcal{P}_\mu$ with $\mu := \sum_{n\in\mathbb{Z}} a_n\delta_{x_n}$ and we may replace in formula (2.8) $\mathcal{E}$ and $\mathcal{P}$ by $\mathbb{D}$ and $\mathcal{P}_\mu$, respectively. Then the assertion on strong resolvent convergence follows from Kato's monotone convergence theorem, cf. (2.10). □

Different choices of the weights a_n in the last example lead to extremely different convergence results. If the a_n go to zero as $n \to \pm\infty$, then the operators $-\Delta + b\sum_{n\in\mathbb{Z}} a_n\delta_{x_n}$ do not converge in the norm resolvent sense, cf. the next example. On the other hand, if $\inf_{n\in\mathbb{Z}} a_n > 0$, then these operators converge in the norm resolvent with maximal rate of convergence, i.e., as fast as $O(1/b)$, cf. Example 3.8 below.

Example 2.17 (Continuation of Example 2.16). We choose $(x_n)_{n\in\mathbb{Z}}$, $(a_n)_{n\in\mathbb{Z}}$, d, Γ, $-\Delta_D^\Gamma$, and μ as in the previous example. Assume, in addition, that

$$\lim_{|n|\to\infty} a_n = 0 \text{ and } D := \sup_{n\in\mathbb{Z}}(x_{n+1} - x_n) < \infty. \tag{2.44}$$

Then the operators $-\Delta + b\sum_{n\in\mathbb{Z}} a_n\delta_{x_n}$ do not converge in the norm resolvent sense.

Proof. The hypothesis (2.44) implies that $\mathcal{P}_\mu$ is an infinitesimal small form perturbation of $\mathbb{D}$, cf. [5], and hence, in particular, $D(J^\mu) = H^1(\mathbb{R})$. In conjunction with Lemma 2.15 and the hypotheses (2.42) and (2.44) this implies that the operator J^μ is compact. In Lemma 2.3 we may replace H, H_b, G and J by $-\Delta$, $-\Delta + b\sum_{n\in\mathbb{Z}} a_n\delta_{x_n}$, $(-\Delta+1)^{-1}$ and J^μ, respectively. Then the resolvent formula (2.12) yields that $(-\Delta+1)^{-1} - (-\Delta + b\sum_{n\in\mathbb{Z}} a_n\delta_{x_n} + 1)^{-1}$ is compact, too. By Weyl's essential spectrum theorem, this implies that

$$\sigma_{\mathrm{ess}}\left(\left(-\Delta + b\sum_{n\in\mathbb{Z}} a_n\delta_{x_n} + 1\right)^{-1}\right) = \sigma_{\mathrm{ess}}((-\Delta+1)^{-1}) = [0,1]. \tag{2.45}$$

Moreover,

$$-\Delta_D^\Gamma \geq \frac{\pi^2}{D^2}$$

and hence

$$\sup \sigma((-\Delta_D^\Gamma + 1)^{-1})) \leq \frac{1}{1+\pi^2/D^2}. \tag{2.46}$$

If the operators $-\Delta + b\sum_{n\in\mathbb{Z}} a_n\delta_{x_n}$ converged in the norm resolvent sense to the Dirichlet Laplacian $-\Delta_D^\Gamma$, then, by (2.45), we would have $\sigma(-\Delta_D^\Gamma + 1)^{-1}) \supset [0,1]$, which contradicts (2.46). Thus the operators $-\Delta + b\sum_{n\in\mathbb{Z}} a_n\delta_{x_n}$ do not converge in the norm resolvent sense. □

In Example 2.17 the operators $(-\Delta + b\mu + 1)^{-1}$ do not converge locally uniformly. In this example μ is a so-called δ-potential and, in particular, singular. In the regular case we can also have absence of convergence with respect to the operator norm, as it is shown by the next example. That the operators $(-\Delta +$

$bV+1)^{-1}$ in the next example do not converge locally uniformly can be shown by mimicking the proof in Example 2.17.

Example 2.18. Let $(a_n)_{n\in\mathbb{Z}}$ and $(b_n)_{n\in\mathbb{Z}}$ be families of real numbers with the following properties:

$$a_n < b_n < a_{n+1} \quad \forall\, n \in \mathbb{Z}, \quad D := \sup_{n\in\mathbb{Z}}(a_{n+1}-b_n) < \infty,$$
$$d := \inf_{n\in\mathbb{Z}}(a_{n+1}-b_n) > 0, \qquad \lim_{|n|\to\infty}(b_n-a_n) = 0. \tag{2.47}$$

Let $V := \sum_{n\in\mathbb{Z}} 1_{[a_n,b_n]}$. Then the operators $(-\Delta + bV + 1)^{-1}$ converge strongly as b goes to infinity, but do not converge locally uniformly.

2.5. Convergence within a Schatten-von Neumann class

Let $p \in [1,\infty)$. Let $\mathcal{H}_i$ be Hilbert spaces with scalar products $(\cdot,\cdot)_i$, $i = 0,1,2,\ldots$ Let C be a compact operator from $\mathcal{H}_1$ to $\mathcal{H}_2$. Then $\mathcal{H}_2$ has an orthonormal basis $\{e_i\}_{i\in I}$ such that, with $|C| := \sqrt{CC^*}$,

$$|C|e_i = \lambda_i e_i \quad \forall i \in I$$

for some suitably chosen family $(\lambda_i)_{i\in I}$ in $[0,\infty)$ which is unique up to permutations. One sets

$$\|C\|_{S_p} := \left(\sum_{i\in I} \lambda_i^p\right)^{1/p}.$$

$S_p(\mathcal{H}_1,\mathcal{H}_2)$ (short S_p) denotes the set of compact operators from $\mathcal{H}_1$ to $\mathcal{H}_2$ such that $\|C\|_{S_p} < \infty$. It is called the Schatten-von Neumann class of order p. S_p is a linear space and $\|\cdot\|_{S_p}$ a norm on it. If $C\colon \mathcal{H}_1 \to \mathcal{H}_2$ belongs to the class $S_p(\mathcal{H}_1,\mathcal{H}_2)$ and $A\colon \mathcal{H}_0 \to \mathcal{H}_1$ and $B\colon \mathcal{H}_2 \to \mathcal{H}_3$ are linear and bounded, then $CA \in S_p(\mathcal{H}_0,\mathcal{H}_2)$ and $BC \in S_p(\mathcal{H}_1,\mathcal{H}_3)$ and

$$\|CA\|_{S_p} \le \|C\|_{S_p}\|A\|, \quad \|BC\|_{S_p} \le \|C\|_{S_p}\|B\|. \tag{2.48}$$

Moreover,

$$\|C\|_{S_p} = \|C^*\|_{S_p} = \||C|\|_{S_p} \tag{2.49}$$

for every compact operator C.

Let $B\colon \mathcal{H}_1 \to \mathcal{H}_2$ be linear and bounded, Q_1 be an orthogonal projection in $\mathcal{H}_1$, and Q_2 be an orthogonal projection in $\mathcal{H}_2$ such that the dimension N of the range of Q_2 is finite. Then $|Q_2BQ_1|^2 = Q_2BQ_1B^*Q_2$ and hence $|Q_2BQ_1|$ is compact and

$$\||Q_2BQ_1|\|_{S_p} = \||Q_2BQ_1| \restriction \operatorname{ran}(Q_2)\|_{S_p}. \tag{2.50}$$

Since $|Q_2BQ_1| \restriction \operatorname{ran}(Q_2)$ belongs to the finite-dimensional space of all linear mappings from $\operatorname{ran}(Q_2)$ into itself and all norms on a finite-dimensional space are equivalent, there exists a finite constant c, depending only on p and N such that

$$\||Q_2BQ_1| \restriction \operatorname{ran}(Q_2)\|_{S_p} \le c\,\||Q_2BQ_1| \restriction \operatorname{ran}(Q_2)\| \le c\,\|B\|. \tag{2.51}$$

By (2.49) to (2.51),

$$\|Q_2BQ_1\|_{S_p} \leq c\|B\| \tag{2.52}$$

for some finite constant c, depending only on p and $N < \infty$, provided the range of Q_1 or the range of Q_2 is at most N-dimensional.

If A is a non-negative bounded self-adjoint operator and dominated by the compact self-adjoint operator B, then A and $B - A$ are also compact and it follows easily from the min-max principle for compact operators that

$$\|A\|_{S_p} \leq \|B\|_{S_p} \text{ and } \|B - A\|_{S_p} \leq \|B\|_{S_p}. \tag{2.53}$$

In the proof of Theorem 2.6 we have used that strong convergence of non-negative self-adjoint operators dominated by a compact self-adjoint operator implies operator-norm convergence. Similarly, strong convergence of non-negative self-adjoint operators dominated by a self-adjoint operator in S_p implies convergence in S_p:

Lemma 2.19. *Let $\{A_n\}_{n\in\mathbb{N}}$ be a sequence of non-negative bounded self-adjoint operators in the Hilbert space $\mathcal{H}$ dominated by the non-negative bounded self-adjoint operator A. Let $1 \leq p < \infty$. If $A \in S_p$ and $\lim_{n\to\infty} \|Au - A_nu\| = 0$ for all $u \in \mathcal{H}$, then*

$$\lim_{n\to\infty} \|A - A_n\|_{S_p} = 0. \tag{2.54}$$

Proof. By Lemma 2.5, $\lim_{n\to\infty} \|A_n - A\| = 0$.

A admits the representation

$$A = \sum_{i\in I} \lambda_i \,(e_i, \cdot)\, e_i$$

for some orthonormal system $(e_i)_{i\in I}$ and some family $(\lambda_i)_{i\in I}$ of non-negative real numbers satisfying

$$\sum_{i\in I} \lambda_i^p = \|A\|_{S_p}^p.$$

Let $\varepsilon > 0$. We choose a finite subset I_0 of I such that

$$\sum_{i\in I\setminus I_0} \lambda_i^p \leq \varepsilon^p$$

and denote by Q the orthogonal projection onto the orthogonal complement of the finite-dimensional space spanned by $\{e_i : i \in I_0\}$. Then

$$QAQ = \sum_{i\in I\setminus I_0} \lambda_i \,(e_i, \cdot)\, e_i$$

and, in particular,

$$\|QAQ\|_{S_p}^p = \sum_{i\in I\setminus I_0} \lambda_i^p \leq \varepsilon^p.$$

Since $Q(A - A_n)Q$ is dominated by QAQ, it follows that

$$\|Q(A - A_n)Q\|_{S_p} \leq \varepsilon \quad \forall n \in \mathbb{N}. \tag{2.55}$$

Since the range of the orthogonal projection $1 - Q$ is finite-dimensional and $\lim_{n\to\infty} \|A - A_n\| = 0$, it follows from (2.52), that

$$\begin{aligned}\lim_{n\to\infty} \|(1 - Q)(A - A_n)Q\|_{S_p} &= \lim_{n\to\infty} \|(1 - Q)(A - A_n)(1 - Q)\|_{S_p} \\ &= \lim_{n\to\infty} \|Q(A - A_n)(1 - Q)\|_{S_p} = 0.\end{aligned}$$

Since $A - A_n = Q(A - A_n)Q + (1 - Q)(A - A_n)Q + Q(A - A_n)(1 - Q) + (1 - Q)(A - A_n)(1 - Q)$, this implies in conjunction with (2.55), that

$$\limsup_{n\to\infty} \|A - A_n\|_{S_p} \leq \varepsilon,$$

and the lemma is proved. □

Corollary 2.20. *Let $1 \leq p < \infty$. Let $D(J) \supset D(H)$ and suppose that the operator $(H + 1)^{-1} - (H_\infty + 1)^{-1}$ belongs to the Schatten-von Neumann ideal of order p. Then $D_b \in S_p(\mathcal{H}, \mathcal{H})$ and*

$$\|D_\infty - D_b\|_{S_p} \leq \|D_\infty\|_{S_p} \text{ and } \|D_b\|_{S_p} \leq \|D_\infty\|_{S_p} \tag{2.56}$$

for all $b \in (0, \infty)$. Moreover,

$$\lim_{b\to\infty} \|D_\infty - D_b\|_{S_p} = 0. \tag{2.57}$$

Proof. It holds $\lim_{b\to\infty} \|D_\infty u - D_b u\| = 0$ for all $u \in \mathcal{H}$. Hence (2.57) follows from Lemma 2.19.

By (2.16) in conjunction with (2.20), D_b is a non-negative bounded self-adjoint operator dominated by the self-adjoint operator D_∞. Hence (2.56) follows from (2.53). □

The following corollary gives a sufficient condition that the operator $D_\infty = (H + 1)^{-1} - (H_\infty + 1)^{-1}$ belongs to a Schatten-von Neumann ideal of finite order and gives an upper bound for the corresponding Schatten-von Neumann norm.

Corollary 2.21. *Let $D(J) \supset D(H)$ and $L(H, P) < \infty$.*

a) *Let $1 \leq p < \infty$. If $JG \in S_p(\mathcal{H}, \mathcal{H}_{\text{aux}})$, then $D_b \in S_p(\mathcal{H}, \mathcal{H})$ and*

$$\|D_\infty\|_{S_p} \leq \sqrt{L(H, P)}\, \|JG\|_{S_p}. \tag{2.58}$$

b) *Let $t \in (3/2, \infty)$. If JJ^* is bounded and JG^t belongs to the Hilbert-Schmidt class $S_2(\mathcal{H}, \mathcal{H}_{\text{aux}})$, then*

$$\|D_\infty\|_{S_{4t-2}} \leq \sqrt{L(H, P)} \left(\|JJ^*\|^{2t-2} \|JG^t\|_{S_2}^2\right)^{\frac{1}{4t-2}}. \tag{2.59}$$

Proof. By Theorem 2.7 and since $L(H, P) < \infty$, we have that $\operatorname{ran}(JG) \subset D(\check{H})$, $\|\check{H}JG\| = \sqrt{L(H, P)}$ and $\lim_{b\to\infty} \|D_\infty - D_b\| = 0$. By Lemma 2.4 b), this implies that

$$D_\infty = (JG)^* \check{H} JG,$$

hence (2.58) follows from (2.48) in conjunction with (2.49).

Suppose, in addition, that JJ^* is bounded. For all $h \in \mathcal{H}_{\rm aux}$ and $f \in D(\mathcal{E})$

$$(f, (JG)^* h) = (JGf, h)_{\rm aux} = \mathcal{E}_1(Gf, J^* h) = (f, J^* h).$$

Thus $J^* h = (JG)^* h$ for all $h \in \mathcal{H}_{\rm aux}$. Thus $JJ^* = JG^{1/2}(JG^{1/2})^*$ and hence

$$\|JJ^*\| = \|JG^{1/2}\|^2.$$

In conjunction with the hypothesis $JG^t \in S_2$ this implies, by [6, Lemma 2], that

$$\|JG\|_{S_{4t-2}}^{4t-2} \leq \|JJ^*\|^{2t-2} \, \|JG^t\|_{S_2}^2,$$

hence (2.59) follows now from (2.58). □

2.6. Compact perturbations

2.6.1. Expansions. We get stronger assertions provided the operator J is compact. Let us assume that J is a compact operator from $(D(\mathcal{E}), \mathcal{E}_1)$ into $\mathcal{H}_{\rm aux}$, that the domain of J equals $D(\mathcal{E})$, and that the range of J is dense in $\mathcal{H}_{\rm aux}$.

Since $J\colon D(\mathcal{E}) \to \mathcal{H}_{\rm aux}$ is compact and $G^{1/2}$ is a unitary mapping from the Hilbert space $\mathcal{H}$ onto the Hilbert space $(D(\mathcal{E}), \mathcal{E}_1)$, the operator $JG^{1/2}\colon \mathcal{H} \to \mathcal{H}_{\rm aux}$ is also compact and there exist a family $(\lambda_k)_{k\in I}$ in $(0,\infty)$, an orthonormal system $(e_k)_{k\in I}$ in $\mathcal{H}$, and an orthonormal system $(g_k)_{k\in I}$ in $\mathcal{H}_{\rm aux}$ with the following properties:

(i) I has only finitely many elements or $I = \mathbb{N}$ and

$$\lambda_k \to 0, \quad k \to \infty.$$

(ii)
$$JG^{1/2} f = \sum_{k\in I} \lambda_k (e_k, f) g_k \quad \forall\, f \in \mathcal{H}. \tag{2.60}$$

We shall call the latter expansion the *canonical expansion* of the operator $JG^{1/2}$ and refer the reader to [24, p. 4], for more details.

It follows that

$$(JG^{1/2})^* h = \sum_{k\in I} \lambda_k (g_k, h)_{\rm aux}\, e_k \quad \forall\, h \in \mathcal{H}_{\rm aux}, \tag{2.61}$$

and, in particular,

$$(JG^{1/2})^* g_k = \lambda_k e_k \quad \forall\, k \in I. \tag{2.62}$$

By (2.60) and (2.61),

$$JG^{1/2}(JG^{1/2})^* h = \sum_{k\in I} \lambda_k^2 (g_k, h)_{\rm aux} g_k \quad \forall\, h \in \mathcal{H}_{\rm aux}. \tag{2.63}$$

In particular,

$$JG^{1/2}(JG^{1/2})^* g_k = \lambda_k^2 g_k \quad \forall\, k \in \mathbb{N}. \tag{2.64}$$

Furthermore, $\ker((JG^{1/2})^*) = (\operatorname{ran}(JG^{1/2}))^\perp = \{0\}$, since $\operatorname{ran}(J)$ is dense in $\mathcal{H}_{\rm aux}$. Thus the compact operator $JG^{1/2}(JG^{1/2})^*$ in $\mathcal{H}_{\rm aux}$ is invertible. Therefore, (2.63) implies that $(\lambda_k^2)_{k\in I}$ is the family of eigenvalues of $JG^{1/2}(JG^{1/2})^*$ counted repeatedly according to their multiplicity, that, for any $k \in I$, the vector g_k is an eigenvector of $JG^{1/2}(JG^{1/2})^*$ corresponding to the eigenvalue λ_k^2, and that $(g_k)_{k\in I}$ is an orthonormal basis of $\mathcal{H}_{\text{aux}}$. (2.63) implies now that

$$\{1/b + JG^{1/2}(JG^{1/2})^*\}^{-1}h = \sum_{k\in I} \frac{1}{\lambda_k^2 + 1/b}\,(g_k, h)_{\text{aux}}\, g_k \quad \forall\, h \in \mathcal{H}_{\text{aux}}. \tag{2.65}$$

By (2.12), (2.60), (2.61), and (2.65),

$$D_b f := ((H+1)^{-1} - (H_b+1)^{-1})f = G^{1/2}\sum_{k\in I} \frac{\lambda_k^2}{\lambda_k^2 + 1/b}(e_k, G^{1/2}f)e_k \quad \forall\, f \in \mathcal{H}.$$

Since $G^{1/2}$ is self-adjoint and bounded, it follows that

$$\begin{aligned} D_b f &= \sum_{k\in I} \frac{\lambda_k^2}{\lambda_k^2 + 1/b}(G^{1/2}e_k, f)G^{1/2}e_k \\ &= \sum_{k\in I} \frac{\lambda_k^2}{\lambda_k^2 + 1/b}\mathcal{E}_1(G^{1/2}e_k, Gf)G^{1/2}e_k \quad \forall\, f \in \mathcal{H}. \end{aligned} \tag{2.66}$$

$(G^{1/2}e_k)_{k\in I}$ is an orthonormal system in $(D(\mathcal{E}), \mathcal{E}_1)$, since $(e_k)_{k\in I}$ is an orthonormal system in $\mathcal{H}$ and the operator $G^{1/2}$ from $\mathcal{H}$ into $(D(\mathcal{E}), \mathcal{E}_1)$ is unitary. Thus the series $\sum_{k\in I} \mathcal{E}_1(G^{1/2}e_k, Gf)G^{1/2}e_k$ converges in $(D(\mathcal{E}), \mathcal{E}_1)$ (and, therefore, also in $\mathcal{H}$),

$$\sum_{k\in I} |\mathcal{E}_1(G^{1/2}e_k, Gf)|^2 \le \mathcal{E}_1(Gf, Gf) < \infty,$$

and

$$\begin{aligned} &\mathcal{E}_1\left(\sum_{k\in I} \mathcal{E}_1(G^{1/2}e_k, Gf)G^{1/2}e_k - D_b f, \sum_{k\in I} \mathcal{E}_1(G^{1/2}e_k, Gf)G^{1/2}e_k - D_b f\right) \\ &\qquad = \sum_{k\in I} \left|\frac{1}{1 + b\lambda_k^2}\right|^2 |\mathcal{E}_1(G^{1/2}e_k, Gf)|^2 \to 0, \quad b \to \infty, \end{aligned} \tag{2.67}$$

for all $f \in \mathcal{H}$. Since convergence in $(D(\mathcal{E}), \mathcal{E}_1)$ implies convergence in $\mathcal{H}$ and the operators D_b strongly converge in $\mathcal{H}$ to D_∞, (2.67) implies that

$$D_\infty f = \sum_{k\in I} \mathcal{E}_1(G^{1/2}e_k, Gf)G^{1/2}e_k = \sum_{k\in I} (G^{1/2}e_k, f)G^{1/2}e_k \quad \forall\, f \in \mathcal{H}. \tag{2.68}$$

Thus we have proved the following theorem.

Theorem 2.22. *Suppose that $D(J) = D(\mathcal{E})$ and that J is compact. Then, with $(\lambda_k)_{k\in I}$ and $(e_k)_{k\in I}$ as in the canonical expansion of $JG^{1/2}$,*

$$((H+1)^{-1} - (H_b+1)^{-1})f = \sum_{k\in I} \frac{\lambda_k^2}{\lambda_k^2 + 1/b} (G^{1/2}e_k, f)\, G^{1/2}e_k \quad \forall f \in \mathcal{H}, \tag{2.69}$$

$$((H+1)^{-1} - (H_\infty+1)^{-1})f = \sum_{k\in I} (G^{1/2}e_k, f)\, G^{1/2}e_k \quad \forall f \in \mathcal{H}, \tag{2.70}$$

$$\|(H_b+1)^{-1} - (H_\infty+1)^{-1}\| = \sup_{\|f\|=1} \sum_{k\in I} \frac{1}{1+b\lambda_k^2} \,|\,(G^{1/2}e_k, f)\,|^2. \tag{2.71}$$

Remark 2.23. The technique of regularizing the singular problem through the use of the canonical expansion is also typical for the theory of generalized pseudo inverses like presented in [21]. In this context the large coupling limits are sometimes called the limits of the large penalty. They are used in numerical analysis to regularize the 'jumping coefficients' differential equations by penalization. A good survey on regularization can be found in [18] and its use in the theory of saddle-point problems can be found in [19].

In Sections 2.3 and 2.5 the operator $\check{H} = (JJ^*)^{-1}$ has played an important role, but did occur neither in the discussion of Schrödinger operators nor in this section. Actually $\check{H}$ is useful in these contexts, too. To begin with let us mention that we can express the singular values λ_k with the aid of $\check{H}$. By (2.14), $JJ^* = J(JG)^* = JG^{1/2}(JG^{1/2})^*$. Thus the orthonormal basis $(g_k)_{k\in I}$ of $\mathcal{H}_{\rm aux}$ is contained in the domain of $\check{H}$ and

$$\check{H}g_k = \frac{1}{\lambda_k^2}\, g_k \quad \forall k \in I. \tag{2.72}$$

In addition, we have, by (2.62), that

$$(JG)^*g_k = G^{1/2}(JG^{1/2})^*g_k = \lambda_k G^{1/2}e_k \quad \forall k \in I. \tag{2.73}$$

In many applications, one can use this formula in order to describe the vectors e_k with the aid of the eigenvectors g_k of $\check{H}$. We demonstrate this in a simple case:

Let $\mathcal{E} = \mathbb{D}$ be the classical Dirichlet form in $L^2(\mathbb{R})$ and μ be a positive Radon measure on $\mathbb{R}$ such that $\text{supp}(\mu) = [0,1]$. The operator $G := (-\Delta+1)^{-1} \colon L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is an integral operator with kernel $g(x-y)$, where $g(x) := \frac{1}{2}\exp(-|x|)$ for all $x \in \mathbb{R}$. Since the function $\int g(\cdot - y)f(y)dy$ is continuous for all $f \in L^2(\mathbb{R})$, the mapping $J^\mu G : L^2(\mathbb{R}) \to L^2(\mathbb{R},\mu)$ is also an integral operator with the same kernel $g(x-y)$. Thus $(J^\mu G)^* : L^2(\mathbb{R},\mu) \to L^2(\mathbb{R})$ is an integral operator with kernel $\overline{g(y-x)} = g(x-y)$. Since the function $\int g(\cdot - y)h(y)\mu(dy)$ is continuous for all $h \in L^2(\mathbb{R},\mu)$, we finally obtain that also $J^\mu(J^\mu G)^* = J^\mu J^{\mu *} : L^2(\mathbb{R},\mu) \to L^2(\mathbb{R},\mu)$ is an integral operator with kernel $g(x-y)$.

By Lemma 2.15, $J^\mu \colon H^1(\mathbb{R}) \to L^2(\mathbb{R},\mu)$ is compact. Thus we can choose an orthonormal system $(e_k)_{k\in\mathbb{N}}$ in $L^2(\mathbb{R})$, an orthonormal basis $(g_k)_{k\in\mathbb{N}}$ of $L^2(\mathbb{R},\mu)$, and a sequence $(\lambda_k)_{k\in\mathbb{N}}$ of strictly positive real numbers such that

$$J^\mu G^{1/2} = \sum_{k=1}^{\infty} \lambda_k (e_k, \cdot) g_k.$$

Of course, the λ_k, e_k and g_k depend on μ, but we suppress this dependence in our notation.

Let $k \in \mathbb{N}$. The function $u_k := \int g(\cdot - y) g_k(y) \mu(dy)$ is continuous and square integrable, and, for $\mathrm{supp}(\mu) = [0,1]$, satisfies the differential equation $-y'' + y = 0$ on $\mathbb{R} \setminus [0,1]$. Thus

$$u_k(x) = \begin{cases} u_k(0) e^x, & x \le 0, \\ u_k(1) e^{1-x}, & x \ge 1. \end{cases}$$

Since u_k is the continuous representative of $\lambda_k G^{1/2} e_k = (J^\mu G)^* g_k$ and $J^\mu (J^\mu G)^* g_k = \lambda_k^2 g_k$ it follows, for the continuous representative $G^{1/2} e_k$ of $G^{1/2} e_k$, that

$$G^{1/2} e_k(x) = \lambda_k \begin{cases} g_k(0) e^x, & x \le 0, \\ g_k(x), & 0 < x < 1, \\ g_k(1) e^{1-x}, & x \ge 1. \end{cases} \tag{2.74}$$

Set

$$\alpha_k(f) := \left| \int_{-\infty}^0 g_k(0) e^x f(x) dx + \int_0^1 g_k(x) f(x) dx + \int_1^\infty g_k(1) e^{1-x} f(x) dx \right|^2. \tag{2.75}$$

By (2.71) and (2.74), we can express the distances between the operators $(-\Delta + b\mu + 1)^{-1}$ and their limit with the aid of the self-adjoint operator $-\check{\Delta}^\mu = (J^\mu J^{\mu *})^{-1}$ in $L^2(\mathbb{R}, \mu)$. Let $b \in (0, \infty)$. Then

$$\|(-\Delta + b\mu + 1)^{-1} - (-\Delta + \infty\mu + 1)^{-1}\| = \sup_{\|f\|=1} \sum_{k=1}^{\infty} \frac{\alpha_k(f)}{E_k + b}, \tag{2.76}$$

where $-\check{\Delta}^\mu g_k = E_k g_k$ for all $k \in \mathbb{N}$, $(g_k)_{k\in\mathbb{N}}$ is an orthonormal basis of $L^2(\mathbb{R}, \mu)$.

2.6.2. Schatten-von Neumann classes. We can use Theorem 2.22 in order to derive estimates for the rate of convergence with respect to S_p-norms.

Lemma 2.24. *Suppose that $D(J) = D(\mathcal{E})$ and J is compact. Let $1 \le p < \infty$. Then with λ_k and e_k as in the canonical expansion of $JG^{1/2}$ the following holds.*

a) *The operator $D_\infty = (H+1)^{-1} - (H_\infty + 1)^{-1}$ belongs to the Schatten-von Neumann class of order p if and only if*

$$\sum_{k\in I} \|D_\infty^{\frac{p-1}{2}} G^{1/2} e_k\|^2 < \infty. \tag{2.77}$$

If this is the case, then

$$\|D_\infty\|_{S_p}^p = \sum_{k\in I} \|D_\infty^{\frac{p-1}{2}} G^{1/2} e_k\|^2. \tag{2.78}$$

b) *Let* $0 < b < \infty$. *The operator* $D_\infty - D_b = (H_b + 1)^{-1} - (H_\infty + 1)^{-1}$ *belongs to the Schatten-von Neumann class of order* p *if and only if*

$$\sum_{k\in I} \frac{1}{1 + b\lambda_k^2} \|(D_\infty - D_b)^{\frac{p-1}{2}} G^{1/2} e_k\|^2 < \infty. \tag{2.79}$$

If this is the case, then

$$\|D_\infty - D_b\|_{S_p}^p = \sum_{k\in I} \frac{1}{1 + b\lambda_k^2} \|(D_\infty - D_b)^{\frac{p-1}{2}} G^{1/2} e_k\|^2. \tag{2.80}$$

Proof. a) Let $(f_j)_{j\in I'}$ be an orthonormal basis for $\mathcal{H}$. Since D_∞ is a non-negative self-adjoint operator, we obtain

$$\begin{aligned} \|D_\infty\|_{S_p}^p &= \operatorname{tr}(D_\infty^p) = \sum_{j\in I'} (D_\infty^p f_j, f_j) = \sum_{j\in I'} (D_\infty D_\infty^{\frac{p-1}{2}} f_j, D_\infty^{\frac{p-1}{2}} f_j) \\ &= \sum_{j\in I', k\in I} |(G^{1/2} e_k, D_\infty^{\frac{p-1}{2}} f_j)|^2 = \sum_{k\in I} \|D_\infty^{\frac{p-1}{2}} G^{1/2} e_k\|^2. \end{aligned} \tag{2.81}$$

b) The proof of b) is quite similar, so we omit it. □

Theorem 2.25. *Let* $p \in \{1, 2\}$. *Suppose that* $JG^{1/2}$ *is compact. Then the following two assertions are equivalent:*

a) $\|(H_b + 1) - (H_\infty + 1)^{-1}\|_{S_p} \to 0$ *as* $b \to \infty$.
b) $(H + 1)^{-1} - (H_\infty + 1)^{-1}$ *belongs to* $S_p(\mathcal{H}, \mathcal{H})$.

Proof. It is always true that $\|(H_b + 1) - (H_\infty + 1)^{-1}\|_{S_p} \to 0$ as $b \to \infty$ if $D_\infty = (H + 1)^{-1} - (H_\infty + 1)^{-1}$ belongs to $S_p(\mathcal{H}, \mathcal{H})$, cf. Corollary 2.20.

Conversely, let first $p = 2$ and assume that

$$\lim_{b\to\infty} \|(H_b + 1) - (H_\infty + 1)^{-1}\|_{S_2} = 0. \tag{2.82}$$

Then, by Lemma 2.24,

$$\begin{aligned} \|D_\infty - D_b\|_{S_2}^2 &= \sum_{k\in I} \frac{1}{1 + b\lambda_k^2} \|(D_\infty - D_b)^{1/2} G^{1/2} e_k\|^2 \\ &= \sum_{k\in I} \frac{1}{1 + b\lambda_k^2} ((D_\infty - D_b) G^{1/2} e_k, G^{1/2} e_k) \\ &= \sum_{k\in I} \frac{1}{1 + b\lambda_k^2} \sum_{j\in I} \frac{1}{1 + b\lambda_j^2} |(G^{1/2} e_j, G^{1/2} e_k)|^2. \end{aligned} \tag{2.83}$$

Similarly, we obtain

$$\sum_{k\in I} \|D_\infty^{\frac{1}{2}} G^{1/2} e_k\|^2 = \sum_{j,k\in I} |(G^{1/2} e_j, G^{1/2} e_k)|^2. \tag{2.84}$$

By (2.82) in conjunction with (2.83), we get for sufficiently large b that

$$1 \geq \|D_\infty - D_b\|_{S_2}^2 = \sum_{j,k\in I} \frac{1}{1+b\lambda_k^2} \frac{1}{1+b\lambda_j^2} |(G^{1/2}e_j, G^{1/2}e_k)|^2$$
$$\geq \frac{1}{1+b^2} \sum_{\lambda_j,\lambda_k<1} |(G^{1/2}e_j, G^{1/2}e_k)|^2 \tag{2.85}$$

and hence

$$\sum_{k\in I} \|D_\infty^{\frac{1}{2}} G^{1/2} e_k\|^2 = \sum_{j,k\in I} |(G^{1/2}e_j, G^{1/2}e_k)|^2$$
$$\leq (1+b)^2 + \sum_{\lambda_k\geq 1} \sum_{j\in I} |(G^{1/2}e_j, G^{1/2}e_k)|^2 + \sum_{\lambda_k<1} \sum_{\lambda_j\geq 1} |(G^{1/2}e_j, G^{1/2}e_k)|^2$$
$$\leq (1+b)^2 + 2 \sum_{\lambda_k\geq 1} \|Ge_k\|^2 < \infty. \tag{2.86}$$

Thus, by Lemma 2.24 a), the proof is complete for the case $p = 2$. The case $p = 1$ can be treated in a similar way. □

As in the previous subsection we can express the distances between the operators $(-\Delta + b\mu + 1)^{-1}$ and their limit with the aid of the operator $-\check{\Delta}^\mu$.

Lemma 2.26. *Let μ be a positive Radon measure on $\mathbb{R}$ and suppose that* $\mathrm{supp}(\mu) = [0, 1]$. *Let (g_k) be an orthonormal basis of $L^2(\mathbb{R}, \mu)$ such that, with the operator $-\check{\Delta}^\mu = (J^\mu J^{\mu*})^{-1}$, the following holds:*

$$-\check{\Delta}^\mu g_k = E_k g_k \quad \forall\, k \in \mathbb{N}.$$

Then

$$\|(-\Delta + b\mu + 1)^{-1} - (-\Delta + \infty\mu + 1)^{-1}\|_{S_1} = \sum_{k=1}^{\infty} \frac{\beta_k}{E_k + b} \quad \forall\, b > 0, \tag{2.87}$$

where

$$\beta_k = \frac{1}{2}|g_k(0)|^2 + \frac{1}{2}|g_k(1)|^2 + \int_0^1 |g_k(x)|^2 dx \quad \forall\, k \in \mathbb{N}. \tag{2.88}$$

Proof. Since $E_k = 1/\lambda_k^2$ for every $k \in \mathbb{N}$, the lemma follows from (2.80) in conjunction with (2.74). □

2.7. Dynkin's formula

We can use (2.70) in order to derive an abstract version of the celebrated Dynkin's formula.

To begin with let us assume that $D(J) = D(\mathcal{E})$ and J is compact. Choose an orthonormal system $(e_k)_{k\in I}$ in $\mathcal{H}$, an orthonormal basis $(g_k)_{k\in I}$ in $\mathcal{H}_{\mathrm{aux}}$, and a family $(\lambda_k)_{k\in I}$ of non-negative real numbers as in (2.60), i.e., such that $JG^{1/2}f = \sum_{k\in I} \lambda_k (e_k, f) g_k$ for all $f \in \mathcal{H}$. Then $JG^{1/2}f = 0$ if and only if $(e_k, f) = 0$ for all $k \in I$.

$G^{1/2}$ is a unitary operator from $\mathcal{H}$ to $(D(\mathcal{E}), \mathcal{E}_1)$. Thus $(G^{1/2}e_k)_{k\in I}$ is an orthonormal system in the Hilbert space $(D(\mathcal{E}), \mathcal{E}_1)$. Moreover, $(e_k, f) = 0$ for all $k \in I$ if and only if $\mathcal{E}_1(G^{1/2}e_k, G^{1/2}f) = 0$ for all $k \in I$. Thus $(G^{1/2}e_k)_{k\in I}$ is an orthonormal basis of $\ker(J)^\perp$; here $\perp$ means orthogonal with respect to the scalar product $\mathcal{E}_1$ on $D(\mathcal{E})$ and "orthonormal" means "orthonormal with respect to $\mathcal{E}_1$". Thus the first equality in (2.68) yields that

$$D_\infty f = P_J G f \quad \forall\, f \in \mathcal{H}, \tag{2.89}$$

where P_J denotes the orthogonal projection in $(D(\mathcal{E}), \mathcal{E}_1)$ onto $\ker(J)^\perp$.

(2.89) holds true under much weaker assumptions on the operator J. It is easy to understand this fact: Let J_1 and J_2 be densely defined closed operators from $(D(\mathcal{E}), \mathcal{E}_1)$ to $\mathcal{H}_{\text{aux}}$. For $i = 1, 2$ denote by $H_b^{J_i}$ the self-adjoint operator in $\mathcal{H}$ associated to $\mathcal{E}^{bJ_i}$ and put

$$D_\infty^{J_i} := (H+1)^{-1} - \lim_{b\to\infty}(H_b^{J_i}+1)^{-1}.$$

By Kato's monotone convergence theorem,

$$\lim_{b\to\infty}(H_b^{J_1}+1)^{-1} = \lim_{b\to\infty}(H_b^{J_2}+1)^{-1}$$

provided $\ker(J_1) = \ker(J_2)$, cf. (2.10). Trivially, we also have $P_{J_1} = P_{J_2}$ in this case and (2.89) holds true for J_1 if and only if it holds true for J_2. Thus in order to prove (2.89) for a given operator J_1 we only have to choose a compact operator J_2 such that $\ker(J_2) = \ker(J_1)$ and $\operatorname{ran}(J_2)$ is dense in $\mathcal{H}_{\text{aux}}$. Hence the next theorem follows from Lemma 2.29 below.

Theorem 2.27. *Suppose that $D(J)$ is dense in the Hilbert space $(D(\mathcal{E}), \mathcal{E}_1)$ and the auxiliary Hilbert space $\mathcal{H}_{\text{aux}}$ is separable. Let P_J be the orthogonal projection in the Hilbert space $(D(\mathcal{E}), \mathcal{E}_1)$ onto the kernel* $\ker J$ *of J. Then the following* abstract Dynkin's formula *holds true*

$$(H+1)^{-1} - (H_\infty+1)^{-1} = P_J G. \tag{2.90}$$

Remark 2.28. Since we choose $\mathcal{H}_{\text{aux}}$ in such a way that $\operatorname{ran}(J)$ is dense in $\mathcal{H}_{\text{aux}}$, the hypothesis that $\mathcal{H}_{\text{aux}}$ be separable is, in particular, satisfied in the case when $D(J) = D(\mathcal{E})$ and J is compact.

Lemma 2.29. *Let J be a densely defined closed operator from the Hilbert space $(\mathcal{H}_1, (\cdot,\cdot)_1)$ into the separable Hilbert space $(\mathcal{H}_2, (\cdot,\cdot)_2))$. Suppose that* $\operatorname{ran}(J)$ *is dense in $\mathcal{H}_2$. Then there exists a compact operator J_2 from $\mathcal{H}_1$ into $\mathcal{H}_2$ such that $D(J_2) = \mathcal{H}_1$, the range of J_2 is dense in $\mathcal{H}_2$, and*

$$\ker(J_2) = \ker(J).$$

Proof. J^* is a closed operator from the separable Hilbert space $\mathcal{H}_2$ to the Hilbert space $\mathcal{H}_1$. Hence the Hilbert space $(D(J^*), (\cdot,\cdot)_{J^*})$ is separable, where $(u, v)_{J^*} := (u, v)_2 + (J^*u, J^*v)_1$.

Since $(D(J^*), (\cdot,\cdot)_{J^*})$ is separable, we can choose a sequence $(f_n)_{n\in\mathbb{N}}$ such that the set $\{f_n : n \in \mathbb{N}\}$ is dense in $(D(J^*), (\cdot,\cdot)_{J^*})$. Selecting a linearly independent subsequence $(g_n)_{n\in\mathbb{N}}$ of $(f_n)_{n\in\mathbb{N}}$ and applying Gram-Schmidt orthogonalization, we get an orthonormal system $(e_n)_{n\in\mathbb{N}}$ in $\mathcal{H}_2$ with

$$\operatorname{span}\{e_n\colon n \in \mathbb{N}\} = \operatorname{span}\{g_n : n \in \mathbb{N}\}$$

and $\operatorname{span}\{e_n\colon n \in \mathbb{N}\}$ is dense in $(D(J^*), (\cdot,\cdot)_{J^*})$.

$D(J^*)$ is dense in $\mathcal{H}_2$, since J is closed. Thus $\operatorname{span}\{e_n\colon n \in \mathbb{N}\}$ is also dense in $\mathcal{H}_2$ and hence an orthonormal basis of $\mathcal{H}_2$. With this basis, we are able to define the compact operator J_2.

Set

$$\lambda_k := 2^{-k}\,\frac{1}{1+\|J^*e_k\|_1} \quad \forall\, k \in \mathbb{N}.$$

Define an operator J_0 by $D(J_0) = D(J)$ and

$$J_0 f := \sum_{k=1}^{\infty} \lambda_k\,(e_k, Jf)_2\, e_k \quad \forall\, f \in D(J_0).$$

J_0 is a bounded operator from $\mathcal{H}_1$ to $\mathcal{H}_2$ and densely defined. Hence its closure J_2 is a bounded operator from $\mathcal{H}_1$ to $\mathcal{H}_2$ and $D(J_2) = \mathcal{H}_2$.

J_2 is a Hilbert-Schmidt operator. To show that take an orthonormal basis $(h_j)_{j\in I}$ of $\mathcal{H}_1$ such that $h_j \in D(J)$ for every $j \in I$. Then

$$\begin{aligned}\sum_{j\in I} \|J_2 h_j\|_2^2 &= \sum_{j\in I} \left\| \sum_{k\in\mathbb{N}} \lambda_k (e_k, Jh_j)_2 e_k \right\|_2^2 \\ &= \sum_{k\in\mathbb{N}} \lambda_k^2 \sum_{j\in I} |(J^*e_k, h_j)_1|^2 = \sum_{k\in\mathbb{N}} \lambda_k^2 \|J^*e_k\|_1^2 < \infty.\end{aligned}$$

Next we show that $\ker(J) = \ker(J_2)$. If $Jf = 0$, then $J_0 f = J_2 f = 0$ and we obtain $\ker(J) \subset \ker(J_2)$. On the other hand, J is densely defined and closed. Hence $\ker(J) = \operatorname{ran}(J^*)^\perp$. Take an $f \in \ker(J_2)$. Then there is a sequence $(f_n)_{n\in\mathbb{N}}$ in $D(J_0)$ such that $f = \lim_{n\to\infty} f_n$ and $J_2 f = \lim_{n\to\infty} J_0 f_n$. Let $(e_k)_{k\in\mathbb{N}}$ be the orthonormal basis in $\mathcal{H}_2$ introduced above. Then

$$\begin{aligned}0 = (J_2 f, e_k)_2 &= \lim_{n\to\infty} (J_0 f_n, e_k)_2 \\ &= \lim_{n\to\infty} \left(\sum_{m\in\mathbb{N}} \lambda_m (e_m, Jf_n)_2 (e_m, e_k)_2 \right) \\ &= \lim_{n\to\infty} \lambda_k (e_k, Jf_n)_2 = \lambda_k (J^*e_k, f)_1.\end{aligned}$$

Therefore, f is orthogonal to J^*e_k for all $k \in \mathbb{N}$. Since $\operatorname{span}\{e_k\colon k \in \mathbb{N}\}$ is dense in $(D(J^*), (\cdot,\cdot)_{J^*})$, its image $\operatorname{span}\{J^*e_k\colon k \in \mathbb{N}\}$ is dense in $\operatorname{ran}(J^*)$. Thus $f \in \operatorname{ran}(J^*)^\perp = \ker(J)$.

It remains to prove that $\operatorname{ran}(J_2)$ is dense in $\mathcal{H}_2$. Fix $k_0 \in \mathbb{N}$ and $\varepsilon > 0$. Since, by hypothesis, $\operatorname{ran}(J)$ is dense in $\mathcal{H}_2$, we can choose $f \in D(J)$ satisfying

$$\left\| Jf - \frac{e_{k_0}}{\lambda_{k_0}} \right\| < \varepsilon.$$

Thus $\|J_2 f - e_{k_0}\| < \varepsilon$, because of

$$\begin{aligned}
\|J_2 f - e_{k_0}\|_2^2 &= \left\| \sum_{k\in\mathbb{N}} \lambda_k (e_k, Jf)_2 e_k - e_{k_0} \right\| \\
&= \sum_{k\in\mathbb{N}, k\neq k_0} \lambda_k^2 \left|(e_k, Jf)_2\right|^2 + \lambda_{k_0}^2 \left|(e_{k_0}, Jf)_2 - \frac{1}{\lambda_{k_0}}\right|^2 \\
&\leq \sum_{k\in\mathbb{N}, k\neq k_0} \left|(e_k, Jf)_2\right|^2 + \left|(e_{k_0}, Jf)_2 - \frac{1}{\lambda_{k_0}}\right|^2 \\
&= \left\| \sum_{k\in\mathbb{N}} (e_k, Jf)_2 e_k - \frac{e_{k_0}}{\lambda_{k_0}} \right\|_2^2 = \left\| Jf - \frac{e_{k_0}}{\lambda_{k_0}} \right\|_2^2 < \varepsilon.
\end{aligned}$$

Thus $e_{k_0} \in \overline{\operatorname{ran}(J_2)}$. Since $\overline{\operatorname{span}\{e_k : k \in \mathbb{N}\}} = \mathcal{H}_2$, we have shown that $\operatorname{ran}(J_2)$ is dense in $\mathcal{H}_2$. $\square$

2.8. Differences of powers of resolvents

In this section we shall use the generalized Dynkin's formula to derive the surprising result that

$$(H_b + 1)^{-k} - (H_\infty + 1)^{-k} = \left((H_b + 1)^{-1} - (H_\infty + 1)^{-1}\right)^k \quad \forall\, k \in \mathbb{N} \tag{2.91}$$

for a large class of operators H and form perturbations $\mathcal{P}$ of H. Let us recall that

$$(H_b + 1)^{-1} \to (H_\infty + 1)^{-1} \oplus 0, \quad b \to \infty,$$

for a suitably chosen non-negative self-adjoint operator H_∞ in a suitably chosen closed subspace $\mathcal{H}_\infty$ of $\mathcal{H}$ and that we abuse notation and write $(H_\infty + 1)^{-1}$ in place of $(H_\infty + 1)^{-1} \oplus 0$. Here we abuse notation again and simply write $(H_\infty + 1)^{-k}$ in place of $(H_\infty + 1)^{-k} \oplus 0$.

Before we derive formula (2.91), let us briefly mention some reasons why one might be interested in this result. Let A and A_0 be non-negative self-adjoint operators. A and A_0 may be differential operators so that passing to higher powers of the resolvents improves regularity. There are also many examples where the resolvent difference $(A + 1)^{-1} - (A_0 + 1)^{-1}$ does not belong to the trace class, but $(A + 1)^{-k} - (A_0 + 1)^{-k}$ is a trace class operator for sufficiently large k. This implies, by the Birman-Kuroda theorem, that the absolutely continuous spectral part A^{ac} of A is unitarily equivalent to A_0^{ac} and, in particular, A and A_0 have the same absolutely continuous spectrum. Estimates of the trace norm of $(A+1)^{-k} - (A_0 + 1)^{-k}$ can also be used to compare the eigenvalue distributions of A and A_0.

Lemma 2.30. *Suppose that* $D(J) \supset D(H)$ *and*

$$JGu = 0 \quad \forall\, u \in \ker(J). \tag{2.92}$$

Then the following holds:

a) $D_b(G - D_\infty) = 0$ *for all* $b > 0$.
b) $D_\infty(G - D_\infty) = 0$.

Proof. a) Let P_J be the orthogonal projection in $(D(\mathcal{E}), \mathcal{E}_1)$ onto the orthogonal complement of $\ker(J)$. Then $1 - P_J$ is the orthogonal projection onto the bi-orthogonal complement and hence onto the closure of $\ker(J)$. Since J is a closed operator, its kernel is closed and hence $1 - P_J$ is the orthogonal projection onto the kernel of J.

By the generalized Dynkin's formula, cf. Theorem 2.27,

$$D_\infty = P_J G.$$

In conjunction with the resolvent formula (2.12) and the hypothesis (2.92), this implies that

$$D_b(G - D_\infty) = (JG)^* \left(\frac{1}{b} + JJ^*\right)^{-1} JG(1 - P_J)G = 0.$$

b) Due to the fact that the operators D_b converge strongly to D_∞, b) follows from a). □

In the proof of the main theorem of this section we shall use the following telescope-sum formula which holds true for arbitrary everywhere defined operators A and B on $\mathcal{H}$.

$$A^k - B^k = \sum_{j=0}^{k-1} A^{k-1-j}\,(A - B)\,B^j. \tag{2.93}$$

If A and B are bounded self-adjoint operators and $AB = 0$, then

$$(BAu, v) = (u, ABv) = 0 \quad \forall\, u, v \in \mathcal{H}$$

and hence $BA = 0$.

Theorem 2.31. *Suppose that* $D(J) \supset D(H)$ *and* $\ker(J)$ *is* G*-invariant. Then*

$$(H_b + 1)^{-k} - (H_\infty + 1)^{-k} = \left((H_b + 1)^{-1} - (H_\infty + 1)^{-1}\right)^k \quad \forall\, k \in \mathbb{N}.$$

Proof. Let $k \in \mathbb{N}$. By formula (2.93) and having Lemma 2.30 in mind, we get

$$\begin{aligned}(H_b+1)^{-k} &- (H_\infty+1)^{-k}\\ &= \sum_{j=0}^{k-1} (H_\infty+1)^{-k-1-j} \left((H_\infty+1)^{-1} - (H_b+1)^{-1}\right) (H_b+1)^{-j}\\ &= \sum_{j=0}^{k-1} (G-D_\infty)^{k-1-j} (D_\infty - D_b) \left((G-D_\infty) + (D_\infty - D_b)\right)^j\\ &= \sum_{j=0}^{k-1} (G-D_\infty)^{k-1-j} (D_\infty - D_b)^{j+1}\\ &= (D_\infty - D_b)^k + \sum_{j=1}^{k-1} (G-D_\infty)^{k-j} (D_\infty - D_b)^j.\end{aligned}$$

Now observing that, by Lemma 2.30, we have, for all $f \in \mathcal{H}$,

$$\left(\sum_{j=1}^{k-1} (G-D_\infty)^{k-j} (D_\infty - D_b)^j f, f\right) = (f, (D_\infty - D_b)^j (G-D_\infty)^{k-j} f) = 0,$$

we get the result. □

Corollary 2.32. *Under the hypotheses of Theorem* 2.31*, the following holds:*

$$\|(H_b+1)^{-k} - (H_\infty+1)^{-k}\| = \|(H_b+1)^{-1} - (H_\infty+1)^{-1}\|^k \quad \forall\, k \in \mathbb{N}. \tag{2.94}$$

In particular, there exists a $c > 0$ *such that*

$$\begin{aligned}\liminf_{b\to\infty}\, & b^k \|(H_b+1)^{-k} - (H_\infty+1)^{-k}\|\\ &= \limsup_{b\to\infty}\, b^k \|(H_b+1)^{-k} - (H_\infty+1)^{-k}\| = c^k > 0 \quad \forall k \in \mathbb{N},\end{aligned} \tag{2.95}$$

and, for any $k \in \mathbb{N}$*, we have the following equivalence:*

$$\lim_{b\to\infty} b^k \|(H_b+1)^{-k} - (H_\infty+1)^{-k}\| < \infty \iff J(D(H)) \subset D(\check{H}). \tag{2.96}$$

Proof. By (2.16) in conjunction with (2.20), the operator $D_\infty - D_b$ is non-negative, bounded, and self-adjoint. By the spectral calculus and Theorem 2.31, this implies formula (2.94). The assertions (2.95) and (2.96), respectively, follow from (2.94) in conjunction with Theorem 2.7. □

We conclude this section with an example which shows that the condition (2.92) is not "artificial" at all.

Example 2.33. Let D be the open unit disc in $\mathbb{R}^2$ and T the unit circle. We consider the form in $L^2(T) = L^2(T, d\theta)$ defined by

$$\dot{\mathcal{F}}(f,f) := \frac{1}{16\pi}\int_0^{2\pi}\int_0^{2\pi} |f(\theta) - f(\theta')|^2 \sin^{-2}\left(\frac{\theta-\theta'}{2}\right) d\theta d\theta',$$
$$D(\dot{\mathcal{F}}) := \{f \in L^2(T) \colon \mathcal{F}(f,f) < \infty\}. \tag{2.97}$$

We define the form $\dot{\mathcal{E}}$ in $L^2(D)$ as follows:

$$\dot{\mathcal{E}}(f,f) := \frac{1}{2}\int_D |\nabla f|^2 dx,$$
$$D(\dot{\mathcal{E}}) := \{f \in L^2(D) \colon f \text{ is harmonic}, \mathcal{E}(f,f) < \infty\}. \tag{2.98}$$

We take

$$\dot{J} \colon (D(\dot{\mathcal{E}}), \dot{\mathcal{E}}) \to (D(\dot{\mathcal{F}}), \dot{\mathcal{F}}), \quad \dot{J}f := f \restriction T \quad \forall f \in D(\dot{\mathcal{E}}),$$

where $f \restriction T$ is the operation of taking the boundary limit of f. It is known, cf. [13, p. 12], that $\dot{J}$ is unitary and it preserves the subspace of constant functions. We define an equivalence relation on both $L^2(D)$ and $L^2(T)$ by $f \sim g \Leftrightarrow f - g$ is a constant function. Accordingly we define the forms

$$\mathcal{F}([f],[f]) := \dot{\mathcal{F}}(f,f), \; D(\mathcal{F}) = \big(D(\dot{\mathcal{F}})\big)/{\sim}, \tag{2.99}$$
$$\mathcal{E}([f],[f]) = \dot{\mathcal{E}}(f,f), \; D(\mathcal{E}) = \big(D(\dot{\mathcal{E}})\big)/{\sim}, \tag{2.100}$$

and

$$J \colon (D(\mathcal{E}), \mathcal{E}) \to (D(\mathcal{F}), \mathcal{F}), \quad J[f] := \dot{J}f \quad \forall [f] \in D(\mathcal{E}).$$

Then both $\mathcal{F}, \mathcal{E}$ and J are well defined and it is well known that $(D(\mathcal{E}), \mathcal{E})$ is a Hilbert space (which we take to be $\mathcal{H}$). Furthermore since $\dot{J}$ is unitary we conclude that J is unitary as well. Thus $\ker(J) = \{0\}$ and trivially the assumption (2.92) is satisfied. Since $\ker(J) = \{0\}$, also $\mathcal{H}_\infty = \{0\}$, cf. (2.8), and hence $(H_\infty + 1)^{-1} = 0$ and $D_\infty = G$. Since J_0 is unitary, $JJ^* = 1$ and, in particular, $\operatorname{ran}(JJ^*) = D(\mathcal{F})$. J is not unitary as an operator from $(D(\mathcal{E}), \mathcal{E}_1)$ onto $(D(\mathcal{F}), \mathcal{F})$, but the norms induced by $\mathcal{E}$ and $\mathcal{E}_1$ are equivalent and hence we still have $\operatorname{ran}(JJ^*) = D(\mathcal{F})$. Thus, by formula (2.96), there exists a constant $c \in (0, \infty)$ such that

$$\lim_{b\to\infty} b^k \|(H_b + 1)^{-k}\| = c^k$$

for all $k \in \mathbb{N}$.

It is also known that $\mathcal{E}$ and $\mathcal{F}$ in the previous example are Dirichlet forms and the perturbation corresponding to J is a so-called jumping term and, in particular, non-local, cf. [13, p. 12]. Moreover, obviously the operator J is not compact. In the next section we shall concentrate on Dirichlet forms and treat certain local perturbations, the so-called killing terms.

3. Dirichlet forms

We can combine our general methods with tools from the theory of Dirichlet forms in order to improve our results in the special, but very important case when $H_b = H + b\mu$ for some Dirichlet operator H and some killing measure μ. It is also possible to treat other kinds of perturbations, for instance, perturbations by jumping terms, as it was demonstrated in Example 2.33.

3.1. Notation and basic results

Throughout this section, X denotes a locally compact separable metric space, m a positive Radon measure on X such that $\mathrm{supp}(m) = X$ and $\mathcal{E}$ a (symmetric) Dirichlet form in $L^2(X,m)$, i.e., a densely defined closed form in $L^2(X,m)$ satisfying

$$\bar{f} \in D(\mathcal{E}) \quad \forall f \in D(\mathcal{E}), \tag{3.1}$$

(this condition is void in the real case) and possessing the contraction property

$$f^c \in D(\mathcal{E}) \text{ and } \mathcal{E}(f^c, f^c) \le \mathcal{E}(f,f) \tag{3.2}$$

for all real-valued $f \in D(\mathcal{E})$, where $f^c := \min(1, f^+)$ and $f^+ := \max(0, f)$. In addition, we require the Dirichlet form be regular, i.e., the following two conditions are satisfied:

a) The set of all f in the space $C_0(X)$ of continuous functions with compact support such that f is a representative of an element of $D(\mathcal{E})$ is dense in $(C_0(X), \|\cdot\|_\infty)$. We shall denote this set by $C_0(X) \cap D(\mathcal{E})$.
b) The set of all f in $D(\mathcal{E})$ with a continuous representative with compact support is dense in $(D(\mathcal{E}), \mathcal{E}_1)$. We shall denote this set by $C_0(X) \cap D(\mathcal{E})$, too.

The capacity (with respect to $\mathcal{E}$) of an open subset U of X and an arbitrary subset B of X is defined as follows:

$$\begin{aligned} \mathrm{cap}(U) &:= \inf\{\mathcal{E}_1(u,u) \colon u \ge 1\, m\text{-a.e. on U}\}, \\ \mathrm{cap}(B) &:= \inf\{\mathrm{cap}(U) \colon U \supset B,\ U \text{ is open}\}, \end{aligned} \tag{3.3}$$

respectively. The classical Dirichlet form $\mathbb{D}$, defined by (2.34), is a regular Dirichlet form in $L^2(\mathbb{R}^d)$ and the definition of capacity in Section 2.4 is equivalent to the definition of capacity for $\mathbb{D}$ in (3.3). As in the classical case, a function $u : X \to \mathbb{C}$ is called quasi-continuous (with respect to $\mathcal{E}$) if and only if for every $\varepsilon > 0$ there exists an open set U_ε such that $u \restriction X \backslash U_\varepsilon$ is continuous and $\mathrm{cap}(U_\varepsilon) < \varepsilon$. Moreover, as in the classical case, every $u \in D(\mathcal{E})$ has a quasi-continuous representative, two quasi-continuous representatives are equal q.e., i.e., everywhere up to a set with capacity zero, and every $\mathcal{E}_1$-convergent sequence has a subsequence converging q.e. For $u \in D(\mathcal{E})$ we denote by u also any quasi-continuous representative of u. We shall denote by H the non-negative self-adjoint operator associated to $\mathcal{E}$.

Remark 3.1. There exists a Markov process $\mathbb{M}$ such that $p_t(\cdot, B)$ is a quasi-continuous representative of $e^{-tH}1_B$ for every Borel set $B \in \mathcal{B}(X)$ with $m(B) < \infty$ and all $t > 0$. Here $p_t(x, B)$ is the transition function of $\mathbb{M}$ and $\mathbb{M}$ is even an m-symmetric Hunt process with state space $X \cup \{\Delta\}$, where Δ is added as an isolated point if X is compact and $X \cup \{\Delta\}$ is the one-point compactification of X otherwise. If $\mathcal{E} = \frac{1}{2}\mathbb{D}$, then the corresponding Markov process $\mathbb{M}$ is the standard Brownian motion.

In the following, let μ be a positive Radon measure on X charging no set with capacity zero. As in the classical case, we set

$$D(\mathcal{P}_\mu) := D(\mathcal{E}) \cap L^2(X, \mu), \tag{3.4}$$

$$\mathcal{P}_\mu(u, v) := \int \bar{u}v \, d\mu \quad \forall\, u, v \in D(\mathcal{E}) \tag{3.5}$$

and obtain that the operator J^μ from $(D(\mathcal{E}), \mathcal{E}_1)$ to $L^2(X, \mu)$, defined by

$$D(J^\mu) := D(\mathcal{P}_\mu), \quad J^\mu u := u \quad \mu\text{-a.e.} \quad \forall\, u \in D(J^\mu), \tag{3.6}$$

is closed and hence $\mathcal{E} + b\mathcal{P}_\mu$ is closed for all $b > 0$. For each $b > 0$, we set $\mathcal{E}^{b\mu} := \mathcal{E} + b\mathcal{P}_\mu$ and denote by $H + b\mu$ the non-negative self-adjoint operator associated with $\mathcal{E}^{b\mu}$. Moreover,

$$(H + \infty\mu + 1)^{-1} := \lim_{b\to\infty} (H + b\mu + 1)^{-1},$$

$$D^\mu_b := (H + 1)^{-1} - (H + b\mu + 1)^{-1} \quad \forall\, b \in [0, \infty].$$

Theorem 3.2. *$\mathcal{E}^\mu$ is a regular Dirichlet form in $L^2(X, m)$.*

$(H + 1)^{-1}$ has a Markovian kernel G, i.e., there exists a mapping

$$G : X \times \mathcal{B}(X) \to [0, 1]$$

such that $G(\cdot, B)$ is measurable for every B in the Borel-algebra $\mathcal{B}(X)$ of X, $G(x, X) \le 1$ and $G(x, \cdot)$ is a measure for every $x \in X$ and

$$x \mapsto \int f(y)G(x, dy)$$

is a quasi-continuous representative of $(H + 1)^{-1}f$ for every $f \in L^2(X, m)$. For every non-negative Borel measurable function f on X the function $Gf : X \to [0, \infty]$, $Gf(x) := \int f(y)G(x, dy)$ for $x \in X$, is well defined. G is also m-symmetric, i.e., $\int Gf\, h dm = \int f\, Gh dm$ for all non-negative Borel measurable functions f and h. $Gf \ge 0$ q.e. if $f \ge 0$ m-a.e. $\mathcal{E}$, H, and G will be called conservative if $G1 = 1$ q.e. We shall abuse notation and denote not only the Markovian kernel of $(H + 1)^{-1}$, but also the operator $(H + 1)^{-1}$ by G. Moreover, we put

$$G^\mu := (H + \mu + 1)^{-1}$$

and denote by G^μ also the m-symmetric Markovian kernel of this operator.

The Dirichlet form $\mathcal{E}$ is strongly local if and only if the following implication holds for all u, $v \in D(\mathcal{E})$:

$$\begin{array}{l}\text{supp}(um) \text{ and supp}(vm) \text{ compact and } v \text{ constant in} \\ \text{a neighborhood of supp}(um) \text{ implies that } \mathcal{E}(u,v) = 0.\end{array} \tag{3.7}$$

Example 3.3. $\mathbb{D}$ is a regular conservative strongly local Dirichlet form in $L^2(\mathbb{R}^d)$.

3.2. Trace of a Dirichlet form

In the remaining part of this note we shall assume that μ is a positive Radon measure on X charging no set with capacity zero (with respect to $\mathcal{E}$) that satisfies

$$D(H) \subset D(J^\mu). \tag{3.8}$$

Recently Chen, Fukushima, and Ying [10] have obtained deep results on the trace of a Dirichlet form and the associated Markov process. It turns out that traces of Dirichlet forms are also very useful for the investigation of large coupling convergence.

Before we give the definition of the trace of a Dirichlet form, we need some preparation. We put

$$F := \text{supp}(\mu)$$

and identify $L^2(X,\mu)$ and $L^2(F,\mu)$ in the canonical way, i.e., via the unitary transformation $u \mapsto u \restriction F$. We further put

$$P_\mu := P_{J^\mu},$$

i.e., P_μ is the orthogonal projection in the Hilbert space $(D(\mathcal{E}),\mathcal{E}_1)$ onto the orthogonal complement of $\ker(J^\mu)$ (with respect to the scalar product $\mathcal{E}_1$). Obviously, the following implications hold:

$$J^\mu u = J^\mu w \implies u - w \in \ker(J^\mu) \implies P_\mu u = P_\mu w.$$

Hence, the following is correctly defined:

Definition 3.4. We define the form $\check{\mathcal{E}}_1^\mu$ in $L^2(F,\mu)$ as follows:

$$\begin{aligned} D(\check{\mathcal{E}}_1^\mu) &:= \text{ran}(J^\mu), \\ \check{\mathcal{E}}_1^\mu(J^\mu u, J^\mu v) &:= \mathcal{E}_1(P_\mu u, P_\mu v) \quad \forall\, u,v \in D(\mathcal{E}). \end{aligned} \tag{3.9}$$

$\check{\mathcal{E}}_1^\mu$ is called the trace of the Dirichlet form $\mathcal{E}_1$ with respect to the measure μ.

Theorem 3.5. *$\check{\mathcal{E}}_1^\mu$ is a regular Dirichlet form in $L^2(F,\mu)$.*

The proof of this theorem can be found in [13, Chapter 6].

Remark 3.6. In the Definition 3.4 we have essentially used that the Dirichlet form $\mathcal{E}_1$ is coercive. One can define the trace $\check{\mathcal{E}}^\mu$ of an arbitrary regular Dirichlet form $\mathcal{E}$ with respect to a measure μ in such a way that for $\mathcal{E}_1$ the Definition 3.5 above is equivalent to the general one. Even in the general case $\check{\mathcal{E}}^\mu$ is a regular Dirichlet form in $L^2(F,\mu)$. We shall not use these extensions in this note and omit the details, but refer the interested reader to [13, Chapter 6.2].

The operator

$$\check{H}^\mu := (J^\mu J^{\mu *})^{-1} \tag{3.10}$$

plays an important role in the discussion of large coupling convergence. It is remarkable that $\check{H}^\mu$ is the self-adjoint operator associated with the Dirichlet form $\check{\mathcal{E}}_1^\mu$.

Lemma 3.7. *$\check{H}^\mu$ is the self-adjoint operator associated with $\check{\mathcal{E}}_1^\mu$.*

Proof. $u - P_\mu u \in \ker(J^\mu)$ for every $u \in D(\mathcal{E})$. Thus

$$P_\mu u \in D(J^\mu) \text{ and } J^\mu P_\mu u = J^\mu u \quad \forall\, u \in D(J^\mu). \tag{3.11}$$

Since the operator $\check{H}^\mu$ is self-adjoint, we only need to prove that it is a restriction of the self-adjoint operator associated with $\check{\mathcal{E}}_1^\mu$. For this it suffices to show that

$$\check{\mathcal{E}}_1^\mu(J^\mu J^{\mu *} f, h) = (f,h)_{L^2(\mu)} \quad \forall\, f \in D(J^\mu J^{\mu *})\,\forall\, h \in D(\check{\mathcal{E}}_1^\mu).$$

By Theorem 3.5, it suffices to prove this equality for all $f \in D(J^\mu J^{\mu *})$ and all $h \in C_0(F) \cap D(\check{\mathcal{E}}_1^\mu)$. Let now $h \in C_0(F) \cap D(\check{\mathcal{E}}_1^\mu)$ and choose $u \in D(\mathcal{E})$ such that $h = J^\mu u$. Then, by (3.11), $J^\mu P_\mu u = J^\mu u = h$. Let $f \in D(J^\mu J^{\mu *})$. Then

$$\check{\mathcal{E}}_1^\mu(J^\mu J^{\mu *} f, h) = \mathcal{E}_1(J^{\mu *} f, P_\mu u) = (f, J^\mu P_\mu u)_{L^2(\mu)} = (f,h)_{L^2(\mu)}.$$

Thus $\check{H}^\mu$ is the self-adjoint operator associated with $\check{\mathcal{E}}_1^\mu$. □

The following example illustrates the strength of the previous lemma for the investigation of large coupling convergence.

Example 3.8 (Continuation of Example 2.16). We choose $(x_n)_{n\in\mathbb{Z}}$, $(a_n)_{n\in\mathbb{Z}}$, d, Γ, $-\Delta_D^\Gamma$, and μ as in the Example 2.16. Assume, in addition, that

$$m_0 := \inf_{n\in\mathbb{Z}} a_n > 0. \tag{3.12}$$

Then the operators $-\Delta + b\sum_{n\in\mathbb{Z}} a_n \delta_{x_n}$ converge in the norm resolvent sense to $-\Delta_D^\Gamma$ with maximal rate of convergence, i.e.,

$$\lim_{b\to\infty} b\,\|(-\Delta + b\sum_{n\in\mathbb{Z}} a_n\delta_{x_n} + 1)^{-1} - (-\Delta_D^\Gamma + 1)^{-1}\| < \infty. \tag{3.13}$$

Proof. Let $\check{\mathbb{D}}_1^\mu$ be the trace of $\mathbb{D}$ with respect to the measure μ. Let $f \in L^2(\mathbb{R},\mu)$. Then

$$\infty > \int |f|^2\,d\mu = \sum_{n\in\mathbb{Z}} a_n |f(x_n)|^2 \ge m_0 \sum_{n\in\mathbb{Z}} |f(x_n)|^2.$$

Choose $\varphi \in C_0^\infty(\mathbb{R})$ such that $\varphi(0) = 1$ and $\varphi(x) = 0$ if $|x| \ge d/2$. Then $f(x_n)\cdot \varphi(\cdot - x_n)$, $n \in \mathbb{Z}$, are pairwise orthogonal elements of $H^1(\mathbb{R})$ and

$$\sum_{n\in\mathbb{Z}} \|f(x_n)\varphi(\cdot - x_n)\|_{H^1(\mathbb{R})}^2 = \sum_{n\in\mathbb{Z}} |f(x_n)|^2 \|\varphi\|_{H^1(\mathbb{R})}^2 < \infty.$$

Thus $u := \sum_{n\in\mathbb{Z}} f(x_n)\varphi(\cdot - x_n) \in H^1(\mathbb{R})$. Since $f = u$ μ-a.e., we obtain $f \in \operatorname{ran}(J^\mu) = D(\check{\mathbb{D}}_1^\mu)$. Thus

$$D(\check{\mathbb{D}}_1^\mu) = L^2(\mathbb{R},\mu).$$

By the previous lemma, $-\check{\Delta}^\mu := (J^\mu J^{\mu *})^{-1}$ is the self-adjoint operator associated with the closed form $\check{\mathbb{D}}_1^\mu$ in $L^2(\mathbb{R},\mu)$. Since the domain of the form associated to $-\check{\Delta}^\mu$ equals the whole Hilbert space $L^2(\mathbb{R},\mu)$, the domain of $D(-\check{\Delta}^\mu)$ equals $L^2(\mathbb{R},\mu)$, too. Thus, trivially,

$$J^\mu(D(-\Delta)) \subset D(-\check{\Delta}^\mu).$$

By Theorem 2.7, this implies the assertion (3.13). □

We shall demonstrate how to use traces of Dirichlet forms for the investigation of large coupling convergence by further examples. First we need some preparation.

Lemma 3.9. *Let μ be a positive Radon measure on $\mathbb{R}$ such that* $\operatorname{supp}(\mu) = [0,1]$. *Then*

$$\check{\mathbb{D}}_1^\mu(f,h) = \int_0^1 (\overline{f'}h' + \bar{f}h)dx + \overline{f(0)}h(0) + \overline{f(1)}h(1) \quad \forall\, f,h \in D(\check{\mathbb{D}}_1^\mu). \tag{3.14}$$

(*We recall that f denotes both an element of $D(\check{\mathbb{D}}_1^\mu)$ and the unique continuous representative of f.*)

Proof. By polarization, it suffices to consider the case $f = h$. Choose $u \in H^1(\mathbb{R})$ such that $f = J^\mu u$. By definition,

$$\check{\mathbb{D}}_1^\mu(f,f) = \mathbb{D}_1(P_\mu u, P_\mu u). \tag{3.15}$$

P_μ is infinitely differentiable on $\mathbb{R}\setminus[0,1]$ and

$$-(P_\mu u)'' + P_\mu u = 0 \text{ on } \mathbb{R}\setminus[0,1], \tag{3.16}$$

since $\mathbb{D}_1(P_\mu u, v) = 0$ for every $v \in C_0^\infty(\mathbb{R})$ with support in $\mathbb{R}\setminus[0,1]$. Since, by (3.11), $J^\mu P_\mu u = J^\mu u = f$, this implies

$$\begin{aligned} P_\mu u(x) &= P_\mu u(0)e^x = f(0)e^x \qquad \forall\, x \le 0,\\ P_\mu u(x) &= P_\mu u(1)e^{1-x} = f(1)e^{1-x} \quad \forall\, x \ge 1. \end{aligned} \tag{3.17}$$

Thus

$$\begin{aligned} \mathbb{D}_1(P_\mu u, P_\mu u) &= \int_{\mathbb{R}\setminus[0,1]} (|(P_\mu u)'|^2 + |(P_\mu u)|^2)dx + \int_0^1 (|f'|^2 + |f|^2)dx \\ &= |f(0)|^2 + |f(1)|^2 + \int_0^1 (|f'|^2 + |f|^2)dx. \end{aligned} \tag{3.18}$$

□

Corollary 3.10. *Let μ be a positive Radon measure on $\mathbb{R}$ such that* $\operatorname{supp}(\mu) = [0,1]$ *and $1_{(0,1)}\mu = 1_{(0,1)}\,dx$. Then each eigenvalue of the self-adjoint operator $-\check{\Delta}^\mu$ in $L^2(\mathbb{R},\mu)$ associated to the trace $\check{\mathbb{D}}_1^\mu$ of $\mathbb{D}_1$ with respect to the measure μ is strictly positive.*

Let $\eta > 0$ and $-\check{\Delta}^\mu f = (\eta^2+1)f$. Then there exist constants $c \in \mathbb{C}$ and $\theta \in [-\pi/2, \pi/2]$ such that (*the continuous representative of*) *f satisfies*

$$f(x) = c\sin(\eta x + \theta) \quad \forall\, x \in [0,1]. \tag{3.19}$$

Proof. Each eigenvalue of $-\check{\Delta}^\mu$ is strictly positive, since $-\check{\Delta}^\mu$ is an invertible non-negative self-adjoint operator.

Let $\eta > 0$ and $-\check{\Delta}^\mu f = (\eta^2 + 1)f$. By (3.14),

$$(-\check{\Delta}^\mu f, h)_{L^2(\mathbb{R},\mu)} = \int_0^1 (\overline{f'}h' + \bar{f}h)\,dx$$

for all infinitely differentiable functions with compact support in $(0,1)$. This implies that f is infinitely differentiable on $(0,1)$ and $-\check{\Delta}^\mu f = -f''(x) + f(x)$ for every $x \in (0,1)$. Thus $-f''(x) = \eta^2 f(x)$ for all $x \in (0,1)$ and hence there exist constants c and θ such that $f(x) = c\sin(\eta x + \theta)$ for all $x \in (0,1)$ and, therefore, by continuity, for all $x \in [0,1]$. $\square$

We can now apply Lemma 2.26 in order to derive results on the rate of trace class convergence. We demonstrate how to do this through the following example.

Example 3.11. Let $\mu_1 := 1_{[0,1]}\,dx$ and $\mu_2 := \mu_1 + \delta_0 + \delta_1$. Then

$$\lim_{b\to\infty} \sqrt{b}\,\|(-\Delta + b\mu_1 + 1)^{-1} - (-\Delta + \infty\mu_1 + 1)^{-1}\|_{S_1} = \frac{3}{2} \tag{3.20}$$

and

$$\lim_{b\to\infty} \sqrt{b}\,\|(-\Delta + b\mu_2 + 1)^{-1} - (-\Delta + \infty\mu_2 + 1)^{-1}\|_{S_1} = \frac{1}{2}. \tag{3.21}$$

Proof. Let $\mu \in \{\mu_1, \mu_2\}$. Let $k \in \mathbb{N}$, $c_k \in \mathbb{R} \setminus \{0\}$, $\eta_k > 0$, $\theta_k \in [-\pi/2, \pi/2]$ and suppose that g_k with $g_k(x) = c_k \sin(\eta_k x + \theta_k)$ for all $x \in [0,1]$ is a normalized eigenfunction of $-\check{\Delta}^\mu$. We have

$$\int_0^1 (g_k' h' + g_k h)\,dx + g_k(1)h(1) + g_k(0)h(0)$$
$$= \check{\mathbb{D}}_1^\mu(g_k, h) = (-\check{\Delta}^\mu g_k, h)_{L^2(\mu)} = (-g_k'' + g_k, h)_{L^2(\mu)} \quad \forall\, h \in D(\check{\mathbb{D}}^\mu).$$

Moreover,

$$(-g_k'' + g_k, h)_{L^2(\mu_1)} = \int_0^1 (g_k' h' + g_k h)\,dx - g_k'(1)h(1) + g_k'(0)h(0),$$

and

$$(-g_k'' + g_k, h)_{L^2(\mu_2)}$$
$$= (-g_k'' + g_k, h)_{L^2(\mu_1)} + (-g_k''(1) + g_k(1))h(1) + (-g_k''(0) + g_k(0))h(0)$$

for all $h \in D(\check{\mathbb{D}}^{\mu_1})$ and $h \in D(\check{\mathbb{D}}^{\mu_2})$, respectively. It follows that

$$g_k'(0) = g_k(0) \quad \text{and} \quad g_k'(1) = -g_k(1) \quad \text{if } \mu = \mu_1,$$

and

$$g_k''(0) = -g_k'(0) \quad \text{and} \quad g_k''(1) = g_k'(1) \quad \text{if } \mu = \mu_2.$$

It follows now by elementary calculus that

$$\lim_{k\to\infty} \theta_k = \pi/2 \quad \text{if } \mu = \mu_1,$$
$$\lim_{k\to\infty} \theta_k = 0 \quad \text{if } \mu = \mu_2,$$

$$\lim_{k\to\infty} (\eta_k - k\pi) = 0 \text{ and } \lim_{k\to\infty} c_k^2 = 2 \text{ in both cases.}$$

Hence

$$\lim_{k\to\infty} g_k^2(0) = \lim_{k\to\infty} g_k^2(1) = 2 \quad \text{if } \mu = \mu_1,$$
$$\lim_{k\to\infty} g_k^2(0) = \lim_{k\to\infty} g_k^2(1) = 0 \quad \text{if } \mu = \mu_2.$$

Inserting these results into Lemma 2.26 and taking Corollary 3.10 into account, we complete the proof by an elementary computation. □

Finally, we want to hint to an interesting fact. Again let $\mu_1 = 1_{[0,1]}\,dx$. Choose an orthonormal system $(g_k)_{k\in\mathbb{N}}$ in $L^2(\mathbb{R},\mu_1)$ and a sequence$(\eta_k)_{k\in\mathbb{N}}$ of strictly positive real numbers such that $-\check{\Delta}^\mu g_k = (1+\eta_k^2)\,g_k$ for all $k\in\mathbb{N}$. Then, by (2.76),

$$\|(-\Delta + b\mu_1 + 1)^{-1} - (-\Delta + \infty\mu_1 + 1)^{-1}\| \geq \sum_{k=1}^{\infty} \frac{\alpha_k(f)}{1+\eta_k^2+b}$$

for any normalized $f\in L^2(\mathbb{R})$, where

$$\alpha_k(f) := |\int_{-\infty}^0 g_k(0)e^x f(x)\,dx + \int_0^1 g_k(x)f(x)\,dx + \int_1^\infty g_k(1)e^{1-x}f(x)\,dx|^2.$$

If we choose $f(x) := \sqrt{2}\,1_{(-\infty,0)}(x)e^x$ for all $x\in\mathbb{R}$, then, by the considerations of the previous example, $\lim_{k\to\infty}\alpha_k(f) = 1$ and hence

$$\lim_{b\to\infty} \sqrt{b}\,\|(-\Delta + b\mu_1 + 1)^{-1} - (-\Delta + \infty\mu_1 + 1)^{-1}\| \geq \frac{1}{2}. \tag{3.22}$$

Thus the operators $(-\Delta + b\mu_1 + 1)^{-1}$ do not converge faster than $O(1/\sqrt{b})$ with respect to the operator norm. On the other hand, the rate of convergence becomes $O(1/b)$, if we add $\varepsilon_0\delta_0 + \varepsilon_1\delta_1$ to the measure μ_1, where ε_1 and ε_2 are any strictly positive real numbers, cf. Example 3.19 below. Thus arbitrarily small changes of the measure can lead to strong changes of the rate of convergence.

Actually, if one combines (2.76), (2.75) and the results from the previous example, then one gets via an elementary computation that

$$\lim_{b\to\infty} \sqrt{b}\,\|(-\Delta + b\mu_1 + 1)^{-1} - (-\Delta + \infty\mu_1 + 1)^{-1}\| = \frac{1}{2}. \tag{3.23}$$

3.3. A domination principle

For positive Radon measures μ on X charging no set with capacity zero let

$$\mathcal{H}_\infty^\mu := \overline{\ker(J^\mu)}$$

be the closure of $\ker(J^\mu)$ in the Hilbert space $\mathcal{H}$. We have

$$(H + \infty\mu + 1)^{-1} = (H + \infty\nu + 1)^{-1}$$

for $\mathcal{H}_\infty^\mu = \mathcal{H}_\infty^\nu$. This can be true even if the measures μ and ν are quite different; in particular, it is not necessary that the measures μ and ν are equivalent.

Intuitively one expects in the case $(H + \infty\mu + 1)^{-1} = (H + \infty\nu + 1)^{-1}$ that the operators $(H + b\mu + 1)^{-1}$ converge at least as fast as $(H + b\nu + 1)^{-1}$ if $\mu \geq \nu$. We shall prove that this is true. In this way we can use known results for one measure ν in order to derive results for another measure μ. For instance, if $(H + b\nu + 1)^{-1}$ converge with maximal rate, i.e., as fast as $O(1/b)$, and $\mu \geq \nu$ and $(H + \infty\mu + 1)^{-1} = (H + \infty\nu + 1)^{-1}$, then $(H + b\mu + 1)^{-1}$ converge with maximal rate, too.

Lemma 3.12. *Let μ and ν be positive Radon measures on X charging no set with capacity (with respect to $\mathcal{E}$) zero. Assume, in addition, that $\mu \geq \nu$. Then the operator $G^\nu - G^\mu$ is positivity preserving, i.e., it holds $(G^\nu - G^\mu)f \geq 0$ m-a.e if $f \geq 0$ m-a.e.*

Proof. Let f, $g \in L^2(X, m)$, $f \geq 0$ m-a.e., and $g \geq 0$ m-a.e. Then $G^\mu f \geq 0$ m-a.e. and $G^\nu g \geq 0$ m-a.e., since G^μ and G^ν are positivity preserving. By [13, Lemma 2.1.5], this implies that all quasi-continuous representatives of $G^\mu f$ and of $G^\nu g$ (with respect to $\mathcal{E}$) are non-negative q.e. and, therefore, also $(\mu - \nu)$-a.e.

We have, with the convention that u denotes both an element of $D(\mathcal{E})$ and any quasi-continuous representative of u, that

$$\begin{aligned}(f, G^\nu g) &= \mathcal{E}_1^\mu(G^\mu f, G^\nu g)\\ &= \mathcal{E}_1^\nu(G^\mu f, G^\nu g) + \int G^\mu f\, G^\nu g\, d(\mu - \nu)\\ &= (G^\mu f, g) + \int G^\mu f\, G^\nu g\, d\mu.\end{aligned}$$

Thus

$$\int (G^\nu f - G^\mu f) g\, dm = \int G^\mu f\, G^\nu g\, d(\mu - \nu).$$

Since the right-hand side is non-negative for every $g \in L^2(X, m)$ satisfying $g \geq 0$ m-a.e., it follows that $G^\nu f - G^\mu f \geq 0$ m-a.e. □

It holds $G = G^0$, where 0 denotes the measure which is identically equal to zero and $b'\mu \leq b\mu$ if $b' \leq b$. Hence it follows from the previous lemma that

$$G(\cdot, B) \geq G^{b'\mu}(\cdot, B) \geq G^{b\mu}(\cdot, B) \quad \forall\, B \in \mathcal{B}(X) \text{ q.e. if } 0 < b' < b. \tag{3.24}$$

Thus $(H + \infty\mu + 1)^{-1}$ has also an m-symmetric Markovian kernel $G^{\infty\mu}$ and

$$G^{b\mu}(\cdot, B) \geq G^{\infty\mu}(\cdot, B) \quad \forall B \in \mathcal{B}(X) \text{ q.e.} \tag{3.25}$$

For each $b \in [0, \infty]$, it follows that D_b^μ has an m-symmetric Markovian kernel, also denoted by D_b^μ, and that

$$D_{b'}^\mu(\cdot, B) \leq D_b^\mu(\cdot, B) \leq D_\infty^\mu(\cdot, B) \quad \forall B \in \mathcal{B}(X) \text{ q.e. if } 0 < b' < b. \tag{3.26}$$

Corollary 3.13. *Under the hypotheses of Lemma* 3.12 *and the additional assumption that*

$$D_\infty^\mu = D_\infty^\nu,$$

it holds that

$$0 \leq D_\infty^\mu f - D_b^\mu f \leq D_\infty^\nu f - D_b^\nu f \quad m\text{-a.e.} \tag{3.27}$$

for all $b > 0$ provided that $f \geq 0$ m-a.e. Moreover,

$$\|D_\infty^\mu - D_b^\mu\| \leq \|D_\infty^\nu - D_b^\nu\| \quad \forall b > 0. \tag{3.28}$$

Proof. (3.27) follows immediately from Lemma 3.12 and (3.28) follows from (3.27), since both the operators $D_\infty^\mu - D_b^\mu$ and the operators $D_\infty^\nu - D_b^\nu$ have m-symmetric Markovian kernels. □

3.4. Convergence with maximal rate and equilibrium measures

First let us recall some known facts from the potential theory of Dirichlet forms, cf. [13]. A positive Radon measure is a measure with finite energy integral (with respect to $\mathcal{E}$) if and only if there exists a constant $c > 0$ such that

$$\int |u|\, d\mu \leq c\sqrt{\mathcal{E}_1(u, u)} \quad \forall u \in C_0(X) \cap D(\mathcal{E}). \tag{3.29}$$

If μ is a measure with finite energy integral, then μ does not charge any set with capacity zero and there exists a unique element $U_1\mu$ (the 1-potential of μ) of $D(\mathcal{E})$ such that

$$\mathcal{E}_1(U_1\mu, v) = \int v\, d\mu \quad \forall v \in D(\mathcal{E}). \tag{3.30}$$

It holds that $U_1\mu \geq 0$ m-a.e. Now let μ be any positive Radon measure on X charging no set with capacity zero. Then, for all $h \in L^2(X, \mu)$ with $h \geq 0$ μ-a.e., the following holds: $h\mu$ is a measure with finite energy integral if and only if $h \in D(J^{\mu*})$. In this case $J^{\mu*}h$ equals the 1-potential $U_1(h\mu)$ of $h\mu$ and hence

$$J^{\mu*}h = U_1(h\mu) \geq 0 \text{ m-a.e. } \forall h \in D(J^{\mu*}) \text{ with } h \geq 0\, \mu\text{-a.e.} \tag{3.31}$$

Let Γ be a closed subset of X such that the 1-capacity $\operatorname{cap}(\Gamma)$ of Γ is finite. There exists a unique $e_\Gamma \in D(\mathcal{E})$ satisfying

$$e_\Gamma = 1 \text{ q.e. on } \Gamma \text{ and } \mathcal{E}_1(e_\Gamma, v) \geq 0\, \forall v \in D(\mathcal{E}) \text{ with } v \geq 0 \text{ q.e. on } \Gamma. \tag{3.32}$$

Moreover, there exists a unique positive Radon measure μ_Γ on X such that μ_Γ has finite energy integral,

$$\mu_\Gamma(\Gamma) = \mu_\Gamma(X) = \operatorname{cap}(\Gamma) \text{ and } e_\Gamma = U_1\mu_\Gamma. \tag{3.33}$$

Thus $1 \in D(J^{\mu_\Gamma *})$ and

$$J^{\mu_\Gamma} J^{\mu_\Gamma *} 1 = 1 \text{ q.e. on } \Gamma. \tag{3.34}$$

The 1-equilibrium potential e_Γ of Γ satisfies, in addition,

$$0 \leq e_\Gamma \leq 1 \quad m\text{-a.e.} \tag{3.35}$$

We recall that $\check{H} = (J^\mu J^{\mu *})^{-1}$ and set

$$\check{K} := J^\mu J^{\mu *} \quad \text{and} \quad \check{K}_\alpha := (\check{H} + \alpha)^{-1} \quad \forall \alpha > 0. \tag{3.36}$$

(3.34) can be used to prove that $J^{\mu_\Gamma} J^{\mu_\Gamma *}$ is a bounded operator with norm one. We prepare the proof through the following lemma.

Lemma 3.14. *Let G be a symmetric Markovian kernel and set*

$$Tf(x) := \int f(y) G(x, dy)$$

whenever the expression on the right-hand side is defined. Then

$$\|Tf\| \leq (\|T1\|_\infty)^{1/2} \|f\| \quad \forall f \in L^2(X, m) \cap L^\infty(X, m)$$

and hence T extends to a bounded operator on $L^2(X, m)$ with

$$\|T\| \leq (\|T1\|_\infty)^{1/2}. \tag{3.37}$$

Proof. Let $f \in L^2(X, m) \cap L^\infty(X, m)$. By Hölder's inequality,

$$|Tf|^2 \leq T1 \int_X f^2(y) G(\cdot, dy) \leq \|T1\|_\infty \int_X f^2(y) G(\cdot, dy). \tag{3.38}$$

This yields, by the Markov property and the symmetry of G, that $\|Tf\|^2 \leq \|T1\|_\infty \|f\|^2$. □

Corollary 3.15. *Let Γ be a closed subset of X such that $0 < \operatorname{cap}(\Gamma) < \infty$. Then*

$$\|J^{\mu_\Gamma} J^{\mu_\Gamma *}\| = 1. \tag{3.39}$$

Proof. By the first resolvent equality and since the operators $\check{K}_\alpha$ are positivity preserving, the sequence $(\check{K}_{1/n} f)_{n=1}^\infty$ is pointwise non-decreasing μ_Γ-a.e. for all $f \in L^2(X, \mu_\Gamma)$ with $f \geq 0$ μ_Γ-a.e.

By (3.36) and (3.34), $1 \in D(\check{K})$ and $\check{K} 1 = 1$ μ_Γ-a.e. and hence $\|\check{K}\| \geq 1$. By spectral calculus,

$$\|\check{K}_{1/n} f - \check{K} f\|_{L^2(X, \mu_\Gamma)} \to 0 \text{ as } n \to \infty \quad \forall f \in D(\check{K}). \tag{3.40}$$

Since the sequence $(\check{K}_{1/n} 1)_{n=1}^\infty$ is non-decreasing μ_Γ-a.e., it follows that it converges to 1 μ_Γ-a.e. and, in particular, $\check{K}_{1/n} 1 \leq 1$ μ_Γ-a.e. for all $n \in \mathbb{N}$, $n \geq 1$. By Lemma 3.14, this implies that

$$\|\check{K}_{1/n}\| \leq 1, \quad n = 1, 2, 3, \ldots$$

By (3.40), it follows that $\|\check{K}\| \leq 1$. □

It is remarkable that the important and large class of equilibrium measures leads to large coupling convergence with maximal rate of convergence.

Theorem 3.16. *Let Γ be a closed subset of X with finite capacity and μ_Γ the equilibrium measure of Γ. Let F be the support of μ_Γ. Assume that $(H+1)^{-1}$ is conservative. Then*

$$\|(H+\beta\mu_\Gamma+1)^{-1}-(H+\infty\mu_\Gamma+1)^{-1}\| \leq \frac{1}{1+b} \quad \forall b>0. \tag{3.41}$$

Proof. By (3.26), $D_\infty^{\mu_\Gamma}-D_b^{\mu_\Gamma}$ possesses an m-symmetric Markovian kernel and, by Lemma 3.14, it suffices to prove that

$$\|(H+b\mu_\Gamma+1)^{-1}1-(H+\infty\mu_\Gamma+1)^{-1}1\|_\infty \leq \frac{1}{1+b} \quad \forall b>0. \tag{3.42}$$

Let $b>0$ and $(f_k)\subset C_0(X)$ such that $f_k \uparrow 1$ everywhere on X. Using the representation of G in terms of its Markovian kernel, we obtain that, by applying the monotone convergence theorem,

$$J^{\mu_\Gamma}Gf_k \to 1 \text{ in } L^2(X,\mu_\Gamma). \tag{3.43}$$

Thus observing that, by (3.34), $\left(\frac{1}{b}+\check{H}^{-1}\right)^{-1}1=\frac{b}{1+b}$, we obtain

$$D_b^{\mu_\Gamma}f_k=(I_{\mu_\Gamma}G)^*\left(\frac{1}{b}+\check{H}^{-1}\right)^{-1}J^{\mu_\Gamma}Gf_k \to \frac{b}{1+b}\,(J^{\mu_\Gamma}G)^*1. \tag{3.44}$$

By monotone convergence again, we get that $D_b^{\mu_\Gamma}f_k \uparrow D_b^{\mu_\Gamma}1$ a.e. Thus, by the latter identity and since

$$\frac{b}{1+b}\,(J^{\mu_\Gamma}G)^*1=\frac{b}{1+b}\,U_1\mu_\Gamma,$$

we arrive at $D_b^{\mu_\Gamma}1=\frac{b}{1+b}U_1\mu_\Gamma$ for all $0<b<\infty$. Since the operators $D_b^{\mu_\Gamma}$ converge to $D_\infty^{\mu_\Gamma}$ strongly, this implies that $D_\infty^{\mu_\Gamma}1=U_1\mu_\Gamma$. Thus

$$\|(H+b\mu_\Gamma+1)^{-1}1-(H+\infty\mu_\Gamma+1)^{-1}1\|_\infty \leq \frac{\|U_1\mu_\Gamma\|_\infty}{1+b} \quad \forall\, b>0. \tag{3.45}$$

Finally, the result follows from (3.33) and (3.35). □

By the previous theorem, $L(H,P_{\mu_\Gamma})\leq 1$ provided that the regular Dirichlet form $\mathcal{E}$ is conservative. For conservative strongly local regular Dirichlet forms, we can even give the exact value of $L(H,P_{\mu_\Gamma})$.

Theorem 3.17. *Suppose that the regular Dirichlet form $\mathcal{E}$ associated to the nonnegative self-adjoint operator H in $L^2(X,m)$ has the strong local property. Let Γ be a closed subset of X with finite capacity. If the interior Γ° of Γ is not empty, then*

$$L(H,P_{\mu_\Gamma})\geq 1. \tag{3.46}$$

If, in addition, the operator $(H+1)^{-1}$ is conservative, then

$$L(H,P_{\mu_\Gamma})=1. \tag{3.47}$$

Proof. (3.47) follows from (3.46) and Theorem 3.16. Thus we only need to prove (3.46).

Since $U_1\mu_\Gamma = 1$ q.e. on Γ and by the strong locality of $\mathcal{E}$,

$$\int u\,dm = (U_1\mu_\Gamma, u) = \mathcal{E}_1(U_1\mu_\Gamma, u) = \int u\,d\mu_\Gamma$$

for all $u \in C_0(\Gamma^\circ) \cap D(\mathcal{E})$. Since $C_0(\Gamma^\circ) \cap D(\mathcal{E})$ is dense in $C_0(\Gamma^\circ)$ with respect to the supremum norm, it follows that

$$\mu_\Gamma = m \text{ on the Borel-Algebra } \mathcal{B}(\Gamma^\circ) \text{ of } B. \tag{3.48}$$

Choose $u \in C_0(\Gamma^\circ) \cap D(\mathcal{E})$ such that $\|u\| = 1$. For all $f \in D(J^{\mu_\Gamma})$

$$\mathcal{E}_1(f, Gu) = (f, u) = (J^{\mu_\Gamma} f, u)_{L^2(\mu_\Gamma)} = \mathcal{E}_1(f, J^{\mu_\Gamma *} u)$$

(in the second step we have used (3.48)). Thus $Gu = J^{\mu_\Gamma *}u$ and hence $\check{H} J^{\mu_\Gamma} Gu = u$. Thus

$$\|\check{H} J^{\mu_\Gamma} H\| \geq \|u\|_{L^2(\mu_\Gamma)} = \|u\| = 1$$

(again, we have used (3.48) in the second step). By Theorem 2.7 (c), this implies (3.46). □

As a consequence of Theorem 3.16 in conjunction with Corollary 3.13, we obtain the next result.

Corollary 3.18. *Let $\mathcal{E}$ be a conservative Dirichlet form. Let Γ be a closed subset of X with finite capacity, $0 < c < \infty$, and let μ be a positive Radon measure on X charging no set with capacity zero and such that $\mu \geq c\,\mu_\Gamma$. Assume, in addition, that*

$$D^\mu_\infty = D^{\mu_\Gamma}_\infty .$$

(*In particular, this is true if μ is absolutely continuous with respect to the equilibrium measure μ_Γ.*) *Then*

$$\|D^\mu_\infty - D^\mu_b\| \leq \frac{1}{1+cb} \quad \forall\, b > 0.$$

If $\mathcal{E}$ equals the classical Dirichlet form $\mathbb{D}$ in $L^2(\mathbb{R})$, then the equilibrium measure of the interval $[0,1]$ equals $1_{[0,1]} = dx + \delta_0 + \delta_1$. Hence the result in the next example follows from the previous corollary. If one compares this result with (3.22), then one sees that the rate of convergence for the operators $(-\Delta + b\mu + 1)^{-1}$ can be changed strongly by an arbitrarily small change of the measure μ.

Example 3.19. Let $\varepsilon_i > 0$ for $i = 0, 1$. Let $\mu = 1_{[0,1]}\,dx + \varepsilon_0\delta_0 + \varepsilon_1\delta_1$. Let $c := \min(\varepsilon_0, \varepsilon_1)$. Then

$$\|(-\Delta + b\mu + 1)^{-1} - (-\Delta + \infty\mu + 1)^{-1}\| \leq \frac{1}{1+cb} \quad \forall\, b > 0.$$

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Smooth Spectral Calculus

Matania Ben-Artzi

Dedicated to the memory of Allen Devinatz (1922–2008)*, who taught me so much in and out of mathematics*

Abstract. A smooth spectral theory is presented in an abstract Hilbert space framework. The main assumption (of smoothness) is the Hölder continuity of the derivative of the spectral measure (*density of states*). A Limiting Absorption Principle (LAP) is derived on the basis of continuity properties of Cauchy-type integrals. This abstract theory is then extended to include short-range perturbations and sums of tensor products. Applications to partial differential operators are presented. In the context of partial differential operators the spectral derivative is closely related to trace operators on compact (for elliptic operators) or non-compact manifolds. A main object of application here is the operator $H = -\sum_{j,k=1}^{n} \frac{\partial}{\partial x_j} a_{j,k}(x) \frac{\partial}{\partial x_k}$, a formally self-adjoint operator in $L^2(\mathbb{R}^n)$, $n \geq 2$. The real coefficients $a_{j,k}(x) = a_{k,j}(x)$ are assumed to be bounded and H is assumed to be uniformly elliptic and to coincide with $-\Delta$ outside of a ball. A suitable LAP is proved in the framework of weighted Sobolev spaces. It is then used for (i) A general eigenfunction expansion theorem and (ii) Global spacetime estimates for the associated (inhomogeneous) generalized wave equation. Finally a number of directions for further study are discussed.

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Keywords. Spectral derivative, tensor products, divergence-type operator, limiting absorption principle, eigenfunction expansion, spacetime estimates.

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1. Introduction

This review deals with *smooth spectral theory*, namely, spectral theory of self-adjoint operators whose spectral families possess certain regularity properties, beyond the properties shared by all spectral families. As we shall see, this situation is typical of broad families of (symmetric) partial differential operators.

Let H be a self-adjoint (bounded or unbounded) operator in a Hilbert space $\mathcal{H}$. The classical spectral theorem [59] gives a representation of H,

$$H = \int_{\mathbb{R}} \lambda \, dE(\lambda),$$

in terms of its (uniquely determined) spectral family (of projections) $\{E(\lambda)\}$.

The knowledge of $\{E(\lambda)\}$ yields valuable information on the spectral structure of H; the location of its singular or absolutely continuous spectrum, as well as its eigenvalues. Also, it leads naturally to a definition of functions $f(H)$, for a wide family of functions f.

On the other hand, there are important issues (typically related to partial differential operators) that cannot be resolved simply on the basis of the spectral theorem. We pick here one important topic and expound it in more detail, so as to illustrate the point at hand.

Assuming that $\{E(\lambda)\}$ is (strongly) continuous from the left, one might think of $E(\lambda+0) - E(\lambda)$ as a projection on the *eigenspace* associated with λ. However, if λ is not an eigenvalue, this projection clearly vanishes. On the other hand, the mathematical foundation of quantum mechanics has turned the *expansion by generalized eigenfunctions* (such as the Fourier transform with respect to the Laplacian) into a basic tool of the theory (see, e.g., [86] for an early treatment). So the question is how (if at all possible) to incorporate such an expansion into the abstract framework of the spectral theorem. We shall address this question in Section 7, where we show how the basic premise of this review, namely, the *smoothness* concept of the spectral family, leads to an eigenfunction expansion theorem for the class of *divergence-type* operators.

Using a formal point of view we can say that the bridge between the spectral theorem and the aforementioned *eigenfunction expansion theorem* is obtained by replacing the above difference $E(\lambda+0) - E(\lambda)$ by its *scaled version*, the (formal, at this stage) derivative $\frac{d}{d\lambda}E(\lambda)$. In fact, this derivative is the cornerstone of the present review.

Certainly, this derivative is far from being a *new object*. In the physical literature it is known as the *density of states* [29, Chapter XIII].

It has appeared implicitly in many mathematical studies of quantum mechanics. Our purpose here is to provide a systematic study of this spectral object and to give some applications of it.

The fact that the spectral derivative is involved explains our use of the term *smooth spectral theory*. It should be distinguished from Kato's theory of *smooth operators* [60, 75]. The latter refers to operators which are smooth *with respect* *to* other operators, while we study here the smoothness of the basic operators. However, the two concepts are certainly related, as Kato's smoothness can be stated in terms of suitable boundedness of an operator with respect to the spectral derivative of another one. Such smoothness plays a crucial role in our treatment of global spacetime estimates in Section 8.

After introducing our basic notational conventions and functional spaces in Section 2, we present the basic abstract setting in Section 3. This structure was first established in a joint work with the late A. Devinatz [15]. It relies on the fundamental hypothesis that the spectral derivative is Hölder continuous in a suitable functional setting. The primary aim is to establish a *Limiting Absorption Principle* (LAP), namely, that the resolvents (from either side of the spectrum) remain continuous up to the (absolutely continuous) spectrum in this setting. Once established for an operator H, we show in Subsection 3.2 that it persists to functions $f(H)$, for a wide family of functions f, with interesting results for operators of mathematical physics, such as the *relativistic Schrödinger* operator. It is pointed out that without the smoothness assumption, the validity of the LAP for H does not necessarily imply its validity even for H^2.

Sections 4 and 5 are devoted to further development of the abstract calculus. The first deals with short-range perturbations and the second with sums of tensor products. The presentation here is based both on [15] and the lecture notes [37]. While the framework is abstract, the applications to partial differential operators are quite concrete. The spectral derivative is closely associated with traces of functions (in Sobolev spaces) on manifolds, which gives a natural explanation to the appearance of weighted L^2 spaces in this context. The classical Schrödinger operator is considered, with either short-range perturbations (the abstract Definition 4.1 leads to the same class of potentials as considered by Agmon [1]) or uniform electric fields (the Stark Hamiltonian). The results derived from the abstract setting include not only the existence of limiting values of the resolvent, but also their Hölder continuity (a fact that cannot be demonstrated readily by other methods), their decay rates at *high energy* and other properties. Using this approach, for example, the study of the Laplacian in $\mathbb{R}^n$ is fully reduced to the one-dimensional case.

The next three sections are devoted to the main application considered in this review, namely, a detailed study of the operator $H = -\sum_{j,k=1}^{n} \frac{\partial}{\partial x_j} a_{j,k}(x) \frac{\partial}{\partial x_k}$, which is assumed to be formally self-adjoint in $L^2(\mathbb{R}^n)$, $n \geq 2$. The real coefficients $a_{j,k}(x) = a_{k,j}(x)$ are assumed to be bounded and H is assumed to be uniformly elliptic and to coincide with $-\Delta$ outside of a ball. In particular, the coefficients can be discontinuous. It is well known that these assumptions imply that $\sigma(H)$, the spectrum of H, is the half-axis $[0, \infty)$, and is entirely continuous. The *threshold* $z = 0$ plays a special role in this setting. Our treatment here follows [11].

In Section 6 we establish the LAP for this operator and, in particular, show that the limiting values of the resolvent remain continuous across the threshold (which is therefore not a resonance). An important corollary is that the spectrum is *entirely absolutely continuous*. While the absolute continuity of the spectrum is known in the case of smooth coefficients (using Mourre's method [68]), its extension to the case at hand (where coefficients are not even assumed to be continuous) appears to be new.

Since its appearance in the classical works of Eidus [40] and Agmon [1], the LAP has proven to be a fundamental tool in the study of spectral and scattering theory. The method of Eidus (for second-order elliptic operators) relied on careful elliptic estimates while the method of Agmon used Fourier analysis (division by symbols with simple zeros), followed by a perturbative ("bootstrap") argument to deal with lower-order terms. This latter method, extended to simply characteristic operators of any order, is expounded in [49, Chapter 14]. The method of Mourre (also known as the "conjugate operator method") [68] paved the way to the breakthrough in the study of the (quantum) N-body problem [70]. We refer to the monographs [4, 36] for the presentation of Mourre's method in an abstract framework. We also refer to the recent paper [41], where the LAP is proved by using a combination of Mourre's method and energy estimates.

The LAP for the divergence-type operator H introduced above cannot be obtained by a straightforward application of either one of these methods. Firstly, the presence of the non-constant coefficients $a_{j,k}(x)$ means that H is not a relatively compact perturbation of the Laplacian, and the perturbation method of Agmon cannot be applied. Secondly, if one insists (as we do here) on assuming only boundedness (and not smoothness) of these coefficients, the method of Mourre, as used in the semiclassical literature [76], cannot be applied (the conjugate operator is related to a generator of the corresponding flow that, in turn, relies on smoothness). In contrast, our approach to the LAP enables us to obtain resolvent estimates for the Laplacian *beyond* the L^2 setting, by using $H^{-1,s}$ weighted Sobolev spaces (see Subsection 6.1). In this context the operator H can be handled as a perturbation of the Laplacian.

We note in addition that both Agmon's and Mourre's methods cannot be applied across the threshold at $z = 0$. Here we obtain continuity of the limiting values of the resolvent across the threshold, at the expense of using a more restrictive weight function. This fact is essential in the treatment of global spacetime estimates in Section 8.

A more detailed discussion of the relevant literature is given in Section 6.

Section 7 is devoted to the eigenfunction expansion theorem (by generalized eigenfunctions) associated with the operator H. We have already touched upon this topic above, illustrating the differences between the general (abstract) spectral theorem and the detailed *Fourier-type* expansion needed in applications. We expand on this issue in the section.

A global spacetime estimate for the associated (inhomogeneous) generalized wave equation is proved in Section 8. We chose to bring this example (instead of the simpler Schrödinger-type equation) in order to stress the various possibilities available with the tool of the spectral derivative. In doing so we need to restrict much further our class of coefficient matrices. In fact, in order to obtain good control on the behavior of the limiting values of the spectral derivative at *high energy*, we need to use geometric assumptions (*non-trapping trajectories*), which are common in semiclassical theory.

Finally, in Section 9 we list a small number of important new directions that can be pursued in order to expand the scope of this *smooth spectral theory*. As an illustration, we outline there the possibility to use the theory for estimates of heat kernels, even beyond the L^2 framework.

Concerning the references cited in this review, an attempt has been made to include items closely related to the topics discussed here – and in the same spirit. Thus, since we do not touch here on the N-body problem, no references are made to papers dealing with this topic, beyond those mentioned above, in connection with the LAP. Similarly, not mentioned are works dealing with the spectral character of Schrödinger operators with more singular potentials, works related to spacetime estimates in the framework of the Strichartz approach, and so on. Even so, the amount of interesting and relevant papers is large, and the author apologizes for any undue omissions.

2. Functional spaces and notation

We collect here some basic notations and functional spaces to be used throughout this paper.

The closure of a set Ω (either in the real line $\mathbb{R}$ or in the complex plane $\mathbb{C}$) is denoted by $\overline{\Omega}$.

For any two normed spaces X, Y, we denote by $B(X,Y)$ the space of bounded linear operators from X to Y, equipped with the operator norm $\| \ \|_{B(X,Y)}$ topology (to which we refer as the *uniform operator topology*). In the case $X = Y$ we simplify to $B(X)$.

The following weighted L^2 and Sobolev spaces will appear frequently. First, for $s \in \mathbb{R}$ and m a non-negative integer, we define

$$L^{2,s}(\mathbb{R}^n) := \Big\{ u(x) \;\Big|\; \|u\|_{0,s}^2 = \int_{\mathbb{R}^n} (1+|x|^2)^s |u(x)|^2 dx < \infty \Big\}$$

$$H^{m,s}(\mathbb{R}^n) := \Big\{ u(x) \;\Big|\; D^\alpha u \in L^{2,s}, \ \ |\alpha| \le m, \ \ \|u\|_{m,s}^2 = \sum_{|\alpha \le m} \|D^\alpha u\|_{0,s}^2 \Big\}$$

(we write L^2 for $L^{2,0}$ and $\|u\|_0 = \|u\|_{0,0}$). More generally, for any $\sigma \in \mathbb{R}$, let $H^\sigma \equiv H^{\sigma,0}$ be the Sobolev space of order σ, namely,

$$H^\sigma = \big\{ \hat{u} \;\big|\; u \in L^{2,\sigma} \big\},$$

$\|\hat{u}\|_{\sigma,0} = \|u\|_{0,\sigma}$, where the Fourier transform is defined as usual by

$$\hat{u}(\xi) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} u(x) \exp(-i\xi x) dx. \tag{2.1}$$

For negative indices, we denote by $\{H^{-m,s}, \|\cdot\|_{-m,s}\}$ the dual space of $H^{m,-s}$. In particular, observe that any function $f \in H^{-1,s}$ can be represented (not uniquely) as

$$f = f_0 + \sum_{k=1}^{n} i^{-1} \frac{\partial}{\partial x_k} f_k, \quad f_k \in L^{2,s}, \ 0 \le k \le n. \tag{2.2}$$

In the case $n = 2$ and $s > 1$, we define

$$L_0^{2,s}(\mathbb{R}^2) = \{u \in L^{2,s}(\mathbb{R}^2) \mid \hat{u}(0) = 0\},$$

and set $H_0^{-1,s}(\mathbb{R}^2)$ to be the space of functions $f \in H^{-1,s}(\mathbb{R}^2)$ which have a representation (2.2), where $f_k \in L_0^{2,s}$, $k = 0, 1, 2$.

3. The basic abstract structure

Let $\mathcal{H}$ be a Hilbert space over $\mathbb{C}$ (the complex numbers), whose scalar product and norm we denote, respectively, by $(\ ,\ )$ and $\|\ \|$.

Let $\mathcal{X}$ be another Hilbert space such that $\mathcal{X} \subseteq \mathcal{H}$, where the embedding is dense and continuous. In other words, $\mathcal{X}$ can be considered as a dense subspace of $\mathcal{H}$, equipped with a stronger norm. Then, of course, $\mathcal{X} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{X}^*$, where $\mathcal{X}^*$ is the anti-dual of $\mathcal{X}$, i.e., the continuous additive functionals l on $\mathcal{X}$, such that $l(\alpha v) = \overline{\alpha}\, l(v)$, $\alpha \in \mathbb{C}$. The (linear) embedding $h \in \mathcal{H} \hookrightarrow x^* \in \mathcal{X}^*$ is obtained as usual by the scalar product (in $\mathcal{H}$), $x^*(x) = (h, x)$.

We use $\|x\|_{\mathcal{X}}$, $\|x^*\|_{\mathcal{X}^*}$ for the norms in $\mathcal{X}$, $\mathcal{X}^*$, respectively, and designate by $\langle\ ,\ \rangle$ the $(\mathcal{X}^*, \mathcal{X})$ pairing.

Let H be a self-adjoint (in general unbounded) operator on $\mathcal{H}$ and let $\{E(\lambda)\}$ be its spectral family. Let

$$R(z) = (H - z)^{-1}, \quad z \in \mathbb{C}^{\pm} = \{z \mid \pm \operatorname{Im} z > 0\},$$

be the associated resolvent operator. We denote by $\sigma(H) \subseteq \mathbb{R}$ the spectrum of H.

Clearly, if $\lambda \in \sigma(H)$, then $R(z)$ cannot converge to a limit in the uniform operator topology of $B(\mathcal{H})$ as $z \to \lambda$. However, a basic notion in our treatment is the fact that such *continuity up to the spectrum* of the resolvent can be achieved in a weaker topology. We begin with the following definition.

Definition 3.1. Let $[\kappa_1, \kappa_2] \subseteq \mathbb{R}$. We say that H satisfies the *Limiting Absorption Principle* (LAP) in $[\kappa_1, \kappa_2]$ if $R(z)$, $z \in \mathbb{C}^{\pm}$, can be extended continuously to $\operatorname{Im} z = 0$, $\operatorname{Re} z \in [\kappa_1, \kappa_2]$, in the uniform operator topology of $B(\mathcal{X}, \mathcal{X}^*)$. In this case we denote the limiting values by $R^{\pm}(\lambda)$, $\kappa_1 \le \lambda \le \kappa_2$.

Remark 3.2. By the well-known Stieltjes formula [59], for all $x \in \mathcal{X}$,

$$((E(\delta) - E(\gamma))x, x) = \frac{1}{2\pi i} \int_{\gamma}^{\delta} \left\langle \left(R^+(\lambda) - R^-(\lambda)\right) x, x \right\rangle d\lambda, \quad [\gamma, \delta] \subseteq [\kappa_1, \kappa_2],$$

it follows that H is absolutely continuous in $[\kappa_1, \kappa_2]$.

Remark that our assumptions readily imply that the uniform operator topology of $B(\mathcal{X}, \mathcal{X}^*)$ is weaker than that of $B(\mathcal{H})$. Also note that the limiting values $R^-(\lambda)$ are, generally speaking, different from $R^+(\lambda)$.

For reasons to become clear later, we introduce still another Hilbert space $\mathcal{X}_H^*$, which is a dense subspace of $\mathcal{X}^*$, equipped with a stronger norm (so that the embedding $\mathcal{X}_H^* \hookrightarrow \mathcal{X}^*$ is continuous). However, we do not require that $\mathcal{H}$ be embedded in $\mathcal{X}_H^*$. As indicated by the notation, $\mathcal{X}_H^*$ may depend on H (see Example 3.5 below). A typical case would be when H can be extended as a densely defined operator in $\mathcal{X}^*$ and $\mathcal{X}_H^*$ would be its domain there, equipped with the graph norm. This will be the case in Theorem 3.11 below.

Let $\{E(\lambda)\}$ be the spectral family of H. When there is no risk of confusion, we also use $E(B)$ to denote the spectral projection on any Borel set B (so that $E(\lambda) = E(-\infty, \lambda)$).

Definition 3.3. Let $U \subseteq \mathbb{R}$ be open and let $0 < \alpha \leq 1$. Assume that U is of *full spectral measure*, namely, $E(\mathbb{R} \setminus U) = 0$. Then H is said to be of *type* $(\mathcal{X}, \mathcal{X}_H^*, \alpha, U)$ if the following conditions are satisfied:

1. The operator-valued function
$$\lambda \to E(\lambda) \in B(\mathcal{X}, \mathcal{X}^*), \quad \lambda \in U,$$
is weakly differentiable with a locally Hölder continuous derivative in $B(\mathcal{X}, \mathcal{X}_H^*)$; that is, there exists an operator-valued function
$$\lambda \to A(\lambda) \in B(\mathcal{X}, \mathcal{X}_H^*), \quad \lambda \in U,$$
so that (recall that $(\ ,\ )$ is the scalar product in $\mathcal{H}$ while $\langle\ ,\ \rangle$ is the $(\mathcal{X}^*, \mathcal{X})$ pairing)
$$\frac{d}{d\lambda}(E(\lambda)x, y) = \langle A(\lambda)x, y\rangle, \quad x,\, y \in \mathcal{X},\, \lambda \in U,$$
and such that for every compact interval $K \subseteq U$, there exists an $M_K > 0$ satisfying
$$\|A(\lambda) - A(\mu)\|_{B(\mathcal{X}, \mathcal{X}_H^*)} \leq M_K \left|\lambda - \mu\right|^\alpha, \quad \lambda,\, \mu \in K.$$
2. For every bounded open set $J \subseteq U$ and for every compact interval $K \subseteq J$, the operator-valued function (defined in the weak sense)
$$z \to \int_{U \setminus J} \frac{A(\lambda)}{\lambda - z}\, d\lambda, \quad z \in \mathbb{C},\, \operatorname{Re} z \in K,\, |\operatorname{Im} z| \leq 1,$$
takes values and is Hölder continuous in the uniform operator topology of $B(\mathcal{X}, \mathcal{X}_H^*)$, with exponent α.

Remark 3.4. We could *localize* this definition and, in particular, relax the assumption that $E(\mathbb{R} \setminus U) = 0$. However, this is not needed for the operators discussed in this review, typically perturbations of operators with absolutely continuous spectrum (see the following example below).

Example 3.5 ($H_0 = -\Delta$). (This example will be continued in Subsections 5.5 and 6.1.)

We take the operator H_0 to be the unique self-adjoint extension of the restriction of $-\Delta$ to smooth compactly supported functions [59]. Let $\{E_0(\lambda)\}$ be the spectral family associated with H_0 so that, using the Fourier notation introduced in Section 2,

$$(E_0(\lambda)h, h) = \int\limits_{|\xi|^2 \le \lambda} |\hat{h}|^2 \, d\xi, \quad \lambda \ge 0, \;\; h \in L^2(\mathbb{R}^n). \tag{3.1}$$

We refer to Section 2 for definitions of the weighted L^2 and Sobolev spaces involved in the sequel. Recall that by the standard trace lemma, we have

$$\int\limits_{|\xi|^2 = \lambda} |\hat{h}|^2 \, d\tau \le C \|\hat{h}\|^2_{H^s}, \quad s > \frac{1}{2}, \; \lambda > 0, \tag{3.2}$$

where $C > 0$ is independent of λ and $d\tau$ is the restriction of the Lebesgue measure (see [15] for the argument that it can be used for the full half-axis, not just compact intervals).

We conclude that the weak derivative $A_0(\lambda) = \frac{d}{d\lambda} E_0(\lambda)$ exists in the space $B(L^{2,s}, L^{2,-s})$ for any $s > \frac{1}{2}$ and $\lambda > 0$ and satisfies

$$\langle A_0(\lambda)h, k\rangle = (2\sqrt{\lambda})^{-1} \int\limits_{|\xi|^2 = \lambda} \hat{h}\bar{\hat{k}} \, d\tau, \quad h, k \in L^{2,s}, \tag{3.3}$$

where $\langle \, , \, \rangle$ is the $(L^{2,-s}, L^{2,s})$ pairing (conjugate linear with respect to the second term) and $d\tau$ is the Lebesgue surface measure (we write $L^{2,s}$ for $L^{2,s}(\mathbb{R}^n)$).

Furthermore, by taking s large in (3.2) (it suffices to take $s > \frac{n}{2} + 2$) and using the Sobolev imbedding theorem we infer that $A_0(\lambda)$ is locally Lipschitz continuous in the uniform operator topology, so that by interpolation it is locally Hölder continuous in the uniform operator topology of $B(L^{2,s}, L^{2,-s})$ for any $s > \frac{1}{2}$.

Finally, since the (distributional) Fourier transform of $A_0(\lambda)h$ is the surface density $(2\sqrt{\lambda})^{-1}\delta_{|\xi|^2 - \lambda}\hat{h}(\xi) \, d\tau$, we conclude that actually $A_0(\lambda)h \in H^{m,-s}$, $s > \frac{1}{2}$, for any $m > 0$, and $A_0(\lambda)$ is locally Hölder continuous in the uniform operator topology of $B(L^{2,s}, H^{m,-s})$ for any $s > \frac{1}{2}$.

Thus, all the requirements of Definition 3.3 are satisfied with $\mathcal{X} = L^{2,s}(\mathbb{R}^n)$, $\mathcal{X}^*_{H_0} = H^{2,-s}(\mathbb{R}^n)$, $s > \frac{1}{2}$.

3.1. The limiting absorption prinicple – LAP

Recall first the classical Privaloff-Korn theorem (see [31] for a proof).

Theorem. *Let* $f : \mathbb{R} \to \mathbb{C}$ *be a compactly supported Hölder continuous function so that, for some* $N > 0$ *and* $0 < \alpha < 1$,

$$|f(\lambda_2) - f(\lambda_1)| \le N \, |\lambda_2 - \lambda_1|^{\alpha}, \quad \lambda_2, \lambda_1 \in \mathbb{R}.$$

Let

$$F^{\pm}(z) = \int_{\mathbb{R}} \frac{f(\lambda)}{\lambda - z}\, d\lambda, \quad z \in \mathbb{C}^{\pm}.$$

Then, for every $\mu \in \mathbb{R}$, the limits

$$F^{\pm}(\mu) = \lim F(z) = \pm i\pi f(\mu) + \mathrm{P.V.} \int_{\mathbb{R}} \frac{f(\lambda)}{\lambda - \mu} d\lambda \quad \text{as } z \to \mu,\ \pm \operatorname{Im} z > 0,$$

exist and moreover, for every compact $K \subseteq \overline{\mathbb{C}^{+}}$ (or $K \subseteq \overline{\mathbb{C}^{-}}$), there exists a constant M_K so that

$$\left|F^{\pm}(z_2) - F^{\pm}(z_1)\right| \leq N M_K \left|z_2 - z_1\right|^{\alpha}, \quad z_1,\, z_2 \in K.$$

We can now state our basic theorem, concerning the LAP in the abstract setting. We remark that a slightly different version will appear in Subsection 5.2.

Theorem 3.6. *Let H be of* type $(\mathcal{X}, \mathcal{X}_H^*, \alpha, U)$ (*where $U \subseteq \mathbb{R}$ is open and* $0 < \alpha \leq 1$). *Then H satisfies the* LAP *in U. More explicitly, the limits*

$$R^{\pm}(\lambda) = \lim_{\epsilon \downarrow 0} R(\lambda \pm i\epsilon), \quad \lambda \in U,$$

exist in the uniform operator topology of $B(\mathcal{X}, \mathcal{X}_H^*)$ and the extended operator-valued function

$$R(z) = \begin{cases} R(z), & z \in \mathbb{C}^{+}, \\ R^{+}(z), & z \in U, \end{cases}$$

is locally Hölder continuous in the same topology (with exponent α).

A similar statement applies when $\mathbb{C}^{+}$ is replaced by $\mathbb{C}^{-}$, but note that the limiting values $R^{\pm}(\lambda)$ are in general different.

Proof. Let $J \subseteq U$ be a bounded open set such that $\overline{J} \subseteq U$ and $K \subseteq J$ be a compact interval. Let $\varphi \in C_0^{\infty}(U)$ be a cutoff function with $\varphi \equiv 1$ on J. Taking $x, y \in \mathcal{X}$, we have, for $\operatorname{Re} z \in K,\ \operatorname{Im} z \neq 0$,

$$\begin{aligned}(R(z)x, y) &= \int_{U} \frac{\varphi(\mu)\, \langle A(\mu)x, y\rangle}{\mu - z}\, d\mu + \int_{U \setminus J} \frac{(1 - \varphi(\mu))\, \langle A(\mu)x, y\rangle}{\mu - z}\, d\mu \\ &= (R_1(z)x, y) + (R_2(z)x, y)\,.\end{aligned}$$

By hypothesis (see Definition 3.3) the operator-valued function

$$R_2(z) = \int_{U \setminus J} \frac{(1 - \varphi(\mu))A(\mu)}{\mu - z}\, d\mu,$$

belongs to $B(\mathcal{X}, \mathcal{X}_H^*)$, and it is locally Hölder continuous for $\operatorname{Re} z \in K$. Thus, we are reduced to considering R_1.

Observe that the integral

$$R_1(z) = \int_{U \setminus J} \frac{\varphi(\mu)A(\mu)}{\mu - z}\, d\mu,$$

is well defined as a Riemann integral, since the integrand is continuous in the uniform norm topology of $B(\mathcal{X}, \mathcal{X}_H^*)$. Thus $R_1(z) \in B(\mathcal{X}, \mathcal{X}_H^*)$. It remains to prove the assertion concerning its Hölder continuity.

Note that the embeddings $\mathcal{X} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{X}^*$ and $\mathcal{X}_H^* \hookrightarrow \mathcal{X}^* \hookrightarrow \mathcal{X}_H^{**}$ are dense and continuous. Thus, we can view $\mathcal{X}$ as embedded in $\mathcal{X}_H^{**}$, so that the pairing $\langle A(\mu)x, y\rangle$ can be regarded as an $(\mathcal{X}_H^*, \mathcal{X}_H^{**})$ pairing.

Suppose now that $\operatorname{Im} z_i > 0$, $\operatorname{Re} z_i \in K$, $i = 1, 2$, so that the Privaloff-Korn theorem yields, for $x, y \in \mathcal{X}$,

$$|([R_1(z_2) - R_1(z_1)]x, y)| \leq M_K \sup_{\mu_1 \neq \mu_2} \frac{|\langle [\varphi(\mu_2)A(\mu_2) - \varphi(\mu_2)A(\mu_2)]\, x, y\rangle|}{|\mu_2 - \mu_1|^\alpha} |z_2 - z_1|^\alpha,$$

and as observed above

$$\begin{aligned}|\langle[\varphi(\mu_2)A(\mu_2) - \varphi(\mu_2)A(\mu_2)]x, y\rangle| &\leq \left\|[\varphi(\mu_2)A(\mu_2) - \varphi(\mu_2)A(\mu_2)]x\right\|_{\mathcal{X}_H^*} \|y\|_{\mathcal{X}_H^{**}} \\ &\leq \left\|\varphi(\mu_2)A(\mu_2) - \varphi(\mu_2)A(\mu_2)\right\|_{B(\mathcal{X}, \mathcal{X}_H^*)} \|x\|_{\mathcal{X}} \|y\|_{\mathcal{X}_H^{**}}.\end{aligned}$$

Thus,

$$\left|([R_1(z_2) - R_1(z_1)]x, y)\right| \leq N M_K |z_2 - z_1|^\alpha \; \|x\|_{\mathcal{X}} \|y\|_{\mathcal{X}_H^{**}},$$

where

$$N = \sup_{\mu_1 \neq \mu_2} \frac{\|\varphi(\mu_2)A(\mu_2) - \varphi(\mu_2)A(\mu_2)\|_{B(\mathcal{X}, \mathcal{X}_H^*)}}{|\mu_2 - \mu_1|^\alpha}.$$

Since $\mathcal{X}$ is dense in $\mathcal{X}_H^{**}$, the last estimate yields

$$\|R_1(z_2) - R_1(z_1)\|_{B(\mathcal{X}, \mathcal{X}_H^*)} \leq N M_K |z_2 - z_1|^\alpha,$$

and the proof is complete. □

Corollary 3.7. *In view of the Stieltjes formula* (*see* Remark 3.2 *above*) *we have*

$$A(\lambda) = \frac{1}{2\pi i}\left(R^+(\lambda) - R^-(\lambda)\right), \quad \lambda \in U.$$

In particular, H is absolutely continuous in U and $R^+(\lambda) - R^-(\lambda)$ cannot vanish on a subset of $\sigma(H) \cap U$ of positive (*Lebesgue*) *measure.*

Remark 3.8. The operator $A(\lambda)$, $\lambda \in [0, \infty)$, is known in the physical literature as the *density of states* [29, Chapter XIII].

Also, combining the theorem with the observations in Example 3.5 we obtain the following corollary, which is Agmon's classical LAP theorem [1].

Corollary 3.9. *Let $H_0 = -\Delta$ and set $R_0(z) = (H_0 - z)^{-1}$, $\operatorname{Im} z \neq 0$. Then the limits*

$$R_0^\pm(\lambda) = \lim_{\epsilon \downarrow 0} R_0(\lambda \pm i\epsilon), \quad \lambda \in (0, \infty),$$

exist in the uniform operator topology of $B(L^{2,s}, H^{2,-s})$, $s > \frac{1}{2}$. *Furthermore, these limiting values are Hölder continuous in this topology.*

Remark 3.10. The considerations of Example 3.5, based on trace estimates, can be applied to a wide range of constant coefficient partial differential operators (so-called *simply characteristic* operators, including all principal-type operators). Hence, a suitable LAP can be established for such operators. We shall not pursue this direction further in this review, but refer the reader to [15].

In general, it is easier to verify the conditions of Definition 3.3 for the operator space $B(\mathcal{X}, \mathcal{X}^*)$ than for $B(\mathcal{X}, \mathcal{X}^*_H)$. However, in some circumstances it is enough to establish the conditions in the latter space. This is expressed in the following theorem.

Theorem 3.11. *Let* H *be densely defined and closable in* $\mathcal{X}^*$, *with closure* $\overline{H}$. *Take* $\mathcal{X}^*_H = D(\overline{H})$ (*its domain*), *equipped with the graph norm*

$$\|x\|^2_{\mathcal{X}^*_H} = \|x\|^2_{\mathcal{X}^*} + \|\overline{H}x\|^2_{\mathcal{X}^*}.$$

Suppose that H *is of type* $(\mathcal{X}, \mathcal{X}^*, \alpha, U)$ (*see* Definition 3.3). *Then in fact* H *is of type* $(\mathcal{X}, \mathcal{X}^*_H, \alpha, U)$.

Proof. In view of Theorem 3.6 (where all assumptions hold in $B(\mathcal{X}, \mathcal{X}^*)$) we know that the limits

$$R^{\pm}(\lambda) = \lim_{\epsilon \downarrow 0} R(\lambda \pm i\epsilon), \quad \lambda \in U,$$

exist in the uniform operator topology, are locally Hölder continuous and, furthermore, for all $x \in \mathcal{X}$,

$$\lim_{\epsilon \downarrow 0} \overline{H} R(\lambda \pm i\epsilon)\, x = x + \lambda R^{\pm}(\lambda) x, \quad \lambda \in U.$$

Since $\overline{H}$ is closed in $\mathcal{X}^*$, we obtain

$$\overline{H} R^{\pm}(\lambda)\, x = x + \lambda R^{\pm}(\lambda) x \in \mathcal{X}^*,$$

so that $R^{\pm}(\lambda)x \in \mathcal{X}^*_H$. From the definition of the graph norm topology we see that $R^{\pm}(\lambda)$ is locally Hölder continuous in $B(\mathcal{X}, \mathcal{X}^*_H)$. Thus, using Eq. (3.7), we conclude that the same is true for $A(\lambda)$, so that the first condition in Definition 3.3 is satisfied.

To establish the second condition, let $J \subseteq U$ be an open set and $K \subseteq J$ compact. Let $z \in \mathbb{C}$ with $\operatorname{Re} z \in K$, and let $F(\lambda; z) = \frac{\chi_{U \setminus J}(\lambda)}{\lambda - z}$ (as usual, χ is the characteristic function of the indicated set). By the standard spectral calculus

$$HF(H; z) = \int_U \lambda F(\lambda; z)\, dE(\lambda) = \int_{U \setminus J} \frac{\lambda A(\lambda)}{\lambda - z}\, d\lambda,$$

so that both $F(H; z) = \int_{U \setminus J} \frac{A(\lambda)}{\lambda - z} d\lambda$ and $\overline{H} F(H; z)$ are in $B(\mathcal{X}, \mathcal{X}^*)$ and are, in fact, locally Lipschitz continuous in the uniform operator topology. Thus $z \to F(H; z)$ is locally Lipschitz continuous in $B(\mathcal{X}, \mathcal{X}^*_H)$, which concludes the proof. $\square$

3.2. Persistence of smoothness under functional operations

For a wide class of functions $f\colon \mathbb{R} \to \mathbb{R}$ the (self-adjoint) operator $f(H)$ is defined via the calculus associated with the spectral theorem [59], namely,

$$f(H) = \int_{\mathbb{R}} f(\lambda)\, dE(\lambda),$$

where $\{E(\lambda)\}$ is the spectral family of H.

Various spectral properties of $f(H)$ (whose spectrum is $\operatorname{Ran} f_{\sigma(H)}$) can be read off from the structure of f. (We use the notation $\operatorname{Ran} f_W$ for the image of $W \subseteq \mathbb{R}$ under f).

However, one important aspect which is missing is the fact that if H satisfies the Limiting Absorption Principle in U, there is no guarantee that $f(H)$ satisfies the same principle in $\operatorname{Ran} f_U$ or any part thereof. This remains true even if f is very smooth, monotone, etc.

In contrast, if H is of type $(\mathcal{X}, \mathcal{X}_H^*, \alpha, U)$, then also $f(H)$ is of that type (with U replaced by $\operatorname{Ran} f_U$ and perhaps a different Hölder exponent), for a rather broad family of functions. This is the content of the next theorem. In particular, in view of Theorem 3.6, also $f(H)$ satisfies the LAP.

We do not attempt to make the most general statement, but instead refer the reader to [20] for further details.

Theorem 3.12. *Let H be of type $(\mathcal{X}, \mathcal{X}_H^*, \alpha, U)$ (where $U \subseteq \mathbb{R}$ is open and $0 < \alpha \le 1$). Let $f\colon \mathbb{R} \to \mathbb{R}$ be a locally Hölder continuous function. Assume, in addition, that the restriction of f to U is continuously differentiable, and that its derivative f' is positive and locally Hölder continuous on U.*

Then the operator $f(H)$ is of type $(\mathcal{X}, \mathcal{X}_H^*, \alpha', \operatorname{Ran} f_U)$, for some $0 < \alpha' \le 1$.

Proof. Let $\{F(\lambda)\}$ be the spectral family of $f(H)$. If $B \subseteq \mathbb{R}$ is a Borel set, the spectral theorem yields

$$F(B) = E(f^{-1}(B)),$$

and since $E(\mathbb{R} \setminus U) = 0$ (see Definition 3.3), we can further write

$$F(B) = E(f^{-1}(B) \cap U).$$

Since $f' > 0$ in U, an easy calculation gives for the (weak) derivative

$$\frac{d}{d\mu} F(\mu) = f'(\lambda)^{-1} \frac{d}{d\lambda} E(\lambda), \quad \lambda = f(\mu) \in U.$$

The assertion of the theorem follows directly from this formula. □

In view of Theorem 3.6 we infer that $f(H)$ satisfies the LAP in $\operatorname{Ran} f_U$.

Remark 3.13. It should be remarked that if H satisfies the LAP in the sense of Definition 3.1 (including all the functional setting mentioned there), there is no guarantee that H^2 satisfies the LAP in $\{\mu = \lambda^2 \mid \lambda \in U\}$. For this to be false, however, one needs to find an example where the limiting values of the resolvent are not Hölder continuous.

Continuing Corollary 3.9 and taking $f(\lambda) = \sqrt{|\lambda|} + 1$, we obtain a LAP for the *relativistic Schrödinger operator* [20].

Corollary 3.14. *Let* $L = \sqrt{-\Delta} + I$ *and set* $P(z) = (L - z)^{-1}$, $\operatorname{Im} z \neq 0$. *The spectrum of* L *is* $\sigma(L) = [1, \infty)$ *and is absolutely continuous. The limits*

$$P^{\pm}(\lambda) = \lim_{\epsilon \downarrow 0} P(\lambda \pm i\epsilon), \quad \lambda \in (1, \infty),$$

exist in the uniform operator topology of $B(L^{2,s}, H^{2,-s})$, $s > \frac{1}{2}$. *Furthermore, these limiting values are Hölder continuous in this topology.*

4. Short-range perturbations

In Subsection 3.2 we have seen that if H satisfies the LAP, then so do various functions of H. The classical work of Agmon [1] showed that the same is true for *short-range* perturbations of H (apart from the possibility of discrete eigenvalues).

Our aim in this section is to introduce the notion of a *short-range perturbation* in the abstract framework constructed in Section 3 and to derive the LAP for the perturbed operator. Our *unperturbed* operator H is assumed to be of type $(\mathcal{X}, \mathcal{X}_H^*, \alpha, U)$ (Definition 3.3). Its spectral family is $\{E(\lambda)\}$, having (weak) derivative $A(\lambda) = \frac{d}{d\lambda} E(\lambda)$, $\lambda \in U$.

Definition 4.1. An operator $V : \mathcal{X}_H^* \to \mathcal{X}$ will be called

1. *Short-range with respect to* H if it is compact.
2. *Symmetric* if $D(H) \cap \mathcal{X}_H^*$ is dense in $\mathcal{H}$ and the restriction of V to $D(H) \cap \mathcal{X}_H^*$ is symmetric.

The following lemma shows that (with some additional assumption) the operator $H + V$ is well defined.

Lemma 4.2. *Let* H *be of type* $(\mathcal{X}, \mathcal{X}_H^*, \alpha, U)$ *and let* V *be short-range and symmetric. Suppose that there exists* $z \in \mathbb{C}$, $\operatorname{Im} z \neq 0$, *and a linear subspace* $D_z \subseteq D(H) \cap \mathcal{X}_H^*$ *such that* $(H - z)(D_z)$, *the image of* D_z *under* $H - z$, *is dense in* $\mathcal{X}$.

Then $P = H + V$, *defined on* $D(H) \cap \mathcal{X}_H^*$, *is essentially self-adjoint.*

Proof. Clearly, P is symmetric in $\mathcal{H}$. Further, $x \in D_z$ implies (with $R(z)$ being the resolvent of H),

$$(P - z)\, x = (I + VR(z))\, (H - z)x.$$

Let $w \in \mathbb{C}$, $\operatorname{Im} w \neq 0$, and define

$$D_w = \text{Range of } R(w)(H - z) \text{ restricted to } D_z.$$

Since the range of $R(w)$ is contained in $D(H) \cap \mathcal{X}_H^*$, we have $D_w \subseteq D(H) \cap \mathcal{X}_H^*$. Also, the range of $H - w$ acting on D_w equals that of $H - z$ acting on D_z, which is dense in $\mathcal{X}$ by assumption, and we can write

$$(P - w)\, x = (I + VR(w))\, (H - w)x, \quad x \in D_w.$$

Thus, if we prove that $I+VR(w)$ is invertible in $\mathcal{X}$, we conclude that P has zero deficiency indices [59], which finishes the proof.

If $I+VR(w)$ is not invertible (in $\mathcal{X}$), then by the Fredholm alternative ($VR(w)$ is compact) there must be $\phi \in \mathcal{X}$, $\phi \neq 0$, such that $\phi = -VR(w)\phi$. Let $\psi = R(w)\phi \neq 0$. We have $\psi \in D(H) \cap \mathcal{X}_H^*$ and $(P-w)\psi = 0$. Thus ψ is an eigenfunction of P, with a non-real eigenvalue w, which is a contradiction, since P is symmetric. □

Example 4.3 ($P = -\Delta + V$). Continuing Example 3.5, let $V\colon H^{2,-s} \to L^{2,s}$, $s > \frac{1}{2}$, be compact. Furthermore, let V be symmetric when restricted to $H^{2,s}$. Then all the assumptions of the lemma are satisfied and the restriction of $-\Delta+V$ to $H^{2,s}$ is essentially self-adjoint. Of course, this conclusion follows also directly from the fact that in this case V is relatively compact [59] with respect to $-\Delta$.

In what follows we always assume that H is of type $(\mathcal{X}, \mathcal{X}_H^*, \alpha, U)$ and that V is short-range and symmetric. Thus, by the lemma, $P = H+V$ can be extended as a self-adjoint operator with domain $D(P) \supseteq D(H) \cap \mathcal{X}_H^*$, and we retain the notation P for this extension.

Our aim is to study the spectral properties of P, particularly the LAP, in this abstract framework.

Denote by $S(z) = (P-z)^{-1}$, $\operatorname{Im} z \neq 0$, the resolvent of P. Our starting point is the resolvent equation

$$S(z)(I+VR(z)) = R(Z), \quad \operatorname{Im} z \neq 0.$$

As noted in the proof of Lemma 4.2, the inverse $(I+VR(z))^{-1}$ exists on $\mathcal{X}$ if $\operatorname{Im} z \neq 0$. This leads to

$$S(z) = R(z)(I+VR(z))^{-1}, \tag{4.1}$$

where the equality is certainly valid from $\mathcal{X} \to \mathcal{X}_H^*$.

Suppose now that $\lambda \in U$. In view of Theorem 3.6 and the assumption on V we have

$$\lim_{\epsilon \downarrow 0} VR(\lambda \pm i\epsilon) = VR^{\pm}(\lambda) \text{ in } B(\mathcal{X}, \mathcal{X}_H^*).$$

Thus, if $(I+VR^{\pm}(\lambda))^{-1}$ exists (in $B(\mathcal{X})$), then Eq. (4.1) implies the existence of the limits

$$S^{\pm}(\lambda) = \lim_{\epsilon \downarrow 0} S(\lambda \pm i\epsilon) = R^{\pm}(\lambda)(I+VR^{\pm}(\lambda))^{-1}, \tag{4.2}$$

in the uniform operator topology of $B(\mathcal{X}, \mathcal{X}_H^*)$.

Let $\lambda \in U$ be a point at which, say, $(I+VR^{+}(\lambda))^{-1}$ does not exist (in $B(\mathcal{X})$). Since $VR^{+}(\lambda)$ is compact in $\mathcal{X}$, there exists a non-zero $\phi \in \mathcal{X}$ so that

$$\phi = -VR^{+}(\lambda)\phi.$$

Let $\psi = R^{+}(\lambda)\phi \in \mathcal{X}_H^*$. Then

$$\langle \psi, \phi \rangle = -\lim_{\epsilon \downarrow 0} \left(R(\lambda+i\epsilon)\phi, VR(\lambda+i\epsilon)\phi \right).$$

By the symmetry of V the right-hand side of this equality is real, so we conclude that $\mathrm{Im}\,\langle R^+(\lambda)\phi, \phi\rangle = 0$, and invoking Eq. (3.7) we conclude that

$$\langle A(\lambda)\phi, \phi\rangle = 0.$$

Now the form $\langle A(\lambda)x, y\rangle = \frac{d}{d\lambda}(E(\lambda)x, y)$ on $\mathcal{X} \times \mathcal{X}$ is symmetric and positive semi-definite. Hence, for every $y \in \mathcal{X}$,

$$|\langle A(\lambda)\phi, y\rangle| \leq \langle A(\lambda)\phi, \phi\rangle^{\frac{1}{2}} \langle A(\lambda)y, y\rangle^{\frac{1}{2}} = 0, \tag{4.3}$$

and we conclude that

$$A(\lambda)\phi = 0. \tag{4.4}$$

In particular, $R^+(\lambda)\phi = R^-(\lambda)\phi$ and

$$\phi = -VR^{\pm}(\lambda)\phi.$$

Remark 4.4. In the case of the operator $H_0 = -\Delta$ (Example 3.5) the condition (4.4) means that the trace of $\hat{\phi}$ on the sphere $|\xi|^2 = \lambda$ vanishes. Thus (4.4) can be viewed as a *generalized* (*vanishing*) *trace condition*.

Definition 4.5. We designate by Σ_P the set

$$\Sigma_P = \big\{\lambda \in U \;\big|\; \text{There exists a non-zero } \phi_\lambda \in \mathcal{X} \text{ such that } \phi_\lambda = -VR^{\pm}(\lambda)\phi_\lambda\big\}.$$

Remark 4.6. The set Σ_P is (relatively) closed in U. Indeed, if $(I + VR^{\pm}(\lambda_0))^{-1}$ exists (in $B(\mathcal{X})$), then $(I + VR^{\pm}(\lambda))^{-1}$ exists for λ close to λ_0.

As a corollary to the discussion above we get

Corollary 4.7. *The operator $P = H+V$ satisfies the* LAP *in $U\setminus\Sigma_P$, in the uniform operator topology of $B(\mathcal{X}, \mathcal{X}_H^*)$, and the limiting values of its resolvent there are given by* Eq. (4.2)*.*

In particular, the spectrum of P in $U\setminus\Sigma_P$ is absolutely continuous. We single out this fact, stated in terms of the eigenvalues, in the following corollary.

Corollary 4.8. *Let $\sigma_p(P)$ be the point spectrum of P. Then*

$$\sigma_p(P) \cap U \subseteq \Sigma_P.$$

4.1. The exceptional set Σ_P

Our aim is to identify the set Σ_P introduced in Definition 4.5. It will turn out that (modulo one additional assumption on the smoothness of the spectral measure of H) we have equality of the sets in the last corollary. In other words, Σ_P is the set of eigenvalues of P embedded in U, and is necessarily discrete.

We start by recalling a variant of a well-known method [22] of constructing a Hilbert space unitarily equivalent to $\mathcal{H}$, which diagonalizes H. Thus, it can be viewed as a *generalized eigenfunction decomposition* of the space $\mathcal{H}$ (we discuss such decompositions in more detail in Section 7).

For $\lambda \in U$ and $x \in \mathcal{X}$, define

$$\widetilde{x}(\lambda) = A(\lambda)x$$

and let $\mathcal{H}'_\lambda \subseteq \mathcal{X}^*_H$ be the linear subspace defined by

$$\mathcal{H}'_\lambda = \{\widetilde{x}(\lambda) \mid x \in \mathcal{X}\}.$$

The form

$$(\widetilde{x}(\lambda), \widetilde{y}(\lambda))_\lambda = \langle A(\lambda)x, y\rangle, \quad x, y \in \mathcal{X}, \lambda \in U,$$

is well defined on $\mathcal{H}'_\lambda$. Indeed, if $y_1, y_2 \in \mathcal{X}$ are such that $A(\lambda)y_1 = A(\lambda)y_2$, then

$$\begin{aligned}\langle A(\lambda)x, y_1\rangle &= \frac{d}{d\lambda}(E(\lambda)x, y_1) = \frac{d}{d\lambda}(x, E(\lambda)y_1) \\ &= \langle A(\lambda)y_1, x\rangle = \langle A(\lambda)y_2, x\rangle = \langle A(\lambda)x, y_2\rangle .\end{aligned}$$

Furthermore, $(\widetilde{x}(\lambda), \widetilde{y}(\lambda))_\lambda$ is a scalar product on $\mathcal{H}'_\lambda$. In fact, the symmetry $(\widetilde{x}(\lambda), \widetilde{y}(\lambda))_\lambda = (\widetilde{y}(\lambda), \widetilde{x}(\lambda))_\lambda$ follows as in the calculation above and, taking note of (4.3),

$$(\widetilde{x}(\lambda), \widetilde{x}(\lambda))_\lambda = 0 \implies \langle A(\lambda)x, y\rangle = 0 \ \forall y \in \mathcal{X} \implies \widetilde{x}(\lambda) = A(\lambda)x = 0.$$

We denote by $\|\widetilde{x}(\lambda)\|_\lambda$ the corresponding norm.

Example 4.9. Continuing Example 3.5, we see that in the case of $H_0 = -\Delta$ the scalar product $(\widetilde{x}(\lambda), \widetilde{y}(\lambda))_\lambda$ is the L^2 scalar product with respect to the Lebesgue surface measure on the sphere of radius $\sqrt{\lambda}$.

We denote by $\mathcal{H}_\lambda$ the Hilbert space obtained as the completion of $\mathcal{H}'_\lambda$, $\lambda \in U$. Next consider the subset $\mathcal{S} \subseteq \prod_{\lambda \in U} \mathcal{H}_\lambda$ given by

$$\mathcal{S} = \{\widetilde{x} \mid \widetilde{x}(\lambda) = A(\lambda)x \text{ for some fixed } x \in \mathcal{X}, \lambda \in U\}.$$

Clearly $\mathcal{S}$ is a linear space over $\mathbb{C}$. We use the *fiberwise* scalar product $(\widetilde{x}(\lambda), \widetilde{y}(\lambda))_\lambda$ to define a scalar product on $\mathcal{S}$ by

$$(\widetilde{x}, \widetilde{y})_{\mathcal{H}^\oplus} = \int_U (\widetilde{x}(\lambda), \widetilde{y}(\lambda))_\lambda \, d\lambda = \int_U (dE(\lambda)x, y) = (x, y). \tag{4.5}$$

This sets up a norm preserving map $x \to \widetilde{x}$ from $\mathcal{X}$ (considered as a dense subspace of $\mathcal{H}$) and $\mathcal{S}$. Let $\mathcal{H}^\oplus$ be the completion of $\mathcal{S}$ under the scalar product $(\widetilde{x}, \widetilde{y})_{\mathcal{H}^\oplus}$. Then $\mathcal{H}$ is unitarily equivalent to $\mathcal{H}^\oplus$ and we retain the notation $x \to \widetilde{x}$, $x \in \mathcal{H}$, for this unitary map.

Observe that if $\widetilde{x}, \widetilde{y} \in \mathcal{H}^\oplus$, then there are sequences $\{x_n\}, \{y_n\} \subseteq \mathcal{X}$ so that, for a.e. (Lebesgue) $\lambda \in U$,

$$\widetilde{x_n}(\lambda) = A(\lambda)x_n \to \widetilde{x}(\lambda), \quad \widetilde{y_n}(\lambda) = A(\lambda)y_n \to \widetilde{y}(\lambda),$$

hence $(\widetilde{x}(\lambda), \widetilde{y}(\lambda))_\lambda = \lim \langle A(\lambda)x_n, y_n\rangle$ is measurable and we continue to have (4.5) for all $x, y \in \mathcal{H}$.

The fact that the representation $\mathcal{H}^\oplus$ diagonalizes the operator H is expressed by the following lemma.

Lemma 4.10. *Let g be a complex-valued Borel measurable function on U. Then*

$$\int_U |g(\lambda)|^2 \, \|\widetilde{x}(\lambda)\|^2_\lambda \, d\lambda < \infty \iff x \in D(g(H)). \tag{4.6}$$

In the event that either side of (4.6) *is true,*

$$\widetilde{g(H)x}(\lambda) = g(\lambda)\widetilde{x}(\lambda), \quad \text{a.e. } \lambda \in U. \tag{4.7}$$

Proof. Let $B \subseteq U$ be a Borel set and $x, y \in \mathcal{X}$. Then

$$(E(B)x, y) = \int_B \langle A(\lambda)x, y\rangle \, d\lambda = \int_B (\widetilde{x}(\lambda), \widetilde{y}(\lambda))_\lambda \, d\lambda.$$

In view of the foregoing comments, this equality can be extended to all $x, y \in \mathcal{H}$.

We conclude that for all $x \in \mathcal{H}$ and g as in the statement

$$\int_U |g(\lambda)|^2 \, \|\widetilde{x}(\lambda)\|_\lambda^2 \, d\lambda = \int_U |g(\lambda)|^2 \, (dE(\lambda)x, x) \, .$$

The right-hand side of this equality is finite if and only if $x \in D(g(H))$. In this case it follows that, for every $y \in \mathcal{H}$,

$$(g(H)x, E(B)y) = \int_B g(\lambda) \, (dE(\lambda)x, y) = \int_B g\,(\lambda)(\widetilde{x}(\lambda), \widetilde{y}(\lambda))_\lambda \, d\lambda,$$

and on the other hand

$$(g(H)x, E(B)y) = \int_B (\widetilde{g(H)x}(\lambda), \widetilde{y}(\lambda))_\lambda \, d\lambda,$$

which proves (4.7). □

Returning to the study of the set Σ_P, let $\mu \in \Sigma_P$, so that by definition there exists a non-zero $\phi \in \mathcal{X}$ satisfying

$$\phi = -VR^\pm(\mu)\phi. \tag{4.8}$$

In view of (4.4) we have $A(\mu)\phi = 0$, and since the form $\langle A(\lambda)\phi, \phi\rangle$ is non-negative we infer that the zero at $\lambda = \mu$ is a minimum. Thus formally this minimum is a second-order zero for the form. However, our smoothness assumption on the spectral measure (Definition 3.3) does not go so far as a second-order derivative. We therefore impose the following additional hypothesis on the spectral derivative near such a minimum.

Assumption S. *Let $K \subseteq U$ be compact and $\phi \in \mathcal{X}$ a solution to* (4.8)*, where $\mu \in K$. Then there exist constants $C, \epsilon > 0$, depending only on K, so that*

$$\langle A(\lambda)\phi, \phi\rangle \, \leq \, C \, |\lambda - \mu|^{1+\epsilon} \, \|\phi\|_{\mathcal{X}}^2 \, , \quad \lambda \in K. \tag{4.9}$$

Remark 4.11. Assumption S is satisfied if the operator-valued function $\lambda \to A(\lambda) \in B(\mathcal{X}, \mathcal{X}_H^*)$ has a Hölder continuous (in the uniform operator topology) Fréchet derivative in a neighborhood of μ. Indeed, in this case we have

$$\langle A(\lambda)\phi, \phi\rangle \, = \, \langle (A(\lambda) - A(\mu))\phi, \phi\rangle \, = \, \frac{d}{d\theta} \, \langle A(\theta)\phi, \phi\rangle_{\theta \in [\mu, \lambda]} \, (\lambda - \mu) \, .$$

Example 4.12 ($H_0 = -\Delta$). Continuing Examples 3.5 and 4.3, and applying the preceding remark, we see that Assumption S is satisfied when ϕ is in a subspace on which the trace map has a Hölder continuous Fréchet derivative. For this we need to restrict further $s > \frac{3}{2}$. In terms of Eq. (4.8), it imposes a faster (than just *short-range*) decay requirement on the perturbation V. We refer to [15] for a *bootstrap* argument that avoids this restriction.

Subject to the additional Assumption S we can identify the set Σ_P.

Theorem 4.13. *Let V be symmetric and short-range, and assume that the condition of* Lemma 4.2 *is satisfied, so that $P = H + V$ is a self-adjoint operator. Assume, in addition, that* Assumption S *holds. Then*

$$\Sigma_P = \sigma_p(P) \cap U.$$

Proof. In view of Corollary 4.8 we need only show that

$$\Sigma_P \subseteq \sigma_p(P) \cap U.$$

Let $\mu \in \Sigma_P$ and let ϕ satisfy Eq. (4.8). Let $\psi = R^{\pm}(\mu)\phi$. We claim that ψ is an eigenvector of P, with eigenvalue μ.

To see this, let $K \subseteq U$ be a compact interval whose interior contains μ. Let χ_K be the characteristic function of K and set

$$\widetilde{\psi}(\lambda) = \chi_K(\lambda)\,\frac{A(\lambda)\phi}{\lambda-\mu} + (1-\chi_K(\lambda))\,\frac{A(\lambda)\phi}{\lambda-\mu}. \tag{4.10}$$

The function $g(\lambda) = \frac{1-\chi_K(\lambda)}{\lambda-\mu}$ is bounded, so by Lemma 4.6 the second term is in $\mathcal{H}^{\oplus}$. Also, using Assumption S,

$$\int_K \frac{\langle A(\lambda)\phi,\phi\rangle}{|\lambda-\mu|^2}\,d\lambda \le C\int_K |\lambda-\mu|^{-1+\epsilon}\,d\lambda\,\|\phi\|_{\mathcal{X}}^2 < \infty,$$

so that the second term is also in $\mathcal{H}^{\oplus}$ and we conclude that $\widetilde{\psi} \in \mathcal{H}^{\oplus}$.

Under the unitary map of $\mathcal{H}$ onto $\mathcal{H}^{\oplus}$, there exists $\psi_0 \in \mathcal{H}$ so that $\psi_0 \to \widetilde{\psi}$. Then we have

$$\|R(\mu \pm i\epsilon)\phi - \psi_0\|^2 = \int_U \left\| \frac{A(\lambda)\phi}{\lambda-\mu\mp i\epsilon} - \frac{A(\lambda)\phi}{\lambda-\mu}\right\|_\lambda^2 d\lambda.$$

(The norm in the left-hand side is that of $\mathcal{H}$.) The right-hand side in the last equality tends to zero as $\epsilon \to 0$, by Lebesgue's dominated convergence theorem. Hence $R(\mu \pm i\epsilon)\phi \to \psi_0$ in $\mathcal{H}$ as $\epsilon \to 0$. But $R(\mu \pm i\epsilon)\phi \to R^{\pm}(\mu)\phi = \psi$ in $\mathcal{X}_H^*$, and since $\mathcal{X}_H^* \subseteq \mathcal{X}^*$ with a stronger norm, this convergence is also in $\mathcal{X}^*$. On the other hand, $\mathcal{H} \hookrightarrow \mathcal{X}^*$ with a stronger norm, so that $R(\mu \pm i\epsilon)\phi \to \psi_0$ in $\mathcal{X}^*$. Hence $\psi_0 = \psi = R^{\pm}(\mu)\phi$.

Next, decomposing as in (4.10),

$$\lambda\widetilde{\psi}(\lambda) = \chi_K(\lambda)\,\frac{\lambda A(\lambda)\phi}{\lambda-\mu} + (1-\chi_K(\lambda))\,\frac{\lambda A(\lambda)\phi}{\lambda-\mu},$$

and using again Lemma 4.6 we obtain that $\{\lambda\widetilde{\psi}(\lambda), \lambda \in U\} \in \mathcal{H}^{\oplus}$ so that $\psi \in D(H) \subseteq \mathcal{H}$.

Now we observe that, by the convergence result above,

$$(H-\mu)R(\mu \pm i\epsilon)\phi = \phi \pm i\epsilon R(\mu \pm i\epsilon)\phi \to \phi \quad \text{in } \mathcal{H} \text{ as } \epsilon \to 0,$$

since $R(\mu \pm i\epsilon)\phi \to \psi$ (in $\mathcal{H}$). From the fact that H is closed we get

$$(H-\mu)\psi = \phi = -V\psi,$$

so that $(P-\mu)\psi = 0$, as claimed. □

We can now give a full characterization of the set of eigenvalues of $P = H + V$ in U.

Theorem 4.14. *Assuming the conditions of* Theorem 4.13, *the set* Σ_P *is discrete. In particular, the spectrum of* P *in* U *is absolutely continuous, except possibly for a discrete set of eigenvalues. Furthermore, every eigenvalue is of finite multiplicity.*

Proof. Suppose that there is a sequence $\{\mu_k\}_{k=1}^{\infty} \subseteq \Sigma_P$ of pairwise disjoint points such that $\mu_k \xrightarrow[k\to\infty]{} \mu \in U$. Then there exists a sequence $\{\phi_k\}_{k=1}^{\infty} \subseteq \mathcal{X}$, $\|\phi_k\|_{\mathcal{X}} = 1$, so that $\phi_k = -VR^{\pm}(\mu_k)\phi_k$, $k = 1, 2, \ldots$ By taking a subsequence, without changing notation, we can assume that $\phi_k \xrightarrow[k\to\infty]{w} \phi$ (weakly in $\mathcal{X}$). We write

$$\phi_m - \phi_n = V[R^{\pm}(\mu_n) - R^{\pm}(\mu)]\phi_n - V[R^{\pm}(\mu_m) - R^{\pm}(\mu)]\phi_m + VR^{\pm}(\mu)[\phi_n - \phi_m].$$

The first two terms vanish as $n, m \to \infty$, because $VR^{\pm}(\mu_k) \xrightarrow[k\to\infty]{} VR^{\pm}(\mu)$ in the uniform operator topology of $B(\mathcal{X})$. The last term vanishes by the compactness of $VR^{\pm}(\mu)$, so that the sequence $\{\phi_k\}$ converges strongly to ϕ in $\mathcal{X}$. Letting $k \to \infty$ in $\phi_k = -VR^{\pm}(\mu_k)\phi_k$ we get $\phi = -VR^{\pm}(\mu)\phi$.

Without loss of generality we may assume that $\{\mu_k\}_{k=1}^{\infty}$ and μ are contained in the interior of some compact interval $K \subseteq U$. Let $\eta > 0$ be given; we may also suppose that for $\epsilon > 0$ as in Assumption S,

$$\int_K |\mu_k - \lambda|^{-1+\epsilon}\, d\lambda < \eta, \quad k = 1, 2, \ldots$$

Let $\psi_n = R^{\pm}(\mu_n)\phi_n$. We decompose as in (4.10),

$$\widetilde{\psi_n}(\lambda) = \chi_K(\lambda)\,\frac{A(\lambda)\phi_n}{\lambda - \mu_n} + (1 - \chi_K(\lambda))\,\frac{A(\lambda)\phi_n}{\lambda - \mu_n} = \widetilde{\psi_n^1}(\lambda) + \widetilde{\psi_n^2}(\lambda).$$

Note that the fact that $\widetilde{\psi_n} \in \mathcal{H}^{\oplus}$ corresponds to ψ_n under the unitary map $\mathcal{H} \to \mathcal{H}^{\oplus}$ was established in the proof of Theorem 4.13.

Assumption S and the smallness assumption on K yield (see computation following Eq. (4.10))

$$\|\widetilde{\psi_n^1}\|_{\mathcal{H}^{\oplus}} \leq C\,\eta, \quad n = 1, 2, \ldots$$

Turning to the difference $\widetilde{\psi_n^2} - \widetilde{\psi_m^2}$ we denote $\delta = \operatorname{dist}\big(\{\mu_k\}_{k=1}^{\infty}, U \setminus K\big) > 0$. Then we have

$$\begin{aligned}
&\left\| (1-\chi_K(\lambda)) \left[\frac{A(\lambda)\phi_n}{\lambda-\mu_n} - \frac{A(\lambda)\phi_m}{\lambda-\mu_m} \right] \right\|_\lambda^2 \\
&\quad \leq 2 \left\| (1-\chi_K(\lambda)) \frac{A(\lambda)(\phi_n-\phi_m)}{\lambda-\mu_n} \right\|_\lambda^2 + 2 \left\| \frac{(1-\chi_K(\lambda))(\mu_n-\mu_m)}{(\lambda-\mu_m)(\lambda-\mu_n)} A(\lambda)\phi_m \right\|_\lambda^2 \\
&\quad \leq 2 \left(\frac{1}{\delta^2} + \frac{1}{\delta^4} \right) \left[\|A(\lambda)(\phi_n-\phi_m)\|_\lambda^2 + |\mu_n-\mu_m|^2 \|A(\lambda)\phi_m\|_\lambda^2 \right].
\end{aligned}$$

Integrating over U and recalling that, for every $\theta \in \mathcal{X}$,

$$\int_U \|A(\lambda)\theta\|_\lambda^2 \, d\lambda = \|\theta\|^2 \leq C \|\theta\|_{\mathcal{X}}^2 ,$$

we see that $\left\{ \widetilde{\psi_k^2} \right\}_{k=1}^{\infty}$ is Cauchy in $\mathcal{H}^{\oplus}$, since $\{\phi_k\}_{k=1}^{\infty}$ converges in $\mathcal{X}$.

Thus (by the unitary equivalence) $\psi_n = R^{\pm}(\mu_n)\phi_n \to \psi \in \mathcal{H}$. Since ψ_n is an eigenvector for P at μ_n (see the proof of Theorem 4.13) it follows that $\|\psi_n - \psi_m\|^2 = \|\psi_n\|^2 + \|\psi_m\|^2 \to 0$ as $n, m \to \infty$ so that $\psi = \lim_{k\to\infty} \psi_k = \lim_{k\to\infty} R^{\pm}(\mu_k)\phi_k = 0$ in $\mathcal{H}$, hence in $\mathcal{X}^*$. On the other hand, $0 = \psi = R^{\pm}(\mu)\phi \in \mathcal{X}_H^*$, so that $0 = -V\psi = -VR^{\pm}(\mu)\phi = \phi$. This contradicts the fact that $\|\phi\|_{\mathcal{X}} = 1$. Thus, Σ_P cannot have a converging subsequence (of distinct elements) in U.

Next we prove that every eigenvalue is of finite multiplicity. The preceding argument, namely, assuming that $\mu \in \Sigma_P$ is of infinite multiplicity and setting there $\mu_n \equiv \mu$, cannot be employed in a straightforward way, because of the following reason: We know from the proof of Theorem 4.13 that $\psi = R^{\pm}(\mu)\phi$ (where ϕ satisfies (4.8)) is an eigenvector of P. However, if $\psi \in D(P)$ is an eigenvector, we do not know if there exists a $\phi \in \mathcal{X}$ such that $\psi = R^{\pm}(\mu)\phi$.

So we proceed as follows. First, we establish two facts:

1. If $\epsilon_n \to 0$, $\epsilon_n \neq 0$, then

$$\epsilon_n R(\mu + i\epsilon_n) \xrightarrow[n\to\infty]{w} 0 \text{ in } \mathcal{H}.$$

   Indeed, for any $\phi \in \mathcal{X}$, $\epsilon_n R(\mu \pm i\epsilon_n)\phi \xrightarrow[n\to\infty]{} 0$ in $\mathcal{X}^*$ and is uniformly bounded in $\mathcal{H}$. By the density of $\mathcal{H} \hookrightarrow \mathcal{X}^*$ every weakly convergent subsequence (in $\mathcal{H}$) must converge to zero.
2. If $\epsilon \neq 0$ then for every $\phi \in \mathcal{X}$, we have $R(\mu + i\epsilon)\phi \in D(H) \cap \mathcal{X}_H^* \subseteq D(V)$.

Now let $\psi \in D(P)$ be an eigenvector of P at μ, and let $\phi \in \mathcal{X}$. Let $\epsilon_n \to 0$, $\epsilon_n \neq 0$. Then

$$\begin{aligned}
0 = ((P-\mu)\psi, R(\mu+i\epsilon_n)\phi) &= (\psi, (H-\mu+V)R(\mu+i\epsilon_n)\phi) \\
&= (\psi, (I + VR(\mu+i\epsilon_n))\phi) + (\psi, i\epsilon_n R(\mu+i\epsilon_n)\phi) \\
&\qquad \to (\psi, (I + VR^{\pm}(\mu))\phi) \quad \text{as } \epsilon_n \to 0.
\end{aligned}$$

Viewing ψ as an element of $\mathcal{X}^*$, we infer that $0 = (I + (VR^{\pm}(\mu))^*)\,\psi \in \mathcal{X}^*$. Since $VR^{\pm}(\mu)$ is compact, the Riesz theory implies that its adjoint is also compact and that the dimension of the kernel of $I+(VR^{\pm}(\mu))^*$ is equal to the (finite) dimension of the kernel of $I + VR^{\pm}(\mu)$. We conclude that the eigenspace associated with $\mu \in \Sigma_P$ is exactly the finite-dimensional subspace

$$\big\{\psi = R^{\pm}(\mu)\phi \;\big|\; \big(I + VR^{\pm}(\mu)\big)\,\phi = 0,\, \phi \in \mathcal{X}\big\},$$

and the proof is complete. □

5. Sums of tensor products

An important class of (self-adjoint) operators is the class of operators which are sums of tensor products of (self-adjoint) operators. In the case of partial differential operators, it is associated with *separation of variables*. For example, the Laplacian is a sum of tensor products of the one-dimensional Laplacian (second-order derivative) with the identity operator (in the remaining coordinates).

In the framework of the present review, we shall see that the smoothness of the spectral derivatives of operators (in the sense of Definition 3.3) leads to similar smoothness of their tensor products, hence in particular the LAP and its ramifications (absolute continuity of the spectrum, etc.).

For the reader's convenience we begin by a brief review of the basic notions concerning tensor products. A more extensive treatment can be found in [22].

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces with scalar products $(\ ,\ )_1$ and $(\ ,\ )_2$, respectively. If $x_1 \in \mathcal{H}_1$, $x_2 \in \mathcal{H}_2$, the *tensor product* $x_1 \otimes x_2$ is the bilinear functional on $\mathcal{H}_1 \times \mathcal{H}_2$ given by

$$x_1 \otimes x_2\,(y_1, y_2) = (y_1, x_1)_1 (y_2, x_2)_2, \quad y_1 \in \mathcal{H}_1,\ y_2 \in \mathcal{H}_2.$$

We extend this to a linear space $\mathcal{H}_0$ over $\mathbb{C}$ by taking sums of such elemental tensor products and defining, for $\alpha \in \mathbb{C}$,

$$\alpha\, x_1 \otimes x_2\,(y_1, y_2) = x_1 \otimes x_2\,(\alpha y_1, y_2) = x_1 \otimes x_2\,(y_1, \alpha y_2)\,.$$

A scalar product on $\mathcal{H}_0$ is defined by

$$\Big(\sum_{k=1}^{n} x_1^k \otimes x_2^k, \sum_{j=1}^{m} x_1^j \otimes x_2^j\Big)_{\mathcal{H}} = \sum_{k=1}^{n}\sum_{j=1}^{m} (x_1^k, y_1^j)_1 (x_2^k, y_2^j)_2.$$

The Hilbert space obtained by completing $\mathcal{H}_0$ with respect to this scalar product is called the *tensor product* of the two spaces and denoted by $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. We retain the notation $(\ ,\ )_{\mathcal{H}}$ for its scalar product.

Suppose now that A and B are densely defined linear operators in the spaces $\mathcal{H}_1$, $\mathcal{H}_2$, respectively. If $(x, y) \in D(A) \times D(B)$ define

$$(A \otimes B)(x \otimes y) = (Ax) \otimes (By),$$

and then extend to finite sums by linearity. The extended operator is well defined in the sense that it is independent of the representation of the finite sums. In this way $A \otimes B$ becomes a densely defined linear operator in $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. Furthermore, if A and B are closable, so is $A \otimes B$ and we continue to use the same symbol for its closure.

If A and B are bounded, then

$$\|A \otimes B\|_{B(\mathcal{H})} = \|A\|_{B(\mathcal{H}_1)} \|B\|_{B(\mathcal{H}_2)} .$$

5.1. The operator $H = H_1 \otimes I_2 + I_1 \otimes H_2$

If H_1, H_2 are self-adjoint operators in $\mathcal{H}_1$, $\mathcal{H}_2$, respectively, and I_1, I_2, are, respectively, the identity operators, then $H_1 \otimes I_2$ and $I_1 \otimes H_2$ are commuting self-adjoint operators in $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. Further, $H = H_1 \otimes I_2 + I_1 \otimes H_2$ has a closure which is self-adjoint for which we retain the same notation. The easy proofs of these facts can be found, e.g., in [22, Chapter IV].

We denote by $R_1(z)$, $R_2(z)$ the resolvents of H_1, H_2, respectively, and by $R(z) = (H - z)^{-1}$ the resolvent of H.

In this subsection, when there is no risk of confusion, we shall simply use $(\, , \,)$ for the scalar product $(\, , \,)_{\mathcal{H}}$.

Let $\{E_1(\lambda)\}$ and $\{E_2(\lambda)\}$ be the spectral families of H_1, H_2, respectively. Then $\big\{E_1(\lambda_1) \otimes E_2(\lambda_2) = (E_1(\lambda_1) \otimes I_2)(I_1 \otimes E_2(\lambda_2))\big\}$ is an orthogonal spectral family in $\mathcal{H}_1 \otimes \mathcal{H}_2$, defined over $\mathbb{R}^2$.

Consider the self-adjoint operator (in $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$)

$$T = \int_{\mathbb{R}^2} (\lambda_1 + \lambda_2) \, d\,(E_1(\lambda_1) \otimes E_2(\lambda_2)) . \tag{5.1}$$

For $f = f_1 \otimes f_2$ and $g = g_1 \otimes g_2$, where $(f_1, f_2) \in D(H_1) \times D(H_2)$, we have

$$\begin{aligned}(Tf, g)_{\mathcal{H}} &= \int_{\mathbb{R}} \lambda_1 \, d\,(E_1(\lambda_1) f_1, g_1)_1 \int_{\mathbb{R}} d\,(E_2(\lambda_2) f_2, g_2)_2 \\ &\qquad + \int_{\mathbb{R}} d\,(E_1(\lambda_1) f_1, g_1)_1 \int_{\mathbb{R}} \lambda_2 \, d\,(E_2(\lambda_2) f_2, g_2)_2 \\ &= (H_1 f_1, g_1)_1 (f_2, g_2)_2 + (f_1, g_1)_1 (H_2 f_2, g_2)_2 \\ &= ([H_1 \otimes I_2 + I_1 \otimes H_2] f, g)_{\mathcal{H}} = (Hf, g)_{\mathcal{H}}.\end{aligned}$$

This equality extends to finite sums of elements $f = f_1 \otimes f_2$, which constitute a dense subspace of $D(H) \subseteq \mathcal{H}$. We conclude that $T = H$.

Going back to (5.1) and making the change of variables $\lambda = \lambda_1 + \lambda_2$, $\nu = \lambda_2$, we get, for $f = f_1 \otimes f_2$, $g = g_1 \otimes g_2$, where $(f_1, f_2) \in D(H_1) \times D(H_2)$,

$$(Hf, g) = \int_{\mathbb{R}} \lambda \, d\lambda \int_{\mathbb{R}} (E_1(\lambda - \nu) f_1, g_1)_1 \, (dE_2(\nu) f_2, g_2)_2 .$$

Since this formula extends to finite sums of elements $f = f_1 \otimes f_2$, we conclude that the spectral family of H is given by

$$E(\lambda) = \int_{\mathbb{R}} E_1(\lambda - \nu) \otimes dE_2(\nu), \tag{5.2}$$

where it suffices to interpret the integral in the weak sense as in the expression above for $(Hf,g)_{\mathcal{H}}$.

We let as usual $R(z) = (H-z)^{-1}$, $\operatorname{Im} z \neq 0$, be the resolvent and use the standard formula (valid for any self-adjoint operator),

$$R(z) = \frac{1}{2\pi i}\int_{\mathbb{R}} \frac{R(\lambda+i\eta)-R(\lambda-i\eta)}{\lambda - z \pm i\eta}\,d\lambda, \quad \pm\operatorname{Im} z > 0,\, \eta>0, \tag{5.3}$$

which can be easily derived from

$$R(\lambda+i\eta)-R(\lambda-i\eta) = 2i\eta\int_{\mathbb{R}} \frac{dE(\mu)}{(\mu-\lambda)^2+\eta^2}, \quad \eta>0. \tag{5.4}$$

We shall also need the formulas (again valid for any self-adjoint operator)

$$\begin{aligned} R(z) &= \pm i\int_0^\infty e^{\pm izt}e^{\mp itH}dt, \quad \pm\operatorname{Im} z>0,\\ e^{itH} &= \frac{1}{2\pi i}e^{\eta|t|}\int_{\mathbb{R}} e^{it\lambda}[R(\lambda+i\eta)-R(\lambda-i\eta)]\,d\lambda, \quad \eta>0. \end{aligned} \tag{5.5}$$

For our purpose it is enough to interpret these formulas in the weak sense.

For notational simplicity we use

$$A(\lambda,\eta) = \frac{1}{2\pi i}\left[R(\lambda+i\eta)-R(\lambda-i\eta)\right], \quad \eta>0,$$

and A_i for the same operators relative to H_i in $\mathcal{H}_i$, $i=1,2$.

Observe that in view of (5.4)

$$\sup_{\eta>0}\int_{\mathbb{R}} |(A(\lambda,\eta)f,g)|\,d\lambda \leq \|f\|\,\|g\|\,.$$

Set $\overline{H_1} = H_1\otimes I_2$, $\overline{H_2} = I_1\otimes H_2$. Since they commute, we have by (5.5)

$$R(\lambda+i\epsilon) = i\int_0^\infty e^{i(\lambda+i\epsilon)t}e^{-it\overline{H_1}}e^{-it\overline{H_2}}\,dt,$$

and a straightforward computation using the second equation in (5.5) yields, for $\epsilon>\eta_1+\eta_2$, $\eta_1>0$, $\eta_2>0$,

$$R(\lambda+i\epsilon) = \int_{\mathbb{R}^2}\frac{A_1(\lambda_1,\eta_1)\otimes A_2(\lambda_2,\eta_2)}{\lambda_1+\lambda_2-\lambda-i(\epsilon-\eta_1-\eta_2)}\,d\lambda_1 d\lambda_2. \tag{5.6}$$

Changing variables to $\mu=\lambda_1+\lambda_2,\ \nu=\lambda_2$ we get

$$R(\lambda\pm i\epsilon) = \int_{\mathbb{R}}\frac{C(\mu,\eta)}{\mu-\lambda\mp i(\epsilon-\eta)}\,d\mu,$$

where $C(\mu,\eta) = \int_{\mathbb{R}} A_1(\mu-\nu,\eta_1)\otimes A_2(\nu,\eta_2)\,d\nu$, $\eta=\eta_1+\eta_2$.

Comparing this equation with (5.3), we infer that

$$C(\mu,\eta) = A(\mu,\eta) = \frac{1}{2\pi i}\left[R(\mu+i\eta)-R(\mu-i\eta)\right].$$

Now using Eq. (5.4) for A_2 we obtain, with $\eta = \eta_1 + \eta_2$,

$$A(\mu,\eta) = \frac{1}{\pi}\int_{\mathbb{R}} A_1(\mu-\lambda,\eta_1) \otimes \int_{\mathbb{R}} \frac{\eta_2\, dE_2(\nu)}{(\nu-\lambda)^2+\eta_2^2}\, d\lambda$$
$$= \int_{\mathbb{R}} \frac{\eta_2}{\pi} \int_{\mathbb{R}} \frac{A_1(\mu-\lambda,\eta_1)}{(\nu-\lambda)^2+\eta_2^2}\, d\lambda \otimes dE_2(\nu).$$

As $\eta_2 \to 0$, the convergence property of the Poisson kernel implies

$$A(\mu,\eta) = \int_{\mathbb{R}} A_1(\mu-\lambda,\eta) \otimes dE_2(\nu). \tag{5.7}$$

The integral ought to be interpreted in the weak (or strong) topology of $B(\mathcal{H})$ as the Stieltjes integral of the continuous function $A_1(\mu-\lambda,\eta)\otimes I_2$ with respect to the spectral measure $I_1 \otimes dE_2(\nu)$.

Finally, using the representation (5.3) for $R_1(z) = (H_1 - z)^{-1}$, we obtain from (5.7)

$$R(\lambda \pm i\epsilon) = \int_{\mathbb{R}} R_1(\lambda \pm i\epsilon - \nu) \otimes dE_2(\nu), \quad \epsilon > 0. \tag{5.8}$$

5.2. Extending the abstract framework of the LAP

In order to fit the operator H of the preceding subsection into the abstract framework, we need to modify somewhat the treatment of Subsection 3.1. We use the same setting as in that subsection. Thus, $\mathcal{H}$ is a Hilbert space, and we assume that $\mathcal{X} \hookrightarrow \mathcal{H}$, $\mathcal{Y} \hookrightarrow \mathcal{H}$ are two densely and continuously embedded subspaces. In particular, their norms, $\|\cdot\|_{\mathcal{X}}$, $\|\cdot\|_{\mathcal{Y}}$, are stronger than $\|\cdot\| = \|\cdot\|_{\mathcal{H}}$.

Referring to Definition 3.3, it is clear what we mean by saying that the self-adjoint operator H is of type $(\mathcal{X},\mathcal{Y}^*,\alpha,U)$ for some $\alpha \in (0,1)$ and an open set $U \subseteq \mathbb{R}$ of full spectral measure.

In particular, for the (weak) spectral derivative $A(\lambda) = \frac{d}{d\lambda}E(\lambda) \in B(\mathcal{X},\mathcal{Y}^*)$, where $\{E(\lambda)\}$ is the spectral family of H.

Our next theorem is very close to Theorem 3.6. However, we need to modify somewhat the proof of that theorem, which at various points relied on the specific embeddings $\mathcal{X} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{X}^*$.

Theorem 5.1. *Let H be of global type $(\mathcal{X},\mathcal{Y}^*,\alpha,\mathbb{R})$ for some $\alpha \in (0,1)$. Thus, suppose that for some constant $C > 0$,*

$$\sup_{\lambda\in\mathbb{R}} \|A(\lambda)\|_{B(\mathcal{X},\mathcal{Y}^*)} < C, \quad \sup_{\lambda_1\neq\lambda_2} \frac{\|A(\lambda_2)-A(\lambda_1)\|_{B(\mathcal{X},\mathcal{Y}^*)}}{|\lambda_2-\lambda_1|^\alpha} < C. \tag{5.9}$$

Then the limits

$$R^\pm(\lambda) = \lim_{\epsilon\downarrow 0} R(\lambda \pm i\epsilon)$$

exist, uniformly in $\lambda \in \mathbb{R}$, in the uniform operator topology of $B(\mathcal{X},\mathcal{Y}^*)$.

Furthermore,

$$\sup_{\lambda\in\mathbb{R}} \left\|R^\pm(\lambda)\right\|_{B(\mathcal{X},\mathcal{Y}^*)} < C, \quad \sup_{\lambda_1\neq\lambda_2} \frac{\|R^\pm(\lambda_2)-R^\pm(\lambda_1)\|_{B(\mathcal{X},\mathcal{Y}^*)}}{|\lambda_2-\lambda_1|^\alpha} < C,$$

and

$$R^{\pm}(\lambda) = \mathrm{P.V.} \int_{\mathbb{R}} \frac{A(\mu)}{\mu - \lambda}\, d\mu \pm i\pi A(\lambda), \quad \lambda \in \mathbb{R}. \tag{5.10}$$

Proof. Let $\phi \in C_0^\infty(\mathbb{R})$ be a cutoff function, where $\phi(\theta) = 1$ for $|\theta| \le 1$.

Denoting the $(\mathcal{Y}^*, \mathcal{Y})$ pairing by $\langle\ ,\ \rangle$ and taking $x \in \mathcal{X}$, $y \in \mathcal{Y}$, we have

$$\left| \int_{\mathbb{R}} \frac{(1 - \phi(\mu - \lambda))\,\langle (A(\mu)x, y\rangle}{\mu - \lambda}\, d\mu \right| \le \|x\|\,\|y\| \le C\,\|x\|_{\mathcal{X}}\,\|y\|_{\mathcal{Y}}\,.$$

Combined with the uniform bounds (5.9), we obtain readily that the integral

$$\int_{\mathbb{R}} \frac{(1 - \phi(\mu - \lambda))A(\mu)}{\mu - z}\, d\mu, \quad z \in \mathbb{C},$$

defines a family of operators in $B(\mathcal{X}, \mathcal{Y}^*)$, which is continuous in the uniform operator topology as $\operatorname{Im} z \to 0$ and $|\operatorname{Re} z - \lambda| < \frac{1}{2}$. Uniform Hölder estimates with respect to $\lambda \in \mathbb{R}$ are readily obtained from (5.9).

Now the integral

$$\int_{\mathbb{R}} \frac{\phi(\mu - \lambda)A(\mu)}{\mu - z}\, d\mu, \quad z \in \mathbb{C},$$

can be treated by the Privaloff-Korn theorem (see Subsection 3.1). □

5.3. The LAP for $H = H_1 \otimes I_2 + I_1 \otimes H_2$

We now return to the context of Subsection 5.1 and consider the LAP for H.

We assume that $\mathcal{X}_i \hookrightarrow \mathcal{H}_i$, $\mathcal{Y}_i \hookrightarrow \mathcal{H}_i$, $i = 1, 2$, are densely and continuously embedded Hilbert spaces.

Theorem 5.2. *Suppose that there exist continuous operator-valued functions* $R_1^{\pm}(\lambda) \in B(\mathcal{X}_1, \mathcal{Y}_1^*)$, $-\infty < \lambda < \infty$, *so that*

$$R_1^{\pm}(\lambda) = \lim_{\epsilon \downarrow 0} R_1(\lambda \pm i\epsilon),$$

in the uniform operator topology of $B(\mathcal{X}_1, \mathcal{Y}_1^*)$, *the convergence being uniform in* $\lambda \in \mathbb{R}$. *Then the limits*

$$R^{\pm}(\lambda) = \lim_{\epsilon \downarrow 0} R(\lambda \pm i\epsilon),$$

exist in the uniform operator topology of $B(\mathcal{X}_1 \otimes \mathcal{H}_2, \mathcal{Y}_1^* \otimes \mathcal{H}_2)$, *uniformly in* $\lambda \in \mathbb{R}$.

Proof. The existence of the limits follows directly from Eq. (5.8). In fact,

$$R^{\pm}(\lambda) = \int_{\mathbb{R}} R_1^{\pm}(\lambda - \nu) \otimes dE_2(\nu). \tag{5.11}$$

The hypothesis on the continuity of $R_1^{\pm}(\lambda)$ implies that this integral can be viewed as a Riemann-Stieltjes integral, either in the weak or strong topology of $B(\mathcal{X}_1 \otimes \mathcal{H}_2, \mathcal{Y}_1^* \otimes \mathcal{H}_2)$. In addition, clearly

$$\left\| R^{\pm}(\lambda) - R(\lambda \pm i\epsilon) \right\|_{B(\mathcal{X}_1 \otimes \mathcal{H}_2, \mathcal{Y}_1^* \otimes \mathcal{H}_2)} \le \sup_{\nu \in \mathbb{R}} \left\| R_1^{\pm}(\nu) - R_1(\nu \pm i\epsilon) \right\|_{B(\mathcal{X}_1, \mathcal{Y}_1^*)}. \quad \square$$

We note that the hypothesis imposed on H_1 in this theorem follows from the hypothesis in Theorem 5.1, with H_1 replacing H. We therefore have

Corollary 5.3. *Let H_1 be of global type $(\mathcal{X}_1, \mathcal{Y}_1^*, \alpha, \mathbb{R})$ for some $\alpha \in (0,1)$. Then it satisfies the condition of* Theorem 5.2. *In particular, the limits $R^{\pm}(\lambda)$ exist, they satisfy* Eq. (5.11) *and are uniformly Hölder continuous in $\mathbb{R}$.*

While for some applications (notably the Stark Hamiltonian considered in Subsection 5.4) the above theorem and corollary are adequate, there are other cases where the spectral derivative *explodes* at the edge of the spectrum, hence the operator is not of global type (for the Laplacian see (3.3) and Subsection 5.5). We therefore formulate the following theorem, that can be viewed as a *localized* version of Theorem 5.2. The basic assumption on the operator H_1 is that its spectral derivative A_1 exists in the sense of Definition 3.3, with $\mathcal{X}_H^*$ (there) replaced by $\mathcal{Y}_1^*$ (here).

Theorem 5.4. *Let $\Lambda \subseteq \mathbb{R}$ be compact and assume that $E_1(\Lambda) = 0$ and that H_1 is of type $(\mathcal{X}_1, \mathcal{Y}_1^*, \alpha, \mathbb{R} \setminus \Lambda)$, $\alpha \in (0,1)$. For any $\delta > 0$, let*

$$\Lambda_\delta = \left\{\mu \;\middle|\; \operatorname{dist}(\mu, \Lambda) \le \delta\right\}.$$

Assume that the spectral derivative $A_1(\lambda) = \frac{d}{d\lambda} E_1(\lambda)$, $\lambda \in \mathbb{R} \setminus \Lambda$ satisfies, for any $\delta > 0$, with a constant M_δ depending only on δ,

(a) $$\|A_1(\lambda_2) - A_1(\lambda_1)\|_{B(\mathcal{X}_1, \mathcal{Y}_1^*)} \le M_\delta \,|\lambda_2 - \lambda_1|^\alpha, \quad \lambda_1, \lambda_2 \in \mathbb{R} \setminus \Lambda_\delta,$$

(b) $$\sup_{\lambda \in \mathbb{R} \setminus \Lambda_\delta} \|A_1(\lambda)\|_{B(\mathcal{X}_1, \mathcal{Y}_1^*)} \le M_\delta.$$

Assume further that there is an open set $U \subseteq \mathbb{R}$, so that the limits

$$R_2^{\pm}(\lambda) = \lim_{\epsilon \downarrow 0} R_2(\lambda \pm i\epsilon), \quad \lambda \in U - \Lambda \text{ (vector sum)}, \tag{5.12}$$

exist in the uniform operator topology of $B(\mathcal{X}_2, \mathcal{Y}_2^*)$, the convergence being uniform in every compact subset of $U - \Lambda$.

Then the limits

$$R^{\pm}(\lambda) = \lim_{\epsilon \downarrow 0} R(\lambda \pm i\epsilon), \quad \lambda \in U,$$

exist in the uniform operator topology of $B(\mathcal{X}_1 \otimes \mathcal{X}_2, \mathcal{Y}_1^* \otimes \mathcal{Y}_2^*)$, and the convergence is uniform in every compact subset of U.

Finally, if the $R_2^{\pm}(\lambda)$ satisfy a local Hölder condition with exponent α' (in the uniform operator topology), then so do the $R^{\pm}(\lambda)$ with exponent $\beta = \min\{\alpha, \alpha'\}$.

Proof. Let $K = [a,b] \subseteq U$ and let $\delta > 0$ be sufficiently small, so that the limits in (5.12) exist uniformly in $K - \Lambda_{2\delta}$. Let $\phi \in C^\infty(\mathbb{R})$ be a cutoff function so that

$$\phi(t) = \begin{cases} 0, & t \in \Lambda_\delta, \\ 1, & t \in \mathbb{R} \setminus \Lambda_{2\delta}. \end{cases}$$

We now rewrite Eq. (5.6) as, taking $\epsilon > 0$ for simplicity,

$$R(\lambda + i\epsilon) = \int_{\mathbb{R}^2} \phi(\omega) \frac{A_1(\omega, \eta_1) \otimes A_2(\nu, \eta_2)}{\omega + \nu - \lambda - i(\epsilon - \eta_1 - \eta_2)} \, d\omega d\nu + \int_{\mathbb{R}^2} (1 - \phi(\omega)) \frac{A_1(\omega, \eta_1) \otimes A_2(\nu, \eta_2)}{\omega + \nu - \lambda - i(\epsilon - \eta_1 - \eta_2)} \, d\omega d\nu, \quad \lambda \in K.$$

Note that $\phi(\omega) A_1(\omega)$ satisfies the assumptions imposed on A_1 in Corollary 5.3 so that, uniformly in $\omega \in \mathbb{R}$,

$$\phi(\omega) A_1(\omega, \eta_1) \xrightarrow[\eta_1 \to 0]{} \phi(\omega) A_1(\omega),$$

in the uniform operator topology of $B(\mathcal{X}_1, \mathcal{Y}_1^*)$.

Also, as in (5.7), we have (weakly in measures), $A_2(\nu, \eta_2) \, d\nu \xrightarrow[\eta_2 \to 0]{} dE_2(\nu)$.

Invoking these facts in the above expression for $R(\lambda + i\epsilon)$, letting $\eta_1, \eta_2 \to 0$ and also using the spectral theorem for R_2 (in the second integral), we get

$$R(\lambda + i\epsilon) = \int_{\mathbb{R}^2} \frac{\phi(\omega) A_1(\omega) d\omega}{\omega + \nu - \lambda - i\epsilon} \otimes dE_2(\nu) + \int_{\mathbb{R}} (1 - \phi(\omega)) dE_1(\omega) \otimes R_2(\lambda - \omega + i\epsilon) = L^1(\lambda, \epsilon) + L^2(\lambda, \epsilon).$$

The integrals can be interpreted in the weak or strong sense of $B(\mathcal{X}_1 \otimes \mathcal{H}_2, \mathcal{Y}_1^* \otimes \mathcal{H}_2)$, $B(\mathcal{H}_1 \otimes \mathcal{X}_2, \mathcal{H}_1 \otimes \mathcal{Y}_2^*)$, respectively.

In the first term, we are precisely in the situation of Corollary 5.3, so as in Eq. (5.11),

$$L^1(\lambda, \epsilon) \xrightarrow[\epsilon \downarrow 0]{} \int_{\mathbb{R}} \left\{ \text{P. V.} \int_{\mathbb{R}} \frac{\phi(\omega) A_1(\omega)}{\omega + \nu - \lambda} d\omega + i\pi \phi(\lambda - \nu) A_1(\lambda - \nu) \right\} \otimes dE_2(\nu), \quad \lambda \in K,$$

in the uniform operator topology of $B(\mathcal{X}_1 \otimes \mathcal{H}_2, \mathcal{Y}_1^* \otimes \mathcal{H}_2)$.

In the second term, we observe that the integrand (in ω) is supported in $K - \Lambda_{2\delta}$ where the limits in (5.12) exist uniformly. We therefore obtain

$$L^2(\lambda, \epsilon) \xrightarrow[\epsilon \downarrow 0]{} \int_{\mathbb{R}} (1 - \phi(\omega)) \, dE_1(\omega) \otimes R_2^+(\lambda - \omega),$$

in the uniform operator topology of $B(\mathcal{H}_1 \otimes \mathcal{X}_2, \mathcal{H}_1 \otimes \mathcal{Y}_2^*)$. Thus both limits exist in the uniform operator topology of $B(\mathcal{X}_1 \otimes \mathcal{X}_2, \mathcal{Y}_1^* \otimes \mathcal{Y}_2^*)$.

To prove the last assertion of the theorem, we note that under the local Hölder continuity of $R_2^+(\lambda)$ in $U - \Lambda$ the limit integral in the last equation is Hölder continuous, with the same exponent α'. The limit integral of the first term is Hölder continuous by virtue of the Privaloff-Korn theorem. □

Corollary 5.5 (corollary to the proof). *We note that the spectral derivative of H is given by*

$$A(\lambda) = i\pi \int_{\mathbb{R}} \phi(\lambda - \nu) A_1(\lambda - \nu) \otimes dE_2(\nu) + \int_{\mathbb{R}} (1 - \phi(\omega))\, dE_1(\omega) \otimes A_2(\lambda - \omega).$$

5.4. The Stark Hamiltonian

The quantum mechanical operator governing (in the Schrödinger equation) the motion of a charged particle subject to a uniform electric field is known as the Stark Hamiltonian. Setting various physical parameters as units, this operator is given by

$$H = -\Delta - x_1, \quad x = (x_1, x_2, \dots, x_n) \in \mathbb{R}^n. \tag{5.13}$$

To represent it in the form of a sum of tensor products, we write it as

$$H = H_1 \otimes I_2 + I_1 \otimes H_2,$$

where

$$H_1 = -\frac{d^2}{dx_1^2} - x_1, \tag{5.14}$$

is self-adjoint in $\mathcal{H}_1 = L^2(\mathbb{R})$ [15, 6] and

$$H_2 = -\Delta, \quad \text{with respect to } x' = (x_2, \dots, x_n) \in \mathbb{R}^{n-1}, \tag{5.15}$$

is self-adjoint in $\mathcal{H}_2 = L^2(\mathbb{R}^{n-1})$.

We are going to deal with the operator H_1 and show that it satisfies the assumptions of Theorem 5.2. We simplify notation by denoting $S = H_1$ and replacing x_1 by a single coordinate $y \in \mathbb{R}$. We take the space $\mathcal{X} = L^{2,s}(\mathbb{R})$, $s > \frac{1}{4}$ (refer to Section 2 for definitions of weighted spaces).

It is easy to verify that S has a closure in $\mathcal{X}^* = L^{2,-s}(\mathbb{R})$. If we take $\mathcal{X}^*_S$ to be the domain of this closure (equipped with the graph norm), then Theorem 3.11 is applicable. It therefore suffices to consider the computations ahead in the framework of $B(\mathcal{X}, \mathcal{X}^*)$.

Lemma 5.6. *Let $S = -\frac{d^2}{dy^2} - y$, viewed as a self-adjoint operator in $L^2(\mathbb{R})$. Denote by $\{E_S(\lambda)\}$ its spectral family. Let $s > \frac{1}{4}$, $\mathcal{X} = L^{2,s}(\mathbb{R})$.*

Then there exists $\alpha \in (0, 1)$ (depending on s) so that S is of global type $(\mathcal{X}, \mathcal{X}^*, \alpha, \mathbb{R})$. In other words, its spectral derivative $A_S(\lambda) = \frac{d}{d\lambda} E_S(\lambda)$ satisfies (5.9) (with $\mathcal{Y} = \mathcal{X}$).

Proof. Let $w(y)$ be the real non-zero function (up to a multiplicative constant) which is a solution of

$$Sw(y) = \left(-\frac{d^2}{dy^2} - y\right) w(y) = 0,$$

and has the following properties:

$$\begin{aligned} &w(y) \text{ decays exponentially as } y \to -\infty, \\ &|w(y)| \le C\,(1 + |y|)^{-\frac{1}{4}}, \quad y \in \mathbb{R}, \\ &|w'(y)| \le C\,(1 + |y|)^{\frac{1}{4}}, \quad y \in \mathbb{R}. \end{aligned} \tag{5.16}$$

This solution is known as the *Airy function*. Its existence is an easy consequence of simple asymptotic theorems for solutions of ordinary differential equations [15].

If $\hat{w}(\xi)$ is the Fourier transform of w (as a tempered distribution), it solves the first-order equation

$$\left(i^{-1}\frac{d}{d\xi}+\xi^2\right)\hat{w}(\xi)=0,$$

hence $\hat{w}(\xi)=\hat{w}(0)\exp(-\frac{1}{3}i\xi^3)$. We normalize by setting $\hat{w}(0)=(2\pi)^{-\frac{1}{2}}$.

For $\lambda\in\mathbb{R}$ we define $w_\lambda(y)=w(y+\lambda)$ so that

$$\hat{w}_\lambda(\xi)=(2\pi)^{-\frac{1}{2}}\exp\left(i\lambda\xi-\frac{1}{3}i\xi^3\right).$$

Let $f\in C_0^\infty(\mathbb{R})$ and define the transformation

$$(\mathcal{A}f)(\lambda)=\int_{\mathbb{R}}f(y)w_\lambda(y)\,dy,\quad \lambda\in\mathbb{R}.$$

By the Parseval equality

$$(\mathcal{A}f)(\lambda)=(2\pi)^{-\frac{1}{2}}\int_{\mathbb{R}}\hat{f}(\xi)\exp\left(\frac{1}{3}i\xi^3\right)e^{-i\lambda\xi}\,d\xi.$$

Since $\left|\exp(\frac{1}{3}i\xi^3)\right|=1$, the transformation $\mathcal{A}$ can be extended to a unitary map on $L^2(\mathbb{R})$, for which we retain the same notation. Using integration by parts, we get

$$(\mathcal{A}Sf)(\lambda)=\int_{\mathbb{R}}f(y)Sw_\lambda(y)\,dy=\lambda\,(\mathcal{A}f)(\lambda),\quad f\in C_0^\infty(\mathbb{R}). \tag{5.17}$$

Thus the transformation $\mathcal{A}$ diagonalizes S, so that (compare Eq. (3.3)),

$$\frac{d}{d\lambda}(E_S(\lambda)f,g)=(\mathcal{A}f)(\lambda)\,\overline{(\mathcal{A}g)(\lambda)},\quad f,g\in C_0^\infty(\mathbb{R}). \tag{5.18}$$

We claim that for $s>\frac{1}{4}$ there is a constant $M>0$ so that

$$|(\mathcal{A}f)(\lambda)|\le M\,\|f\|_{0,s}\,. \tag{5.19}$$

Indeed, using the estimates in (5.16) and the Schwartz and Hölder inequalities,

$$\begin{aligned}|(\mathcal{A}f)(\lambda)|&\le C\int_{\mathbb{R}}(1+|y+\lambda|)^{-\frac{1}{4}}\left(1+y^2\right)^{-\frac{s}{2}}\left(1+y^2\right)^{\frac{s}{2}}|f(y)|\,dy\\&\le C\left\{\int_{\mathbb{R}}(1+|y+\lambda|)^{-\frac{1}{2}}\left(1+y^2\right)^{-s}dy\right\}^{\frac{1}{2}}\|f\|_{0,s}\\&\le C\left\{\int_{\mathbb{R}}(1+|y+\lambda|)^{-\frac{p}{2}}\,dy\right\}^{\frac{1}{2p}}\left\{\int_{\mathbb{R}}\left(1+y^2\right)^{-sq}\,dy\right\}^{\frac{1}{2q}}\|f\|_{0,s}\,,\end{aligned}$$

where $\frac{1}{p}+\frac{1}{q}=1$.

We can choose $p > 2$ so that $sq > \frac{1}{2}$. The integrals in the above inequality converge and are bounded uniformly in $\lambda \in \mathbb{R}$, which proves (5.19). In view of (5.18) this establishes the first inequality in (5.9). We therefore have $A_S(\lambda) = \frac{d}{d\lambda} E_S(\lambda) \in B(\mathcal{X}, \mathcal{X}^*)$ (and is uniformly bounded).

As for the Hölder condition of (5.9), we write (using $\langle\ ,\ \rangle$ for the $(\mathcal{X}^*, \mathcal{X})$ pairing),

$$\begin{aligned}\langle [A_S(\lambda+h) - A_S(\lambda)]\, f, g\rangle = \ & (\mathcal{A}f)(\lambda+h)\, \overline{[(\mathcal{A}g)(\lambda+h) - (\mathcal{A}g)(\lambda)]} \\ & + \overline{(\mathcal{A}g)(\lambda)}\, [(\mathcal{A}f)(\lambda+h) - (\mathcal{A}f)(\lambda)]\,. \end{aligned} \tag{5.20}$$

For $|h| < 1$ we have from (5.16)

$$|w(y+h) - w(y)| \le C \min\big\{(1+|y|)^{-\frac{1}{4}}, (1+|y|)^{\frac{1}{4}}\, |h|\big\},$$

so that by interpolation, for any $0 \le \gamma \le 1$,

$$|w(y+h) - w(y)| \le C\, (1+|y|)^{-\frac{1}{4}+\frac{\gamma}{2}}\, |h|^{\gamma}\,.$$

We now estimate as before,

$$\begin{aligned} &|(\mathcal{A}f)(\lambda+h) - (\mathcal{A}f)(\lambda)| \\ &\quad \le C\, |h|^{\gamma} \int_{\mathbb{R}} (1+|y+\lambda|)^{-\frac{1}{4}+\frac{\gamma}{2}} \left(1+y^2\right)^{-\frac{s}{2}} \left(1+y^2\right)^{\frac{s}{2}} |f(y)|\, dy \\ &\quad \le C\, |h|^{\gamma} \left\{\int_{\mathbb{R}} (1+|y+\lambda|)^{-\frac{p}{2}+\gamma p}\, dy\right\}^{\frac{1}{2p}} \left\{\int_{\mathbb{R}} \left(1+y^2\right)^{-sq}\, dy\right\}^{\frac{1}{2q}} \|f\|_{0,s}\,. \end{aligned}$$

We can choose $p > 2$ and $\gamma > 0$ sufficiently small so that $p(\frac{1}{2} - \gamma) > 1$, while $sq > \frac{1}{2}$. This yields

$$|(\mathcal{A}f)(\lambda+h) - (\mathcal{A}f)(\lambda)| \le C\, |h|^{\gamma}\, \|f\|_{0,s}\,,$$

with a similar estimate for g. Inserting these estimates in (5.20) and noting the uniform boundedness of $(\mathcal{A}f)(\lambda)$ we obtain the second required estimate in (5.9).

□

Turning back to the Stark Hamiltonian H given in (5.13), we have the following theorem.

Theorem 5.7. *The spectrum of H is all of $\mathbb{R}$, and is entirely absolutely continuous.*

The resolvent limits

$$(H - \lambda \pm i\cdot 0)^{-1} = \lim_{\epsilon \downarrow 0} (H - \lambda \pm i\epsilon)^{-1}\,, \quad \lambda \in \mathbb{R},$$

exist in the uniform operator topology of $B\left(L^{2,s}(\mathbb{R}) \otimes L^2(\mathbb{R}^{n-1}), \mathcal{X}_S^* \otimes L^2(\mathbb{R}^{n-1})\right)$, for any $s > \frac{1}{4}$, where $\mathcal{X}_S^*$ is the domain of the operator $H_1 = -\frac{d^2}{dx_1^2} - x_1$ in $L^{2,-s}(\mathbb{R})$, equipped with the graph norm. These limits are locally Hölder continuous in this operator topology.

Furthermore, these limits are attained uniformly in $\lambda \in \mathbb{R}$ and are uniformly Hölder continuous in $B\left(L^{2,s}(\mathbb{R}) \otimes L^2(\mathbb{R}^{n-1}), L^{2,-s}(\mathbb{R}) \otimes L^2(\mathbb{R}^{n-1})\right)$.

Proof. The fact that the spectrum of H_1 in (5.14) is the full line follows from the expansion (5.17). In fact, it shows that it is unitarily equivalent to multiplication by the variable in $L^2(\mathbb{R})$. Thus, the spectrum of H is also $\mathbb{R}$.

In view of Lemma 5.6, the operator H_1 in (5.14) satisfies the conditions of Corollary 5.3, which yields all the statements of the theorem, with $\mathcal{X}_S^*$ replaced by $L^{2,-s}(\mathbb{R})$. The statement in $B(L^{2,s}(\mathbb{R}) \otimes L^2(\mathbb{R}^{n-1}), \mathcal{X}_S^* \otimes L^2(\mathbb{R}^{n-1}))$ is obtained by invoking Theorem 3.11. Note, however, that the uniform estimates in (5.9) are lost in the graph norm space, due to the extra multiplication by λ in (5.19).

The absolute continuity of the spectrum is implied by the LAP. □

Remark 5.8 (transversal perturbations). Note that the specific character of the operator $H_2 = -\Delta$ in $L^2(\mathbb{R}^{n-1})$ (see (5.15)) plays no role in the theorem and it could be replaced by *any self-adjoint operator* with respect to the $n-1$ coordinates x', without changing anything in the statement of this theorem. In the quantum mechanical setting, it means that any perturbation, depending only on directions which are transversal to the electric field, can be added to the Stark Hamiltonian, without having any effect on the spectrum and the resolvent.

Remark 5.9 (short-range perturbations). It can be shown [15] that a short-range symmetric perturbation in the sense of Definition 4.1 satisfies Assumption S, hence Theorem 4.14 is applicable to such perturbations.

5.5. The operator $H_0 = -\Delta$ and some wild perturbations

In Example 3.5 and Corollary 3.9 we obtained a representation of the spectral derivative of H_0, from which the LAP could be established, using the trace lemma in Sobolev spaces.

We now investigate further these objects, with the aim of singling out two aspects:

- Deriving the n-dimensional estimates from the one-dimensional estimates, as a straightforward application of our general theorems about sums of tensor products.
- Finding an *optimal* weight for the LAP, depending only on three coordinates.

In analogy with the Stark Hamiltonian (5.13), we have here

$$H_0 = H_1 \otimes I_2 + I_1 \otimes H_2, \tag{5.21}$$

where

$$H_1 = -\frac{d^2}{dx_1^2}, \tag{5.22}$$

and

$$H_2 = -\Delta, \quad \text{with respect to } x' = (x_2, \ldots, x_n) \in \mathbb{R}^{n-1}, \tag{5.23}$$

are self-adjoint in $\mathcal{H}_1 = L^2(\mathbb{R})$ and $\mathcal{H}_2 = L^2(\mathbb{R}^{n-1})$, respectively (closures of their restrictions to test functions, see [59]).

The following lemma is the analog to Lemma 5.6.

Lemma 5.10. *Let $Q = -\frac{d^2}{dy^2}$, viewed as a self-adjoint operator in $L^2(\mathbb{R})$. Denote by $\{E_Q(\lambda)\}$ its spectral family. Let $s > \frac{1}{2}$, $\mathcal{X} = L^{2,s}(\mathbb{R})$. Then there exists $\alpha \in (0,1)$ (depending on s) so that Q is of type $\big(\mathcal{X}, \mathcal{X}_Q^*, \alpha, \mathbb{R} \setminus \{0\}\big)$. In other words, its spectral derivative $A_Q(\lambda) = \frac{d}{d\lambda} E_Q(\lambda)$ satisfies the conditions of* Definition 3.3, *where $\mathcal{X}_Q^* = H^{2,-s}(\mathbb{R})$ is the domain of (the closure of) Q in $L^{2,-s}(\mathbb{R})$, equipped with the graph norm.*

Furthermore, instead of the estimates (5.9) *we now have the following estimates, presented in the framework of operators from $\mathcal{X} = L^{2,s}(\mathbb{R})$ to $\mathcal{X}^* = L^{2,-s}(\mathbb{R})$:*

$$\begin{aligned} \|A_Q(\lambda)\|_{B(\mathcal{X},\mathcal{X}^*)} &\le C_s\, \lambda^{-\frac{1}{2}}, \quad \lambda > 0, \\ \|A_Q(\lambda_2) - A_Q(\lambda_1)\|_{B(\mathcal{X},\mathcal{X}^*)} &\le C_{s,\delta} \left(\lambda_1^{-\frac{1+\alpha}{2}} + \lambda_2^{-\frac{1+\alpha}{2}}\right) |\lambda_2 - \lambda_1|^{\alpha}, \end{aligned} \tag{5.24}$$

where $\lambda_1,\, \lambda_2 > \delta > 0$.

Proof. The proof is similar (but simpler) to that of Lemma 5.6 and we outline it briefly.

For $f,\, g \in C_0^\infty(\mathbb{R})$ we have, in terms of their Fourier transforms (compare Eq. (5.18)),

$$\frac{d}{d\lambda}(E_Q(\lambda) f, g) = \frac{1}{2}\lambda^{-\frac{1}{2}} \left[\hat{f}(\sqrt{\lambda})\, \overline{\hat{g}(\sqrt{\lambda})} + \hat{f}(-\sqrt{\lambda})\, \overline{\hat{g}(-\sqrt{\lambda})}\right], \quad \lambda > 0. \tag{5.25}$$

This is indeed Eq. (3.3) in the one-dimensional case.

Since we have, for any $\mu \in \mathbb{R}$,

$$\left|\hat{f}(\mu)\right| \le (2\pi)^{-\frac{1}{2}} \left\{\int_{\mathbb{R}} \left(1 + y^2\right)^{-s} dy\right\}^{\frac{1}{2}} \|f\|_{0,s},$$

the estimates (5.24) follow by a suitable interpolation as in the proof of Lemma 5.6. □

Note that $E_Q(\lambda) = 0$ for $\lambda < 0$. Denote by $R_Q(z) = (Q - z)^{-1}$ the resolvent of Q (recall that $Q = H_1$).

From the lemma we obtain the following corollary.

Corollary 5.11. *Let $U = \mathbb{R} \setminus \{0\}$ and $\mathcal{X}_Q^* = H^{2,-s}(\mathbb{R})$ for $s > \frac{1}{2}$. The limits*

$$R_Q^{\pm}(\lambda) = \lim_{\epsilon \downarrow 0} R_Q(\lambda \pm i\epsilon), \quad \lambda \in U,$$

exist in the uniform operator topology of $B(\mathcal{X}, \mathcal{X}_Q^*)$, and the extended operator-valued function

$$R_Q(z) = \begin{cases} R_Q(z), & z \in \mathbb{C}^+, \\ R_Q^+(z), & z \in U, \end{cases}$$

is locally Hölder continuous in the same topology (with exponent α). A similar statement holds when $\mathbb{C}^+$ is replaced by $\mathbb{C}^-$.

Finally, the following estimates hold true, for any $\delta > 0$:

$$\left\| R_Q^{\pm}(\lambda) \right\|_{B(\mathcal{X},\mathcal{X}^*)} < C_s\, \lambda^{-\frac{1}{2}}, \quad \lambda > 0,$$
$$\left\| R_Q^{\pm}(\lambda_2) - R_Q^{\pm}(\lambda_1) \right\|_{B(\mathcal{X},\mathcal{X}^*)} \le C_{s,\delta} \left(\lambda_1^{-\frac{1+\alpha}{2}} + \lambda_2^{-\frac{1+\alpha}{2}} \right) |\lambda_2 - \lambda_1|^{\alpha}, \tag{5.26}$$

where $\lambda_1,\, \lambda_2 > \delta > 0$.

Proof. All the statements, except for the estimates (5.26), follow directly from Theorems 3.6 and 3.11, since all the requirements in these theorems are established in the last lemma.

The estimates (5.26) do not follow directly from the estimates (5.25) for the spectral derivative. In fact, in the case of the Stark Hamiltonian the uniform estimates for the spectral derivative (see Lemma 5.6) enabled similar estimates for the limiting values of the resolvent (see Theorem 5.7). However, using the corresponding estimates (5.24) for the spectral derivative here, the estimates for the resolvent should follow from an inspection of the principal value integral in (a suitably modified form of) Eq. (5.10). Indeed, this can be done, but a simpler way would be simply to resort to the well-known resolvent kernel of Q, namely,

$$K_Q(x, y; z) = (2i\sqrt{z})^{-1} \exp(i\sqrt{z}|x - y|), \quad \operatorname{Im} \sqrt{z} \ge 0. \qquad \square$$

We now assume the dimension $n = 2$ and take in (5.23) $H_2 = -\frac{d^2}{dx_2^2}$, $x_2 \in \mathbb{R}$.

We get, for the spectral derivatives A_1, A_2, the estimates (5.24), as well as the resolvent estimates (5.26).

Let $\lambda > 0$. We take a function $\phi \in C^\infty(\mathbb{R})$, $0 \le \phi(\omega) \le 1$ such that $\phi(\omega) = 0$ for $\omega \in \left(-\infty, \frac{\lambda}{3}\right)$ and $\phi(\omega) = 1$ for $\omega \in \left(\frac{2\lambda}{3}, \infty\right)$. Using this function in the proof of Theorem 5.4 and Corollary 5.5 we obtain similar estimates for the spectral derivative and resolvent of H_0. By induction, we conclude:

Theorem 5.12. *Let* $U = \mathbb{R} \setminus \{0\}$ *and* $\mathcal{X}_{H_0}^* = H^{2,-s}(\mathbb{R}^n)$ *for* $s > \frac{1}{2}$. *The limits*

$$R_0^{\pm}(\lambda) = \lim_{\epsilon \downarrow 0} R_0(\lambda \pm i\epsilon), \quad \lambda \in U,$$

exist in the uniform operator topology of $B(\mathcal{X}, \mathcal{X}_{H_0}^*)$, *and the extended operator-valued function*

$$R_0(z) = \begin{cases} R_0(z), & z \in \mathbb{C}^+, \\ R_0^+(z), & z \in U, \end{cases}$$

is locally Hölder continuous in the same topology (with exponent α*). A similar statement holds when* $\mathbb{C}^+$ *is replaced by* $\mathbb{C}^-$.

Finally, for $\mathcal{X}^* = L^{2,-s}(\mathbb{R}^n)$, *the following estimates hold true, for any* $\delta > 0$:

$$\left\| R_0^{\pm}(\lambda) \right\|_{B(\mathcal{X},\mathcal{X}^*)} < C_s\, \lambda^{-\frac{1}{2}}, \quad \lambda > 0,$$
$$\left\| R_0^{\pm}(\lambda_2) - R_0^{\pm}(\lambda_1) \right\|_{B(\mathcal{X},\mathcal{X}^*)} \le C_{s,\delta} \left(\lambda_1^{-\frac{1+\alpha}{2}} + \lambda_2^{-\frac{1+\alpha}{2}} \right) |\lambda_2 - \lambda_1|^{\alpha}, \tag{5.27}$$

where $\lambda_1,\, \lambda_2 > \delta > 0$.

The above estimates blow up as $\lambda \to 0+$. This is because we took an *optimal* weight $s > \frac{1}{2}$. However, as is shown in Proposition 6.4 below, taking $s > 1$ (for dimension $n \geq 3$) we see that the resolvent $R_0(z)$ can be extended continuously from $\mathcal{C}^\pm$ to $\overline{\mathcal{C}^\pm}$, in the respective uniform operator topologies. Certainly the estimates (5.27) continue to hold (for large λ).

It therefore follows that the operator $H_0 = -\Delta$ is of global type $\big(L^{2,s}(\mathbb{R}^3), L^{2,-s}(\mathbb{R}^3), \alpha, \mathbb{R}\big)$ and Theorem 5.1 can be applied to yield the following theorem:

Theorem 5.13. *Let $n \geq 4$ and set $x = (x', x'')$ where $x' = (x_1, x_2, x_3)$ and $x'' = (x_4, \ldots, x_n) \in \mathbb{R}^{n-3}$. Let $H = -\Delta_{x'} + L(x'')$, where $\Delta_{x'}$ is the Laplacian with respect to the three coordinates x' and $L(x'')$ is any (unbounded) self-adjoint operator in $L^2(\mathbb{R}^{n-3})$. Let $R(z) = (H - z)^{-1}$ be the resolvent.*

The resolvent limits

$$R^\pm(\lambda \pm i \cdot 0) = \lim_{\epsilon \downarrow 0} R(\lambda \pm i\epsilon), \quad \lambda \in \mathbb{R},$$

exist, uniformly in $\lambda \in \mathbb{R}$, in the uniform operator topology of $B\big(L^{2,s}(\mathbb{R}^3) \otimes L^2(\mathbb{R}^{n-3}), L^{2,-s}(\mathbb{R}^3) \otimes L^2(\mathbb{R}^{n-3})\big)$, for any $s > 1$. They are also uniformly Hölder continuous in this topology.

Furthermore, these limits exist and are locally Hölder continuous in the uniform operator topology of $B\big(L^{2,s}(\mathbb{R}) \otimes L^2(\mathbb{R}^{n-3}), H^{2,-s}(\mathbb{R}^3) \otimes L^2(\mathbb{R}^{n-3})\big)$.

Remark 5.14 (*wild* perturbations). We have here the same situation as pointed out in Remark 5.14; the specific character of the operator $L(x'')$ in $L^2(\mathbb{R}^{n-3})$ plays no role in the theorem. In the title of this subsection we referred to this fact as *wild* perturbations.

The special case of the Schrödinger operator for the N-body problem was established in [43].

6. The limiting absorption principle for second-order divergence-type operators

In the previous sections we have shown how various constructions, such as functions of operators or short-range perturbations, fit into the general abstract framework. In the following sections we consider *divergence-type* second-order operators. As perturbations of the Laplacian they do not belong to any of the above categories; the difference between such an operator and the Laplacian is not even compact. However, our aim is to show that we can still deal with such operators, starting from the smoothness properties of (the spectral derivative of) the Laplacian.

Let $H = -\sum_{j,k=1}^{n} \partial_j a_{j,k}(x) \partial_k$, where $a_{j,k}(x) = a_{k,j}(x)$, be a formally self-adjoint operator in $L^2(\mathbb{R}^n)$, $n \geq 2$. The notation $\partial_j = \frac{\partial}{\partial x_j}$ is used throughout the following sections.

We assume that the real measurable matrix function $a(x) = \{a_{j,k}(x)\}_{1\le j,k\le n}$ satisfies, with some positive constants $a_1 > a_0 > 0$, $\Lambda_0 > 0$,

$$a_0 I \le a(x) \le a_1 I, \qquad x \in \mathbb{R}^n, \tag{6.1}$$

$$a(x) = I, \qquad |x| > \Lambda_0. \tag{6.2}$$

In what follows we shall use the notation $H = -\nabla \cdot a(x)\nabla$.

We retain the notation H for the self-adjoint (Friedrichs) extension associated with the form $(a(x)\nabla\varphi, \nabla\psi)$, where $(\, , \,)$ is the scalar product in $L^2(\mathbb{R}^n)$. When $a(x) \equiv I$, we get $H = H_0 = -\Delta$.

We refer to Section 2 for definitions of the various functional spaces that will appear in what follows.

Let

$$R_0(z) = (H_0 - z)^{-1}, \;\; R(z) = (H - z)^{-1}, \quad z \in \mathcal{C}^{\pm} = \big\{ z \;\big|\; \pm \operatorname{Im} z > 0 \big\},$$

be the associated resolvent operators.

We note that the operator H can be extended in an obvious way (retaining the same notation) as a bounded operator $H\colon H^1_{\text{loc}} \to H^{-1}_{\text{loc}}$. In particular, $H\colon H^{1,-s} \to H^{-1,-s}$, for all $s \ge 0$. Furthermore, the graph norm of H in $H^{-1,-s}$ is equivalent to the norm of $H^{1,-s}$.

Similarly, we can consider the resolvent $R(z)$ as defined on $L^{2,s}$, $s \ge 0$, where $L^{2,s}$ is densely and continuously embedded in $H^{-1,s}$.

The fundamental result presented in this section is that H satisfies the LAP over the *whole real axis*. The exact formulation is as follows:

Theorem 6.1. *Suppose that* $a(x)$ *satisfies* (6.1), (6.2)*. Then the operator* H *satisfies the* LAP *in* $\mathbb{R}$*. More precisely, let* $s > 1$ *and consider the resolvent* $R(z) = (H - z)^{-1}$, $\operatorname{Im} z \ne 0$, *as a bounded operator from* $L^{2,s}(\mathbb{R}^n)$ *to* $H^{1,-s}(\mathbb{R}^n)$.

Then:

(a) $R(z)$ *is bounded with respect to the* $H^{-1,s}(\mathbb{R}^n)$ *norm. Using the density of* $L^{2,s}$ *in* $H^{-1,s}$*, we can therefore view* $R(z)$ *as a bounded operator from* $H^{-1,s}(\mathbb{R}^n)$ *to* $H^{1,-s}(\mathbb{R}^n)$.

(b) *The operator-valued functions, defined respectively in the lower and upper half-planes,*

$$z \to R(z) \in B(H^{-1,s}(\mathbb{R}^n), H^{1,-s}(\mathbb{R}^n)), \quad s > 1, \pm \operatorname{Im} z > 0, \tag{6.3}$$

can be extended continuously from $\mathcal{C}^{\pm} = \big\{ z \;\big|\; \pm \operatorname{Im} z > 0 \big\}$ *to* $\overline{\mathcal{C}^{\pm}} = \mathcal{C}^{\pm} \bigcup \mathbb{R}$ (*with respect to the uniform operator topology of* $B(H^{-1,s}(\mathbb{R}^n), H^{1,-s}(\mathbb{R}^n))$). *In the case* $n = 2$ *replace* $H^{-1,s}$ *by* $H_0^{-1,s}$.

We denote the limiting values of the resolvent on the real axis by

$$R^{\pm}(\lambda) = \lim_{z \to \lambda, \, \pm \operatorname{Im} z > 0} R(z). \tag{6.4}$$

Remark 6.2. Since $L^{2,s}$ (resp. $H^{1,-s}$) is densely and continuously embedded in $H^{-1,s}$ (resp. $L^{2,-s}$), we conclude that the resolvents $R_0(z)$, $R(z)$ can be extended continuously to $\overline{\mathcal{C}^{\pm}}$ in the $B(L^{2,s}(\mathbb{R}^n), L^{2,-s}(\mathbb{R}^n))$ uniform operator topology.

The spectrum of H is therefore entirely absolutely continuous. In particular, it follows that the limiting values $R^{\pm}(\lambda)$ are continuous at $\lambda = 0$ and H has no resonance there.

The study of the resolvent near the threshold $\lambda = 0$ is sometimes referred to as *low energy estimates*. Following the proof of the theorem, at the end of Subsection 6.2, we review some of the existing literature concerning such estimates, as well as some other results pertaining to the LAP in *non short-range* settings.

Before proceeding to the proof of the theorem, we need to obtain more information on the resolvent of the Laplacian.

6.1. The operator $H_0 = -\Delta$ – revisited

The basic properties of this operator have already been discussed in Example 3.5 and Corollary 3.9. In particular, the explicit form of $\{E_0(\lambda)\}$, its spectral family, is given in Eq. (3.1), and the spectral derivative A_0 is given explicitly in Eq. (3.3). See also the treatment by sums of tensor products in Subsection 5.5.

The weighted L^2 estimates for A_0 were obtained by using the trace estimate (3.2).

However, we can refine this estimate near $\lambda = 0$ as follows.

Proposition 6.3. *Let $\frac{1}{2} < s < \frac{3}{2}$, $h \in L^{2,s}$. For $n = 2$ assume further that $s > 1$ and $h \in L_0^{2,s}$. Then*

$$\int\limits_{|\xi|^2=\lambda} |\hat{h}|^2 \, d\tau \leq C \min\{\lambda^\gamma, 1\} \|\hat{h}\|_{H^s}^2, \tag{6.5}$$

where

$$\begin{aligned} 0 < \gamma = s - \frac{1}{2}, \quad n \geq 3, \\ 0 < \gamma < s - \frac{1}{2}, \quad n = 2, \end{aligned} \tag{6.6}$$

and $C = C(s, \gamma, n)$.

Proof. If $n \geq 3$, the proof follows as in [19, Appendix], when we take into account the fact (*generalized Hardy inequality*) that multiplication by $|\xi|^{-s}$ is bounded from H^s into L^2 [45] (see also [64, Section 9.4]).

If $n = 2$ and $1 < s < \frac{3}{2}$ we have, for $h \in L_0^{2,s}$,

$$|\hat{h}(\xi)| = |\hat{h}(\xi) - \hat{h}(0)| \leq C_{s,\delta} \, |\xi|^\delta \, \|\hat{h}\|_{H^s},$$

for any $0 < \delta < \min\{1, s-1\}$. Using this estimate in the integral in the right-hand side of (6.5), the claim follows also in this case. □

Combining Eqs. (3.3),(3.2) and (6.5), we conclude that

$$\begin{aligned} |\langle A_0(\lambda)f, g\rangle| &\leq \langle A_0(\lambda)f, f\rangle^{\frac{1}{2}} \, \langle A_0(\lambda)g, g\rangle^{\frac{1}{2}} \\ &\leq C \min\{\lambda^{-\frac{1}{2}}, \lambda^\eta\} \, \|f\|_{0,s} \, \|g\|_{0,\sigma}, \quad f \in L^{2,s}, \, g \in L^{2,\sigma}, \end{aligned} \tag{6.7}$$

where

$$\text{(i)}\quad n \geq 3, \quad \frac{1}{2} < s, \sigma < \frac{3}{2}, \quad s+\sigma > 2 \quad \text{and} \quad 0 < 2\eta = s+\sigma-2,$$

or (6.8)

$$\text{(ii)}\quad n = 2, \quad 1 < s < \frac{3}{2}, \quad \frac{1}{2} < \sigma < \frac{3}{2}, \quad s+\sigma > 2, \quad 0 < 2\eta < s+\sigma-2 \quad \text{and} \quad \hat{f}(0) = 0.$$

In both cases, $A_0(\lambda)$ is Hölder continuous and vanishes at $0, \infty$, so we obtain as in [15]:

Proposition 6.4. *The operator-valued function*

$$z \to R_0(z) \in \begin{cases} B(L^{2,s}, L^{2,-\sigma}), & n \geq 3, \\ B(L_0^{2,s}, L^{2,-\sigma}), & n = 2, \end{cases} \tag{6.9}$$

where s, σ satisfy (6.8), *can be extended continuously from $\mathcal{C}^{\pm}$ to $\overline{\mathcal{C}^{\pm}}$, in the respective uniform operator topologies.*

Remark 6.5. We note that the conditions (6.8) yield the continuity of $A_0(\lambda)$ *across the threshold* $\lambda = 0$ and hence the continuity property of the resolvent as in Proposition 6.4. However, for the local continuity at any $\lambda_0 > 0$, it suffices to take $s, \sigma > \frac{1}{2}$, as has been stated in Theorem 5.12, which is Agmon's original result [1].

This remark applies equally to the statements below, where the resolvent is considered in other functional settings.

We shall now extend this proposition to more general function spaces. Let $g \in H^{1,\sigma}$, where s, σ satisfy (6.8). Let $f \in H^{-1,s}$ have a representation of the form (2.2). Eq. (3.3) can be extended to yield an operator (for which we retain the same notation)

$$A_0(\lambda) \in B(H^{-1,s}, H^{-1,-\sigma}),$$

defined by (where now $\langle\ ,\ \rangle$ is used for the $(H^{-1,s}, H^{1,\sigma})$ pairing),

$$\left\langle A_0(\lambda)\left[f_0 + i^{-1}\sum_{k=1}^{n}\frac{\partial}{\partial x_k}f_k\right], g\right\rangle = (2\sqrt{\lambda})^{-1}\int_{|\xi|^2=\lambda}\left[\hat{f}_0(\xi) + \sum_{k=1}^{n}\xi_k\hat{f}_k(\xi)\right]\overline{\hat{g}(\xi)}\,d\tau, \quad f \in H^{-1,s},\ g \in H^{1,\sigma}. \tag{6.10}$$

(replace $H^{-1,s}$ by $H_0^{-1,s}$ if $n = 2$).

Observe that this definition makes good sense even though the representation (2.2) is not unique, since

$$f = f_0 + \sum_{k=1}^{n} i^{-1}\frac{\partial}{\partial x_k}f_k = \tilde{f}_0 + \sum_{k=1}^{n} i^{-1}\frac{\partial}{\partial x_k}\tilde{f}_k,$$

implies

$$\hat{f}_0(\xi) + \sum_{k=1}^{n} \xi_k \hat{f}_k(\xi) = \hat{\hat{f}}_0(\xi) + \sum_{k=1}^{n} \xi_k \hat{\hat{f}}_k(\xi)$$

(as tempered distributions).

To estimate the operator-norm of $A_0(\lambda)$ in this setting we use (6.10) and the considerations preceding Proposition 6.4, to obtain, instead of (6.7), for $k = 1, 2, \ldots, n$,

$$\begin{aligned} &\left| \left\langle A_0(\lambda) \frac{\partial}{\partial x_k} f_k, g \right\rangle \right| \\ &\qquad \le C \min\{\lambda^{-\frac{1}{2}}, \lambda^{\eta}\} \, \|f\|_{-1,s} \, \|g\|_{1,\sigma}, \quad f \in H^{-1,s}, \, g \in H^{1,\sigma}, \end{aligned} \tag{6.11}$$

where s, σ satisfy (6.8) (replace $H^{-1,s}$ by $H_0^{-1,s}$ if $n = 2$).

We now define the extension of the resolvent operator by

$$R_0(z) = \int_0^{\infty} \frac{A_0(\lambda)}{\lambda - z} \, d\lambda, \quad \operatorname{Im} z \neq 0. \tag{6.12}$$

The convergence of the integral (in the operator norm) follows from the estimate (6.11).

The LAP in this case is given in the following proposition.

Proposition 6.6. *The operator-valued function $R_0(z)$ is well defined (and analytic) for non-real z in the following functional setting.*

$$z \to R_0(z) \in \begin{cases} B(H^{-1,s}, H^{1,-\sigma}), & n \ge 3, \\ B(H_0^{-1,s}, H^{1,-\sigma}), & n = 2, \end{cases} \tag{6.13}$$

where s, σ satisfy (6.8). Furthermore, it can be extended continuously from $\mathcal{C}^{\pm}$ to $\overline{\mathcal{C}^{\pm}}$, in the respective uniform operator topologies. The limiting values are denoted by $R_0^{\pm}(\lambda)$.

The extended function satisfies

$$(H_0 - z) \, R_0(z) f = f, \quad f \in H^{-1,s}, \, z \in \overline{\mathcal{C}^{\pm}}, \tag{6.14}$$

where for $z = \lambda \in \mathbb{R}$, $R_0(z) = R_0^{\pm}(\lambda)$.

Proof. For simplicity we assume $n \ge 3$. By Definition (6.12) and estimate (6.11), we get readily $R_0(z) \in B(H^{-1,s}, H^{-1,-\sigma})$ if $\operatorname{Im} z \neq 0$ as well as the analyticity of the map $z \to R_0(z)$, $\operatorname{Im} z \neq 0$. Furthermore, the extension to $\operatorname{Im} z = 0$ is carried out as in [15].

Eq. (6.14) is obvious if $\operatorname{Im} z \neq 0$ and $f \in L^{2,s}$. By the density of $L^{2,s}$ in $H^{-1,s}$, the continuity of $R_0(z)$ on $H^{-1,s}$ and the continuity of $H_0 - z$ (in the sense of distributions) we can extend it to all $f \in H^{-1,s}$.

As $z \to \lambda \pm i \cdot 0$ we have $R_0(z) f \to R_0^{\pm}(\lambda) f$ in $H^{-1,-\sigma}$. Applying the (constant coefficient) operator $H_0 - z$ yields, in the sense of distributions, $f = (H_0 - z) \, R_0(z) f \to (H_0 - \lambda) \, R_0^{\pm}(\lambda) f$ which establishes (6.14) also for $\operatorname{Im} z = 0$.

Finally, the established continuity of $z \to R_0(z) \in B(H^{-1,s}, H^{-1,-\sigma})$ (up to the real boundary) and Eq. (6.14) imply the continuity of the map $z \to H_0\, R_0(z) \in B(H^{-1,s}, H^{-1,-\sigma})$.

The stronger continuity claim (6.13) follows, since the norm of $H^{1,-\sigma}$ is equivalent to the graph norm of H_0 as a map of $H^{-1,-\sigma}$ to itself. □

Remark 6.7. The main point here is the fact that the limiting values can be extended continuously to the threshold at $\lambda = 0$.

In the neighborhood of any $\lambda > 0$ this proposition follows from [79, Theorem 2.3], where a very different proof is used. In fact, using the terminology there, the limit functions $R_0^{\pm}(\lambda)f$ are the unique (on either side of the positive real axis) radiative functions and they satisfy a suitable *Sommerfeld radiation condition*. We recall it here for the sake of completeness, since we will need it in the next section.

Let $z = k^2 \in \mathcal{C} \setminus \{0\}$, $\operatorname{Im} k \geq 0$. For $f \in H^{-1,s}$ let $u = R_0(z)f \in H^{1,-\sigma}$ be as defined above. Then

$$\mathcal{R}u = \int\limits_{|x|>\Lambda_0} \left| r^{-\frac{n-1}{2}} \frac{\partial}{\partial r}\left(r^{\frac{n-1}{2}} u\right) - iku \right|^2 dx < \infty, \tag{6.15}$$

where $r = |x|$. We shall refer to $\mathcal{R}u$ as the radiative norm of u.

Furthermore, we can take $s,\, \sigma > \frac{1}{2}$, as in Remark 6.5.

6.2. Proof of the LAP for the operator *H*

We start with some considerations regarding the behavior of the resolvent near the spectrum.

Fix $[\alpha, \beta] \subset \mathbb{R}$ and let

$$\Omega = \left\{ z \in \mathcal{C}^+ \;\middle|\; \alpha < \operatorname{Re} z < \beta,\, 0 < \operatorname{Im} z < 1 \right\}. \tag{6.16}$$

Let $z = \mu + i\varepsilon \in \Omega$ and consider the equation

$$(H - z)\, u = f \in H^{-1,s}, \quad u \in H^{1,-\sigma} \ (f \in H_0^{-1,s} \text{ if } n = 2). \tag{6.17}$$

(Observe that in the case $n = 2$ also $u \in L_0^{2,\sigma}$).

With Λ_0 as in (6.2), let $\chi(x) \in C^\infty(\mathbb{R}^n)$ be such that

$$\chi(x) = \begin{cases} 0, & |x| < \Lambda_0 + 1, \\ 1, & |x| > \Lambda_0 + 2. \end{cases} \tag{6.18}$$

Eq. (6.17) can be written as

$$(H_0 - z)\,(\chi u) = \chi f - 2\nabla\chi \cdot \nabla u - u\Delta\chi. \tag{6.19}$$

Letting $\psi(x) = 1 - \chi(\frac{x}{2}) \in C_0^\infty(\mathbb{R}^n)$ and using Proposition 6.6 and standard elliptic estimates, we obtain from (6.19)

$$\|u\|_{1,-\sigma} \leq C \left[\|f\|_{-1,s} + \|\psi u\|_{0,-s} \right], \tag{6.20}$$

where s, σ satisfy (6.8), $\sigma' > \sigma$ and $C > 0$ depends only on Λ_0, σ, s, n.

We note that, since ψ is compactly supported, the term $\|\psi u\|_{0,-s}$ can be replaced by $\|\psi u\|_{0,-s'}$ for any real s'.

In fact, the second term in the right-hand side can be dispensed with, as is demonstrated in the following proposition.

Proposition 6.8. *The solution to* (6.17) *satisfies,*

$$\|u\|_{1,-\sigma} \leq C\,\|f\|_{-1,s}\,, \tag{6.21}$$

where s, σ satisfy (6.8) *and $C > 0$ depends only on σ, s, n, Λ_0.*

Proof. In view of (6.20) we only need to show that

$$\|\psi u\|_{0,-s} \leq C\,\|f\|_{-1,s}\,. \tag{6.22}$$

Since $L^{2,s}(\mathbb{R}^n)$ is dense in $H^{-1,s}(\mathbb{R}^n)$, it suffices to prove this inequality for $f \in L^{2,s}(\mathbb{R}^n) \cap H^{-1,s}(\mathbb{R}^n)$ (using the norm of $H^{-1,s}$).

We argue by contradiction. Let

$$\{z_k\}_{k=1}^{\infty} \subseteq \Omega, \quad \{f_k\}_{k=1}^{\infty} \subseteq L^{2,s}(\mathbb{R}^n) \cap H^{-1,s}(\mathbb{R}^n)$$

(with $\hat{f}_k(0) = 0$ if $n = 2$) and

$$\{u_k = R(z_k) f_k\}_{k=1}^{\infty} \subseteq H^{1,-\sigma}(\mathbb{R}^n)$$

be such that

$$\begin{gathered} \|\psi u_k\|_{0,-s} = 1, \quad \|f_k\|_{-1,s} \leq k^{-1}, \quad k = 1, 2, \ldots, \\ z_k \to z_0 \in \overline{\Omega} \quad \text{as } k \to \infty. \end{gathered} \tag{6.23}$$

By (6.20), $\{u_k\}_{k=1}^{\infty}$ is bounded in $H^{1,-\sigma}$. Replacing the sequence by a suitable subsequence (without changing notation) and using the Rellich compactness theorem we may assume that there exists a function $u \in L^{2,-\sigma'}$, $\sigma' > \sigma$, such that

$$u_k \to u \quad \text{in } L^{2,-\sigma'} \text{ as } k \to \infty. \tag{6.24}$$

Furthermore, by weak compactness we actually have (restricting again to a subsequence if needed)

$$u_k \xrightarrow{w} u \quad \text{in } H^{1,-\sigma} \text{ as } k \to \infty. \tag{6.25}$$

Since H maps continuously $H^{1,-\sigma}$ into $H^{-1,-\sigma}$, we have

$$Hu_k \xrightarrow{w} Hu \quad \text{in } H^{-1,-\sigma} \text{ as } k \to \infty,$$

so that from $(H - z_k)\,u_k = f_k$ we infer that

$$(H - z_0)\,u = 0. \tag{6.26}$$

In view of (6.19) and Remark 6.7 the functions χu_k are *radiative functions*. Since they are uniformly bounded in $H^{1,-\sigma}$, their *radiative norms* (6.15) are uniformly bounded.

Suppose first that $z_0 \neq 0$. In view of Remark 6.7 we can take s, $\sigma > \frac{1}{2}$. Then the limit function u is a radiative solution to $(H_0 - z_0)\,u = 0$ in $|x| > \Lambda_0 + 2$ and hence must vanish there (see [79]). By the unique continuation property of solutions to (6.26) we conclude that $u \equiv 0$. Thus by (6.24) we get $\|\psi u_k\|_{0,-\sigma'} \to 0$ as $k \to \infty$, which contradicts (6.23).

We are therefore left with the case $z_0 = 0$. In this case $u \in H^{1,-\sigma}$ satisfies the equation

$$\nabla \cdot (a(x)\nabla u) = 0. \tag{6.27}$$

In particular, $\Delta u = 0$ in $|x| > \Lambda_0$ and

$$\int_{\Lambda_0}^{\infty} \int_{|x|=r} r^{-2\sigma} \left(|u|^2 + |\frac{\partial u}{\partial r}|^2 \right) d\tau dr < \infty. \tag{6.28}$$

Consider first the case $n \geq 3$. We may then use the representation of u by spherical harmonics so that, with $x = r\omega$, $\omega \in S^{n-1}$,

$$u(x) = r^{-\frac{n-1}{2}} \left\{ \sum_{j=0}^{\infty} b_j r^{\mu_j} h_j(\omega) + \sum_{j=0}^{\infty} c_j r^{-\nu_j} h_j(\omega) \right\}, \quad r > \Lambda_0, \tag{6.29}$$

where

$$\mu_j(\mu_j - 1) = \nu_j(\nu_j + 1) = \lambda_j + \frac{(n-1)(n-3)}{4}, \tag{6.30}$$
$$0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \cdots$$

being the eigenvalues of the Laplace-Beltrami operator on S^{n-1}, and $h_j(\omega)$ the corresponding spherical harmonics. Since $\lambda_1 = n - 1$, it follows that

$$\mu_0 = \frac{n-1}{2}, \quad \mu_0 + 1 \leq \mu_1 \leq \mu_2 \leq \cdots, \quad \frac{n-3}{2} = \nu_0 < \nu_1 \leq \nu_2 \leq \cdots . \tag{6.31}$$

We now observe that (6.28) forces

$$b_0 = b_1 = \cdots = 0.$$

Also, by (6.29)

$$\int_{|x|=r} \frac{\partial u}{\partial r} d\tau = -(n-2)\left|S^{n-1}\right| c_0, \quad r > \Lambda_0, \tag{6.32}$$

($\left|S^{n-1}\right|$ is the surface measure of S^{n-1}), while integrating (6.27) we get

$$\int_{|x|=r} \frac{\partial u}{\partial r} d\tau = 0, \quad r > \Lambda_0. \tag{6.33}$$

Thus $c_0 = 0$. It now follows from (6.29) that, for $r > \Lambda_0$,

$$\int_{|x|=r} \left(|u|^2 + \left|\frac{\partial u}{\partial r}\right|^2 \right) d\tau \leq \left(\frac{r}{\Lambda_0}\right)^{-2\nu_1} \int_{|x|=\Lambda_0} \left(|u|^2 + \left|\frac{\partial u}{\partial r}\right|^2 \right) d\tau. \tag{6.34}$$

Multiplying (6.27) by $\overline{u}$ and integrating by parts over the ball $|x| \leq r$, we infer from (6.34) that the boundary term vanishes as $r \to \infty$. Thus $\nabla u \equiv 0$, in contradiction to (6.23)–(6.24).

It remains to deal with the case $n = 2$. Instead of (6.29) we now have

$$u(x) = r^{-\frac{1}{2}} \left\{ \widetilde{b_0} r^{\frac{1}{2}} \log r + \sum_{j=0}^{\infty} b_j r^{\mu_j} h_j(\omega) + \sum_{j=1}^{\infty} c_j r^{-\nu_j} h_j(\omega) \right\}, \quad r > \Lambda_0, \quad (6.35)$$

where $\mu_0 = \frac{1}{2}$, $\mu_1 = \frac{3}{2}$, $\nu_1 = \frac{1}{2}$. As in the derivation above, the condition (6.28) yields $b_0 = b_1 = \cdots = 0$. Also, we get $\widetilde{b_0} = 0$ in view of (6.33). It now follows that

$$\int\limits_{|x|=r} \overline{u} \frac{\partial u}{\partial r} d\tau = -2\pi \sum_{j=1}^{\infty} \left(\nu_j + \frac{1}{2} \right) |c_j|^2 r^{-2\nu_j - 1}, \quad r \geq \Lambda_0, \qquad (6.36)$$

from which, as in the argument following (6.34), we deduce that $u \equiv 0$, again in contradiction to (6.23)–(6.24). □

Proof of Theorem 6.1. Part (a) of the theorem is actually covered by Proposition 6.8. Moreover, the proposition implies that the operator-valued function

$$z \to R(z) \in B(H^{-1,s}(\mathbb{R}^n), H^{1,-\sigma}(\mathbb{R}^n)), \quad s > 1,\, z \in \Omega,$$

is uniformly bounded, where s, σ satisfy (6.8). Here and below replace $H^{-1,s}$ by $H_0^{-1,s}$ if $n = 2$.

We next show that the function $z \to R(z)$ can be continuously extended to $\overline{\Omega}$ in the *weak topology* of $B(H^{-1,s}(\mathbb{R}^n), H^{1,-\sigma}(\mathbb{R}^n))$. To this end, we take $f \in H^{-1,s}(\mathbb{R}^n)$ and $g \in H^{-1,\sigma}(\mathbb{R}^n)$ and consider the function

$$z \to \langle g, R(z)f \rangle, \quad z \in \Omega,$$

where $\langle \,,\, \rangle$ is the $(H^{-1,\sigma}, H^{1,-\sigma})$ pairing. We need to show that it can be extended continuously to $\overline{\Omega}$.

In view of the uniform boundedness established in Proposition 6.8, we can take f, g in dense sets (of the respective spaces). In particular, we can take $f \in L^{2,s}(\mathbb{R}^n)$ and $g \in L^{2,\sigma}(\mathbb{R}^n)$, so that the continuity property in Ω is obvious.

Consider therefore a sequence $\{z_k\}_{k=1}^{\infty} \subseteq \Omega$ such that $z_k \xrightarrow[k \to \infty]{} z_0 \in [\alpha, \beta]$. The sequence $\{u_k = R(z_k)f\}_{k=1}^{\infty}$ is bounded in $H^{1,-\sigma}(\mathbb{R}^n)$. Therefore there exists a subsequence $\{u_{k_j}\}_{j=1}^{\infty}$ which converges to a function $u \in L^{2,-\sigma'}$, $\sigma' > \sigma$.

We can further assume that $u_{k_j} \xrightarrow[j \to \infty]{w} u$ in $H^{1,-\sigma}$. It follows that

$$\langle g, u_{k_j} \rangle \xrightarrow[j \to \infty]{} \langle g, u \rangle .$$

Passing to the limit in $(H - z_{k_j})\, u_{k_j} = f$ we see that the limit function function satisfies

$$(H - z_0)\, u = f.$$

We now repeat the argument employed in the proof of Proposition 6.8. If $z_0 \neq 0$ we note that the functions $\{\chi u_k\}_{k=1}^{\infty}$ are radiative functions with uniformly bounded *radiative norms* (6.15) in $|x| > \Lambda_0 + 2$. The same is therefore true for the limit function u.

If $z_0 = 0$, then the function $u \in H^{1,-\sigma}$ solves $Hu = f$.

In both cases this function is unique and we get the convergence

$$\langle g, R(z_k)f\rangle = \langle g, u_k\rangle \xrightarrow[k\to\infty]{} \langle g, u\rangle .$$

We can now define

$$R^+(z_0)f = u, \tag{6.37}$$

with an analogous definition for $R^-(z_0)$.

At this point we can readily deduce the following extension of the resolvent $R(z)$ as the inverse of $H - z$.

$$(H - z)\, R(z)f = f, \quad f \in H^{-1,s},\, z \in \overline{\mathcal{C}^{\pm}}, \tag{6.38}$$

where $R(z) = R^{\pm}(\lambda)$ when $z = \lambda \in \mathbb{R}$.

Indeed, observe that if $\operatorname{Im} z \neq 0$ then $(H - z)R(z)f = f$ for $f \in L^{2,s}(\mathbb{R}^n)$ and $(H - z)R(z) \in B(H^{-1,s}, H^{-1,-\sigma})$, so the assertion follows from the density of $L^{2,s}(\mathbb{R}^n)$ in $H^{-1,s}(\mathbb{R}^n)$. For $z = \lambda \in \mathbb{R}$ we use the (just established) weak continuity of the map $z \hookrightarrow (H - z)R(z)$ from $H^{-1,s}$ into $H^{-1,-\sigma}$ in $\overline{\mathcal{C}^{\pm}}$.

The passage *from weak to uniform continuity* (in the operator topology) is a classical argument due to Agmon [1]. In [9] we have applied it in the case $n = 1$. Here we outline the proof in the case $n > 1$.

We establish first the continuity of the operator-valued function $z \to R(z)$, $\overline{\Omega}$, in the *uniform operator topology* of $B(H^{-1,s}(\mathbb{R}^n), L^{2,-\sigma}(\mathbb{R}^n))$.

Let $\{z_k\}_{k=1}^{\infty} \subseteq \overline{\Omega}$ and $\{f_k\}_{k=1}^{\infty} \subseteq H^{-1,s}(\mathbb{R}^n)$ be sequences such that $z_k \xrightarrow[k\to\infty]{} z \in \overline{\Omega}$ and f_k converges weakly to f in $H^{-1,s}(\mathbb{R}^n)$. It suffices to prove that the sequence $u_k = R(z_k)f_k$, which is bounded in $H^{1,-\sigma}(\mathbb{R}^n)$, converges strongly in $L^{2,-\sigma}(\mathbb{R}^n)$. Since this is clear if $\operatorname{Im} z \neq 0$, we can take $z \in [\alpha, \beta]$.

Note first that we can take $\frac{1}{2} < \sigma' < \sigma$ so that s, σ' satisfy (6.8). Then the sequence $\{u_k\}_{k=1}^{\infty}$ is bounded in $H^{1,-\sigma'}(\mathbb{R}^n)$ and there exists a subsequence $\{u_{k_j}\}_{j=1}^{\infty}$ which converges to a function $u \in L^{2,-\sigma}$.

We can further assume that $u_{k_j} \xrightarrow[j\to\infty]{w} u$ in $H^{1,-\sigma}$.

It follows that the limit function function satisfies (see Eq. (6.38))

$$(H - z)\, u = f.$$

Once again we consider separately the cases $z \neq 0$ and $z = 0$.

In the first case, in view of (6.38) and Remark 6.7, the functions χu_k are *radiative functions*. Since they are uniformly bounded in $H^{1,-\sigma}$ their *radiative norms* (6.15) are uniformly bounded, and we conclude that also $\mathcal{R}u < \infty$.

In the second case, we simply note that $u \in H^{1,-\sigma}$ solves $Hu = f$.

As in the proof of Proposition 6.8 we conclude that in both cases the limit is unique, so that the whole sequence $\{u_k\}_{k=1}^{\infty}$ converges to u in $L^{2,-\sigma}(\mathbb{R}^n)$.

Thus, the continuity in the uniform operator topology of $B(H^{-1,s}(\mathbb{R}^n), L^{2,-\sigma}(\mathbb{R}^n))$ is proved.

Finally, we claim that the operator-valued function $z \to R(z)$ is continuous in the *uniform operator topology* of $B(H^{-1,s}(\mathbb{R}^n), H^{1,-\sigma}(\mathbb{R}^n))$. Indeed, if we invoke Eq. (6.38), we get that also $z \to HR(z)$ is continuous in the uniform operator topology of $B(H^{-1,s}(\mathbb{R}^n), H^{-1,-\sigma}(\mathbb{R}^n))$.

Since the domain of H in $H^{-1,-\sigma}(\mathbb{R}^n)$ is $H^{1,-\sigma}(\mathbb{R}^n)$, the claim follows. The conclusion of the theorem follows by taking $\sigma = s$. □

Remark 6.9. In view of (6.19) and Remark 6.7 it follows that for $\lambda > 0$ the functions $R^{\pm}(\lambda)f$, $f \in H^{-1,s}$, are *radiative*, i.e., satisfy a Sommerfeld radiation condition.

The fact that the limiting values of the resolvent are continuous across the threshold at $\lambda = 0$ has been established in the case $H = H_0$ [14, Appendix A], and in the one-dimensional case ($n = 1$) in [9, 12, 30]. The paper [74] deals with the two-dimensional ($n = 2$) case, but the resolvent $R(z)$ is restricted to continuous compactly supported functions f, thus enabling the use of pointwise decay estimates of $R(z)f$ at infinity. In the case of the closely related *acoustic propagator*, where the matrix $a(x) = b(x_1)I$ is scalar and dependent on a single coordinate, there are in general countably many thresholds embedded in the continuous spectrum. Any study of the LAP must therefore deal with this difficulty. We mention here the papers [12, 24, 23, 39, 32, 34, 57, 58, 63, 85], as well as the *anisotropic* case where $b(x_1)$ is a general positive matrix [13].

We mention next some related studies concerning the LAP where, however, the threshold has been avoided. Our discussion is restricted, however, to operators that can be characterized as "perturbations of the Laplacian". The extensive literature concerning the N-body operators is omitted, apart from the monographs [4, 36] that have already been mentioned in the Introduction in connection with Mourre's approach to the LAP.

The pioneering works of Eidus and Agmon have already been mentioned in the Introduction. Under assumptions close to ours here (but also assuming that $a(x)$ is continuously differentiable) a weaker version (roughly, *strong* instead of *uniform* convergence of the resolvents) was obtained by Eidus [40, Theorem 4 and Remark 1]. For $H = H_0$ the LAP has been established by Agmon [1]. Indeed, it was established for operators of the type $H_0 + V$, where V is a short-range perturbation. The short-range potential V was later replaced by a long-range or Stark-like potential [53, 6], a potential in $L^p(\mathbb{R}^n)$ [44, 55], a potential depending only on direction $x/|x|$ [46] and a perturbation of such a potential [71, 72]. In these latter cases the condition $\alpha > 0$ is replaced by $\alpha > \limsup_{|x|\to\infty} V(x)$.

We refer to [20] for the LAP for operators of the type $f(-\Delta)+V$ for a certain class of functions f.

We refer to [76] and references therein for the case of perturbations of the Laplace-Beltrami operator Δ_g on noncompact manifolds. The LAP (still in $(0,\infty)$) holds under the assumption that g is a smooth metric on $\mathbb{R}^n$ that vanishes at infinity. We make use of this result in the proof of Theorem 8.1 (see Section 8).

The LAP for the periodic case (namely, $a(x)$ is symmetric and periodic) has recently been established in [69]. Note that in this case the spectrum is absolutely continuous and consists of a union of intervals (*bands*).

6.3. An application: Existence and completeness of the wave operators $W_\pm(H, H_0)$

A nice consequence of Theorem 6.1 is the existence and completeness of the wave operators. We recall first the definition [59, Chapter X].

Consider the family of unitary operators

$$W(t) = \exp(itH)\exp(-itH_0), \quad -\infty < t < \infty.$$

The strong limits $W_\pm(H, H_0) = s\text{-}\lim_{t\to\pm\infty} W(t)$, if they exist, are called the *wave operators* (relating H, H_0). They are clearly isometries. If their ranges are equal, we say that they are *complete*.

Using a well-known theorem of Kato and Kuroda [61], we have the following corollary.

Corollary 6.10. *The wave operators $W_\pm(H, H_0)$ exist and are complete.*

Indeed, all that is needed is that H, H_0 satisfy the LAP in $\mathbb{R}$, with respect to the same operator topologies.

We refer to [54], where the existence and completeness of the wave operators $W_\pm(H, H_0)$ is established under suitable smoothness assumptions on $a(x)$. (However, $a(x) - I$ is not assumed to be compactly supported and H can include also magnetic and electric potentials.)

7. An eigenfunction expansion theorem

In the Introduction we mentioned the connection (as well as the *gap*) between the spectral theorem (for self-adjoint operators) in its functional-analytic formulation and the *generalized eigenfunction theorem*, a fundamental tool in the study of partial differential operators (and scattering theory). It was mentioned there that these theorems should be connected through the Limiting Absorption Principle. This is indeed the purpose of this section.

We derive an eigenfunction expansion theorem for a divergence-type operator H, the operator considered in Section 6.

Let $\{E(\lambda),\ \lambda \in \mathbb{R}\}$ be the spectral family associated with H and $A(\lambda) = \frac{d}{d\lambda}E(\lambda)$ be its weak derivative. We use the formula (3.7),

$$A(\lambda) = \frac{1}{2\pi i}\lim_{\epsilon\downarrow 0}\left(R(\lambda + i\epsilon) - R(\lambda - i\epsilon)\right) = \frac{1}{2\pi i}\left(R^+(\lambda) - R^-(\lambda)\right).$$

By Theorem 6.1 we know that $A(\lambda) \in B(L^{2,s}(\mathbb{R}^n), L^{2,-s}(\mathbb{R}^n))$, for values of s as given in the theorem.

The formal relation $(H - \lambda)\,A(\lambda) = 0$ can be given a rigorous meaning if, for example, we can find a bounded operator T such that $T^*A(\lambda)T$ is bounded in $L^2(\mathbb{R}^n)$ and has a complete set (necessarily at most countable) of eigenvectors. These will serve as *generalized eigenvectors* for H. We refer to [22, Chapters V, VI] and [25] for a development of this approach for self-adjoint elliptic operators. Note that by this approach we have at most a countable number of such generalized eigenvectors for any fixed λ. In the case of $H_0 = -\Delta$ they correspond to

$$|x|^{-\frac{n-3}{2}} J_{\sqrt{\kappa_j}}\big(\sqrt{\lambda}\,|x|\big)\psi_j(\omega),$$

where $\kappa_j = \lambda_j + \frac{(n-1)(n-3)}{4}$, λ_j being the jth eigenvalue of the Laplace-Beltrami operator on the unit sphere S^{n-1}, ψ_j the corresponding eigenfunction and J_ν is the Bessel function of order ν.

On the other hand, the inverse Fourier transform

$$g(x) = (2\pi)^{-\frac{n}{2}} \int\limits_{\mathbb{R}^n} \hat{g}(\xi) e^{i\xi x}\, d\xi, \tag{7.1}$$

can be viewed as expressing a function in terms of the *generalized eigenfunctions* $\exp(i\xi x)$ of H_0. Observe that now there is a continuum of such functions corresponding to $\lambda > 0$, namely, $|\xi|^2 = \lambda$.

From the physical point-of-view this expansion in terms of *plane waves* proves to be more useful for many applications. In particular, replacing $-\Delta$ by the Schrödinger operator $-\Delta + V(x)$ one can expect, under certain hypotheses on the potential V, a similar expansion in terms of *distorted plane waves*. This has been accomplished, in increasing order of generality (more specifically, decay assumptions on $V(x)$ as $|x| \to \infty$) in [73, 52, 1, 79, 2]. See also [87] for an eigenfunction expansion for relativistic Schrödinger operators.

Here we use the LAP result of Theorem 6.1 in order to derive a similar expansion for the operator H. In fact, our generalized eigenfunctions are given by the following definition.

Definition 7.1. For every $\xi \in \mathbb{R}^n$, let

$$\begin{aligned}\psi_\pm(x,\xi) &= -R^\mp\left(|\xi|^2\right)\big((H - |\xi|^2)\exp(i\xi x)\big)\\ &= R^\mp(|\xi|^2)\left(\sum_{l,j=1}^n \partial_l(a_{l,j}(x) - \delta_{l,j})\partial_j\right)\exp(i\xi x).\end{aligned} \tag{7.2}$$

The *generalized eigenfunctions* of H are defined by

$$\varphi_\pm(x,\xi) = \exp(i\xi x) + \psi_\pm(x,\xi). \tag{7.3}$$

We assume $n \geq 3$ in order to simplify the statement of the theorem. As we show below (see Proposition 7.3) the generalized eigenfunctions are (at least) continuous in x, so that the integral in the statement makes sense.

Theorem 7.2. *Suppose that $n \geq 3$ and that $a(x)$ satisfies* (6.1), (6.2). *For any compactly supported $f \in L^2(\mathbb{R}^n)$ define*

$$(\mathbb{F}_{\pm} f)(\xi) = (2\pi)^{-\frac{n}{2}} \int\limits_{\mathbb{R}^n} f(x)\overline{\varphi_{\pm}(x,\xi)}\, dx, \quad \xi \in \mathbb{R}^n. \tag{7.4}$$

Then the transformations $\mathbb{F}_{\pm}$ can be extended as unitary transformations (for which we retain the same notation) of $L^2(\mathbb{R}^n)$ onto itself. Furthermore, these transformations diagonalize H in the following sense:

$f \in L^2(\mathbb{R}^n)$ is in the domain $D(H)$ if and only if $|\xi|^2(\mathbb{F}_{\pm} f)(\xi) \in L^2(\mathbb{R}^n)$ and

$$H = \mathbb{F}_{\pm}^* M_{|\xi|^2} \mathbb{F}_{\pm}, \tag{7.5}$$

where $M_{|\xi|^2}$ is the multiplication operator by $|\xi|^2$.

Before starting the proof of the theorem, we collect some basic properties of the generalized eigenfunctions in the following proposition.

Proposition 7.3. *The generalized eigenfunctions*

$$\varphi_{\pm}(x,\xi) = \exp(i\xi x) + \psi_{\pm}(x,\xi)$$

(see (7.3)*) are in $H^1_{\text{loc}}(\mathbb{R}^n)$ for each fixed $\xi \in \mathbb{R}^n$ and satisfy the equation*

$$\left(H - |\xi|^2\right) \varphi_{\pm}(x,\xi) = 0. \tag{7.6}$$

In addition, these functions have the following properties:

(i) *The map*

$$\mathbb{R}^n \ni \xi \to \psi_{\pm}(\cdot,\xi) \in H^{1,-s}(\mathbb{R}^n), \quad s > 1,$$

is continuous.

(ii) *For any compact $K \subseteq \mathbb{R}^n$, the family of functions $\left\{\varphi_{\pm}(x,\xi) \;\middle|\; \xi \in K\right\}$ is uniformly bounded and uniformly Hölder continuous in $x \in \mathbb{R}^n$.*

Proof. Since $(H - |\xi|^2)\exp(i\xi x) \in H^{-1,s}$, $s > 1$, Eq. (7.6) follows from the definition (7.2) in view of Eq. (6.38).

Furthermore, the map

$$\mathbb{R}^n \ni \xi \to \left(H - |\xi|^2\right)\exp(i\xi x) \in H^{-1,s}(\mathbb{R}^n), \quad s > 1,$$

is continuous, so the continuity assertion (i) follows from Theorem 6.1.

For $s > 1$, the set of functions $\left\{\psi_{\pm}(\cdot,\xi) \;\middle|\; \xi \in K\right\}$ is uniformly bounded in $H^{1,-s}$. Thus, in view of (7.6), it follows from the De Giorgi-Nash-Moser Theorem [42, Chapter 8] that the set $\left\{\varphi_{\pm}(x,\xi) \;\middle|\; \xi \in K\right\}$ is uniformly bounded and uniformly Hölder continuous in $\{|x| < R\}$ for every $R > 0$. In particular, we can take $R > \Lambda_0$ (see Eq. (6.2)). In the exterior domain $\{|x| > R\}$ the set $\left\{\psi_{\pm}(x,\xi) \;\middle|\; \xi \in K\right\}$ is bounded in $H^{1,-s}$, $s > 1$, and we have $\left(H_0 - |\xi|^2\right)\psi_{\pm}(x,\xi) = 0$.

In addition, the boundary values $\left\{\psi_{\pm}(x,\xi) \;\middle|\; |x| = R,\, \xi \in K\right\}$ are uniformly bounded. From well-known properties of solutions of the Helmholtz equation we conclude that this set is uniformly bounded and therefore, invoking once again the De Giorgi-Nash-Moser Theorem, uniformly Hölder continuous. □

Proof of Theorem 7.2. We use the LAP proved in Theorem 6.1, adapting the methodology of Agmon's proof [1] for the eigenfunction expansion in the case of Schrödinger operators with short-range potentials. To simplify notation, we prove for $\mathbb{F}_+$.

Let $u \in H^1$ be compactly supported. For any z such that $\operatorname{Im} z \neq 0$ we can write its Fourier transform as

$$\hat{u}(\xi) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} u(x) \exp(-i\xi x)\, dx = \frac{(2\pi)^{-\frac{n}{2}}}{|\xi|^2 - z} \int_{\mathbb{R}^n} u(x)\, (H_0 - z) \exp(-i\xi x)\, dx.$$

Let $\theta \in C_0^\infty(\mathbb{R}^n)$ be a (real) cutoff function such that $\theta(x) = 1$ for x in a neighborhood of the support of u.

We can rewrite the above equality as

$$\hat{u}(\xi) = \frac{(2\pi)^{-\frac{n}{2}}}{|\xi|^2 - z} \left\langle (H_0 - z)\, u(x), \theta(x) \exp(i\xi x) \right\rangle,$$

where $\langle\ ,\ \rangle$ is the $(H^{-1,s}, H^{1,-s})$-sesquilinear pairing (conjugate linear with respect to the second term).

We have therefore, with $f = (H - z)\, u$,

$$\begin{aligned} \hat{u}(\xi) &= \frac{(2\pi)^{-\frac{n}{2}}}{|\xi|^2 - z} \Big(\langle (H - z)\, u(x), \theta(x) \exp(i\xi x) \rangle + \overline{\langle (H_0 - H) \exp(i\xi x), u(x) \rangle} \Big) \\ &= \frac{(2\pi)^{-\frac{n}{2}}}{|\xi|^2 - z} \left(\langle f(x), \theta(x) \exp(i\xi x) \rangle + \langle f(x), R(\bar{z})\, (H_0 - H) \exp(i\xi x) \rangle \right). \end{aligned} \tag{7.7}$$

Introducing the function

$$\widetilde{f}(\xi, z) = \hat{f}(\xi) + (2\pi)^{-\frac{n}{2}} \langle f(x), R(\bar{z})\, (H_0 - H) \exp(i\xi x) \rangle,$$

we have

$$\hat{u}(\xi) = \widehat{R(z)f}(\xi) = \frac{\widetilde{f}(\xi, z)}{|\xi|^2 - z}, \quad \operatorname{Im} z \neq 0. \tag{7.8}$$

We now claim that this equation is valid for all compactly supported $f \in H^{-1}$.

Indeed, let $u = R(z)f \in H^{1,-s}$, $s > 1$. Let $\psi(x) = 1 - \chi(x)$, where $\chi(x)$ is defined in (6.18). We set

$$u_k(x) = \psi(k^{-1}x)u(x), \quad f_k(x) = (H - z) \left(\psi(k^{-1}x)u(x) \right), \quad k = 1, 2, 3, \ldots$$

The equality (7.8) is satisfied with u, f replaced, respectively, by u_k, f_k. Since

$$\psi(k^{-1}x)u(x) \xrightarrow[k \to \infty]{} u(x)$$

in $H^{1,-s}$, we have

$$(H - z)\, (\psi(k^{-1}x)u(x)) \xrightarrow[k \to \infty]{} (H - z)\, u = f(x)$$

in $H^{-1,-s}$, where in the last step we have used Eq. (6.38).

In addition, since $(H_0 - H)\exp(i\xi x)$ is compactly supported

$$\langle f_k(x), R(\bar{z})\,(H_0 - H)\exp(i\xi x)\rangle \;=\; \overline{\langle (H_0 - H)\exp(i\xi x), R(z) f_k(x)\rangle}$$
$$\xrightarrow[k\to\infty]{} \overline{\langle (H_0 - H)\exp(i\xi x), R(z) f\rangle} = \langle f, R(\bar{z})\,(H_0 - H)\exp(i\xi x)\rangle\,.$$

Combining these considerations with the continuity of the Fourier transform (on tempered distributions) we establish that (7.8) is valid for all compactly supported $f \in H^{-1}$.

Let $\{E(\lambda),\ \lambda \in \mathbb{R}\}$ be the spectral family associated with H. Let $A(\lambda) = \frac{d}{d\lambda}E(\lambda)$ be its weak derivative. More precisely, we use the relation (3.7), to get (using Theorem 6.1), for any $f \in H^{-1,s}$, $s > 1$,

$$\langle f, A(\lambda) f\rangle \;=\; \frac{1}{2\pi i}\left\langle f, \left(R^+(\lambda) - R^-(\lambda)\right) f\right\rangle.$$

We now take $f \in L^2$ and compactly supported. From the resolvent equation we infer

$$R(\lambda + i\epsilon) - R(\lambda - i\epsilon) = 2i\epsilon R(\lambda + i\epsilon) R(\lambda - i\epsilon), \quad \epsilon > 0,$$

so that

$$\langle f, A(\lambda) f\rangle = \lim_{\epsilon\downarrow 0} \frac{\epsilon}{\pi}\, \|R(\lambda + i\epsilon) f\|_0^2\,, \quad \epsilon > 0.$$

Using Eq. (7.8) and Parseval's theorem, we therefore have

$$\langle f, A(\lambda) f\rangle \;=\; \lim_{\epsilon\to 0+} \frac{\epsilon}{\pi} \left\| \left(|\xi|^2 - (\lambda + i\epsilon)\right)^{-1} \widetilde{f}(\xi, \lambda + i\epsilon)\right\|_0^2, \quad \epsilon > 0. \tag{7.9}$$

Note that $\widetilde{f}(\xi, z)$ can be extended continuously as $z \to \lambda + i\cdot 0$ by

$$\widetilde{f}(\xi, \lambda) = \hat{f}(\xi) + (2\pi)^{-\frac{n}{2}} \left\langle f(x), R^-(\lambda)\,(H_0 - H)\exp(i\xi x)\right\rangle. \tag{7.10}$$

In order to study properties of $\widetilde{f}(\xi, z)$ as a function of ξ we compute

$$\widetilde{f}(\xi, z) = \hat{f}(\xi) + (2\pi)^{-\frac{n}{2}} \overline{\left\langle \left(\sum_{l,j=1}^{n} \partial_l (a_{l,j}(x) - \delta_{l,j})\partial_j\right) \exp(i\xi x), R(z) f(x)\right\rangle}$$
$$= \hat{f}(\xi) + (2\pi)^{-\frac{n}{2}} i \sum_{l,j=1}^{n} \xi_j \int_{\mathbb{R}^n} (a_{l,j}(x) - \delta_{l,j})\, \partial_l (R(z) f(x)) \exp(-i\xi x)\, dx, \tag{7.11}$$

where in the last step we have used that both $\partial_l(R(z)f(x))$ and $(a_{l,j}(x) - \delta_{l,j})$ $\exp(-i\xi x)$ are in L^2.

Consider now the integral

$$g(\xi, z) = \int_{\mathbb{R}^n} (a_{l,j}(x) - \delta_{l,j})\, \partial_l (R(z) f(x)) \exp(-i\xi x)\, dx, \quad z \in \Omega,$$

where Ω is as in (6.16).

In view of Theorem 6.1, the family $\{\partial_l R(z)f(x)\}_{z\in\Omega}$ is uniformly bounded in $L^{2,-s}$, $s>1$, so by Parseval's theorem we get

$$\|g(\cdot,z)\|_0 < C, \quad z\in\Omega,$$

where C only depends on f.

This estimate and (7.11) imply that, if $f\in L^2$ is compactly supported,

(i) The function

$$\mathbb{R}^n \times \overline{\Omega} \ni (\xi,z) \to \widetilde{f}(\xi,z)$$

is continuous. For real z it is given by (7.10).

(ii)
$$\lim_{k\to\infty} \int_{|\xi|>k} \left(|\xi|^2 - z\right)^{-1} |\widetilde{f}(\xi,z)|^2\, d\xi = 0,$$

uniformly in $z\in\Omega$.

As $z\to|\xi|^2+i\cdot 0$, we have by Theorem 6.1 and Eq. (7.3),

$$\lim_{z\to|\xi|^2+i\cdot 0} \widetilde{f}(\xi,z) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} f(x)\,\overline{\varphi_+(x,\xi)}\,dx = \mathbb{F}_+ f(\xi),$$

so that, taking (i) and (ii) into account, we obtain from (7.9), for any compactly supported $f\in L^2$,

$$\langle f, A(\lambda)f\rangle = \frac{1}{2\sqrt{\lambda}} \int_{|\xi|^2=\lambda} |\mathbb{F}_+ f(\xi)|^2\, d\sigma, \quad \lambda>0, \tag{7.12}$$

where $d\sigma$ is the surface Lebesgue measure.

It follows that, for any $[\alpha,\beta]\subset(0,\infty)$,

$$((E(\beta)-E(\alpha))f,f) = \int_\alpha^\beta \langle f, A(\lambda)f\rangle\, d\lambda = \int_{\alpha\le|\xi|^2\le\beta} |\mathbb{F}_+ f(\xi)|^2\, d\xi. \tag{7.13}$$

Letting $\alpha\to 0$, $\beta\to\infty$, we get

$$\|f\|_0 = \|\mathbb{F}_+ f\|_0\,. \tag{7.14}$$

Thus $f\to\mathbb{F}_+ f\in L^2(\mathbb{R}^n)$ is an isometry for compactly supported functions, which can be extended by density to all $f\in L^2(\mathbb{R}^n)$.

Furthermore, since the spectrum of H is entirely absolutely continuous, it follows that for every $f\in L^2$, Eq. (7.12) holds for almost all $\lambda>0$ (with respect to the Lebesgue measure).

Let $f\in D(H)$. By the spectral theorem

$$\langle Hf, A(\lambda)Hf\rangle = \lambda^2\langle f, A(\lambda)f\rangle = \frac{1}{2\sqrt{\lambda}} \int_{|\xi|^2=\lambda} \left||\xi|^2\,\mathbb{F}_+ f(\xi)\right|^2 d\sigma, \quad \lambda>0.$$

In particular,

$$\|Hf\|_0^2 = \int_{\mathbb{R}^n} \left||\xi|^2\,\mathbb{F}_+ f(\xi)\right|^2 d\xi. \tag{7.15}$$

Conversely, if the right-hand side of (7.15) is finite, then $\int_0^\infty \lambda^2 \langle f, A(\lambda)f\rangle \, d\lambda < \infty$, so $f \in D(H)$.

The adjoint operator $\mathbb{F}_+^*$ is a partial isometry (on the range of $\mathbb{F}_+$). If $f(x) \in L^2(\mathbb{R}^n)$ is compactly supported and $g(\xi) \in L^2(\mathbb{R}^n)$ is likewise compactly supported, then

$$(\mathbb{F}_+ f, g) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^n} f(x)\, \overline{\varphi_+(x,\xi)}\, dx \right) \overline{g(\xi)}\, d\xi$$
$$= (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} f(x) \left(\int_{\mathbb{R}^n} \overline{g(\xi)\, \varphi_+(x,\xi)}\, d\xi \right) dx,$$

where in the change of order of integration Proposition 7.3 was taken into account.

It follows that, for a compactly supported $g(\xi) \in L^2(\mathbb{R}^n)$,

$$(\mathbb{F}_+^* g)(x) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} g(\xi)\, \varphi_+(x,\xi)\, d\xi, \tag{7.16}$$

and the extension to all $g \in L^2(\mathbb{R}^n)$ is obtained by the fact that $\mathbb{F}_+^*$ is a partial isometry.

Now if $f \in D(H)$, $g \in L^2(\mathbb{R}^n)$, we have

$$(Hf, g) = \int_{\mathbb{R}^n} |\xi|^2\, \mathbb{F}_+ f(\xi)\, \overline{\mathbb{F}_+ g(\xi)}\, d\xi = \int_{\mathbb{R}^n} \mathbb{F}_+^* \left(|\xi|^2\, \mathbb{F}_+ f(\xi) \right) \overline{g(\xi)}\, d\xi,$$

which is the statement (7.5) of the theorem.

It follows from the spectral theorem that, for every interval $J = [\alpha, \beta] \subseteq [0, \infty)$ and for every $f \in L^2(\mathbb{R}^n)$, we have, with $E_J = E(\beta) - E(\alpha)$ and χ_J the characteristic function of J,

$$E_J f(x) = \mathbb{F}_+^* \left(\chi_J(|\xi|^2)\, \mathbb{F}_+ f(\xi) \right)$$

or

$$\mathbb{F}_+ E_J f(\xi) = \chi_J(|\xi|^2)\, \mathbb{F}_+ f(\xi).$$

It remains to prove that the isometry $\mathbb{F}_+$ is onto (and hence unitary). So, suppose to the contrary that, for some nonzero $g(\xi) \in L^2(\mathbb{R}^n)$,

$$(\mathbb{F}_+^* g)(x) = 0.$$

In particular, for any $f \in L^2(\mathbb{R}^n)$ and any interval J as above,

$$0 = \left(E_J f, \mathbb{F}_+^* g\right) = (\mathbb{F}_+ E_J f, g) = \left(\chi_J(|\xi|^2)\mathbb{F}_+ f(\xi), g(\xi)\right) = \left(\mathbb{F}_+ f(\xi), \chi_J(|\xi|^2) g(\xi)\right),$$

so that $\mathbb{F}_+^* \left(\chi_J(|\xi|^2)\, g(\xi)\right) = 0$.

By Eq. (7.16) we have, for any $0 \le \alpha < \beta$,

$$\int_{\alpha < |\xi|^2 < \beta} g(\xi)\, \varphi_+(x,\xi)\, d\xi = 0$$

so that, in view of the continuity properties of $\varphi_+(x,\xi)$ (see Proposition 7.3), for a.e. $\lambda \in (0,\infty)$,

$$\int_{|\xi|^2=\lambda} g(\xi)\,\varphi_+(x,\xi)\,d\sigma = 0. \tag{7.17}$$

From the definition (7.3) we get

$$\int_{|\xi|^2=\lambda} g(\xi)\exp(i\xi x)\,d\sigma - \int_{|\xi|^2=\lambda} g(\xi)R^-(\lambda)\left((H-\lambda)\exp(i\xi x)\right)d\sigma = 0. \tag{7.18}$$

Since $(H-\lambda)\exp(i\xi x)$ is compactly supported (when $|\xi|^2 = \lambda$), the continuity property of $R^-(\lambda)$ enables us to write

$$\int_{|\xi|^2=\lambda} g(\xi)\,R^-(\lambda)\left((H-\lambda)\exp(i\xi x)\right)d\sigma = R^-(\lambda)\int_{|\xi|^2=\lambda} g(\xi)\,(H-\lambda)\exp(i\xi x)\,d\sigma,$$

which, by Remark 6.9, satisfies a Sommerfeld radiation condition. We conclude that the function

$$G(x) = \int_{|\xi|^2=\lambda} g(\xi)\exp(i\xi x)\,d\sigma \in H^{1,-s}, \quad s > \frac{1}{2},$$

is a radiative solution (see Remark 6.7) of $(-\Delta-\lambda)\,G = 0$ and hence must vanish. Since this holds for a.e. $\lambda > 0$, we get $\hat{g}(\xi) = 0$, hence $g = 0$. □

8. Global spacetime estimates for a generalized wave equation

The Strichartz estimates [83] have become a fundamental ingredient in the study of nonlinear wave equations. They are L^p spacetime estimates that are derived for operators whose leading part has constant coefficients. We refer to the books [81, 82] and [5] for detailed accounts and further references.

Here we focus on spacetime estimates pertinent to the framework of this review, namely, weighted L^2 estimates.

We recall first some results related to the Cauchy problem for the classical wave equation,

$$\Box u = \frac{\partial^2 u}{\partial t^2} - \Delta u = 0, \tag{8.1}$$

subject to the initial data

$$u(x,0) = u_0(x), \quad \partial_t u(x,0) = v_0(x), \quad x \in \mathbb{R}^n. \tag{8.2}$$

The Morawetz estimate [66] yields

$$\int_{\mathbb{R}}\int_{\mathbb{R}^n} |x|^{-3}|u(x,t)|^2\,dxdt \le C\left(\|\nabla u_0\|_0^2 + \|v_0\|_0^2\right), \quad n \ge 4,$$

while in [8] we gave the estimate

$$\int_{\mathbb{R}}\int_{\mathbb{R}^n} |x|^{-2\alpha-1}\,|u(x,t)|^2\,dxdt \le C_\alpha\left(\||\nabla|^\alpha u_0\|_0^2 + \left\||\nabla|^{\alpha-1}v_0\right\|_0^2\right), \quad n\ge 3,$$

for every $\alpha\in(0,1)$.

Related results were obtained in [65] (allowing also dissipative terms), [50] (with some gain in regularity), [88] (with short-range potentials) and [47] for spherically symmetric solutions.

Here we consider the equation

$$\frac{\partial^2 u}{\partial t^2} + Hu = \frac{\partial^2 u}{\partial t^2} - \sum_{i,j=1}^{n} \partial_i a_{i,j}(x)\partial_j u = f(x,t), \tag{8.3}$$

subject to the initial data (8.2).

We first replace the assumptions (6.1), (6.2) by stronger ones as follows:

(H1) $$a(x) = g^{-1}(x) = \left(g^{i,j}(x)\right)_{1\le i,j\le n}, \tag{8.4}$$

where $g(x) = (g_{i,j}(x))_{1\le i,j\le n}$ is a smooth Riemannian metric on $\mathbb{R}^n$ such that

$$g(x) = I, \quad |x| > \Lambda_0.$$

(H2) The Hamiltonian flow associated with $h(x,\xi) = (g(x)\xi,\xi)$ is nontrapping for any (positive) value of h. (8.5)

Recall that (H2) means that the flow associated with the Hamiltonian vectorfield $\mathcal{H} = \frac{\partial h}{\partial \xi}\frac{\partial}{\partial x} - \frac{\partial h}{\partial x}\frac{\partial}{\partial \xi}$ leaves any compact set in $\mathbb{R}^n_x$.

Identical hypotheses are imposed in the study of resolvent estimates in semiclassical theory [26, 27].

In our estimates we use *homogeneous Sobolev spaces* associated with the operator H.

We let $G = H^{\frac{1}{2}}$ which is a positive self-adjoint operator. Note that $\|G\theta\|_0$ is equivalent to the homogeneous Sobolev norm $\|\nabla\theta\|_0$.

Theorem 8.1. *Suppose that $n\ge 3$ and that $a(x)$ satisfies* Hypotheses (H1)–(H2). *Let $s>1$.*

(a) (*local energy decay*) *There exists a constant $C_1 = C_1(s,n) > 0$ such that the solution to* (8.3), (8.2) *satisfies*

$$\int_{\mathbb{R}}\int_{\mathbb{R}^n} \left(1+|x|^2\right)^{-s}\left[|Gu(x,t)|^2 + |u_t(x,t)|^2\right]dxdt$$
$$\le C_1\left\{\|Gu_0\|_0^2 + \|v_0\|_0^2 + \int_{\mathbb{R}}\int_{\mathbb{R}^n} |f(x,t)|^2\,dxdt\right\}. \tag{8.6}$$

(b) (*amplitude decay*) *Assume that* $f = 0$. *There exists a constant* $C_2 = C_2(s,n) > 0$ *such that the solution to* (8.3), (8.2) *satisfies,*

$$\int_{\mathbb{R}}\int_{\mathbb{R}^n} \left(1+|x|^2\right)^{-s} |u(x,t)|^2 \, dxdt \le C_2 \left[\|u_0\|_0^2 + \|G^{-1}v_0\|_0^2\right]. \tag{8.7}$$

This estimate generalizes similar estimates obtained for the classical ($g = I$) wave equation [8, 65].

Remark 8.2. The estimate (8.6) is an *energy decay estimate* for the wave equation (8.3). A localized (in space) version of the estimate has served to obtain global (small amplitude) existence theorems for the corresponding nonlinear equation [27, 48].

The weighted L^2 spacetime estimates for the *dispersive* equation

$$i^{-1}\frac{\partial}{\partial t}u = Lu,$$

have been extensively treated in recent years. In general, in this case there is also a gain of derivatives (so-called *smoothing*) in addition to the energy decay. For the Schrödinger operator $L = -\Delta + V(x)$, with various assumptions on the potential V, we refer to [3, 7, 8, 17, 19, 50, 62, 78, 80, 89] and references therein. In [33] the case of magnetic potentials is considered. The Schrödinger operator on a Riemannian manifold is treated in [26, 38]. For more general operators see [16, 20, 28, 51, 67, 77, 84] and references therein.

Proof of Theorem 8.1. (a) Define, with $G = H^{\frac{1}{2}}$,

$$u_\pm = \frac{1}{2}\left(Gu \pm iu_t\right).$$

Then

$$\partial_t u_\pm = \mp i\, Gu_\pm \pm \frac{i}{2}f. \tag{8.8}$$

Defining

$$U(t) = \begin{pmatrix} u_+(t) \\ u_-(t) \end{pmatrix}, \tag{8.9}$$

we have

$$i^{-1}U'(t) = -KU + F, \tag{8.10}$$

where

$$K = \begin{pmatrix} G & 0 \\ 0 & -G \end{pmatrix}, \quad F(t) = \begin{pmatrix} \frac{1}{2}f(\cdot,t) \\ -\frac{1}{2}f(\cdot,t) \end{pmatrix}.$$

Note that, as is common when treating evolution equations, we write $U(t)$, $F(t)$, etc. for $U(x,t)$, $F(x,t)$, etc. when there is no risk of confusion.

The operator K is a self-adjoint operator on $\mathcal{D} = L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n)$. Its spectral family $E_K(\lambda)$ is given by $E_K(\lambda) = E_G(\lambda) \oplus (I - E_G(-\lambda))$, $\lambda \in \mathbb{R}$, where E_G is the spectral family of G.

Let $E(\lambda)$ be the spectral family of H, and let $A(\lambda) = \frac{d}{d\lambda}E(\lambda)$ be its weak derivative (3.7). By the definition of G we have

$$E_G(\lambda) = E(\lambda^2),$$

hence its weak derivative is given by

$$A_G(\lambda) = \frac{d}{d\lambda}E_G(\lambda) = 2\lambda\, A(\lambda^2), \quad \lambda > 0. \tag{8.11}$$

In view of the LAP (Theorem A) we therefore have that the operator-valued function

$$A_G(\lambda) \in B(L^{2,s}(\mathbb{R}^n), L^{2,-s}(\mathbb{R}^n))$$

is continuous for $\lambda \geq 0$.

Denoting $\mathcal{D}^s = L^{2,s}(\mathbb{R}^n) \oplus L^{2,s}(\mathbb{R}^n)$, it follows that

$$A_K(\lambda) = \frac{d}{d\lambda}E_K(\lambda) = A_G(\lambda) \oplus A_G(-\lambda), \quad \lambda \in \mathbb{R},$$

is continuous with values in $B(\mathcal{D}^s, \mathcal{D}^{-s})$ for $s > 1$.

Making use of Hypotheses (H1)–(H2), we invoke [76, Theorem 5.1] to conclude that $\limsup_{\mu\to\infty} \mu^{\frac{1}{2}} \|A(\mu)\|_{B(L^{2,s},L^{2,-s})} < \infty$, so that by (8.11) there exists a constant $C > 0$ such that

$$\|A_G(\lambda)\|_{B(L^{2,s},L^{2,-s})} < C, \quad \lambda \geq 0. \tag{8.12}$$

It follows that also

$$\|A_K(\lambda)\|_{B(\mathcal{D}^s,\mathcal{D}^{-s})} < C, \quad \lambda \in \mathbb{R},\ s > 1,\ \lambda \in \mathbb{R}. \tag{8.13}$$

Let $\langle\ ,\ \rangle$ be the sesquilinear pairing between $\mathcal{D}^{-s}$ and $\mathcal{D}^s$ (conjugate linear with respect to the second term).

For any $\psi,\ \chi \in \mathcal{D}^s$ we have, in view of the fact that $A_K(\lambda)$ is a weak derivative of a spectral measure,

$$\begin{aligned} &\text{(i)} \qquad |\langle A_K(\lambda)\psi, \chi\rangle|^2 \leq \langle A_K(\lambda)\psi, \psi\rangle \cdot \langle A_K(\lambda)\chi, \chi\rangle\,, \\ &\text{(ii)} \qquad \int_{-\infty}^{\infty} \langle A_K(\lambda)\psi, \psi\rangle\, d\lambda = \|\psi\|^2_{L^2(\mathbb{R}^n)\oplus L^2(\mathbb{R}^n)}\,. \end{aligned} \tag{8.14}$$

We first treat the pure Cauchy problem, i.e., $f \equiv 0$.

To estimate $U(x,t) = e^{-itK}U(x,0)$ we use a duality argument. Some of the following computations will be rather formal, but they can easily be justified by a density argument, as in [8, 20]. We shall use $((\ ,\ ))$ for the scalar product in $L^2(\mathbb{R}^{n+1}) \oplus L^2(\mathbb{R}^{n+1})$.

Take $w(x,t) \in C_0^\infty(\mathbb{R}^{n+1}) \oplus C_0^\infty(\mathbb{R}^{n+1})$. Then,

$$\begin{aligned}((U,w)) &= \int\limits_{-\infty}^{\infty} e^{-itK}U(x,0)\cdot\overline{w(x,t)}\,dxdt \\ &= \int\limits_{-\infty}^{\infty}\left\langle A_K(\lambda)U(x,0), \int\limits_{-\infty}^{\infty} e^{it\lambda}w(\cdot,t)dt\right\rangle d\lambda \\ &= (2\pi)^{1/2}\int\limits_{-\infty}^{\infty}\langle A_K(\lambda)U(x,0),\tilde{w}(\cdot,\lambda)\rangle\,d\lambda,\end{aligned}$$

where

$$\tilde{w}(x,\lambda) = (2\pi)^{-\frac{1}{2}}\int\limits_{\mathbb{R}} w(x,t)e^{it\lambda}dt.$$

Noting (8.14), (8.13) and using the Cauchy-Schwartz inequality

$$\begin{aligned}\big|((U,w))\big| &\le (2\pi)^{1/2}\,\|U(x,0)\|_0\left(\int\limits_{-\infty}^{\infty}\langle A_K(\lambda)\tilde{w}(\cdot,\lambda),\tilde{w}(\cdot,\lambda)\rangle\,d\lambda\right)^{1/2} \\ &\le C\,\|U(x,0)\|_0\left(\int\limits_{-\infty}^{\infty}\|\tilde{w}(\cdot,\lambda)\|^2_{\mathcal{D}^s}\,d\lambda\right)^{\frac{1}{2}}.\end{aligned}$$

It follows from the Plancherel theorem that

$$\big|((U,w))\big| \le C\,\|U(x,0)\|_0\left(\int\limits_{\mathbb{R}}\|w(\cdot,t)\|^2_{\mathcal{D}^s}\,dt\right)^{1/2}.$$

Let $\phi(x,t) \in C_0^\infty(\mathbb{R}^{n+1}) \oplus C_0^\infty(\mathbb{R}^{n+1})$ and take $w(x,t) = \left(1+|x|^2\right)^{-\frac{s}{2}}\phi(x,t)$ so that

$$\Big|\Big(\Big(\left(1+|x|^2\right)^{-\frac{s}{2}}U,\phi\Big)\Big)\Big| \le C\ \|U(x,0)\|_0\cdot\|\phi\|_{L^2(\mathbb{R}^{n+1})}.$$

This concludes the proof of the part involving the Cauchy data in (8.6), in view of (8.9).

To prove the part concerning the inhomogeneous equation, it suffices to take $u_0 = v_0 = 0$. In this case the Duhamel principle yields, for $t > 0$,

$$U(t) = \int_0^t e^{-i(t-\tau)K}F(\tau)d\tau,$$

where we have used the form (8.10) of the equation.

Integrating the inequality

$$\|U(t)\|_{\mathcal{D}^{-s}} \le \int_0^t \left\|e^{-i(t-\tau)K}F(\tau)\right\|_{\mathcal{D}^{-s}}\,d\tau,$$

we get

$$\int_0^\infty \|U(t)\|_{\mathcal{D}^{-s}}\, dt \le \int_0^\infty \int_\tau^\infty \left\| e^{-i(t-\tau)K} F(\tau) \right\|_{\mathcal{D}^{-s}} dt\, d\tau.$$

Invoking the first part of the proof we obtain

$$\int_0^\infty \|U(t)\|_{\mathcal{D}^{-s}}\, dt \le C \int_0^\infty \|F(\tau)\|_0\, d\tau,$$

which proves the part related to the inhomogeneous term in (8.6).

(b) Define

$$v_\pm(x,t) = \exp(\pm itG)\, \phi_\pm(x),$$

where

$$\phi_\pm(x) = \frac{1}{2}\left[u_0(x) \mp G^{-1} v_0(x)\right].$$

Then clearly

$$u(x,t) = v_+(x,t) + v_-(x,t).$$

We establish the estimate (8.7) for v_+.

Taking $w(x,t) \in C_0^\infty(\mathbb{R}^{n+1})$ we proceed as in the first part of the proof. Let $\langle\ ,\ \rangle$ be the $(L^{2,-s}(\mathbb{R}^n), L^{2,s}(\mathbb{R}^n))$ pairing. Then

$$\begin{aligned}(v_+, w) &= \int_{-\infty}^{\infty} e^{itG}\phi_+(x)\, \overline{w(x,t)}\, dx dt \\ &= \int_0^\infty \left\langle A_G(\lambda)\phi_+, \int_{-\infty}^{\infty} e^{-it\lambda} w(\cdot,t) dt \right\rangle d\lambda \\ &= (2\pi)^{1/2} \int_0^\infty \langle A_G(\lambda)\phi_+, \tilde{w}(\cdot,\lambda)\rangle\, d\lambda,\end{aligned}$$

where

$$\tilde{w}(x,\lambda) = (2\pi)^{-\frac{1}{2}} \int_{\mathbb{R}} w(x,t) e^{-it\lambda}\, dt.$$

Noting (8.12) as well as the inequalities (8.14) (with A_G replacing A_K) and using the Cauchy-Schwartz inequality

$$\begin{aligned}|(v_+, w)| &\le (2\pi)^{1/2} \|\phi_+\|_0 \left(\int_0^\infty \langle A_G(\lambda)\tilde{w}(\cdot,\lambda), \tilde{w}(\cdot,\lambda)\rangle\, d\lambda \right)^{1/2} \\ &\le C \|\phi_+\|_0 \left(\int_0^\infty \|\tilde{w}(\cdot,\lambda)\|_{0,s}^2\, d\lambda \right)^{\frac{1}{2}}.\end{aligned}$$

The Plancherel theorem yields

$$|(v_+, w)| \leq C \|\phi_+\|_0 \left(\int_{\mathbb{R}} \|w(\cdot, t)\|_{0,s}^2 \, dt \right)^{1/2} .$$

Let $\omega \in C_0^\infty(\mathbb{R}^{n+1})$ and take $w(x,t) = \left(1+|x|^2\right)^{-\frac{s}{2}} \omega(x,t)$ so that

$$\left| \left(\left(1+|x|^2\right)^{-\frac{s}{2}} v_+, \omega \right) \right| \leq C \|\phi_+\|_0 \|\omega\|_{L^2(\mathbb{R}^{n+1})} .$$

This (with the similar estimate for v_-) concludes the proof of the estimate (8.7). □

Remark 8.3 (optimality of the requirement $s > 1$). A key point in the proof was the use of the uniform bound (8.13). In view of the relation (8.11), this is reduced to the uniform boundedness of $\lambda A(\lambda^2)$, $\lambda \geq 0$, in $B(L^{2,s}, L^{2,-s})$. By [76, Theorem 5.1] the boundedness at infinity, $\limsup_{\mu \to \infty} \mu^{\frac{1}{2}} \|A(\mu)\| < \infty$, holds already with $s > \frac{1}{2}$. Thus the further restriction $s > 1$ is needed in order to ensure the boundedness at $\lambda = 0$ (Theorem A).

Remark 8.4. Clearly we can take $[0, T]$ as the time interval, instead of $\mathbb{R}$, for any $T > 0$.

9. Further directions and open problems

We conclude this review with a number of suggestions for new directions and developments in this domain of smooth spectral theory.

This section is by no means intended to be exhaustive. Indeed, some of the topics we touched upon in this review, from eigenfunction expansion through spectral structure of differential operators to global estimates in spacetime, are still areas of very intensive research, not only within pure mathematics, but also in various areas of applied mathematics. As an illustration of the latter, we mention the role of the acoustic propagator (resp. the Maxwell equations) in the study of sound waves in media with variable speed of sound (resp. fiber optics). For the latter, see [18, 21].

1. Estimating the heat kernel in Lebesgue spaces

Recall that by Eq. (3.3) the spectral derivative $A_0(\lambda)$ of $H_0 = -\Delta$ satisfies ($\langle \, , \, \rangle$ is the $(L^{2,s}, L^{2,-s})$ pairing, $s > \frac{1}{2}$),

$$\langle A_0(\lambda) f, g \rangle \; = \; \lambda^{-\frac{1}{2}} \int_{|\xi|^2 = \lambda} \hat{f}(\xi) \, \overline{\hat{g}(\xi)} \, d\tau .$$

Now using this formula with functions f, $g \in C_0^\infty$, we can estimate the integral in various norms. Thus, using the L^∞ estimate of $\hat{f}$ in terms of $\|f\|_{L^1(\mathbb{R}^n)}$,

$$\langle A_0(\lambda) f, f \rangle \; \leq \; C \, \lambda^{-\frac{1}{2}} \lambda^{\frac{n-1}{2}} \, \|f\|_{L^1(\mathbb{R}^n)}^2 , \quad f \in L^1(\mathbb{R}^n). \tag{9.1}$$

Also, the spectral theorem yields

$$\int_0^\infty \langle A_0(\lambda)g, g\rangle \, d\lambda = \|g\|^2_{L^2(\mathbb{R}^n)}, \quad g \in L^2(\mathbb{R}^n).$$

Thus, for $t > 0$,

$$\left(e^{t\Delta} f, g\right)_{L^2(\mathbb{R}^n)} = \int_0^\infty e^{-t\lambda} \, d\left(E_0(\lambda)f, g\right) = \int_0^\infty e^{-t\lambda} \, \langle A_0(\lambda)f, g\rangle \, d\lambda.$$

It follows that, using the fact that $\langle A_0 f, g\rangle$ is positive semi-definite (see (4.3)),

$$\begin{aligned} |(e^{t\Delta} f, g)|^2 &\le \int_0^\infty e^{-2t\lambda} \, \langle A_0(\lambda)f, f\rangle \, d\lambda \int_0^\infty \langle A_0(\lambda)g, g\rangle \, d\lambda \\ &\le Ct^{-\frac{n}{2}} \|f\|^2_{L^1(\mathbb{R}^n)} \|g\|^2_{L^2(\mathbb{R}^n)}. \end{aligned}$$

We obtain therefore the familiar formula

$$\left\|e^{t\Delta}\right\|_{B(L^1(\mathbb{R}^n), L^2(\mathbb{R}^n))} \le Ct^{-\frac{n}{4}},$$

from which we also have, by duality

$$\left\|e^{t\Delta}\right\|_{B(L^2(\mathbb{R}^n), L^\infty(\mathbb{R}^n))} \le Ct^{-\frac{n}{4}}.$$

By interpolation we can then obtain various L^p, L^q estimates.

Observe that the same considerations can be applied to other operators, say Δ^2 (and indeed any elliptic operator with constant coefficients) for which explicit kernel formulas are not available.

An essential ingredient in the above argument is the estimate (9.1), which leads to the following problem:

Find methods to estimate the spectral derivatives in Lebesgue spaces L^p or weighted spaces based on them, instead of the weighted L^2 estimates employed throughout this review.

We remark further that such estimates could bring different insights into the Strichartz estimates, as already mentioned in Section 8.

2. Abstract approach to long-range perturbations

In Section 4 the abstract approach to short-range perturbations was developed, within the framework of the smooth spectral theory. Definition 4.1 is very natural in this framework and, indeed, leads to the same class of short-range potentials as in Agmon's work [1].

Thus, a natural problem is the following:

Develop a similar definition for long-range perturbations. Such a definition should cover the long-range potentials in the Schrödinger operator, as discussed in [79].

3. Discreteness of eigenvalues of short-range perturbations

In the course of the proof of the discreteness of the eigenvalues (embedded in the continuous spectrum) of short-range perturbations (Theorem 4.14), we needed to impose Assumption S on the regularity of the spectral derivative. This assumption is satisfied in many concrete examples, including the case of the Schrödinger operator, due to the fact that in these cases the derivative is more regular than the minimal assumption required in Definition 3.3. However, it might be desirable to find alternative assumptions or, in fact:

Try to see if Assumption S *could be dispensed with completely.*

4. High energy estimates of divergence-type operators

In establishing the global spacetime estimates for the generalized wave equation (Theorem 8.1), we needed the uniform estimate (8.12). For this we needed the strong assumptions (H1)–(H2) (8.4) concerning the smoothness of the coefficients and the non-trapping character of the metric. However, it is of great interest to try and *minimize* the smoothness assumptions, so as to stay only with the assumptions imposed in Theorem 6.1 for the LAP (and continuity of the spectral derivative at the threshold at zero). Thus, we can formulate this problem as follows:

Find conditions on the matrix $a(x)$ (*see* (6.1)) *so that the limiting values* $R^{\pm}(\lambda)$ *of the resolvent* (*see* (6.4)) *are uniformly bounded in* $\lambda \in \mathbb{R}$, *with respect to the uniform operator topology of* $B(L^{2,s}(\mathbb{R}^n), L^{2,-s}(\mathbb{R}^n))$, $s > 1$. *Furthermore, what are the additional conditions needed to establish a decay of these values as* $\lambda \to \infty$, *similar to the decay of the resolvent of the Laplacian* (*see* (5.27))?

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Spectral Analysis and Geometry of Sub-Laplacian and Related Grushin-type Operators

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Abstract. In this article, we discuss three topics in the area of sub-Riemannian geometry and analysis.

First, we recall the notion of a sub-Riemannian structure in the strong sense and its sub-Laplacian. We define an operator, called Grushin-type operator, on the base manifold of a submersion under an additional compatibility condition. Then a relation between the bicharacteristic flows of the sub-Laplacian and the Grushin-type operator is proved. In particular, we give the explicit forms of all Grushin-type operators defined from a sub-Riemannian structure on the three-dimensional Heisenberg group which will serve as typical examples of our analysis. As a main example we study Grushin-type operators on the two- and four-dimensional spheres defined from a sub-Riemannian structures on S^3 and S^7, respectively. For this purpose we construct a sub-Riemannian structure in the strong sense on the seven-dimensional sphere based on the quaternionic structure of $\mathbb{R}^8$.

Next, we apply the relation between the bicharacteristic curves of a sub-Laplacian and a Grushin-type operator to determine the singular geodesics on the Grushin sphere, which is the two-dimensional sphere with a singular metric. Here we use the isoperimetric interpretation of the sub-Riemannian geodesics on the three-dimensional sphere via Stoke's theorem and the double fibration structure defined by the left and right quaternionic vector space structure on $\mathbb{R}^4$.

Then, we explicitly determine the heat kernels of a sub-Laplacian on the six-dimensional free nilpotent Lie group and all related Grushin-type operators including a sub-Laplacian on a five-dimensional nilpotent Lie group. Using the explicit integral forms of these heat kernels we obtain the spectra of certain five- and six-dimensional compact nilmanifolds via the Selberg trace formula and determine the poles and residues of the corresponding spectral zeta functions which have close relations to the Epstein zeta function.

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1. Introduction

There are many geometric structures on manifolds which define differential operators (linear and non-linear). The Riemannian structure gives the Laplace-Beltrami operator acting on the space of differential forms, a spin structure defines Dirac operators acting on spinors and some fiber bundle structures induce Fourier integral operators like a Radon transformation. These operators mostly are elliptic. In this paper, our main concern are hypo-elliptic (not elliptic) operators on a class of sub-Riemannian manifolds and closely related operators such as sub-Laplacian and Grushin-type operators.

Let $\mathcal{H}$ be a sub-bundle in the tangent bundle of a manifold M. In the case the space $\mathcal{X}_{\mathcal{H}}$ of vector fields taking values in $\mathcal{H}$ is closed under the bracket operation the sub-bundle $\mathcal{H}$ defines a foliation structure on M. If $\mathcal{X}_{\mathcal{H}}$ is not closed under the bracket operation, then after adding higher Lie brackets of vector fields in $\mathcal{X}_{\mathcal{H}}$, one obtains a stable Lie algebra of vector fields. In general, by localizing this procedure, we obtain a (pre-)sheaf $\mathcal{S}_{\mathcal{H}}$ of Lie algebras of vector fields:

$$\begin{aligned} M \supset U \longmapsto \mathcal{S}_{\mathcal{H}}(U) \\ = \big\{\text{sums of vector fields: } fX, [fX, gY], \big[\, [fX, gY], hZ \,\big] \cdots \ \big| \\ f, g, h, \ldots \in C^\infty(U),\ X, Y, Z \ldots \text{ vector fields on } U \text{ taking values in } \mathcal{H} \,\big\}. \end{aligned}$$

It might happen that this sheaf comes from another sub-bundle $\tilde{\mathcal{H}}$ of the tangent bundle which includes $\mathcal{H}$. More precisely, it is the sheaf of germs of vector fields taking values in $\tilde{\mathcal{H}}$ and $\tilde{\mathcal{H}}$ defines a foliation structure on the manifold. It follows that the sub-bundle $\mathcal{H}$ restricted to each integral sub-manifold of $\tilde{\mathcal{H}}$ is non-holonomic. In particular, $\mathcal{H}$ defines a sub-Riemannian structure on each leaf by installing a suitable metric.

Roughly speaking, the study of foliated manifolds is focused on the study of how the leaves are piling or can be piling in a manifold. In classical mechanics the manifold is considered as a configuration space of the physical states, a classical free particle is trapped on a connected leaf and cannot jump from one to another. From the theory of C^*-algebras on foliated manifolds it is apparent that many interesting analytic problems arise once one drops the restriction of only studying mechanics on each single leaf.

However, in the present text we assume from the beginning that the manifold has a non-holonomic sub-bundle and we impose two additional strong conditions. Our aim is it to give explicit forms of various analytic and geometric quantities.

In our general framework we fix smooth vector fields $\{X_i\}_{i=1}^N$ on a manifold M such that there is an open dense subset W in M on which $\{X_i\}_{i=1}^N$ are linearly independent. Moreover, we assume that the vector fields $\{X_i\}_{i=1}^N$ together with all their Lie brackets and coefficients in the space of smooth functions span the whole tangent space at each point (the Hörmander condition). In our examples the complement $M \backslash W$ is at most of codimension one. The beginning of sub-Riemannian geometry goes back to the 17th century being motivated by physical phenomena such as thermodynamics. Theorem 2.3 by Chow [Ch-39] is one of the most fundamental results in this area which expresses physical phenomena in a geometrical picture. Subsequently, it was proved by Hörmander [Hö1-67] that the sub-Laplacian (cf. §2) is always hypo-elliptic. Recently, lots of studies have been done surrounding these two basic theorems on sub-Riemannian manifolds from a geometric and analytic point of view (e.g., [St-86], [ABGR-09], [ABS-08], [CC2-09], [Mo2-02], [CCFI-10], [BGG3-97], [Ag-07], and the references therein).

In the realm of Chow's theorem, one of the most interesting and basic problems in sub-Riemannian geometry is to answer the question how the configurations of a physical system are realized as a sub-Riemannian manifold and how to develop a control theory on it (see [Ag-07], [CC2-09]).

Based on Hörmander's theorem which can be seen as a quantum version of Chow's theorem also the spectral analysis of a sub-Laplacian is of importance. In this paper, we mostly deal with hypo-elliptic operators on 2-step nilpotent Lie groups. Note that the definition of the nilpotency ensures the existence of a sub-Riemannian structure on any nilpotent Lie group. On such groups the sub-Laplacian roughly speaking forms the *core of the Laplace operator* and therefore it seems to be more fundamental. The expressions for the heat kernel of both, the Laplace and the sub-Laplace operator, are given as integrals over the characteristic variety of the sub-Laplace operator. However, the corresponding action functions, which appear in the integrand of the heat kernel expression, differ. These action functions can be given explicitly according to the results in [BGG1-96], cf. Remark 15.1.

We study spectral properties and the geometry of sub-Laplacians on manifolds having a non-holonomic sub-bundle as well as operators defined from a sub-Laplacian through a submersion compatible with the sub-Riemannian structure. Such operators act on the base space of the submersion and we call them Grushin type operators. We will discuss:

(I) Operators defined by sub-Riemannian structures and a relation between their bicharacteristic flows,

(II) Isoperimetric interpretation of the geodesics in the sense of sub-Riemannian and singular Riemannian geodesics together with Stoke's theorem and a double fibration,

(III) Explicit integral expressions of heat kernels of a class of sub-Laplacians and related Grushin-type operators, and

(IV) Determination of the spectrum of sub-Laplacians on low-dimensional (≤ 6) compact 2-step nilmanifolds and the analytic continuation of their spectral zeta function.

Our main goal is it to give explicit expressions of various analytic and geometric quantities such as the construction of sub-Riemannian structures, heat kernels and spectra of the corresponding sub-Laplacians, geodesics in the sub-Riemannian and the singular Riemannian sense.

In §2, we recall the notion of a sub-Riemannian structure and we define Grushin-type operators. A manifold together with a singular metric is introduced. Important examples of this construction which will be treated in this text are the *Grushin plane* (defined from a Heisenberg group) and the *Grushin sphere* (defined from S^3).

In §3, we discuss a relation between the bicharacteristic flows of a sub-Laplacian and a Grushin-type operator (cf. Theorem 3.1). This gives us one basic method for constructing geodesics on the Grushin plane and the Grushin sphere which are given in §4.2 and §6. The former will serve as a model example.

In §4, we deal with a sub-Laplacian on the three-dimensional Heisenberg group. We study related operators and their bicharacteristic curves as a typical example. In §4.1, we start from the classical Grushin operator and we list all possible Grushin-type operators coming from the three-dimensional Heisenberg group H_3, although most of them are transformed into each other by a group automorphism of H_3. In §4.2 and applying Theorem 3.1 together with the isoperimetric interpretation of sub-Riemannian geodesic on H_3 via Stoke's theorem, we determine geodesics (in the sense of the Grushin metric) connecting two points on the Grushin plane and sitting on the singular set (see [AB-08]).

In §5, we define a sub-Laplacian on the space $SL(2,\mathbb{R})$ of 2×2 real matrices with determinant one. It naturally defines a Grushin-type metric on the Poincaré upper half-plane and a related Grushin-type operator. In this case we have no singular set, i.e., the Grushin-type operator is elliptic (note that it does not coincide with the Laplacian). We discuss problems similar to those arising in case of the three-dimensional Heisenberg group in section §4.2. However, we do not give a precise descriptions of the geodesics for the Grushin upper half-plane. It is only mentioned that they can be constructed from circles (in the Euclidean sense) on the Poincaré upper half-plane through the correspondence between the geodesics on $SL(2,\mathbb{R})$ in the sub-Riemannian sense and its isoperimetric interpretation on the Poincaré upper half-plane via Stoke's theorem (see (5.7)).

In §6, we deal with the three-dimensional sphere S^3 equipped with a sub-Riemannian structure. Through the Hopf fibration we define a Grushin-type operator on S^2. Geodesics on S^2 connecting two points on the singular set are constructed in form of an explicit integral expression with respect to a singular metric. They arise as projections of a class of bicharacteristic curves of the Grushin-type operator. Again our method uses an isoperimetric interpretation of sub-Riemannian geodesics on S^3 and the double fibration (Hopf fibration). The spectrum and analytic continuation of the spectral zeta function of the sub-Laplacian for this case was given in [BF3-08] (see also [Ba-05], [CC2-09]).

In §7, we construct sub-Riemannian structures on S^7 based on the quaternionic structure on $\mathbb{R}^8$. Several operators related to a codimension 3 sub-Riemannian structure on S^7 in the strong sense are defined. Similar to the case of S^3 and for defining a Grushin-type operator we use the Hopf bundle with the one-dimensional quaternion projective line as a base space. However, we remark that there are essential differences between the three- and seven-dimensional setting. In particular, on S^7 we have no elliptic operators corresponding to the horizontal Laplacians defined in the S^3-case. We show that a sub-Riemannian structure on $S^3 \times S^3$ (see Proposition 7.16) and an elliptic operator on the three-dimensional ball (see Proposition 7.9) are induced from the sub-Laplacian on S^7. The eigenvalue problems of sub-Laplacians on S^7, $S^3 \times S^3$ and an elliptic operator on the three-dimensional ball with the Dirichlet boundary condition will be discussed elsewhere. In [BF3-08] we have determined the spectrum of a sub-Laplacian on S^7 corresponding to a codimension one sub-Riemannian structure and partly we have discussed the analytic continuation of its spectral zeta function.

In §8, we explain the standard sub-Riemannian structure on nilpotent Lie groups. As a typical 3-step case we specialize to such kind of structures and related Grushin-type operators on the *Engel group* in §9. Solutions of the bicharacteristic flow for a Grushin-type operator of step three are presented. However, it is not clear whether we can construct the heat kernel of the sub-Laplacian on the Engel group in an integral form by a method similar the 2-step nilpotent cases.

In §10, we explain the notion of free nilpotent Lie groups of step 2. They can be considered as a universal type, since any 2-step nilpotent Lie group is isomorphic to a quotient of such a group by a subgroup of the center. The heat kernels for any 2-step nilpotent Lie groups are obtained via a fiber integration of the heat kernel of a free nilpotent Lie group.

In §11, we give an explicit expression of the heat kernels for nilpotent Lie groups (of 2-step) dimension less than 6 and of non-decomposable type and their Grushin-type operators.

In §12 and §13, the heat kernel trace of a sub-Laplacian on a five- and six-dimensional nilmanifold is calculated based on the data given in §11 and by fixing typical lattices in the free nilpotent Lie group of dimension 5 and 6, respectively. Although we provide the details of these calculations only for the five-dimensional case, the method we employ is the Selberg trace formula calculation (see Appendix D) and can be applied to the six-dimensional case, as well.

In the final section §14, we analyze the spectral zeta-function for the sub-Laplacians on a five- and six-dimensional compact nilmanifold. We show that in both cases these spectral zeta-functions are meromorphic on the complex plane with only one simple pole on the positive real axis and we give explicit values of the corresponding residues (see Remark 15.1). This follows from the short time asymptotic expansion of the corresponding heat kernel traces.

In particular, and similar to the case of elliptic operators on closed manifolds, complex analyticity of the spectral zeta function in a zero-neighbourhood follows and in a standard way the regularized determinants can be defined from the derivative of the spectral zeta-function at $s = 0$. By different methods, it is possible to calculate an integral form of the spectral zeta-functions above. This leads to an expression of its derivative in $s = 0$ and therefore gives the zeta-regularized determinant of the corresponding operators. The details will be given in a forthcoming paper (see [BFI]).

In the Appendices A-C, we sum up a general theorem for constructing a fundamental solution of a degenerate parabolic equation by means of Weyl calculus. This guarantees the existence of the heat kernel and it includes the class of our sub-Laplacians (see [II1-79], [II2-81], [Mu1-82]). Note that the existence of the heat kernels also is guaranteed by the functional-analytic framework based on the essentially self-adjointness of the sub-Laplacians on sub-Riemannian manifolds with a metric that can be extended to a complete Riemannian metric, cf. [St-86]. In fact, all our cases satisfy this condition. Finally, in Appendix D we recall the algebraic and geometric aspects of the Selberg trace formula.

2. Sub-Riemannian manifolds

First, we recall the notion of a sub-Riemannian structure. The book [Mo2-02] treats various topics on sub-Riemannian geometry, starting from the basic definitions to various geometric aspects. Also the recent books [CC1-09], [CC2-09], [CCFI-10] and the present text deal with similar aspects. In particular, in the last reference the authors discuss the construction of heat kernels for various hypo-elliptic operators by different methods.

Definition 2.1. A manifold M is called a *sub-Riemannian manifold* if its tangent bundle $T(M)$ has a sub-bundle $\mathcal{H}$ such that all linear combinations of the vector fields taking values in the sub-bundle $\mathcal{H}$ and a finite numbers of their Lie brackets span the whole tangent space at each point. This property of the sub-bundle $\mathcal{H}$ is called *bracket generating*. Usually we equip the sub-bundle with metric in a suitable way.

A sub-bundle $\mathcal{H}$ having the bracket generating property is also called *non-holonomic* and the number $\dim M - \dim \mathcal{H}$ gives the *co-dimension of the sub-Riemannian structure.*

Remark 2.2.

1. If $\mathcal{H}$ is a non-holonomic sub-bundle, then any sub-bundle including $\mathcal{H}$ is also non-holonomic.

2. If there is no non-holonomic sub-bundle properly included in a non-holonomic sub-bundle $\mathcal{H}$, then we call the sub-Riemannian structure defined by this sub-bundle *minimal*.
3. The minimal number plus one of the bracket order of vector fields with values in a non-holonomic sub-bundle $\mathcal{H}$, which is needed to span the whole tangent space, is called the *step of the sub-Riemannian structure.*

If we consider a manifold as configuration space of a physical system, then a Riemannian structure means that any state can move to any direction, so that any two states can be joined by a geodesic. However, if the system is sub-Riemannian, classical states can move only along the curves whose tangent vectors are in the given sub-bundle $\mathcal{H}$ (the horizontal directions). Even so, they might not be directly joined by a geodesic, the bracket generating property allows them to be reached from any state through another state. In fact, we have:

Theorem 2.3 (Chow's Theorem [Ch-39]). *Any two points on a sub-Riemannian manifold can be joined by a piece-wise smooth horizontal curve.*

As we discussed in the introduction, opposite to the sub-Riemannian structure, if a physical system is not sub-Riemannian, then we have an integrable system (a foliation structure) which does not coincide with the whole tangent bundle. Curves having tangent vectors in this integrable system remain in the connected leaf. Hence a Chow type theorem does not hold.

In this paper we always require two additional conditions (A-1) and (A-2) of the non-holonomic sub-bundle $\mathcal{H}$.

(A-1) *The sub-bundle is trivial as a vector bundle.* Then we can take globally defined and nowhere vanishing vector fields $\{X_i\}_{i=1}^{\dim \mathcal{H}}$, which are linearly independent at each point of the manifold M and satisfy the *Hörmander condition.* This guarantees that the second-order operator

$$\sum_{i=1}^{\dim \mathcal{H}} X_i^* X_i$$

is hypo-elliptic. (The adjoint operation $*$ can be introduced by fixing a suitable inner product on the function space $C_0^\infty(M)$.) See [Hö1-67].

(A-2) *There exists a volume form Ω_M on the manifold M such that the vector fields $\{X_i\}$ trivializing the sub-bundle $\mathcal{H}$ are all skew-symmetric with respect to Ω_M:*

$$\int_M f(x)X_i(g)(x)\,\Omega_M(x) = -\int_M X_i(f)(x)g(x)\,\Omega_M(x), \quad f,\, g \in C_0^\infty(M).$$

In this case we call this sub-Riemannian structure *trivializable* or sub-Riemannian structure *in a strong sense* and the formally symmetric operator

$$\Delta^{\text{sub}} = -\sum_{i=1}^{\dim \mathcal{H}} {X_i}^2$$

is called the *sub-Laplacian*. Usually we equip the sub-bundle $\mathcal{H}$ with a metric in such a way that the vector fields $\{X_i\}$ are orthonormal at each point.

Remark 2.4.

1. Under the assumption (A-1) we can construct a volume form in a natural way, cf. [Mo2-02], [CCFI-10]. However, the existence of skew-symmetric vector fields trivializing the non-holonomic sub-bundle can not be deduced. In the examples we deal with in this paper, the volume form which we assume to exist coincides with this natural form (apart from a constant).
2. Contact manifolds are typical sub-Riemannian manifolds, but rather rarely they are trivializable.

Examples of manifolds which have a sub-Riemannian structure in the strong sense are:

1. Nilpotent Lie groups,
2. Compact Lie groups,
3. Non-compact semi-simple Lie groups with a finite center,
4. Direct products of a semi-simple Lie group (compact or non-compact),
5. S^7 carries a sub-Riemannian structure in the strong sense of codimension three and step 2, which is minimal.
6. All odd-dimensional spheres carry a contact structure. Based on the famous result by Adams [Adm-62] we know that most of them are not in the strong sense. Besides S^3 and S^7 which are trivializable the spheres S^{15}, S^{23} and S^{31} are the only candidates for carrying a sub-Riemannian structure in the strong sense of codimension ≥ 2.

   We will discuss some aspects of the construction of such sub-Riemannian structures on the seven-dimensional sphere S^7 in §7 (see also [BF3-08]).

We do not explain the sub-Riemannian structure for all these examples in general. Lie group cases are described in terms of the Lie algebra structure (nilpotency or root space decompositions). So we have a left (or right) invariant sub-Riemanian structure of step 2 and codimension one. As typical cases of the examples 1, 2 and 3 (nilpotent, compact simple and non-compact simple) we deal with the lowest-dimensional cases (Heisenberg group, $S^3 \cong SU(2)$ and $SL(2,\mathbb{R})$). The sphere S^7 provides a typical case for example 4.

Under the assumptions (A-1) and (A-2) and an additional assumption (G-1) below, we explain the notion of a *Grushin-type* operator.

Let a surjective map $\varphi\colon M \longrightarrow N$ be a submersion and assume that the non-holonomic sub-bundle $\mathcal{H}$ defines a sub-Riemannian structure on M in the strong sense. Also we assume that this non-holonomic sub-bundle is trivialized by vector fields $\{X_i\}_{i=1}^{\dim \mathcal{H}}$ in such a way that each X_i can be descended to the manifold N by the map φ. This means that

$$\text{(G-1)} \qquad d\varphi_x(X_i) = d\varphi_{x'}(X_i) \text{ if } \varphi(x) = \varphi(x').$$

Then the vector fields $\{d\varphi(X_i)\}_{i=1}^{\dim \mathcal{H}}$ on the manifold N satisfy the bracket generating property. In particular:

Proposition 2.5. *Let φ be a proper map*[1] *and X_i be skew-symmetric with respect to a volume form Ω_M. Then $d\varphi(X_i)$ is also skew-symmetric with respect to the volume form $\varphi_*(\Omega_M)$.*

Proof.

$$\begin{aligned}\int_N d\varphi(X_i)(f)\cdot g\,\varphi_*(\Omega_M) &= \int_M \varphi^*\big(d\varphi(X_i)(f)\big)\cdot\varphi^*(g)\,\Omega_M\\ &= \int_M X_i\big(\varphi^*(f)\big)\cdot\varphi^*(g)\,\Omega_M\\ &= -\int_M \varphi^*(f)\cdot X_i\big(\varphi^*(g)\big)\,\Omega_M\\ &= -\int_M \varphi^*(f)\cdot\varphi^*\big(d\varphi(X_i)(g)\big)\,\Omega_M\\ &= -\int_N f\cdot d\varphi(X_i)(g)\,\varphi_*(\Omega_M),\quad f \text{ or } g\in C_0^\infty(N).\end{aligned}$$ □

Remark 2.6. In case the fibers of the submersion $\varphi\colon M\to N$ are not compact, then we often have a volume form Ω_N on N and a $(\dim M-\dim N)$-form θ on M such that

$$\theta\wedge\varphi^*(\Omega_N)=\Omega_M$$

and with respect to the volume form Ω_N the descended vector fields $\{d\varphi(X_i)\}$ are skew-symmetric (see examples in §4, §7 and §10). If the map φ is proper, then there is a $(\dim M-\dim N)$-form θ on M such that $\theta\wedge\varphi^*\big(\varphi_*(\Omega_M)\big)=\Omega_M$ (at least, if M and N both are orientable).

Definition 2.7. Under the assumptions (A-1), (A-2) and (G-1), we call the operator

$$\mathcal{G}=-\sum_i\big(d\varphi(X_i)\big)^2$$

on N a *Grushin-type operator.*

The operator $\mathcal{G}$ is hype-elliptic, since all brackets $[X_i,X_j]$, $[X_i,\ [X_j,X_k]]$, … of the vector fields $\{X_i\}$ descend through the map φ. This means that the vector fields$\{d\varphi(X_i)\}$ satisfy the bracket generating property (= Hörmander condition). Assume that

(G-2) $$\dim\mathcal{H}=\dim N,$$

and denote by $\mathcal{S}$ the subset on which the kernel of the differential $d\varphi$ and the subbundle $\mathcal{H}$ have a non-trivial intersection. It holds $\varphi^{-1}(\varphi(\mathcal{S}))=\mathcal{S}$ and we assume that $N\backslash\varphi(\mathcal{S})$ is open dense. In this case we introduce a Riemannian metric in N in such a way that:

[1]That is, the inverse image by φ of any compact set in N is compact.

Definition 2.8. $\{d\varphi(X_i)\}_{i=1}^{\dim N}$ are orthonormal at each point in $N \backslash \varphi(\mathcal{S})$, and we call the manifold N with this Riemannian metric a *singular Riemannian manifold* (in case $\mathcal{S} \neq \phi$) and the set $\varphi(\mathcal{S})$ the *singular set* (or singular manifold if it is a non-empty manifold).

Remark 2.9. The Laplacian with respect to the (singular) Riemannian metric being described in Definition 2.8 above can be considered on the outside of the possible singular set. In general, this Laplacian and the Grushin-type operator do not coincide. However, their principal symbols always coincide. Hence the geodesics with respect to the (singular) Riemannian metric are projections of bicharacteristic curves of the Laplacian at least outside of the singular set. In particular, the principal symbol of the Laplacian can be seen as a function defined on all the cotangent bundle.

In sections §4 *and* §6*, we construct geodesics connecting two points on the singular set via an isoperimetric interpretation of sub-Riemannian geodesics together with Stoke's theorem and a double fibration in particular examples.*

3. Bicharacteristic flow of Grushin-type operator

We discuss a relation between the bicharacteristic flows of a sub-Laplacian and a Grushin-type operator.

Let M be a sub-Riemannian manifold with a non-holonomic sub-bundle $\mathcal{H}$ and nowhere vanishing vector fields $\{X_i\}_{i=1}^{\dim \mathcal{H}}$ which trivialize $\mathcal{H}$. Let $\varphi\colon M \to N$ be a surjective submersion such that the conditions (A-1), (A-2) and (G-1) with respect to the vector fields $\{X_i\}$ are fulfilled. We denote the singular set by $\mathcal{S} \subset M$, if it is non-empty. Also we assume that $\dim N = \dim \mathcal{H}$ $(= n)$ and that there are volume forms Ω_M on M, Ω_N on N and a ℓ-form θ ($\ell = \dim M - \dim N$) on M such that $\theta \wedge \varphi^*(\Omega_N) = \Omega_M$. With respect to these volume forms Ω_M and Ω_N we assume that the vector fields X_i and $d\varphi(X_i)$, respectively, are skew-symmetric. Since there exists no natural global map

$$T^*(M) \longrightarrow T^*(N)$$

making the diagram

$$\begin{array}{ccc} T^*(M) & \xrightarrow{\pi_M} & M \\ \big\downarrow & & \big\downarrow \varphi \\ T^*(N) & \xrightarrow{\pi_N} & N \end{array}$$

commutative, there is no global correspondence between the bicharacteristic flows of the sub-Laplacian

$$\Delta^{\text{sub}} = -\sum_{i=1}^{n} {X_i}^2$$

on M and the Grushin-type operator

$$\mathcal{G} = -\sum_{i=1}^{n} \big(d\varphi(X_i)\big)^2$$

on N. So we consider each bi-characteristic curve locally:

Let $x \in N$ and $y \in M$ such that $\varphi(y) = x$ and take local coordinates

$$\big(U; x_1, x_2, \ldots, x_n\big)$$

about a point x. Then by the implicit function theorem we can find local coordinates

$$\big(W \cong U \times V; x_1, x_2, \ldots, x_n; y_1, y_2, \ldots, y_\ell\big)$$

$(n + \ell = \dim M)$ about the point y such that

$$\varphi(x_1, x_2, \ldots, x_n; y_1, y_2, \ldots, y_\ell) = (x_1, x_2, \ldots, x_n).$$

Let $(\xi,\ \eta)$ be the dual coordinates of (x, y) in W,

$$(x, y; \xi, \eta) \longleftrightarrow \sum \xi_i dx_i + \sum \eta_j dy_j \in T^*(W),$$

then

$$(x, \xi) \longleftrightarrow \sum \xi_i dx_i \in T^*(U).$$

are the dual coordinates in $T^*(U)$. Let $\mathbb{L} = \{(x, y; \xi, 0) \ \in \ T^*(W)\}$ and $\mathcal{L} : \mathbb{L} \to T^*(U)$ be the map

$$\mathcal{L} : (x, y; \xi, 0) \mapsto (x, \xi) \in T^*(U).$$

Then $\mathcal{L}$ should be understood as the composition

$$\mathcal{L} : \mathbb{L} = T^*(U) \times V \hookrightarrow T^*(U) \times T^*(V) \cong T^*(U \times V) \xrightarrow{\text{projection}} T^*(U)$$

and the diagram

$$\begin{array}{ccc} U \times V & \xleftarrow{\ \pi_M\ } & \mathbb{L} \subset T^*(U \times V) \\ {\scriptstyle\varphi}\big\downarrow & & \big\downarrow{\scriptstyle\mathcal{L}} \\ U & \xleftarrow{\ \pi_N\ } & T^*(U) \end{array}$$

is commutative.

Theorem 3.1. *Let $\{\gamma(t)\}$ be any local bicharacteristic curve of the Grushin-type operator included in $T^*(U)$. Then there exists a bicharacteristic curve $\{\tilde{\gamma}(t)\}$ in $\mathbb{L}$ such that $\mathcal{L}(\tilde{\gamma}(t)) = \gamma(t)$. There are many such curves, but if we choose the initial condition $\tilde{\gamma}(0) = (\gamma(0); \xi_0, 0)$, then such a curve is unique. We call them* lifts of the curve *$\{\gamma(t)\}$. So any local geodesic curve $\{g(t)\}$ outside of $\varphi(\mathcal{S})$ is the image of a bicharacteristic curve of the sub-Laplacian in $\mathbb{L}$ by the map $\varphi \circ \pi_M = \pi_N \circ \mathcal{L}$.*

Remark 3.2. There exist geodesic curves (abnormal geodesic) in a sub-Riemannian manifold which are not a projection of any bicharacteristic curve of a sub-Laplacian. However, all geodesic curves in our examples will be such a projection. In our cases and on the subset $N \backslash \varphi(\mathcal{S})$ it is enough to consider only this type of curves, since the principal symbol of the Grushin-type operator and the metric tensor coincide according to the definition of the singular metric on N. It is described in [Mo2-02] (p. 70) that, if a sub-Riemannian structure is *fat*, then any sub-Riemannian geodesics come from a bicharacteristic curve of the sub-Laplacian. Our examples below always satisfy the *fatness* condition and we will consider only curves on the sub-Riemannian manifold induced from a bicharacteristic curve. See [Mo1-94, LS-95] for the case of an abnormal geodesic.

Proof. We express the vector fields in local coordinates:

$$X_k = \sum_{i=1}^{n} a_i{}^{(k)}(x)\frac{\partial}{\partial x_i} + \sum_{j=1}^{\ell} b_j{}^{(k)}(x,y)\frac{\partial}{\partial y_j},$$

$$d\varphi(X_k) = \sum_{i=1}^{n} a_i{}^{(k)}(x)\frac{\partial}{\partial x_i}.$$

Then the principal symbols of the sub-Laplacian and the Grushin-type operator are given by

$$\sigma(\Delta^{\mathrm{sub}})(x,y;\xi,\eta) = \sum_{k=1}^{n}\Big(\sum_{i=1}^{n} a_i{}^{(k)}(x)\xi_i + \sum_{j=1}^{\ell} b_j{}^{(k)}(x,y)\eta_j\Big)^2,$$

$$\sigma(\mathcal{G})(x,\xi) = \sum_{k=1}^{n}\Big(\sum_{i=1}^{n} a_i{}^{(k)}(x)\,\xi_i\Big)^2,$$

and the Hamilton vector fields with the Hamiltonian given by the principal symbols of the sub-Laplacian and the Grushin-type operator are expressed in the local coordinates by

$$\begin{aligned}
\mathcal{X}_{\sigma(\Delta^{\mathrm{sub}})} &= \sum_{\alpha=1}^{n}\Big[\sum_{k=1}^{n}\Big(\sum_{i=1}^{k} a_i{}^{(k)}(x)\xi_i + \sum_{j=1}^{\ell} b_j{}^{(k)}(x,y)\eta_j\Big)\cdot\Big(a_\alpha{}^{(k)}(x)\Big)\Big]\frac{\partial}{\partial x_\alpha}\\
&+ \sum_{\beta=1}^{\ell}\Big[\sum_{k=1}^{n}\Big(\sum_{i=1}^{k} a_i{}^{(k)}(x)\xi_i + \sum_{j=1}^{\ell} b_j{}^{(k)}(x,y)\eta_j\Big)\cdot\Big(b_\beta{}^{(k)}(x,y)\Big)\Big]\frac{\partial}{\partial y_\beta}\\
&- \sum_{\alpha=1}^{n}\Big[\sum_{k=1}^{n}\Big(\sum_{i=1}^{k} a_i{}^{(k)}(x)\xi_i + \sum_{j=1}^{\ell} b_j{}^{(k)}(x,y)\eta_j\Big)\\
&\qquad\times\Big(\sum_{i=1}^{k}\frac{\partial a_i{}^{(k)}(x)}{\partial x_\alpha}\xi_i + \sum_{j=1}^{\ell}\frac{\partial b_j{}^{(k)}(x,y)}{\partial x_\alpha}\eta_j\Big)\Big]\frac{\partial}{\partial \xi_\alpha}\\
&- \sum_{\beta=1}^{n}\Big[\sum_{k=1}^{n}\Big(\sum_{i=1}^{k} a_i{}^{(k)}(x)\xi_i + \sum_{j=1}^{\ell} b_j{}^{(k)}(x,y)\eta_j\Big)\Big(\sum_{j=1}^{\ell}\frac{\partial b_j{}^{(k)}(x,y)}{\partial y_\beta}\eta_j\Big)\Big]\frac{\partial}{\partial \eta_\beta},
\end{aligned}$$

$$\mathcal{X}_{\sigma(\mathcal{G})} = \sum_{\alpha=1}^{n}\Big[\sum_{k=1}^{n}\Big(\sum_{i=1}^{k} a_i{}^{(k)}(x)\xi_i\Big)\cdot\Big(a_\alpha{}^{(k)}(x)\Big)\Big]\frac{\partial}{\partial x_\alpha} - \sum_{\alpha=1}^{n}\Big[\sum_{k=1}^{n}\Big(\sum_{i=1}^{k} a_i{}^{(k)}(x)\xi_i\Big)\Big(\sum_{i=1}^{k}\frac{\partial a_i{}^{(k)}(x)}{\partial x_\alpha}\xi_i\Big)\Big]\frac{\partial}{\partial \xi_\alpha}.$$

From these expressions, it is apparent that the vector field $\mathcal{X}_{\sigma(\Delta^{\mathrm{sub}})}$ cannot be descended to $T^*(U)$, even locally, without some additional vanishing conditions on the coefficients $b_j{}^{(k)}$. The restriction of the Hamilton vector field $\mathcal{X}_{\sigma(\Delta^{\mathrm{sub}})}$ to $\mathbb{L}$ is given by

$$\begin{aligned}\mathcal{X}_{\sigma(\Delta^{\mathrm{sub}})}(x,y;\xi,0) &= \sum_{\alpha=1}^{n}\Big[\sum_{k=1}^{n}\Big(\sum_{i=1}^{k} a_i{}^{(k)}(x)\xi_i\Big)\cdot\Big(a_\alpha{}^{(k)}(x)\Big)\Big]\frac{\partial}{\partial x_\alpha}\\ &+ \sum_{\beta=1}^{\ell}\Big[\sum_{k=1}^{n}\Big(\sum_{i=1}^{k} a_i{}^{(k)}(x)\xi_i\Big)\cdot\Big(b_\beta{}^{(k)}(x,y)\Big)\Big]\frac{\partial}{\partial y_\beta}\\ &- \sum_{\alpha=1}^{n}\Big[\sum_{k=1}^{n}\Big(\sum_{i=1}^{k} a_i{}^{(k)}(x)\xi_i\Big)\Big(\sum_{i=1}^{k}\frac{\partial a_i{}^{(k)}(x)}{\partial x_\alpha}\xi_i\Big)\Big]\frac{\partial}{\partial \xi_\alpha}.\end{aligned}$$

From this expression we see that the vector field $\mathcal{X}_{\sigma(\Delta^{\mathrm{sub}})}$ on $\mathbb{L}$ is tangential to $\mathbb{L}$ and can be descended to $T^*(U)$ by the map $\mathcal{L}$. The descended vector field coincides with the Hamilton vector field $\mathcal{X}_{\sigma(\mathcal{G})}$. This implies that an integral curve of the Hamilton vector field $\mathcal{X}_{\sigma(\mathcal{G})}$ in $T^*(U)$ (i.e., a local bicharacteristic curve of the Grushin operator in $T^*(U)$) has a unique lift to a bicharacteristic curve of the sub-Laplacian when we fix the initial point $(\gamma(0);\xi_0,0)$ in $\mathbb{L}$. □

Remark 3.3. We consider two kinds of *lifts of a curve* in this article. One is in the sense of the above theorem and another type is in the sense of a connection, i.e., horizontal lifts of a curve in the base space of a principal bundle and appears in sections §4, §5 and §6.

Remark 3.4. It can be easily checked that in the proof of the above theorem we only use the property (G-1) for the (local) correspondence of the bicharacteristic curves. In this article we treat examples satisfying the conditions (A-1), (A-2), (G-1) and often condition (G-2) which is needed to prove that the geodesics are realized as the projection of bicharacteristic curves.

We restate the above theorem in an extended form. Let U be an open set in N and assume that there exists a manifold F and a diffeomorphism $\mathcal{D}\colon U\times F\to\varphi^{-1}(U)$ such that $\varphi\circ\mathcal{D}=\pi_U$ = projection onto U. Then through the identification

$$T^*(U)\times F\subset T^*(U)\times T^*(F)\cong T^*(U\times F)\xleftarrow{(d\mathcal{D})^*}T^*\big(\varphi^{-1}(U)\big),$$

let $\mathcal{F}$ be the image of $T^*(U)\times F$ in $T^*\big(\varphi^{-1}(U)\big)$.

Corollary 3.5. *The Hamilton vector field* $\mathcal{X}_{\sigma(\Delta^{\mathrm{sub}})}$ *restricted to a sub-manifold* $\mathcal{F}$ *is tangential to* $\mathcal{F}$*. It can be descended to* $T^*(U)$ *and* $d\varphi\left(\mathcal{X}_{\sigma(\Delta^{\mathrm{sub}})}\big|_{\mathcal{F}}\right)$ *coincides with the Hamilton vector field* $\mathcal{X}_{\sigma(\mathcal{G})}$ *on* $T^*(U)$*. Hence bicharacteristic curves in* $\mathcal{F}$ *are mapped to bicharacteristic curves in* $T^*(U)$ *of the Grushin-type operator* $\mathcal{G}$*.*

By Theorem 3.1, Corollary 3.5 and an isoperimetric interpretation of sub-Riemannian geodesics through double fibrations, we can describe geodesics connecting two points on the image of the singular manifold $\varphi(\mathcal{S})$ in the case of $M =$ *Heisenberg group* and S^3 ($N = \mathbb{R}^2$ and S^2).

4. Heisenberg group case

The classical *Grushin operator* is obtained in the way explained in the last section. We deduce various Grushin-type operators by fixing subgroups in the three-dimensional Heisenberg group H_3. Geodesic curves on the Grushin plane connecting two singular points are determined via an isoperimetric interpretation of sub-Riemannian geodesics on H_3 (see [AB-08]) and a double fibration structure. In these cases we can solve the Hamilton system of the bicharacteristic curves explicitly. As a model case it gives us a geometric aspect of sub-Riemannian geodesics and a relation between singular geodesics defined by a Grushin operator in the framework of a double fibration.

4.1. Grushin-type operators

Let H_3 be the Heisenberg group of dimension three identified with $\mathbb{R}^3$, where the product is given by the formula

$$\begin{aligned}\mathbb{R}^3 \times \mathbb{R}^3 \ni <(x,y,z),(\tilde{x},\tilde{y},\tilde{z})> &\longmapsto (x,y,z) * (\tilde{x},\tilde{y},\tilde{z}) \\ &= \big(x+\tilde{x}, y+\tilde{y}, z+\tilde{z}+(x\tilde{y}-\tilde{y}x)/2\big) \in \mathbb{R}^3.\end{aligned}$$

The left-invariant vector fields X, Y and Z are defined as

$$X = \frac{\partial}{\partial x} - \frac{y}{2}\frac{\partial}{\partial z}, \qquad Y = \frac{\partial}{\partial y} + \frac{x}{2}\frac{\partial}{\partial z}, \qquad \text{and} \qquad Z = \frac{\partial}{\partial z}.$$

The bracket relation $[X,Y] = Z$ implies that the sub-bundle $\mathcal{H}$ spanned by $\{X,Y\}$ defines a left-invariant sub-Riemannian structure on H_3 with the sub-Riemannian metric:

$$<X,Y> = 0, \quad <X,X> = <Y,Y> = 1,$$

and we have a sub-Laplacian

$$\Delta_{H_3}^{\mathrm{sub}} = -(X^2+Y^2) = -\left(\frac{\partial}{\partial x} - \frac{y}{2}\frac{\partial}{\partial z}\right)^2 - \left(\frac{\partial}{\partial y} + \frac{x}{2}\frac{\partial}{\partial z}\right)^2,$$

which is symmetric with respect to the volume form

$$dx \wedge dy \wedge dz.$$

Of course this volume form coincides with the Haar measure of the group H_3.

Let $N_Y = \{(0,y,0) \mid y \in \mathbb{R}\}$ be the subgroup generated by Y and consider the left coset space $\pi_L \colon H_3 \to N_Y \backslash H_3$ which is realized as

$$\pi_L : H_3 \cong \mathbb{R}^3 \to N_Y \backslash H_3 \cong \mathbb{R}^2,$$
$$\pi_L(x,y,z) = (u,v) = \left(x, z + \frac{xy}{2}\right).$$

The left-invariant vector fields X and Y are descended by the projection map π_L to vector fields

$$d\pi_L(X) = \frac{\partial}{\partial u}, \quad d\pi_L(Y) = u\,\frac{\partial}{\partial v},$$
$$\text{Grushin operator} = \mathcal{G} = -\left(\frac{\partial^2}{\partial u^2} + u^2\frac{\partial^2}{\partial v^2}\right).$$

It is clear that this operator is symmetric with respect to the volume form $du \wedge dv$ and we have $\pi_L^*(du \wedge dv) \wedge dy = dx \wedge dz \wedge dy$, where dy is a left N_Y-invariant one-form on H_3. In this case, let $\mathcal{S} = \{(0,y,z) \mid y,z \in \mathbb{R}\}$. Then the subset $\pi_L(\mathcal{S})$ on which $\pi_L(X)$ and $\pi_L(Y)$ are not linearly independent is given by $\{(0,v) \mid v \in \mathbb{R}\}$, i.e., it is the v-axis. On $N_Y \backslash H_3 \cong \mathbb{R}^2$ we define a singular metric g_G by

$$g_G = \begin{pmatrix} g\left(\frac{\partial}{\partial u}, \frac{\partial}{\partial u}\right) & g\left(\frac{\partial}{\partial u}, \frac{\partial}{\partial v}\right) \\ g\left(\frac{\partial}{\partial v}, \frac{\partial}{\partial u}\right) & g\left(\frac{\partial}{\partial v}, \frac{\partial}{\partial v}\right) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1/u^2 \end{pmatrix}.$$

We call the plane $N_Y \backslash H_3 \cong \mathbb{R}^2$ with this singular metric the *Grushin plane*. Now, we consider new coordinates on H_3,

$$\mathbb{R} \times \mathbb{R}^2 \ni (t,u,v) \xrightarrow{\mathcal{D}} (x,y,z) = \left(u, t, v - \frac{tu}{2}\right) \in \mathbb{R}^3 \cong H_3. \tag{4.1}$$

Then we have $\pi_L \circ \mathcal{D}(t,u,v) = (u,v)$ which shows that we have a global splitting of H_3 compatible with the projection π_L as described in Corollary 3.5.

In these new coordinates (t,u,v) and their dual coordinates $(t,u,v;\delta,\alpha,\beta) \in \mathbb{R}^3 \times \mathbb{R}^3 \cong T^*(H_3)$, the principal symbol $\sigma(\Delta_{H_3}^{\mathrm{sub}})$ of the sub-Laplacian is given by

$$\sigma(\Delta_{H_3}^{\mathrm{sub}})(t,u,v;\delta,\alpha,\beta) = \alpha^2 + (\delta + u\beta)^2$$

and the Hamilton vector field $\mathcal{X}_{\sigma(\Delta^{\mathrm{sub}})}$ is expressed as

$$\mathcal{X}_{\sigma(\Delta^{\mathrm{sub}})} = \alpha\frac{\partial}{\partial u} + (\delta + u\beta)\frac{\partial}{\partial t} + (\delta + u\beta)u\frac{\partial}{\partial v} - (\delta + u\beta)\beta\frac{\partial}{\partial \alpha}.$$

Let $\mathbb{L}$ be the following sub-manifold in $T^*(H_3)$,

$$\mathbb{L} = \{(t,u,v;0,\alpha,\beta) \in \mathbb{R}^3 \times \mathbb{R}^3\} \subset T^*(H_3). \tag{4.2}$$

Then the restriction of the vector field $\mathcal{X}_{\sigma(\Delta^{\mathrm{sub}})}$ to $\mathbb{L}$ is given by

$$\mathcal{X}_{\sigma(\Delta^{\mathrm{sub}})} = \alpha\frac{\partial}{\partial u} + u\beta\frac{\partial}{\partial t} + u^2\beta\frac{\partial}{\partial v} - u\beta^2\frac{\partial}{\partial \alpha}.$$

Hence it can be descended to the space $T^*(N_Y \backslash H_3) \cong \mathbb{R}^2 \times \mathbb{R}^2$ by the map

$$(t,u,v;0,\alpha,\beta) \longmapsto (u,v;\alpha,\beta). \tag{4.3}$$

The descended vector field is given by

$$\alpha\frac{\partial}{\partial u}+u^2\beta\frac{\partial}{\partial v}-u\beta^2\frac{\partial}{\partial\alpha},$$

and it coincides with the Hamilton vector field where the Hamiltonian is the principal symbol of the Grushin operator ($=\alpha^2+u^2\beta^2$). In this case, all integral curves of $\mathcal{X}_{\sigma(\mathcal{G})}$ come from the bicharacteristic curves of $\mathcal{X}_{\sigma(\Delta^{\mathrm{sub}}_{H_3})}$ passing through the sub-manifold $\mathbb{L}$.

4.2. Isoperimetric interpretation and double fibration: Grushin plane case

We construct geodesic curves connecting two points on the singular set of the Grushin plane $N_Y\backslash H_3$.

Let $N_Z=\big\{(0,0,z)\ \big|\ z\in\mathbb{R}\big\}=$ *the center of the Heisenberg group*. Then the vector fields X and Y can be descended to the quotient space $\pi_R\colon H_3\to H_3/N_Z$ and the resulting vector fields on $\pi_R\colon H_3\to H_3/N_Z\cong\mathbb{R}^2$, $(x,y,z)\mapsto\pi_R(x,y,z)=(x,y)$, are

$$d\pi_R(X)=\frac{\partial}{\partial x}\quad\text{and}\quad d\pi_R(Y)=\frac{\partial}{\partial y}.$$

Hence, in this case the Grushin-type operator is just the Euclidean Laplacian and there are no singular points. The metric we install on H_3/N_Z by assuming that $\pi_R(X)$ and $\pi_R(Y)$ are orthonormal, is the standard Euclidean metric.

Remark 4.1. Note that the left multiplication of the group H_3 is isometric with respect to this sub-Riemannian metric and induces the parallel displacement on the plane.

The invariance of the two vector fields X and Y under the action of the group $N_Z=\{e^{tZ}\}_{t\in\mathbb{R}}=\big\{(0,0,t)\ \big|\ t\in\mathbb{R}\big\}$ enables us to define a connection on the principal bundle,

$$\pi_R\colon H_3\to H_3/\{(0,0,t)\}\cong\mathbb{R}^2$$

with the horizontal subspace $\mathcal{H}=[\{X,Y\}]$. With this connection, let

$$\mathbb{R}\ni s\mapsto\tilde{\gamma}(s)=\big(x(s),y(s),z(s)\big)\in H_3,$$
$$\dot{\tilde{\gamma}}(s)=\dot{x}(s)\frac{\partial}{\partial x}+\dot{y}(s)\frac{\partial}{\partial y}+\dot{z}(s)\frac{\partial}{\partial z}\in\mathcal{H}$$

be a horizontal curve. It can be expressed as

$$\dot{\tilde{\gamma}}(s)=\dot{x}(s)X+\dot{y}(s)Y,$$

and so

$$\dot{z}(s)=\frac{\dot{y}(s)x(s)-\dot{x}(s)y(s)}{2}.$$

The curve $\{\tilde{\gamma}\}$ is realized as the lift of a curve $\big\{\gamma(s)=(x(s),y(s))\big\}$ in the base space $\mathbb{R}^2$ with the same length

$$z(s)=z(0)+\frac{1}{2}\int_0^s\dot{y}(\theta)x(\theta)-\dot{x}(\theta)y(\theta)\,d\theta,\quad\|\tilde{\gamma}\|=\|\gamma\|=\int_0^s\sqrt{\dot{x}(\theta)^2+\dot{y}(\theta)^2}\,d\theta.$$

Let us take any point $(x_1, y_1, z_1) \in H_3$ and let $\{\gamma(s) = (x(s), y(s))\}_{s\in[0,1]}$ be a smooth curve with $\gamma(0) = (0,0)$ and $\gamma(1) = (x_1, y_1)$. We assume that it does not intersect with the line segment $\ell = \{(sx_1, sy_1) \,|\, 0 \le s \le 1\}$ and denote by D_γ the domain in $H_3/N_Z \cong \mathbb{R}^2$ surrounded by the curve $\{\gamma(s)\}$ and the line segment ℓ. Let $\{\tilde{\gamma}(s) = (x(s), y(s), z(s))\}$ be the horizontal lift of the curve $\{\gamma(s)\}$ with the initial point $\tilde{\gamma}(0) = (0,0,0)$. Then we have

$$\begin{aligned}\mathrm{area}(D_\gamma) &= \int_{D_\gamma} dx \wedge dy = \frac{1}{2}\int_{\partial D_\gamma} xdy - ydx \qquad (4.4)\\ &= -\int_0^1 \frac{x(s)\dot{y}(s) - y(s)\dot{x}(s)}{2} ds + \int_0^1 \frac{x(s)\dot{y}(s) - y(s)\dot{x}(s)}{2} ds = z(1).\end{aligned}$$

Hence we have:

Proposition 4.2. *If we choose a suitable curve $\{\gamma\}$, then* $\mathrm{area}(D_\gamma)$*, the area of the domain D_γ, can take any value. This implies that we can connect any point in H_3 with the point $(0,0,0)$ by a smooth horizontal curve. Hence also any two points can be joined by a smooth horizontal curve (see Remark 4.1).*

Moreover, as a solution to the isoperimetric problem on the Euclidean plane for a domain (like D_γ) with a fixed line segment as a part of the boundary, we have:

Proposition 4.3. *We can connect any two points $p_0 = (x_0, y_0, z_0)$ and $p_1 = (x_1, y_1, z_1)$ in H_3 by a smooth geodesic with respect to the sub-Riemannian metric. That is, let a curve $\{(x(s), y(s))\}$ connecting two points $\pi_R(p_0)$ and $\pi_R(p_1)$ be a half-circle with a suitable radius determined by the area (which coincides with the value $z_1 - z_0$, see (4.4)). Then its lift to H_3 is a geodesic with respect to the sub-Riemannian metric connecting the two points p_0 and p_1. In fact, it is a projection onto the space H_3 of a bicharacteristic curve of the sub-Laplacian and there exist many such geodesics connecting two points.*

Again take two points $E_0 = (0,0)$ and $E_1 = (0, v_1)$ $(v_1 > 0)$ on the singular set $\pi_L(\mathcal{S}) = \{(0,v)\} = \pi_L(\{(0,y,z) \mid y,z \in \mathbb{R}\})$ in the Grushin plane, where we cannot define the Riemannian metric. However, assume that there exists a bicharacteristic curve

$$\{c(s) = (u(s), v(s); \alpha(s), \beta(s))\}_{0\le s\le 1}$$

of the Grushin operator $\mathcal{G} = \frac{\partial^2}{\partial u^2} + u^2\frac{\partial^2}{\partial v^2}$ satisfying the conditions

$$u(0) = 0,\ v(0) = 0,\ \text{and}\ u(1) = 0,\ v(1) = v_1,$$

which says that the curve $\{\ell(s) = (u(s), v(s))\}$ is connecting two points E_0 and E_1. So the curve $\{\ell\}$ outside of $\pi_L(\mathcal{S})$ is a geodesic curve with respect to the Grushin metric. The curve $\{c(s)\}$ satisfies the equations

$$\dot{u}(s) = \alpha,\ \dot{v}(s) = u^2\beta,\ \dot{\alpha}(s) = -u\beta^2,\ \dot{\beta}(s) = 0$$

with the initial-boundary conditions

$$u(0) = 0,\ u(1) = 0,\ v(0) = 0,\ v(1) = v_1.$$

Note that $\alpha(0)$ and $\beta(0)$ are not determined uniquely. Now, let $\{\tilde{c}(s)\}$ be a *unique* lift of the curve $\{c(s)\}$,

$$\big\{\tilde{c}(s) = \big(t(s), u(s), v(s); 0, \alpha(s), \beta(s)\big)\big\}_{0\le s\le 1},$$

as a bicharacteristic curve of the sub-Laplacian on the Heisenberg group H_3 in the subspace $\mathbb{L} = \big\{t, u, v\,;\, 0, \alpha, \beta)\big\}$ and starting from the initial point

$$\big(t(0), u(0), v(0)\,;\, 0, \alpha(0), \beta(0)\big) = \big((0, 0, 0\,;\, 0, \alpha(0), \beta(0)\big),$$

(see Theorem 3.1). Let $\{\tilde{\gamma}(s)\} = \big\{\big(d(\mathcal{D}^{-1})\big)^*\big(\tilde{c}(s)\big)\big\}$ be expressed in the coordinates $(x, y, z\,;\, \xi, \eta, \tau)$,

$$x(s) = u(s),\ y(s) = t(s),\ z(s) = v(s) - \frac{u(s)t(s)}{2},$$

$$\xi(s) = \alpha(s) + \frac{t(s)\beta(s)}{2},\ \eta(s) = \frac{u(s)\beta(s)}{2},\ \tau(s) = \beta(s),$$

and denote the curve $\{(x(s), y(s))\}$ by $\{\gamma(s)\}$. Then this curve $\{\gamma(s)\}$ must be a (possibly iterated) *circle* or *iterated circles + a sector of the circle* (with the same radius) starting from the point $(x(0), y(0)) = (u(0), t(0)) = (0, 0)$ and ending at $\gamma(1) = (x(1), y(1)) = (u(1), t(1)) = (0, t(1))$ (we can show this fact by solving the bicharacteristic equation for the sub-Laplacian on H_3). Since $\dot{t}(s) = u(s)\beta(s) = \dot{y}(s)$, and especially $\dot{t}(0) = u(0)\beta(0) = \dot{y}(0) = 0$, $\dot{t}(1) = u(1)\beta(1) = \dot{y}(1) = 0$, this circle or a part of a circle intersects with the v-axis perpendicular at the points $(x(0), y(0)) = (0, 0)$ and $(x(1), y(1)) = (u(1), y(1)) = (0, v_1)$. Therefore, the curve $\{\gamma(s)\}$ is an *iterated circle* or an *iterated circle + a half of the circle*. There is the relation

$$\begin{aligned} z(1) = v(1) - \frac{u(1)t(1)}{2} &= \frac{1}{2}\int_0^1 \dot{y}(r)x(r) - \dot{x}(r)y(r)dr \\ &= \frac{1}{2}\int_{\partial D_\gamma} \gamma^*(xdy - ydx) = \int\int_{D_\gamma} dx \wedge dy \\ &= \{\text{area of } D_\gamma\} \times\ \{\text{number of the iteration of the curve}\}\ = v_1, \end{aligned}$$

where D_γ is a domain surrounded by a iterated circle $\{\gamma(s)\}$ (or in case of a iterated circle + half of the circle, then by a line segment connecting $(0, 0)$ and $(0, t_1)$). It determines the radius of the circle and gives a relation between v_1 and $t(1)$ (for example, $\frac{1}{2}\pi\big(\frac{t(1)}{2}\big)^2 = v_1$). Note that the integral of the one form $xdy - ydx$ on the line segment passing through the origin always vanishes. Here we state the inverse procedure as a proposition:

Proposition 4.4. *First we take circles in the (x, y)-Euclidean plane ($\cong H_3/N_Z$) which pass through the origin and are perpendicular to the y-axis at the origin. These are solutions of the isoperimetric problem on the Euclidean plane. Then we determine the horizontal lifts of the circles starting from the point* $(0, 0, 0)$ *with* *respect to the connection defined by the sub-bundle $\mathcal{H} = [\{X, Y\}]$ of the principal bundle $\pi_R \colon H_3 \to H_3/N_Z \cong \mathbb{R}^2$. These lifts are geodesics with respect to the sub-Riemannian metric and they are projections of bicharacteristic curves of the sub-Laplacian. Next we take their projections to the Grushin plane (u, v) by the map $(x, y, z) \mapsto (u, v) = (x, z + \frac{xy}{2})$. From this we obtain curves connecting $(0, 0)$ and an arbitrary fixed point $(0, v_1)$ on the singular manifold $\pi_L(\mathcal{S})$ ($= v$-axis) in the Grushin plane explicitly. The resulting curves are geodesic curves outside of the singular manifold $\mathcal{S}$.*

Following this procedure we determine such curves explicitly. So let

$$\left\{\gamma(s) = (x(s), y(s)) = \left(\frac{\dot{x}(0)}{\tau}\sin\tau s, \frac{\dot{x}(0)}{\tau}(1 - \cos\tau s)\right)\right\}_{0\le s\le 1}$$

be a circle passing through the origin and being perpendicular to the y-axis at the origin. Since the curves must be an iterated circle or an iterated circle + a half-circle there are two cases:

(I) When $\gamma(1) = (0, 0)$, then $\tau = 2\pi n$ with $n \in \mathbb{Z}$.

For each fixed $n \in \mathbb{Z}$, let

$$\gamma(s) = (x(s), y(s)) = \left(\frac{\dot{x}(0)}{2n\pi}\sin 2n\pi s, \frac{\dot{x}(0)}{2n\pi}\left(1 - \cos 2n\pi s\right)\right).$$

Then the lift $\{\tilde{\gamma}(s) = (x(s), y(s), z(s))\}$ to H_3 is

$$\tilde{\gamma}(s) = \left(\frac{\dot{x}(0)}{2n\pi}\sin 2n\pi s, \frac{\dot{x}(0)}{2n\pi}\left(1 - \cos 2n\pi s\right), \frac{\dot{x}(0)^2 s}{2\cdot 2n\pi} - \frac{\dot{x}(0)^2\sin 2n\pi s}{2\cdot(2n\pi)^2}\right),$$

since $z(s)$ must be given by the integral

$$z(s) = \frac{1}{2}\int_0^s \dot{y}(r)x(r) - \dot{x}(r)y(r)\,dr.$$

Now, from $z(1) = v(1) - \frac{u(1)t(1)}{2}$ we have

$$v_1 = \frac{\dot{x}(0)^2}{2\cdot 2\pi n}, \quad \dot{x}(0) = \pm 2\sqrt{n\pi v_1}.$$

Hence, for each $n \in \mathbb{Z}$, we have the curves

$$\begin{aligned}\left\{c_{2n}^{\pm}(s)\right\} &= \left\{\left(x_{2n}(s), z_{2n}(s) + \frac{x_{2n}(s)y_{2n}(s)}{2}\right)\right\} \\ &= \left\{\left(u_{2n}(s), v_{2n}(s)\right)\right\} = \left\{\left(\pm\sqrt{\frac{v_1}{n\pi}}\sin 2\pi ns, v_1\left(s - \frac{\sin 4n\pi s}{4n\pi}\right)\right)\right\}\end{aligned}$$

connecting the points $(0, 0)$ and $(0, v_1)$ on the singular manifold $\{(0, v)\}$ in the Grushin plane. Note that the curve

$$\{\tilde{\gamma}(s)\} = \left\{(x_{2n}(s), y_{2n}(s), z_{2n}(s)\right\}$$

is the projection of the bicharacteristic curves

$$(x_{2n}(s), y_{2n}(s), z_{2n}(s); \xi_{2n}(s), \eta_{2n}(s), \tau_{2n}(s)),$$

where

$$\xi_{2n}(s) = \xi_{2n}(0) + x_{2n}(s) \cdot \frac{\tau_{2n}(s)}{2} = \dot{x}_{2n}(0) + x_{2n}(s) \cdot \frac{\tau_{2n}(s)}{2},$$
$$\eta_{2n}(s) = \eta_{2n}(0) + x_{2n}(s) \cdot \frac{\tau_{2n}(s)}{2}, \quad \tau_{2n}(s) \equiv 2n\pi$$

with $\eta_{2n}(0) = \dot{y}_{2n}(0) - \dfrac{x_{2n}(0)\tau_{2n}(0)}{2} = 0$. In the coordinates $(t, u, v; \delta, \alpha, \beta)$, it always holds

$$\delta(0) = \eta_{2n}(0) - \frac{x_{2n}(0)\tau_{2n}(0)}{2} = 0$$

and they stay in the sub-manifold $\mathbb{L}$ (see (4.2)). Hence the projection of these bicharacteristic curves by the map (4.3) are bicharacteristic curves of the Grushin operator (see Corollary 3.5).

(II) When $\gamma(1) = (0, t_1)$ with $t_1 > 0$, then $\tau = (2n+1)\pi$ with $n \in \mathbb{Z}$ (the case $t_1 < 0$ can be treated the same way). The resulting curves $\{c_{2n+1}(s)\}$ are given by

$$c^{\pm}_{2n+1}(s) = \left(\pm\sqrt{\frac{2v_1}{(2n+1)\pi}} \sin(2n+1)\pi s, v_1 \left(s - \frac{\sin 2(2n+1)\pi s}{2(2n+1)\pi} \right) \right).$$

5. Sub-Riemannian structure on $SL(2, \mathbb{R})$

On the three-dimensional sphere we have three linearly independent vector fields which trivialize the tangent bundle. Each pair among them defines a sub-Riemannian structure, but they are all essentially the same. In case of the group $SL(2, \mathbb{R})$ we have three types of sub-Riemannian structures. In this section we treat one case among them which leads to the *Poincaré upper half-plane*. We do not construct the geodesics explicitly. This problem will be treated elsewhere together with the study of two other sub-Riemannian structures, see [ABGR-09], [Ju-01].

5.1. A sub-Riemannian structure and Grushin-type operator

Let $SL(2, \mathbb{R})$ denote the group of real 2×2-matrices with determinant 1 and let $\mathfrak{sl}(2, \mathbb{R})$ be its Lie algebra consisting of real 2×2-matrices with trace zero. We fix a basis of $\mathfrak{sl}(2, \mathbb{R})$ as follows:

$$X = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad K = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

Then we have

$$[X, Y] = 2K, \quad [X, K] = 2Y, \quad [Y, K] = -2X.$$

Put

$$\mathfrak{p} = [\{X, Y\}] = \big\{\text{subspace generated by } X \text{ and } Y\big\} \text{ and } \mathfrak{k} = [\{K\}].$$

Then we have a decomposition of

$$\mathfrak{sl}(2,\mathbb{R}) = \mathfrak{p} + \mathfrak{k} \ \text{(Cartan decomposition)}$$

with the properties

$$[\mathfrak{p},\mathfrak{p}] = \mathfrak{k}, \quad [\mathfrak{k},\mathfrak{p}] = \mathfrak{p}, \quad [\mathfrak{k},\mathfrak{k}] = \{0\}.$$

We denote the left-invariant vector fields by $\tilde{X}$, $\tilde{Y}$, $\tilde{K}$, where $\tilde{X}$ is given by

$$\tilde{X}(f)(g) = \frac{df(g\exp tX)}{dt}\Big|_{t=0}, \quad f \in C^\infty\left(SL(2,\mathbb{R})\right),$$

and so forth. At $g = \begin{pmatrix} x & y \\ w & z \end{pmatrix} \in SL(2,\mathbb{R})$, these vector fields are expressed as

$$\begin{aligned}
\tilde{X}_g &= x\frac{\partial}{\partial x} - y\frac{\partial}{\partial y} + w\frac{\partial}{\partial w} - z\frac{\partial}{\partial z}, \\
\tilde{Y}_g &= y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y} + z\frac{\partial}{\partial w} + w\frac{\partial}{\partial z}, \\
\tilde{K}_g &= -y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y} - z\frac{\partial}{\partial w} + w\frac{\partial}{\partial z}.
\end{aligned}$$

The relation $[X,Y] = 2K$ indicates that the sub-bundle $\mathcal{H}_{SL} = \left[\{\tilde{X},\tilde{Y}\}\right]$ in the tangent bundle $T(SL(2,\mathbb{R}))$ spanned by the vector fields $\tilde{X}$ and $\tilde{Y}$ defines a left-invariant sub-Riemannian structure on $SL(2,\mathbb{R})$. We assume that $\tilde{X}$ and $\tilde{Y}$ are *orthonormal* at each point. The sub-Laplacian is expressed as

$$\begin{aligned}
\Delta_{SL}^{\mathrm{sub}} &= -\left(\tilde{X}^2 + \tilde{Y}^2\right) \\
&= -\left(x\frac{\partial}{\partial x} - y\frac{\partial}{\partial y} + w\frac{\partial}{\partial w} - z\frac{\partial}{\partial z}\right)^2 - \left(y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y} + z\frac{\partial}{\partial w} + w\frac{\partial}{\partial z}\right)^2.
\end{aligned}$$

We also have a left-invariant one-form θ_C on $SL(2,\mathbb{R})$,

$$\theta_C = \frac{1}{2}\left(wdx + zdy - xdw - ydz\right), \tag{5.1}$$

which satisfies

$$\theta_C(\tilde{X}) = 0, \quad \theta_C(\tilde{Y}) = 0 \quad \text{and} \quad \theta_C(\tilde{K}) = 1$$

and gives us a volume form Ω_{SL}, i.e.,

$$\Omega_{SL} = \theta_C \wedge d\theta_C$$

never vanishes on $SL(2,\mathbb{R})$. This is a Haar measure on $SL(2,\mathbb{R})$ (left- and also right-invariant) and with respect to this volume form left- (or right-) invariant vector fields are always anti-symmetric. Set

$$K = \left\{\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}\right\}$$

then we describe an identification of the right coset space $SL(2,\mathbb{R})/K$ with the upper half-plane,

$$H_+ = \{\sigma = u + \sqrt{-1}v \in \mathbb{C} \mid v > 0\},$$

in the following way: Consider the map $\pi_R\colon SL(2,\mathbb{R}) \longrightarrow H_+$,

$$\pi_R\left(\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right) = \frac{a\sqrt{-1}+b}{c\sqrt{-1}+d},$$

$$u = \frac{ac+bd}{c^2+d^2}, \quad v = \frac{1}{c^2+d^2},$$

which can be seen as the projection map to the space of right cosets by the subgroup K,

$$SL(2,\mathbb{R}) \longrightarrow SL(2,\mathbb{R})/K.$$

The right action R_λ of an element $\lambda \in K$ induces the action on the sub-bundle $\mathcal{H}_{SL}$ in the following way:

Proposition 5.1. *It holds*

$$dR_\lambda(\tilde{X}) = \cos 2\theta\ \tilde{X} + \sin 2\theta\ \tilde{Y},$$
$$dR_\lambda(\tilde{Y}) = -\sin 2\theta\ \tilde{X} + \cos 2\theta\ \tilde{Y}$$

for $\lambda = \left(\begin{smallmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{smallmatrix}\right) \in K$.

Proof. This is proved through the adjoint action of K on $\mathfrak{sl}(2,\mathbb{R})$,

$$Ad_\lambda(X) = \lambda X \lambda^{-1} = \cos 2\theta\ X + \sin 2\theta\ Y$$
$$Ad_\lambda(Y) = \lambda Y \lambda^{-1} = -\sin 2\theta\ X + \cos 2\theta\ Y. \qquad \square$$

This proposition implies that the sub-bundle $\mathcal{H}_{SL}$ in $T(SL(2,\mathbb{R}))$ defines a connection of the principal bundle

$$\pi_R : SL(2,\mathbb{R}) \to SL(2,\mathbb{R})/K \cong H_+.$$

Moreover, the right action R_λ is *orthogonal* with respect to the metric installed in $\mathcal{H}_{SL}$ so that we can descend the sub-Riemannian metric onto the base space $SL(2,\mathbb{R})/K \cong H_+$, as a Riemannian metric. The left action of $SL(2,\mathbb{R})$ onto itself also leaves invariant the sub-Riemannian metric and so its left action on the space of right cosets $SL(2,\mathbb{R})/K \cong H_+$ leaves invariant the descended metric. Hence we know that the descended metric is the metric with constant negative curvature (= Poincaré metric) so that it has the form of a constant times the metric

$$\frac{du^2+dv^2}{v^2} \quad \text{(modulo constants)}.$$

The constant will be determined in (5.6) and we denote the upper half-plane with this metric – identified with the right coset space $SL(2,\mathbb{R})/K$ – by H_+^R.

Next, we consider the principal bundle on the left cosets space by the subgroup K,

$$\pi_L\colon SL(2,\mathbb{R}) \longrightarrow K\backslash SL(2,\mathbb{R}).$$

Again, we identify this space with the upper half-plane H_+ by the map

$$\pi_L \colon g = \begin{pmatrix} x & y \\ w & z \end{pmatrix} \mapsto (u, v) = \left(-\frac{xy + wz}{x^2 + w^2}, \frac{1}{x^2 + w^2} \right) \in H_+.$$

Since the vector fields $\tilde{X}$ and $\tilde{Y}$ are left-invariant, we can descend them to the plane H_+ by the map π_L.

Proposition 5.2. *At any point in $SL(2, \mathbb{R})$, we have*

$$\operatorname{Ker}(d\pi_L) \cap \mathcal{H}_{SL} = \{0\}.$$

Proof. This is proved by determining the descended vector fields $d\pi_L(\tilde{X})$ and $d\pi_L(\tilde{Y})$ explicitly,

$$d\pi_L(\tilde{X}) = -2u \frac{\partial}{\partial u} - 2v \frac{\partial}{\partial v},$$
$$d\pi_L(\tilde{Y}) = \left(1 + v^2 - u^2\right) \frac{\partial}{\partial u} - 2uv \frac{\partial}{\partial v}.$$

The matrix

$$\begin{pmatrix} -2u & -2v \\ 1 + v^2 - u^2 & -2uv \end{pmatrix}$$

is invertible for $v > 0$, which implies that the vector fields $d\pi_L(\tilde{X})$ and $d\pi_L(\tilde{Y})$ are always linearly independent in the upper half-plane. □

We define the metric in the upper half-plane by assuming that the two vectors $d\pi_L(\tilde{X})$ and $d\pi_L(\tilde{Y})$ are orthonormal at every point. In this case we will denote the left coset space $K \backslash SL(2, \mathbb{R})$ with this Riemannian metric by H_+^L and call it the *Grushin upper half-plane*.

The metric tensor g^L is given by

$$g^L = \begin{pmatrix} g^L\left(\frac{\partial}{\partial u}, \frac{\partial}{\partial u}\right) & g^L\left(\frac{\partial}{\partial v}, \frac{\partial}{\partial u}\right) \\ g^L\left(\frac{\partial}{\partial u}, \frac{\partial}{\partial v}\right) & g^L\left(\frac{\partial}{\partial v}, \frac{\partial}{\partial v}\right) \end{pmatrix} = \begin{pmatrix} \frac{1+u^2}{(1+v^2+u^2)^2} & \frac{u(v^2-u^2-1)}{2v(1+v^2+u^2)^2} \\ \frac{u(v^2-u^2-1)}{2v(1+v^2+u^2)^2} & \frac{4u^2+(u^2-v^2-1)^2}{4v^2(1+v^2+u^2)^2} \end{pmatrix}.$$

We call the operator

$$\mathcal{G}_{SL} = -\left(\left(d\pi_L(\tilde{X}) \right)^2 + \left(d\pi_L(\tilde{Y}) \right)^2 \right)$$

a *SL-Grushin operator*. Although this is not the *Laplacian* with respect to this metric g^L, the principal symbol $\sigma(\mathcal{G}_{SL})$ of this operator coincides with that of the Laplacian and is given by

$$\sigma(\mathcal{G}_{SL})(u, v, \xi, \eta) = 4\left(u\xi + v\eta\right)^2 + \left((1 + v^2 - u^2)\xi - 2uv\eta\right)^2.$$

5.2. Horizontal curves: $SL(2,\mathbb{R})$

Since the sub-Riemannian distribution $\mathcal{H}_{SL}$ defines also a *connection* on the principal bundle

$$\pi_R \colon SL(2,\mathbb{R}) \longrightarrow H_+^R = \text{right coset space},$$

we can parametrize horizontal curves in $SL(2,\mathbb{R})$ as lifts of curves in the base space H_+^R. In this section we describe these lifts. We only consider curves starting from the point $\sqrt{-1} = (0,1) \in H_+^R$ and its lift starting from the point $\left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$.

Let $\tilde{\gamma} = \{\tilde{\gamma}(t)\}_{t\in[0,1]}$ be a smooth curve in $SL(2,\mathbb{R})$. Then $\tilde{\gamma}$ is horizontal if and only if

$$\theta_C\left(\frac{d\tilde{\gamma}(t)}{dt}\right) = 0 \tag{5.2}$$

everywhere, where

$$\theta_C = \frac{1}{2}\big(wdx + zdy - xdw - ydz\big).$$

So, when we write

$$\tilde{\gamma}(t) = \begin{pmatrix} x(t) & y(t) \\ w(t) & z(t) \end{pmatrix},$$

then the horizontality condition is expressed as:

Proposition 5.3.

$$w(t)\,\frac{dx(t)}{dt} + z(t)\,\frac{dy(t)}{dt} - x(t)\,\frac{dw(t)}{dt} - y(t)\,\frac{dz(t)}{dt} = 0.$$

If the curve $\tilde{\gamma}$ is horizontal, then the tangent vector $\frac{d\tilde{\gamma}(t)}{dt}$ is expressed as

$$\begin{aligned}\frac{d\tilde{\gamma}(t)}{dt} &= \frac{dx(t)}{dt}\left(\frac{\partial}{\partial x}\right)_{\tilde{\gamma}(t)} + \frac{dy(t)}{dt}\left(\frac{\partial}{\partial y}\right)_{\tilde{\gamma}(t)} + \frac{dw(t)}{dt}\left(\frac{\partial}{\partial w}\right)_{\tilde{\gamma}(t)} + \frac{dz(t)}{dt}\left(\frac{\partial}{\partial z}\right)_{\tilde{\gamma}(t)} \\ &= \alpha(t)\tilde{X}_{\tilde{\gamma}(t)} + \beta(t)\tilde{Y}_{\tilde{\gamma}(t)},\end{aligned}$$

with two functions $\alpha(t)$ and $\beta(t)$. The functions $\alpha(t)$ and $\beta(t)$ satisfy:

Proposition 5.4.

$$\begin{aligned}\alpha(t) &= \frac{x(t)\,\frac{dx(t)}{dt} - y(t)\,\frac{dy(t)}{dt}}{x(t)^2 + y(t)^2} = \frac{w(t)\,\frac{dw(t)}{dt} - z(t)\,\frac{dz(t)}{dt}}{w(t)^2 + z(t)^2},\\ \beta(t) &= \frac{x(t)\,\frac{dy(t)}{dt} + y(t)\,\frac{dx(t)}{dt}}{x(t)^2 + y(t)^2} = \frac{w(t)\,\frac{dz(t)}{dt} + z(t)\,\frac{dw(t)}{dt}}{w(t)^2 + z(t)^2}.\end{aligned}$$

Let $\mathcal{S} \colon H_+^R \to SL(2,\mathbb{R})$ be the global section (i.e., it satisfies $\pi_R \circ \mathcal{S} = \mathrm{Id}$) defined by

$$\mathcal{S} \colon u + \sqrt{-1}v \mapsto \begin{pmatrix} \frac{u}{\sqrt{v}} & -\sqrt{v} \\ \frac{1}{\sqrt{v}} & 0 \end{pmatrix}.$$

Then the curve $\tilde{\gamma}$ is written as

$$\tilde{\gamma}(t) = \begin{pmatrix} x(t) & y(t) \\ w(t) & z(t) \end{pmatrix} = \begin{pmatrix} u(t)/\sqrt{v(t)} & -\sqrt{v(t)} \\ 1/\sqrt{v(t)} & 0 \end{pmatrix} \begin{pmatrix} \cos\theta(t) & -\sin\theta(t) \\ \sin\theta(t) & \cos\theta(t) \end{pmatrix}$$
$$= \begin{pmatrix} \frac{u(t)\cos\theta(t)}{\sqrt{v(t)}} - \sqrt{v(t)}\sin\theta(t) & -\frac{u(t)\sin\theta(t)}{\sqrt{v(t)}} - \sqrt{v(t)}\cos\theta(t) \\ \frac{\cos\theta(t)}{\sqrt{v(t)}} & -\frac{\sin\theta(t)}{\sqrt{v(t)}} \end{pmatrix},$$

where $\{(u(t), v(t))\}$ is an arbitrary given smooth curve in H_+^R starting from the point $(0,1) \in H_+^R$. Then we have an equation, after a somewhat lengthy calculation, satisfied by the function $\theta(t)$ ($\theta(0) = 0$):

Proposition 5.5.

$$\frac{d\,\theta(t)}{dt} = \frac{\frac{d\,u(t)}{dt}}{2v(t)}.$$

If we take suitable functions $u(t)$ and $v(t)$ under the conditions

$$u(0) = 0, \;\; v(0) = 1, \;\; u(1) = u_1 \;\text{ and }\; v(1) = v_1 > 0,$$

(where (u_1, v_1) is an arbitrary fixed point in H_+^R), then it will be apparent that the integral

$$\theta(1) \;=\; \int_0^1 \frac{\frac{d\,u(t)}{dt}}{2v(t)} dt$$

can assume an arbitrary value.

Corollary 5.6. *Any two points in $SL(2,\mathbb{R})$ can be joined with a smooth horizontal curve (a strong version of Chow's theorem).*

If the curve $\tilde{\gamma}$ is horizontal, we express the coefficients $\alpha(t)$ and $\beta(t)$ in terms of the functions $u(t)$ and $v(t)$ by making use of the formulas for $\alpha(t)$ and $\beta(t)$ and the equation in Proposition 5.5,

$$\alpha(t) = \frac{\frac{dv(t)}{dt}}{2v(t)}\left(\sin^2\theta(t) - \cos^2\theta(t)\right) - \frac{\frac{du(t)}{dt}}{v(t)}\sin\theta(t)\cos\theta(t), \tag{5.3}$$

$$\beta(t) = \frac{\frac{du(t)}{dt}}{2v(t)}\left(\sin^2\theta(t) - \cos^2\theta(t)\right) + \frac{\frac{dv(t)}{dt}}{v(t)}\sin\theta(t)\cos\theta(t). \tag{5.4}$$

Therefore, the sub-Riemannian length $\|\tilde{\gamma}\|$ of the horizontal curve $\tilde{\gamma}$ is given by the integral

$$\|\tilde{\gamma}\| = \int_0^1 \sqrt{\alpha(t)^2 + \beta(t)^2}dt = \int_0^1 \frac{\sqrt{\frac{du(t)}{dt}^2 + \frac{dv(t)}{dt}^2}}{2v(t)}\,dt. \tag{5.5}$$

Now, we can determine the metric tensor on the right coset space $SL(2,\mathbb{R})/K \cong H_+^R$,

$$g_P = \begin{pmatrix} g_P\left(\frac{\partial}{\partial u}, \frac{\partial}{\partial u}\right) & g_P\left(\frac{\partial}{\partial v}, \frac{\partial}{\partial u}\right) \\ g_P\left(\frac{\partial}{\partial u}, \frac{\partial}{\partial v}\right) & g_P\left(\frac{\partial}{\partial v}, \frac{\partial}{\partial v}\right) \end{pmatrix} = \begin{pmatrix} \frac{1}{4v^2} & 0 \\ 0 & \frac{1}{4v^2} \end{pmatrix}. \tag{5.6}$$

5.3. Isoperimetric interpretation: $SL(2,\mathbb{R}) \to$ Upper half-plane

Let τ_R be the one-form

$$\tau_R = \frac{du}{4v}$$

on H_+^R. Then it is easy to see that the two-form $d\tau_R$ coincides with the Riemannian volume form $\frac{1}{4v^2}\, du \wedge dv$ with respect to the Poincaré metric determined in (5.6).

Let $\gamma = \left\{\gamma(t) = (u(t), v(t))\right\}_{t\in[0,1]}$ be a smooth curve in H_+^R with $\gamma(0) = (0,1)$ and end point on the imaginary axis $\gamma(1) = (0, v_1)$. Consider a domain D_γ in H_+^R surrounded by the curve γ and a straight line $\ell = \{\ell(t)\}_{1\le t\le v_1}$ from $(0, v_1)$ to $(0,1)$ (with $v_1 \le 1$). Then the oriented area of the domain D_γ is given by:

$$\begin{aligned} \operatorname{area}(D_\gamma) &= \int_{D_\gamma} d\tau_R = \int_{\partial D_\gamma} \tau_R \qquad (5.7) \\ &= \int_0^1 \gamma^*(\tau_R) + \int_{v_1}^1 \ell^*(\tau_R) = \int_0^1 \gamma^*(\tau_R) = \frac{1}{2}\int_0^1 \frac{\frac{du(t)}{dt}}{v(t)}\, dt = \frac{\theta_1}{2}. \end{aligned}$$

Therefore the horizontal lift $\tilde{\gamma}$ of a curve γ,

$$\tilde{\gamma}(0) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad \tilde{\gamma}(1) = \begin{pmatrix} x_1 & y_1 \\ w_1 & z_1 \end{pmatrix} = \begin{pmatrix} -\sqrt{v_1}\sin\theta_1 & -\sqrt{v_1}\cos\theta_1 \\ \cos\theta_1/\sqrt{v_1} & -\sin\theta_1/\sqrt{v_1} \end{pmatrix},$$

is a sub-Riemannian geodesic in $SL(2,\mathbb{R})$ if and only if the curve $\gamma = \{(u(t), v(t))\}$ is a minimizing curve of the isoperimetric problem under the conditions that the oriented area $\int_{D_\gamma} d\tau$ is constant $= \theta_1$ and $\gamma(0) = (0,1)$, $\gamma(1) = (0, v_1)$.

If the end point (u_1, v_1) of the given curve γ in H_+^R is not on the imaginary axis, then we reduce the problem by rotating the point onto the imaginary axis by an element of the form

$$g(\theta) = \begin{pmatrix} \cos\eta & -\sin\eta \\ \sin\eta & \cos\eta \end{pmatrix}.$$

We can consider the same problem again and obtain the solution via going back by the element $g(\theta)^{-1}$. Without going into details we mention that the isoperimetric problem of the Poincaré upper half-plane has also circles (in the sense of Euclidean geometry) as solutions (see [Sa-42]). So it is possible to construct both the geodesics on $SL(2,\mathbb{R})$ with respect to the sub-Riemannian structure induced from $\mathcal{H}_{SL}$ and the geodesics on the Grushin upper half-plane H_+^L.

6. The $S^3 \to P^1(\mathbb{C})$ case

In this section, first we explain a sub-Riemannian structure on the three-dimensional sphere S^3 which is well known and studied in various contexts (cf. [CC1-09], [BF3-08], and so on). Through the Hopf fibration we define a Grushin-type operator on the two-dimensional sphere S^2. We call this operator a *spherical Grushin operator*, and we define a singular metric on the two sphere ($\cong P^1(\mathbb{C})$). We call the two-dimensional sphere with such a singular metric the *Grushin sphere* and denote it by $S^2_{\mathcal{G}}$. Then we construct geodesic curves on the Grushin sphere connecting two points located on the singular set by a method similar to the case of the Grushin plane. In the previous paper [BF3-08] (see also [Ba-05]) we have studied the spectral zeta-function of the sub-Laplacian on S^3. This section is partly a continuation of [BF3-08].

6.1. Spherical Grushin operator and Grushin sphere

Let $\mathbb{H} = \{x_0\mathbf{1} + x_1\mathbf{i} + x_2\mathbf{j} + x_3\mathbf{k} \mid x_i \in \mathbb{R}\}$ be the quaternion number field with the standard basis $\{\mathbf{1}, \mathbf{i}, \mathbf{j}, \mathbf{k}\}$. Their multiplications are given as follows: $\mathbf{1i} = \mathbf{i} = \mathbf{i1}$, $\mathbf{1j} = \mathbf{j} = \mathbf{j1}$, $\mathbf{1k} = \mathbf{k} = \mathbf{k1}$, $\mathbf{ij} = \mathbf{k} = -\mathbf{ji}$, $\mathbf{jk} = \mathbf{i} = -\mathbf{kj}$, $\mathbf{ki} = \mathbf{j} = -\mathbf{ik}$, $\mathbf{i}^2 = -\mathbf{1}$, $\mathbf{j}^2 = -\mathbf{1}$, $\mathbf{k}^2 = -1$.

We consider the three sphere S^3 as

$$S^3 = \left\{x_0\mathbf{1} + x_1\mathbf{i} + x_2\mathbf{j} + x_3\mathbf{k} \in \mathbb{H} \;\middle|\; \sum {x_i}^2 = 1\right\},$$

which we regard as a Lie group with the multiplication coming from the product law in $\mathbb{H}$. The corresponding Lie algebra is given by

$$\mathfrak{sp}(1) = \left\{h = x_1\mathbf{i} + x_2\mathbf{j} + x_3\mathbf{k} \;\middle|\; x_i \in \mathbb{R}\right\},$$

with Lie brackets $[h, h'] = hh' - h'h$. Then left-invariant vector fields on S^3 corresponding to the element $\mathbf{i}$, $\mathbf{j}$ and $\mathbf{k}$ are defined with $\varphi \in C^\infty(S^3)$ by

$$X_{\mathbf{i}}(\varphi)(h) = \frac{d}{dt}\varphi\big(h \cdot \exp\, t\mathbf{i}\big)\Big|_{t=0},$$

and so on. In global coordinates they can be expressed as

$$\begin{aligned} X_{\mathbf{i}} &= -x_1 \frac{\partial}{\partial x_0} + x_0 \frac{\partial}{\partial x_1} + x_3 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_3}, \\ X_{\mathbf{j}} &= -x_2 \frac{\partial}{\partial x_0} - x_3 \frac{\partial}{\partial x_1} + x_0 \frac{\partial}{\partial x_2} + x_1 \frac{\partial}{\partial x_3}, \\ X_{\mathbf{k}} &= -x_3 \frac{\partial}{\partial x_0} + x_2 \frac{\partial}{\partial x_1} - x_1 \frac{\partial}{\partial x_2} + x_0 \frac{\partial}{\partial x_3}. \end{aligned}$$

These 3 vector fields trivialize the tangent bundle $T(S^3)$. Since $[X_{\mathbf{k}}, X_{\mathbf{i}}] = 2X_{\mathbf{j}}$, we can consider a co-dimension one sub-Riemannian structure on S^3 in the strong sense and of step 2, which is generated by the two vector fields $\{X_{\mathbf{i}}, X_{\mathbf{k}}\}$. We denote it by $\mathcal{H}_S = [\{X_{\mathbf{i}}, X_{\mathbf{k}}\}]$ and we write $\Delta^{\mathrm{sub}}_{S^3} = -{X_{\mathbf{i}}}^2 - {X_{\mathbf{k}}}^2$ for the corresponding sub-Laplacian. An inner product on $\mathcal{H}_S$ is defined as the restriction of the standard inner product on the three sphere S^3.

In the next step we form the Hopf bundle with a connection. By considering the orbit space of the right action R_λ of $\lambda \in \{\lambda = a + b\mathbf{j} \mid a^2 + b^2 = 1\} \cong U(1)$ on S^3 given by

$$R_\lambda : S^3 \times U(1) \to S^3,\ (h, \lambda) \to h \cdot \lambda$$

we have a principal bundle (Hopf bundle)

$$\pi_R\colon S^3 \longrightarrow P^1(\mathbb{C}).$$

The space $P^1(\mathbb{C})$ is realized in $\mathbb{R}^3$ as 2-sphere with radius 1/2:

$$\pi_R\colon S^3 \ni h \mapsto (u_1, u_2, u_3) \in S^2{}_{(1/2)} = \left\{\sum u_i^2 = 1/4\right\},$$

where

$$u_1 + \sqrt{-1}u_2 = (x_0 - x_2\sqrt{-1})(x_1 + x_3\sqrt{-1}) = \overline{z}w,$$
$$u_3 = |x_0 + x_2\sqrt{-1}|^2 - 1/2 = |z|^2 - 1/2,$$

and we put $z = x_0 + x_2\sqrt{-1},\ w = x_1 + x_3\sqrt{-1}$. The right actions R_λ (where $\lambda = a\mathbf{1} + b\mathbf{j}, a^2 + b^2 = 1$) on $X_\mathbf{i}$ and $X_\mathbf{k}$ are given by

$$dR_\lambda(X_\mathbf{i}) = (a^2 - b^2)X_\mathbf{i} + 2abX_\mathbf{k}, \tag{6.1}$$
$$dR_\lambda(X_\mathbf{k}) = (a^2 - b^2)X_\mathbf{k} - 2abX_\mathbf{i}. \tag{6.2}$$

They leave the subspace $\mathcal{H}_S$ invariant and therefore induce orthogonal actions on $\mathcal{H}_S$. Hence we know that the sub-bundle $\mathcal{H}_S$ defines not only a connection on the principal bundle

$$\pi_R\colon S^3 \to S^2{}_{(1/2)},$$

but also naturally gives a metric on the base space $S^2{}_{(1/2)}$. This coincides with the standard metric induced from $\mathbb{R}^3$. In order to define an operator on S^2, which we call a *spherical Grushin operator*, we consider the left action L_λ of the group $U(1) \cong \left\{\lambda = a + b\mathbf{j} \;\middle|\; a^2 + b^2 = 1\right\}$ on S^3,

$$U(1) \times S^3 \to S^3, (\lambda, h) \mapsto \lambda \cdot h = (a + b\mathbf{j})(x_0\mathbf{1} + x_1\mathbf{i} + x_2\mathbf{j} + x_3\mathbf{k})$$

and denote the projection map to the orbit space by $\pi_L\colon xS^3 \to P^1(\mathbb{C})$.

Both vector fields $X_\mathbf{i}$ and $X_\mathbf{k}$ are L_λ-action invariant and can be descended to the base space $P^1(\mathbb{C})$ through the map π_L. The base space again is realized as a sphere of radius 1/2 in $\mathbb{R}^3$ through the map

$$\pi_L\colon S^3 \ni x_0\mathbf{1} + x_1\mathbf{i} + x_2\mathbf{j} + x_3\mathbf{k} \longmapsto (v_1, v_2, v_3) \in S^2_{(1/2)},$$
$$v_1 + v_2\sqrt{-1} = (x_0 - x_1\sqrt{-1})(x_1 - x_3\sqrt{-1}),\ \ v_3 = x_0^2 + x_2^2 - 1/2.$$

The vector fields $d\pi_L(X_\mathbf{i})$ and $d\pi_L(X_\mathbf{k})$ have the form

$$d\pi_L(X_\mathbf{i}) = -2v_1\frac{\partial}{\partial v_3} + 2v_3\frac{\partial}{\partial v_1},$$
$$d\pi_L(X_\mathbf{k}) = -2v_2\frac{\partial}{\partial v_3} + 2v_3\frac{\partial}{\partial v_2}.$$

From these expressions we find:

Proposition 6.1. *Let $\mathcal{S}$ be the following sub-manifold in S^3:*

$$\mathcal{S} = \left\{ (x_0\mathbf{1} + x_1\mathbf{i} + x_2\mathbf{j} + x_3\mathbf{k}) \;\middle|\; {x_0}^2 + {x_2}^2 = 1/2 \right\}.$$

Then it always holds that $\dim \mathcal{H}_S \cap T(\mathcal{S}) = 1$ *and so the vector fields* $d\pi_L(X_{\mathbf{i}})$ *and* $d\pi_L(X_{\mathbf{k}})$ *are linearly dependent on* $\pi_L(\mathcal{S}) = \left\{ (v_1, v_2, 0) \in S^2_{(1/2)} \right\}$.

We install a metric (denoted by g_{G_S}) on $S^2 = \pi_L(S^3)$ outside the sub-manifold $\pi_L(\mathcal{S}) = \left\{ (a,b,0) \;\middle|\; a^2 + b^2 = 1/4 \right\}$ in such a way that $d\pi_L(X_{\mathbf{i}})$ and $d\pi_L(X_K)$ are orthonormal. The two-sphere equipped with this metric is called *Grushin sphere* and we denote it by $S^2_{\mathcal{G}}$. The operator

$$\mathcal{G}_S = -d\pi_L(X_{\mathbf{i}})^2 - d\pi_L(X_{\mathbf{k}})^2$$

is referred to as *spherical Grushin operator*. Let us describe this metric g_{G_S} in terms of local coordinates,

$$\overline{\mathcal{D}}_L \colon \mathbb{C} \ni z = x + y\sqrt{-1} \longmapsto (v_1, v_2, v_3) \in S^2_{\mathcal{G}} \tag{6.3}$$

$$v_1 = \frac{x}{1 + x^2 + y^2}, \quad v_2 = \frac{y}{1 + x^2 + y^2}, \quad v_3 = \frac{1 - x^2 - y^2}{2(1 + x^2 + y^2)}.$$

Then the metric tensor is given by

$$g_{G_S} = \begin{pmatrix} \frac{(x^2+y^2)^2 - 2(x^2-y^2) + 1}{\left((x^2+y^2)^2 - 1\right)^2} & \frac{-4xy}{\left((x^2+y^2)^2 - 1\right)^2} \\ \frac{-4xy}{\left((x^2+y^2)^2 - 1\right)^2} & \frac{(x^2+y^2)^2 + 2(x^2-y^2) + 1}{\left((x^2+y^2)^2 - 1\right)^2} \end{pmatrix}.$$

Here we provide an expression of the spherical Grushin operator in this coordinates,

$$\begin{aligned} -\mathcal{G}_S &= \left(1 + 2(x^2 - y^2) + (x^2 + y^2)^2\right) \frac{\partial^2}{\partial x^2} \\ &\quad + \left(1 - 2(x^2 - y^2) + (x^2 + y^2)^2\right) \frac{\partial^2}{\partial y^2} + 8xy \frac{\partial^2}{\partial x \partial y} + 4x \frac{\partial}{\partial x} + 4y \frac{\partial}{\partial y}. \end{aligned} \tag{6.4}$$

Also the spherical Grushin operator $\mathcal{G}_S$ is the restriction of

$$\begin{aligned} -\frac{1}{4}\mathcal{G}_S &= \frac{1}{4}\left\{ d\pi_L(X_{\mathbf{i}})^2 + d\pi_L(X_{\mathbf{k}})^2 \right\} \\ &= ({v_1}^2 + {v_2}^2) \frac{\partial^2}{\partial {v_3}^2} + {v_3}^2 \left(\frac{\partial^2}{\partial {v_1}^2} + \frac{\partial^2}{\partial {v_2}^2} \right) \\ &\qquad - 2v_3 \frac{\partial}{\partial v_3} - v_1 \frac{\partial}{\partial v_1} - v_2 \frac{\partial}{\partial v_2} - 2v_1 v_3 \frac{\partial^2}{\partial v_1 \, \partial v_3} - 2v_2 v_3 \frac{\partial^2}{\partial v_2 \, \partial v_3} \end{aligned}$$

to the sphere $S^2_{\mathcal{G}} = \left\{ (v_1, v_2, v_3) \;\middle|\; {v_1}^2 + {v_2}^2 + {v_3}^2 = 1/4 \right\}$.

6.2. Geodesics on the Grushin sphere

We construct geodesic curves on the Grushin sphere $S^2_{\mathcal{G}}$ connecting two points on the singular set $\pi_L(\mathcal{S})$ by the same method as in the Grushin plane case. To apply Theorem 3.1 (and Corollary 3.5) we describe local trivializations $\mathcal{D}_L$ and $\mathcal{D}_R$ of the double fibration

$$\begin{array}{ccc} S^3 & \xrightarrow[\pi_R]{} & S^2_{(1/2)} \\ {\scriptstyle \pi_L}\big\downarrow & & \\ S^2_{\mathcal{G}}. & & \end{array}$$

Let $\mathcal{D}_L : U(1) \times \mathbb{C} \to S^3$ be defined by

$$\mathcal{D}_L\colon (\lambda, z) = \left(e^{\sqrt{-1}t}, x + \sqrt{-1}y\right) \mapsto \left(\frac{\lambda}{\sqrt{1+|z|^2}}, \frac{\lambda z}{\sqrt{1+|z|^2}}\right). \tag{6.5}$$

Then

$$\pi_L \circ \mathcal{D}_L(\lambda, z) = \left(\frac{x}{\sqrt{1+x^2+y^2}}, \frac{y}{\sqrt{1+x^2+y^2}}, \frac{1}{\sqrt{1+x^2+y^2}} - \frac{1}{2}\right) = \overline{\mathcal{D}}_L(z).$$

Although we have the same (local) trivialization $\mathcal{D}_R\colon \mathbb{C} \times U(1) \to S^3$ for the map π_R, we distinguish them through their compatibility with the $U(1)$-action and the actions of the group $\left\{(a + \mathbf{j}b) \mid a^2 + b^2 = 1\right\}$ in the quaternion number field from the right and the left. Then $\mathcal{D}_L(\lambda, z) = \mathcal{D}_R(w, \mu)$ if and only if

$$w = \overline{\lambda}^2 \overline{z} \quad \text{and} \quad \lambda = \mu. \tag{6.6}$$

In the coordinates $\left(e^{\sqrt{-1}t}, z\right) \xrightarrow{\mathcal{D}_L} S^3$ the vector field $X_{\mathbf{i}}$ and $X_{\mathbf{k}}$ are expressed as

$$\begin{aligned} X_{\mathbf{i}} &= -y\,\frac{\partial}{\partial t} + (x^2 - y^2 + 1)\,\frac{\partial}{\partial x} + 2xy\,\frac{\partial}{\partial y}, \\ X_{\mathbf{k}} &= -x\,\frac{\partial}{\partial t} - 2xy\,\frac{\partial}{\partial x} + (x^2 - y^2 - 1)\,\frac{\partial}{\partial y}. \end{aligned}$$

Hence the principal symbol $\sigma(\Delta^{\mathrm{sub}}_{S^3})$ of the sub-Laplacian is given in terms of the coordinates $(t, x, y\ ;\ \delta, \alpha, \beta) \in T^*(\mathbb{R} \times \mathbb{C}) \cong \mathbb{R} \times \mathbb{R}^2 \times \mathbb{R} \times \mathbb{R}^2$ by

$$\begin{aligned} &2\sigma(\Delta^{\mathrm{sub}}_{S^3})(t, x, y\ ;\ \delta, \alpha, \beta) \\ &\quad = \big(-y\delta + (x^2 - y^2 + 1)\alpha + 2xy\beta\big)^2 + \big(-x\delta - 2xy\alpha + (x^2 - y^2 - 1)\beta\big)^2. \end{aligned}$$

Moreover, by the expression (6.4) of the spherical Grushin operator in terms of the coordinates $z = x + \sqrt{-1}y$ in (6.3), the principal symbol $\sigma(\mathcal{G}_S)$ is given by

$$\begin{aligned} 2\sigma(\mathcal{G}_S)(x, y; \alpha, \beta) = \big(1 &+ 2(x^2 - y^2) + (x^2 + y^2)^2\big)\alpha^2 \\ &+ \big(1 - 2(x^2 - y^2) + (x^2 + y^2)^2\big)\beta^2 + 8xy\alpha\beta. \end{aligned}$$

So, our purpose is to find the solutions of the Hamilton system

$$\begin{aligned}\dot{x}(s) &= \big((x^2-y^2+1)\alpha+2xy\beta\big)\big(x^2-y^2+1\big)\\ &\qquad+\big(-2xy\alpha+(x^2-y^2-1)\beta\big)\big(-2xy\big),\\ \dot{y}(s) &= \big((x^2-y^2+1)\alpha+2xy\beta\big)\big(2xy\big)\\ &\qquad+\big(-2xy\alpha+(x^2-y^2-1)\beta\big)\big(x^2-y^2-1\big),\\ \dot{\alpha}(s) &= -\big((x^2-y^2+1)\alpha+2xy\beta\big)\big(2x\alpha+2y\beta\big)\\ &\qquad-\big(-2xy\alpha+(x^2-y^2-1)\beta\big)\big(-2y\alpha+2x\beta\big),\\ \dot{\beta}(s) &= -\big((x^2-y^2+1)\alpha+2xy\beta\big)\big(-2y\alpha+2x\beta\big)\\ &\qquad+\big(-2xy\alpha+(x^2-y^2-1)\beta\big)\big(2x\alpha+2y\beta\big)\end{aligned}$$

under the boundary conditions

$$x(0)=1,\ \ y(0)=0,\ \ x(1)=a_1,\ \ y(1)=b_1,\ \ {a_1}^2+{b_1}^2=1 \tag{6.7}$$

(although $\alpha(0)$ and $\beta(0)$ will not be determined uniquely), where a point $E_1 = a_1+\sqrt{-1}\,b_1$ on the singular set $\overline{\mathcal{D}_L}^{-1}\big(\pi_L(\mathcal{S})\big)=\big\{a+\sqrt{-1}b \mid a^2+b^2=1\big\}$ is given arbitrarily. We treat the case $a_1+b_1\sqrt{-1}=e^{-\sqrt{-1}\,\epsilon_1}$ with $0<\epsilon_1<\pi$.

Remark 6.2. Since the right action of the element $a+b\mathbf{j}$ $(a^2+b^2=1)$ is isometric with respect to the sub-Riemannian metric (see (6.1) and (6.2)) and compatible with the projection map π_L, it induces the rotation on $\pi_L(S^3)\cong S^2$ along the axis v_3. So it is enough to consider the initial point to be $x(0)=1$, $y(0)=0$ or $\overline{\mathcal{D}}_L(x(0)+\sqrt{-1}y(0))=\overline{\mathcal{D}}_L(1)=(v_1(0),v_2(0),v_3(0))=(1/2,0,0)$.

If there exists such a curve

$$\{c(s)\}=\big\{\big(x(s),y(s)\,;\,\alpha(s),\beta(s)\big)\big\}$$

passing through the singular set $\overline{\mathcal{D}_L}^{-1}\big(\pi_L(\mathcal{S})\big)$ at $s=0$, then we have:

Proposition 6.3.

$$\begin{aligned}\dot{x}(0)&=4x(0)\big(x(0)\alpha(0)+y(0)\beta(0)\big),\\ \dot{y}(0)&=4y(0)\big(x(0)\alpha(0)+y(0)\beta(0)\big).\end{aligned}$$

Proof. From

$$\dot{x}(s)=\big((x^2-y^2+1)\alpha+2xy\beta\big)(x^2-y^2+1)+\big(-2xy\alpha+(x^2-y^2-1)\beta\big)(-2xy),$$

and putting $x^2+y^2=1$ we have

$$\dot{x}(s)=(2x^2\alpha+2xy\beta)\cdot 2x^2(-2xy\alpha+(-2y^2)\beta)(-2xy)=4x(x\alpha+y\beta).$$

To calculate $\dot{y}(0)$ note that in the same way it holds $\dot{y}(s)=4y(x\alpha+y\beta)$. □

Assuming the existence of such a curve $\{c(s)\}$ we denote by

$$\{\tilde{c}(s)\}=\Big\{\Big(e^{\sqrt{-1}t(s)},x(s),y(s)\ ;\ 0,\alpha(s),\beta(s)\Big)\Big\},$$

the lift of the curve $\{c(s)\}$ to $T^*(U(1)\times\mathbb{C})$ which is included in the sub-manifold $\mathbb{L}=\big\{(\lambda,x,y;\,0,\alpha,\beta)\big\}$ starting from the point

$$\big(1,1,0\,;\,0,\alpha(0),\beta(0)\big)\in\mathbb{L}\subset T^*\big(U(1)\times\mathbb{C}\big).$$

(We can assume that $t(0)=1$, see Theorem 3.1 for the existence of the lift.) Note that the solution $\delta(s)$ of the equation

$$\dot\delta(s)=-\frac{\partial\sigma(\Delta^{\mathrm{sub}}_{S^3})}{\partial t}\equiv 0$$

is always zero if we choose the initial value of δ to be 0, so it must stay in $\mathbb{L}$. Let $\{\gamma(s)\}$ be the image of the curve $\{\tilde c(s)\}$ by the projection π_R,

$$\{\gamma(s)\}=\pi_R\circ\mathcal{D}_R^{-1}\circ\mathcal{D}_L\big(\{\tilde c(s)\}\big)=\overline{\mathcal{D}}_R\left(\left\{e^{-2\sqrt{-1}t(s)}\cdot\overline{\big(x(s)+\sqrt{-1}y(s)\big)}\right\}\right).$$

Then:

Proposition 6.4.

$$\frac{d}{ds}\left(e^{-2\sqrt{-1}t(s)}\cdot\overline{\big(x(s)+\sqrt{-1}y(s)\big)}\right)(0)=4\overline{z(0)}(x\alpha+y\beta).$$

Proof. From

$$\begin{aligned}\dot t(s)&=\big(-y\delta+(x^2-y^2+1)\alpha+2xy\beta\big)(-y)\\&\quad+\big(-x\delta-2xy\alpha+(x^2-y^2-1)\beta\big)(-x)\\&=\alpha((x^2-y^2+1)(-y)+-2xy(-x))+\beta(-2xy^2+(x^2-y^2-1)(-x))=0\end{aligned}$$

on $\mathbb{L}_S$, with the condition $x^2+y^2=1$ and by Proposition 6.3, we have

$$\begin{aligned}&\frac{d}{ds}\big(e^{-2\sqrt{-1}t(s)}\cdot\overline{(x(s)+\sqrt{-1}y(s))}\big)(0)\\&\qquad=-2\sqrt{-1}\dot t(0)\cdot(x(0)-\sqrt{-1}y(0))+\dot x(0)-\sqrt{-1}\dot y(0)\\&\qquad=\overline{\dot z(0)}=4\overline{z(0)}(x\alpha+y\beta).\end{aligned}$$

□

If we return back on the sphere $S^2_{(1/2)}$ in $\mathbb{R}^3$ by the map $\overline{\mathcal{D}}_R\colon\mathbb{C}\to S^2_{(1/2)}$, then this means:

Corollary 6.5. *The curve $\{\gamma(s)\}$ is perpendicular to the equator $\mathcal{E}=\big\{(a,b,0)\mid a^2+b^2=1/4\big\}$.*

Since the sub-Riemannian structure $\mathcal{H}_S$ on S^3 defines a connection on the bundle $\pi_R:S^3\to S^2_{(1/2)}$, we can prove:

Theorem 6.6 ([BF3-08]). *Any horizontal curve on S^3 is the lift of a curve in the base space $S^2_{(1/2)}$.*

Also according to a classical theorem (F. Bernstein, 1905) we have:

Theorem 6.7. *The solutions of the isoperimetric problem for loops* (*or the case where a part of the loops is always a fixed part of a big circle*) *on the two sphere with the standard metric are given by circles* (*or a half-circle*) *and their horizontal lifts are sub-Riemannian geodesics.*

Now we describe the horizontal lift of a curve $\{\ell(s)\}$ starting from the point $P_N = (0,0,1/2) \in S^2{}_{(1/2)}$ by making use of the local trivialization of the bundle $\pi_R\colon S^3 \to S^2{}_{(1/2)}$:

$$\begin{array}{ccc} S^3 & \xleftarrow{\ \mathcal{D}_R\ } & \mathbb{C}\times U(1) \\ {\scriptstyle\pi_R}\big\downarrow & & \big\downarrow \\ S^2{}_{(1/2)} & \xleftarrow[\ \overline{\mathcal{D}_R}\ ]{} & \mathbb{C} \end{array},$$

$$\begin{array}{ccc} S^3 \ni \left(\frac{\mu}{\sqrt{1+|w|^2}}, \frac{\mu w}{\sqrt{1+|w|^2}}\right) & \xleftarrow{\ \mathcal{D}_R\ } & (w,\mu) \in \mathbb{C}\times U(1) \\ {\scriptstyle\pi_R}\big\downarrow & & \big\downarrow \\ S^2{}_{(1/2)} \ni \left(\frac{w}{1+|w|^2}, \frac{1}{1+|w|^2} - \frac{1}{2}\right) & \xleftarrow[\ \overline{\mathcal{D}_R}\ ]{} & w = x + y\sqrt{-1} \in \mathbb{C}. \end{array}$$

If a curve $\{\tilde{\ell}(s) = \big(w(s),\mu(s)\big)\} = \big\{\big(x(s)+\sqrt{-1}y(s), e^{\sqrt{-1}\,\theta(s)}\big)\big\}$ in $\mathbb{C}\times U(1)$ with $(w(0),\mu(0)) = (0,1)$ and $\theta(0) = 0$ is the lift of $\{\ell(s)\}$, then it satisfies

$$\sqrt{-1}\,\dot{\theta}(s) = \frac{1}{\mu(s)}\frac{d\mu(s)}{ds} = \frac{\sqrt{-1}}{1+|w|^2}\left(\frac{dx(s)}{ds}y(s) - \frac{dy(s)}{ds}x(s)\right).$$

This can be seen as follows: Since the tangent vectors of the curve

$$\big\{\mathcal{D}_R(\tilde{\ell}(s))\big\} = \big\{(x_0(s),x_1(s),x_2(s),x_3(s)) = x_0(s)\mathbf{1} + x_1(s)\mathbf{i} + x_2(s)\mathbf{j} + x_3(s)\mathbf{k}\big\},$$

where

$$x_0(s) + \sqrt{-1}x_2(s) = \frac{\mu(s)}{\sqrt{1+|w(s)|^2}} \quad \text{and} \quad x_1(s) + \sqrt{-1}x_3(s) = \frac{\mu(s)w(s)}{\sqrt{1+|w(s)|^2}},$$

are linear spans of the vector fields $X_{\mathbf{i}}$ and $X_{\mathbf{k}}$ at any points $\mathcal{D}_R(\tilde{\ell}(s))$, there exist functions $A(s)$ and $B(s)$ such that

$$\begin{aligned} \sum \frac{dx_i(s)}{ds}\frac{\partial}{\partial x_i} &= A(s)X_{\mathbf{i}} + B(s)X_{\mathbf{k}}, \\ &= A(s)\left(-x_1(s)\frac{\partial}{\partial x_0} + x_0(s)\frac{\partial}{\partial x_1} + x_3(s)\frac{\partial}{\partial x_2} - x_2(s)\frac{\partial}{\partial x_3}\right) \\ &\quad + B(s)\left(-x_3(s)\frac{\partial}{\partial x_0} + x_2(s)\frac{\partial}{\partial x_1} - x_1(s)\frac{\partial}{\partial x_2} + x_0(s)\frac{\partial}{\partial x_3}\right). \end{aligned}$$

Then we have

$$\begin{aligned}&\dot{x}_0(s)+\sqrt{-1}\,\dot{x}_2(s)\\&\qquad=-A(s)x_1(s)-B(s)x_3(s)+\sqrt{-1}\,\big(A(s)x_3(s)-B(s)x_1(s)\big),\end{aligned}\tag{6.8}$$

$$\begin{aligned}&\dot{x}_1(s)+\sqrt{-1}\,\dot{x}_3(s)\\&\qquad=A(s)x_0(s)+B(s)x_2(s)+\sqrt{-1}\,\big(-A(s)x_2(s)+B(s)x_0(s)\big).\end{aligned}\tag{6.9}$$

If we put $x_0(s)+\sqrt{-1}x_2(s)=w_0(s)$ and $x_1(s)+\sqrt{-1}x_3(s)=w_1(s)$, then (6.8) and (6.9) are rewritten as

$$\begin{aligned}\dot{w}_0(s)&=-\big(A(s)+\sqrt{-1}B(s)\big)\overline{w_1(s)},\\ \dot{w}_1(s)&=\big(A(s)+\sqrt{-1}B(s)\big)\overline{w_0(s)}.\end{aligned}$$

Hence we have

$$\dot{w}_0(s)\overline{w_0(s)}+\dot{w}_1\overline{w_1(s)}=0,\tag{6.10}$$

and by inserting $w_0(s)=\dfrac{\mu(s)}{\sqrt{1+|w(s)|^2}}$ and $w_1(s)=\dfrac{\mu(s)w(s)}{\sqrt{1+|w(s)|^2}}$ into the above equation (6.10), we obtain

$$\frac{\dot{\mu}(s)}{\mu(s)}=\sqrt{-1}\,\frac{\dot{x}(s)y(s)-\dot{y}(s)x(s)}{1+x(s)^2+y(s)^2}.$$

Hence we have:

Proposition 6.8.

$$\mu(s)=e^{\sqrt{-1}\,\theta(s)}=\exp\left\{\sqrt{-1}\,\int_0^s\frac{\dot{x}y-\dot{y}x}{1+x^2+y^2}dr\right\},$$

and the lift $\{\tilde{\ell}(s)\}$ *is given by*

$$\begin{aligned}\tilde{\ell}(s)&=(w(s),\mu(s))\\&=\left(x(s)+\sqrt{-1}y(s),\exp\left\{\sqrt{-1}\,\int_0^s\frac{\dot{x}y-\dot{y}x}{1+x^2+y^2}dr\right\}\right).\end{aligned}$$

By Corollary 6.5 and Theorem 6.7, it is enough for our purpose to consider a circle in $S^2_{(1/2)}=\{(u_1,u_2,u_3)\mid u_1^2+u_2^2+u_3^2=1/4\}$ that is the intersection with the plane perpendicular to the (u_1,u_2)-plane and passes through the points $(1/2,0,0)$ and $Q=(q_1,q_2,0)$, $q_1^2+q_2^2=1/4$. This circle $\{\gamma_Q(s)=(u_1^Q(s),u_2^Q(s),u_3^Q(s))\}$ is parametrized by

$$u_1^Q(s)=\frac{1+2q_1+(1-2q_1)\cos s}{4},\tag{6.11}$$

$$u_2^Q(s)=\frac{q_2(1-\cos s)}{2},\tag{6.12}$$

$$u_3^Q(s)=\sqrt{\frac{1-2q_1}{2}}\,\frac{\sin s}{2}.\tag{6.13}$$

According to Theorem 3.1:

Proposition 6.9. *Let* $\{\tilde{\gamma}_Q\}$ *be the horizontal lift of an iterated circle* $\{\gamma_Q\}$ *(or an iterated circle + half of the circle) to* S^3 *with respect to the sub-Riemannian structure* $\mathcal{H}_S$ *and take the projection* $\pi_L(\tilde{\gamma}_Q)$*. Then it is a geodesic curve (it is a projection of a bicharacteristic curve of the spherical Grushin operator) connecting two points on the singular set* $\pi_L(\mathcal{S})$*.*

We describe the curve $\pi_L(\tilde{\gamma}_Q)$ explicitly. There are many geodesic curves connecting two points $E_0 = (1/2, 0, 0)$ and $E_1 = (a_1/2, b_1/2, 0) \in \pi_L(\mathcal{S}) \subset S^2_{\mathcal{G}}$ (for the sake of simplicity, we only consider the end point $a_1 + \sqrt{-1}b_1 = \frac{1}{2}e^{-\sqrt{-1}\,\epsilon_1}$ with $0 < \epsilon_1 < \pi$). If they come from *iterated circles + a half-circle* in $S^2{}_{(1/2)} = \pi_R(S^3)$ starting from $Q_0 = (1/2, 0, 0)$ and being perpendicular to the (u_1, u_2)-plane, then the end point $(p_1, p_2, 0)$ of such circles must be located on the equator $\big\{(a, b, 0) \,\big|\, a^2 + b^2 = 1/4\big\}$ (see Corollary 6.5). So we only consider E_0 as an end point (if it is different from E_0 similar arguments can be used). As it was noted in (6.6) the end point satisfies

$$e^{-2\sqrt{-1}t(1)}e^{\sqrt{-1}\,\epsilon_1} = 1 \tag{6.14}$$

if the curve $\mathcal{D}_L^{-1}(\tilde{\gamma}_Q)\}$ is expressed as

$$\big\{\mathcal{D}_R^{-1}\big(\tilde{\gamma}_Q(s)\big)\big\} = \big\{\big(e^{\sqrt{-1}t(s)}, z(s)\big)\big\},$$

and so we may assume that

$$t(1) = \frac{\epsilon_1}{2}. \tag{6.15}$$

From (6.15) the explicit description of the curve $\pi_L(\tilde{\gamma}_Q)$ is given in several steps.

Step 1: *Description of the horizontal lift of the circle* $\{\gamma_Q(s)\}$*.*
We transform $\{\gamma_Q(s)\}$ to a circle $\big\{\gamma_Q^{\perp}(s) = (-u_3^Q(s), u_2^Q(s), u_1^Q(s))\big\}$ in $S^2_{(1/2)}$ and consider the loop $\{\overline{\mathcal{D}_R}^{\,-1}(\gamma_Q^{\perp})\}$ in the complex plane, which we denote by $\{\Gamma_Q\}$. Then by Proposition 6.8 we can express the lift $\{\tilde{\Gamma}_Q\}$ of this loop $\{\Gamma_Q\}$ as follows:

Proposition 6.10.

$$\begin{aligned}\tilde{\Gamma}_Q(s) &= \big(w^Q(s), \mu^Q(s)\big)\\ &= \Bigg(\frac{-\sqrt{1/2 - q_1}\cdot\sin s + \sqrt{-1}\cdot 2q_1\cdot\sin^2(s/2)}{1 + 2q_1\sin^2(s/2) + \cos^2(s/2)},\\ &\qquad \exp\left\{\sqrt{-1}\cdot q_2\cdot\sqrt{1/2 - q_1}\cdot\int_0^s \frac{\sin^2(r/2)}{1 + 2q_1\sin^2(r/2) + \cos^2(r/2)}dr\right\}\Bigg).\end{aligned}$$

Proof. Since

$$\overline{\mathcal{D}}_R^{\,-1}(-u_3^Q, u_2^Q, u_1^Q) = \frac{-u_3^Q}{\frac{1}{2} + u_1^Q} + \sqrt{-1}\cdot\frac{u_2^Q}{\frac{1}{2} + u_1^Q} = x(s) + \sqrt{-1}y(s)$$

by (6.11), (6.12) and (6.13) we have:

$$\begin{aligned}\frac{\dot{x}(s)y(s)-\dot{y}(s)x(s)}{1+x(s)^2+y(s)^2} &= \frac{\dot{u}_3^Q(s)u_2^Q(s)-\dot{u_2}^Q(s)u_3^Q(s)}{1/2+u_1^Q(s)}\\ &= \frac{q_2\sqrt{1/2-q_1}\,\sin^2(s/2)}{1+2q_1\sin^2(s/2)+\cos^2(s/2)}.\end{aligned}$$ □

Step 2: *We transform the curve* $\{\mathcal{D}_R(\tilde{\Gamma}_Q)\}$ *by a transformation in* $\mathbb{H}$ *defined by the left multiplication* $L_{(\mathbf{1}+\mathbf{i})/\sqrt{2}}\colon h \mapsto \frac{\mathbf{1}+\mathbf{i}}{\sqrt{2}}\cdot h$ *with the element* $\frac{\mathbf{1}+\mathbf{i}}{\sqrt{2}}$,

$$\begin{array}{ccc}\mathbb{C}\times\mathbb{C} & \longrightarrow & \mathbb{H}\\ {\scriptstyle T}\big\downarrow & & \big\downarrow{\scriptstyle L_{(\mathbf{1}+\mathbf{i})/\sqrt{2}}}\\ \mathbb{C}\times\mathbb{C} & \longrightarrow & \mathbb{H},\end{array}$$

$$\begin{array}{ccc}(w_0,w_1)=(x_0+\sqrt{-1}x_2,\ x_1+\sqrt{-1}x_3) & \longleftarrow & h=x_0\mathbf{1}+x_1\mathbf{i}+x_2\mathbf{j}+x_3\mathbf{k}\\ {\scriptstyle T}\big\downarrow & & \big\downarrow{\scriptstyle L_{(\mathbf{1}+\mathbf{i})/\sqrt{2}}}\\ \frac{1}{\sqrt{2}}(w_0-w_1,w_0+w_1) & \longleftarrow & L_{(\mathbf{1}+\mathbf{i})/\sqrt{2}}(h)=(\mathbf{1}+\mathbf{i})/\sqrt{2}\cdot h.\end{array}$$

Proposition 6.11. *Let* $\mathcal{D}_R(w,\mu)=(w_0,w_1)$ *and* $\mathcal{D}_R(\tilde{w},\tilde{\mu})=\frac{1}{\sqrt{2}}(w_0-w_1,w_0+w_1)=T(w_0,w_1)$. *Then*

$$\tilde{\mu}=\frac{\mu(1-w)}{|1-w|} \quad \textit{and} \quad \tilde{w}=\frac{1+w}{1-w}.$$

Proof. We assume that $w\neq 1$. Then by comparison

$$\frac{1}{\sqrt{2}}\left(\frac{\mu-\mu w}{\sqrt{1+|w|^2}},\frac{\mu+\mu w}{\sqrt{1+|w|^2}}\right)=\left(\frac{\tilde{\mu}}{\sqrt{1+|\tilde{w}|^2}},\frac{\tilde{\mu}\tilde{w}}{\sqrt{1+|\tilde{w}|^2}}\right)$$

the relation follows. □

By Propositions 6.10 and 6.11, we put

$$\tilde{\Gamma}_Q(s)=\mathcal{D}_R^{-1}(\tilde{\gamma}_Q(s))=\big(\tilde{w}(s),\tilde{\mu}(s)\big).$$

Then by taking account the correspondence $\mathcal{D}_L^{-1}\circ\mathcal{D}_R$ (see (6.6)) if we write $\mathcal{D}_L^{-1}\circ\mathcal{D}_R(\tilde{w}(s),\tilde{\mu}(s))$ as $(\lambda(s),z(s))$, then the resulting curve is

$$z(s)=\overline{\mu}^2\frac{1+\overline{w}(s)}{1-w(s)}. \tag{6.16}$$

Step 3: *Then the curve is given as*:

Proposition 6.12.

$$\begin{aligned}\left\{\pi_L\left(\mathcal{D}_L^{-1}(\tilde{\gamma}_Q)\right)\right\} &= \left(\frac{z(s)}{\sqrt{1+|z(s)|^2}}, \frac{1}{\sqrt{1+|z(s)|^2}} - \frac{1}{2}\right) \\ &= \left(\overline{\mu}^2 \frac{1-\overline{w}^2}{2(1+|w|^2)}, -\frac{\overline{w}+w}{2(1+|w|^2)}\right), \end{aligned} \tag{6.17}$$

where

$$\overline{\mu}^2\,\frac{1-\overline{w}^2}{2(1+|w|^2)} = e^{-2\sqrt{-1}\cdot q_2(\sqrt{1/2-q_1})\int_0^s \frac{\sin^2(r/2)}{1+2q_1\sin^2(r/2)+\cos^2(r/2)}dr} \\ \times\left(\frac{1}{2}+\left(\frac{1}{2}-q_1\right)\frac{\sin^2(s/2)\cos^2(s/2)-\sqrt{-1}\left(\frac{1}{2}+q_1\right)\sin^3(s/2)\cos(s/2)}{1+2q_1\sin^2(s/2)+\cos^2(s/2)}\right), \tag{6.18}$$

$$-\frac{\overline{w}+w}{2(1+|w|^2)} = \sqrt{\frac{1}{2}-q_1}\cdot\frac{1+2q_1\sin^2(s/2)+\cos^2(s/2)}{2}\cdot\frac{\sin s}{2},$$

is the curve we aimed to construct in $\pi_L(S^3) = S^2_{\mathcal{G}}$.

The final form of the geodesic $\{\pi_L(\tilde{\gamma}_Q(s))\}$ is given by replacing the value q_1 in the above formulas (6.18) and (6.12) by $q_1(n)$ (see the notation in (6.20)) after determining it according to the number of the iteration of the circle $\{\gamma_Q\}$, which is given in Proposition 6.14 below.

Following the procedure explained above we give the expression of the geodesics $\left\{\pi_L\left(\mathcal{D}_L^{-1}(\tilde{\gamma}_Q)\right)\right\}$ including the curves coming from iterations of this circle. So, for each fixed $n\in\mathbb{N}$, let $\{\gamma_Q^n(s)\}_{0\le s\le 1}$ be an iterated circle

$$\gamma_Q^n(s) = \left(u_1^Q(2n\pi s), u_2^Q(2n\pi s), u_3^Q(2n\pi s)\right)$$

(or we consider $0\le s\le 2n\pi$), and we assume that the end point $\gamma_Q^n(1)=\gamma_Q^n(0)$ of this iterated circle corresponds to $E_1=(a_1/2, b_1/2, 0)\in\pi_L(\mathcal{S})$ ($e^{-\sqrt{-1}\,\epsilon_1} = a_1+b_1\sqrt{-1}$, $0<\epsilon_1<\pi$ or $b_1<0$). According to the equality $0<t_n(1)=\frac{\epsilon_1}{2}<\pi/2$ we have

$$\begin{aligned} t_n(1) &= \int_0^1 \frac{\dot{x}_n(r)y_n(r)-\dot{y}_n(r)x_n(r)}{1+x_n(r)^2+y_n(r)^2}\,dr \\ &= q_2\cdot\sqrt{1/2-q_1}\cdot\int_0^1\frac{2n\pi\cdot\sin^2 n\pi r}{1+2q_1\sin^2 n\pi r+\cos^2 n\pi r}\,dr. \end{aligned} \tag{6.19}$$

Let

$$\tau_R = \frac{ydx-xdy}{2(1+x^2+y^2)}$$

be a one-form on $\mathbb{C} \cong \mathbb{R}^2$. Then the volume form $d_R(x,y)$ on $\mathbb{C}$ with respect to the metric induced by the Riemannian metric on $S^2_{(1/2)}$ through the map $\overline{\mathcal{D}_R}$ coincides with the two-form $d\tau_R$,

$$d\tau_R = d_R(x,y) = \frac{dy \wedge dx}{(1+x^2+y^2)^2}.$$

Proposition 6.13. *In case $\{\ell\}$ is a loop, we have by Stokes theorem that*

$$\int_{D_\ell} d\tau_R = \int_{\partial D_\ell} \tau_R = \int_0^1 \ell^*(\tau_R),$$

where D_ℓ is the domain surrounded by the loop $\{\ell\}$ (we assume that the loop $\{\ell\}$ has no self-intersection).

Now we take a circle $\{\gamma_Q^n\}$ on the sphere ${S^2}_{(1/2)}$. Let $D(q_1)$ be the domain in $S^2_{(1/2)}$ surrounded by a circle $\{\gamma_Q(s)\}_{0\leq s\leq 2\pi}$ including the point $(0,u_2,u_3)$ with $u_2 > 0$. Since the area of the domain $D(q_1)$ is given by

$$\textit{area of the domain } D(q_1) = 2\pi(1/2)^2\left(1-\sqrt{1/2+q_1}\right),$$

we have:

Proposition 6.14.

$$\begin{aligned} t_n(1) &= \int d\tau_R = \int \left(\gamma_Q^n\right)^*(\tau_R) = 2n \cdot \text{area of } D(q_1) \\ &= 2n\cdot 2\pi(1/2)^2\left(1-\sqrt{q_1+1/2}\right) = \frac{\epsilon_1}{2}. \end{aligned}$$

So

$$q_1 = q_1(n) = \left(1-\frac{\epsilon_1}{2n\pi}\right)^2 - \frac{1}{2}. \tag{6.20}$$

Corollary 6.15. *For $0<\epsilon<\pi$, we have the identity*

$$2n\pi\left(\frac{1}{2}-q(n)\right)\sqrt{\frac{1}{2}+q(n)}\int_0^1 \frac{\sin^2 n\pi r}{1+2q(n)\sin^2 n\pi r+\cos^2 n\pi r}\,dr = \frac{\epsilon}{2}$$

if $q(n) = \left(1-\frac{\epsilon}{2n\pi}\right)^2 - \frac{1}{2}$.

7. Quaternionic structure on $\mathbb{R}^8$ and sub-Riemannian structures

It is standard to describe seven vector fields on S^7 based on the Octanion structure on $\mathbb{R}^8$, which give the trivialization of the tangent bundle $T(S^7)$. Here we describe vector fields based on the left and right quaternionic vector space structures of $\mathbb{R}^8$ similar to the S^3 case. Then we can define sub-Riemannian structures on S^7 in the strong sense and of codimensions 3, 2 and 1. Correspondingly there is an operator on the quaternion projective line $P^1\mathbb{H}$ which is called a *spherical Grushin operator*. We have another hypo-elliptic (and not elliptic) operator on $P^1\mathbb{H}$, corresponding to the horizontal Laplacian in the case of S^3.

7.1. Vector fields on S^7 and sub-Riemannian structures

As in §6, let $\mathbb{H}$ be the quaternion number field over $\mathbb{R}$ with the usual basis $\{\mathbf{1} = \mathbf{e}_0, \mathbf{i} = \mathbf{e}_1, \mathbf{j} = \mathbf{e}_2, \mathbf{k} = \mathbf{e}_3\}$. We identify $\mathbb{R}^8$ with $\mathbb{H} \oplus \mathbb{H} = \mathbb{H}^2$ through the correspondence

$$\mathbb{R}^8 \ni x = (x_0, \ldots, x_3, x_4, \ldots, x_7) \longleftrightarrow$$

$$\big(x_0\mathbf{e}_0 + x_1\mathbf{e}_1 + x_2\mathbf{e}_2 + x_3\mathbf{e}_3, x_4\mathbf{e}_0 + x_5\mathbf{e}_1 + x_6\mathbf{e}_2 + x_7\mathbf{e}_3\big) = (h_1, h_2) \in \mathbb{H} \oplus \mathbb{H}$$

together with the standard Euclidean metric

$$< x,\, y >_{\mathbb{R}} = \frac{1}{2}\left(h_1\overline{k_1} + k_1\overline{h_1} + h_2\overline{k_2} + k_2\overline{h_2}\right), \;\; x = (h_1, h_2),\, y = (k_1, k_2), \tag{7.1}$$

where $\overline{h} = x_0\mathbf{1} - \sum_{i=1,2,3} x_i\mathbf{e}_i$ is the quaternion conjugate of $h = \sum x_i\mathbf{e}_i \in \mathbb{H}$.

Let

$$A_0 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad A_1 = \begin{pmatrix} \mathbf{i} & 0 \\ 0 & -\mathbf{i} \end{pmatrix}, \quad A_2 = \begin{pmatrix} \mathbf{j} & 0 \\ 0 & -\mathbf{j} \end{pmatrix}, \quad A_3 = \begin{pmatrix} \mathbf{k} & 0 \\ 0 & -\mathbf{k} \end{pmatrix}$$

be 2×2 quaternion matrices which act on $\mathbb{H}^2$ as

$$\begin{aligned} A_0 &: \mathbb{H}^2 \ni (h_1, h_2) \longmapsto (h_2, -h_1), \\ A_1 &: \mathbb{H}^2 \ni (h_1, h_2) \longmapsto (\mathbf{i}h_1, -\mathbf{i}h_2), \\ A_2 &: \mathbb{H}^2 \ni (h_1, h_2) \longmapsto (\mathbf{j}h_1, -\mathbf{j}h_2), \\ A_3 &: \mathbb{H}^2 \ni (h_1, h_2) \longmapsto (\mathbf{k}h_1, -\mathbf{k}h_2). \end{aligned}$$

Also let A_4, A_5 and A_6 be left $\mathbb{H}$-linear maps on $\mathbb{H}^2$ defined as

$$\begin{aligned} A_4 &: \mathbb{H}^2 \ni (h_1, h_2) \longmapsto (h_2\mathbf{i}, h_1\mathbf{i}), \\ A_5 &: \mathbb{H}^2 \ni (h_1, h_2) \longmapsto (h_2\mathbf{j}, h_1\mathbf{j}), \\ A_6 &: \mathbb{H}^2 \ni (h_1, h_2) \longmapsto (h_2\mathbf{k}, h_1\mathbf{k}). \end{aligned}$$

Then A_0 is *left* and *right* $\mathbb{H}$-linear and A_1, A_2, A_3 are *right* $\mathbb{H}$-linear, while A_4, A_5, A_6 are *left* $\mathbb{H}$-linear. All maps are $\mathbb{R}$-linear, *anti-symmetric* with respect to the standard inner product (7.1) and satisfy the commutation relations

$$0 \le i,\, j \le 6, \;\; A_iA_j + A_jA_i = -2\delta_{i\,j}. \tag{7.2}$$

We define seven vector fields X_i on $\mathbb{H}^2$ by:

$$X_i(\varphi)(h_1, h_2) = \frac{d}{dt}\left\{\varphi\left(\sum_{k \ge 0} \frac{t^k {A_i}^k}{k!}(h_1, h_2)\right)\right\}\Big|_{t=0},$$

where $\varphi \in C^\infty(\mathbb{H}^2)$. Identifying the tangent bundles $T(\mathbb{H}^2) \cong \mathbb{H}^2 \times \mathbb{H}^2$ and

$$T(S^7) \cong \Big\{(h_1, h_2; k_1, k_2) \in \mathbb{H}^2 \times \mathbb{H}^2 \;\Big|\; |h|_1^2 + |h_2|^2 = 1,$$
$$\langle (h_1, h_2),\, (k_1, k_2)\rangle_{\mathbb{R}} = \frac{1}{2}\left(h_1\overline{k_1} + k_1\overline{h_1} + h_2\overline{k_2} + k_2\overline{h_2}\right) = 0\Big\},$$

these seven vector fields $X_0, X_1, \dots, X_6$ are expressed as

$$\begin{aligned} X_0 &= (h_1, h_2; h_2, -h_1) &&= (h_1, h_2; A_0(h_1, h_2)),\\ X_1 &= (h_1, h_2; \mathbf{i}h_1, -\mathbf{i}h_2) &&= (h_1, h_2; A_1(h_1, h_2)),\\ X_2 &= (h_1, h_2; \mathbf{j}h_1, -\mathbf{j}h_2) &&= (h_1, h_2; A_2(h_1, h_2)),\\ X_3 &= (h_1, h_2; \mathbf{k}h_1, -\mathbf{k}h_2) &&= (h_1, h_2; A_3(h_1, h_2)),\\ X_4 &= (h_1, h_2; h_2\mathbf{i}, h_1\mathbf{i}) &&= (h_1, h_2; A_4(h_1, h_2)),\\ X_5 &= (h_1, h_2; h_2\mathbf{j}, h_1\mathbf{j}) &&= (h_1, h_2; A_5(h_1, h_2)),\\ X_6 &= (h_1, h_2; h_2\mathbf{k}, h_1\mathbf{k}) &&= (h_1, h_2; A_6(h_1, h_2)). \end{aligned}$$

All of them are tangent to the sphere and mutually orthonormal at any point on S^7 with respect to the standard Euclidean metric $\langle \cdot, \cdot \rangle_{\mathbb{R}}$. So they trivialize the tangent bundle of S^7 (cf. [Adm-62]) and we also regard them as first-order skew-symmetric differential operators with respect to the inner product defined by the Riemannian volume form $dS(x)$,

$$dS(x) = \sum_{i=0}^{7} (-1)^i x_i dx_0 \wedge \cdots \wedge \widehat{dx_i} \wedge \cdots \wedge dx_7.$$

Here we recall:

Theorem 7.1 ([Adm-62]). *Let* $n + 1 = 2^{a+4b} \times \text{odd integer}$, $0 \le a < 4$, $b \ge 0$ *and put* $\gamma(n) = 2^a + 8b - 1$. *Then the maximal dimension of a trivial sub-bundle in* $T(S^n)$ *is* $\gamma(n)$.

In small dimensions these numbers are given as $\gamma(\text{even}) = 0$, $\gamma(3) = 3$, $\gamma(5) = 1$, $\gamma(7) = 7$, $\gamma(9) = 1$, $\gamma(11) = 3$, $\gamma(13) = 1$, $\gamma(15) = 8$, $\gamma(23) = 7$, …, $\gamma(31) = 13$.

Remark 7.2. In general, the realizations of $\gamma(n)$-vector fields on S^n are given by a Clifford module structure on $\mathbb{R}^{n+1}$. According to Theorem 7.1 we know that the spheres which possibly admit a sub-Riemannian structure in the strong sense are S^3, S^7, S^{15}, S^{23} and S^{31}. Note that all odd-dimensional sphere have a contact structure (see [BF3-08]).

Proposition 7.3. *By the commutation relations* (7.2) *we have*

$$[X_i, X_j](\varphi)(h_1, h_2) = \frac{d}{dt} \left\{ \varphi \left(\sum \frac{t^k [A_i, A_j]^k}{k!} (h_1, h_2) \right) \right\} \Big|_{t=0}.$$

Hence $[X_i, X_j]$ *corresponds to*

$$[X_i, X_j] = (h_1, h_2; 2A_iA_j(h_1, h_2)) \quad \text{for } i \neq j.$$

Now we prove:

Proposition 7.4 (cf. [BF3-08]). *Let* C_1, C_2, C_3, C_4 *be any four among the seven linear transformations* $\{A_i\}_{i=0}^{6}$. *Then for any* $x \in S^7$ *the vectors* $C_i(x)$, $C_iC_j(x)$ $(0 \le i, j \le 4, i < j)$ *span the tangent space* $T_x(S^7)$.

Proof. Let $x \in S^7$. For $i \neq j$, first we remark that $C_iC_j(x)$ is tangent to the sphere at $x \in S^7$, since

$$\begin{aligned}\langle C_iC_j(x),\, x\rangle_{\mathbb{R}} &= -\,\langle C_j(x),\, C_i(x)\rangle_{\mathbb{R}} \\ &= \langle x,\, C_jC_i(x)\rangle_{\mathbb{R}} = -\,\langle x,\, C_iC_j(x)\rangle_{\mathbb{R}}\,.\end{aligned}$$

The five vectors $\{x,\, C_1(x),\, C_2(x),\, C_3(x),\, C_4(x)\}$ are linearly independent. If we assume all the vectors $C_1C_i(x)$ $(i = 2,3,4)$ are linearly dependent with $\{x,\, C_1(x),$ $C_2(x),\, C_3(x),\, C_4(x)\}$, then the five-dimensional subspace spanned by $\{x,\, C_1(x),$ $C_2(x),\, C_3(x),\, C_4(x)\}$ is C_1 invariant, which leads to a contradiction, since C_1 is non-singular skew-symmetric. Hence there is at least one of $C_1C_j(x)$ $(j = 2,3,4)$ which is linearly independent with $\{x,\, C_1(x),\, C_2(x),\, C_3(x),\, C_4(x)\}$. By reordering we may assume it is $C_1C_2(x)$. Now, again we assume all the vectors $C_1C_3(x)$, $C_1C_4(x)$, $C_2C_3(x)$, $C_2C_4(x)$ are linearly dependent with the vectors $\{x,\, C_1(x),$ $C_2(x),\, C_3(x),\, C_4(x),\, C_1C_2(x)\}$. Then the transformations C_1 and C_2 leave the six-dimensional subspace spanned by $\{x,\, C_1(x),\, C_2(x),\, C_3(x),\, C_4(x),\, C_1C_2(x)\}$ invariant. Now by J. Adam's Theorem 7.1 (see [Adm-62]) this also leads to a contradiction. Hence there is at least one vector in $\{C_1C_3(x),\, C_1C_4(x),\, C_2C_3(x),$ $C_2C_4(x)\}$ linearly independent with $\{x,\, C_1(x),\, C_2(x),\, C_3(x),\, C_4(x),\, C_1C_2(x)\}$. If it is $C_1C_3(x)$ or $C_1C_4(x)$, we may assume it is $C_1C_3(x)$. If it is $C_2C_3(x)$ or $C_2C_4(x)$, we reorder C_1 to C_2 and C_2 to C_1 and again we can assume that the seven vectors $\{x,\, C_1(x),\, C_2(x),\, C_3(x),\, C_4(x),\, C_1C_2(x),\, C_1C_3(x)\}$ are linearly independent. If $C_1C_4(x)$ is included in the seven-dimensional subspace spanned by these seven vectors, then again we have a contradiction, since it must be invariant under the anti-symmetric non-singular transformation C_1. Hence at any point $x \in S^7$ the vectors $\{C_1(x),\, C_2(x),\, C_3(x),\, C_4(x),\, C_1C_2(x),\, C_1C_3(x),\, C_1C_4(x),\, C_2C_3(x),$ $C_2C_4(x),\, C_3C_4(x)\}$ span the tangent space $T_x(S^7)$. □

From the previous proposition we know that there are sub-Riemannian structures in the strong sense on the seven-dimensional sphere, of codimension 3 and of step 2. However, contrary to the three-dimensional case not all the 7 vector fields are simultaneously left (or right) invariant under the action of the group $Sp(1)$, i.e., some of them are defined by the right-$\mathbb{H}$ linear transformation (so we have left-$Sp(1)$-invariant vector fields) and some are defined by the left-$\mathbb{H}$ linear transformations (hence we have right-$Sp(1)$-invariant vector fields).

In order to work with the Hopf bundle $S^7 \to \mathbb{H}P^1$ we consider a non-holonomic sub-bundle, denoted by $\mathcal{H}_4$ and spanned by the vector fields X_0, X_4, X_5 and X_6 (they all are left-$Sp(1)$-invariant). On this sub-bundle $\mathcal{H}_4$ we install the metric as the restriction of the standard metric to S^7, i.e., we assume that the vector fields X_0, X_4, X_5 and X_6 are mutually orthonormal at each point on S^7. Then $\mathcal{H}_4$ gives a sub-Riemannian structure on S^7, in the strong sense, of co-dimension 3 and of step 2. Likewise we denote the sub-bundles spanned by $\mathcal{H}_4$ and X_1 by $\mathcal{H}_5$, and the one spanned by $\mathcal{H}_5$ and X_2 by $\mathcal{H}_6$. We always assume that the metric on $\mathcal{H}_i$ $(i = 4,5,6)$ is the restriction of the standard metric on the sphere. Then by Proposition 7.4 above the order of the brackets needed to span the tangent space is always 1.

The operators

$$\begin{aligned}\Delta^{\mathrm{sub}}_{(4)} &= -\left({X_0}^2 + {X_4}^2 + {X_5}^2 + {X_6}^2\right),\\ \Delta^{\mathrm{sub}}_{(5)} &= -\left({X_0}^2 + {X_4}^2 + {X_5}^2 + {X_6}^2 + {X_1}^2\right),\\ \Delta^{\mathrm{sub}}_{(6)} &= -\left({X_0}^2 + {X_4}^2 + {X_5}^2 + {X_6}^2 + {X_1}^2 + {X_2}^2\right)\end{aligned}$$

are sub-Laplacians with respect to the sub-Riemannian structures $\mathcal{H}_4$, $\mathcal{H}_5$ and $\mathcal{H}_6$, respectively. Each sub-Laplacian is hypo-elliptic and positive symmetric with respect to the Riemannian volume form $dS(x)$. The sum of squares of all vector fields

$$\Delta_{S^7} = -\left({X_0}^2 + {X_4}^2 + {X_5}^2 + {X_6}^2 + {X_1}^2 + {X_2}^2 + {X_3}^2\right)$$

gives the Laplace operator with respect to the standard metric.

7.2. Hopf fibration and a sub-Riemannian structure

Let R_g be the *right* action of the symplectic group $Sp(1)$ on S^7,

$$R_g\colon S^7 \ni (h_1, h_2) \longmapsto (h_1 g^{-1}, h_2 g^{-1}),$$

$$g = \sum_{i=0}^{3} g_i \mathbf{e}_i \in Sp(1) = \left\{g \in \mathbb{H} \;\middle|\; g\overline{g} = |g|^2 = 1\right\}.$$

Then we have:

Proposition 7.5. *For $g \in Sp(1)$,*

$$\begin{aligned}&dR_g(X_0) = X_0,\\ &dR_g(X_4) = ({g_0}^2 + {g_1}^2 - {g_2}^2 - {g_3}^2)X_4 + 2(g_0g_3 + g_1g_2)X_5 - 2(g_0g_2 - g_1g_3)X_6,\\ &dR_g(X_5) = 2(g_1g_2 - g_0g_3)X_4 + ({g_0}^2 - {g_1}^2 + {g_2}^2 - {g_3}^2)X_5 + 2(g_0g_1 + g_2g_3)X_6,\\ &dR_g(X_6) = 2(g_0g_2 + g_1g_3)X_4 - 2(g_0g_1 - g_2g_3)X_5 + ({g_0}^2 - g_1^2 - {g_2}^2 + {g_3}^2)X_6.\end{aligned}$$

Proof. Let $g = \sum g_i \mathbf{e}_i \in Sp(1),\ g_i \in \mathbb{R}$. Then

$$\begin{aligned}g\mathbf{i}g^{-1} &= ({g_0}^2 + {g_1}^2 - {g_2}^2 - {g_3}^2)\mathbf{i} + 2(g_0g_3 + g_1g_2)\mathbf{j} - 2(g_0g_2 - g_1g_3)\mathbf{k}\\ g\mathbf{j}g^{-1} &= 2(g_1g_2 - g_0g_3)\mathbf{i} + ({g_0}^2 - {g_1}^2 + {g_2}^2 - {g_3}^2)\mathbf{j} + 2(g_0g_1 + g_2g_3)\mathbf{k}\\ g\mathbf{k}g^{-1} &= 2(g_0g_2 + g_1g_3)\mathbf{i} - 2(g_0g_1 - g_2g_3)\mathbf{j} + ({g_0}^2 - g_1^2 - {g_2}^2 + {g_3}^2)\mathbf{k}.\end{aligned}$$

These give the desired formulas. □

Corollary 7.6. *Let $\Lambda = \sum_{i=4}^{6} {X_i}^2$. Then we have*

$$\sum_{i=4}^{6} \Big(dR_g(X_i)\Big)^2 = \sum_{i=4}^{6} {X_i}^2,$$

i.e., the operator Λ and the sub-Laplacian $\Delta^{\mathrm{sub}}_{(4)}$ are right-$Sp(1)$-invariant.

The orbit space of the *right-$Sp(1)$*-action of R_g on S^7 ($g \in Sp(1)$) is the one-dimensional quaternion projective space $P^1(\mathbb{H})$ and we denote the resulting Hopf bundle by $\pi_R\colon S^7 \longrightarrow P^1(\mathbb{H})$. We identify $P^1(\mathbb{H})$ with the sphere S^4 of radius $1/2$ through the map

$$S^7 \longrightarrow P^1(\mathbb{H}) \cong S^4, \quad \big(h_1, h_2\big) \longmapsto$$
$$\big(|h_1|^2 - 1/2, h_1\overline{h_2}\big) \in \left\{ (a_0, \sum_{i=0}^{3} y_i \mathbf{e}_i) \mid {a_0}^2 + \sum_{i=0}^{3} {y_i}^2 = 1/4 \right\} \subset \mathbb{R} \times \mathbb{H}.$$

Proposition 7.7. *Let $\mathcal{S}$ be the following sub-manifold in S^7:*

$$\mathcal{S} = \big\{(h_1, h_2) \in S^7 \;\big|\; |h_1|^2 = |h_2|^2 = 1/2,\; h_1\overline{h_2} + h_2\overline{h_1} = 0\big\} \;(\cong S^3 \times S^2).$$

Then $\mathcal{S}$ is right-$Sp(1)$*-invariant and*

$$\pi_R(\mathcal{S}) = \Big\{(0, y_1\mathbf{i} + y_2\mathbf{j} + y_3\mathbf{k}) = (0, 0, y_1, y_2, y_3), \Big| \sum {y_i}^2 = 1/4\Big\}.$$

Moreover, the vector field X_0 is tangent to $\mathcal{S}$, that is, $d\pi_R(X_0) = 0$.

Proof. Since the curve $\{e^{tA_0} \cdot (h_1, h_2)\} = \{(\cos t h_1 + \sin t h_2, -\sin t h_1 + \cos t h_2)\}$ $= \{\big(h_1^0(t), h_2^0(t)\big)\}$ on $\mathcal{S}$ satisfies

$$\begin{aligned} &h_1^0(t)\overline{h_1^0(t)} - 1/2 \\ &\qquad = \cos^2 t \cdot |h_1|^2 + \cos t \sin t \cdot h_1\overline{h_2} + \sin^2 t \cdot |h_2|^2 + \cos t \sin t \cdot h_2\overline{h_1} - 1/2 \\ &\qquad = 0, \end{aligned}$$

and

$$\begin{aligned} &h_1^0(t)\overline{h_2^0}(t) \\ &\quad = -\cos t \sin t |h_1|^2 + \cos^2 t \cdot h_1\overline{h_2} - \sin^2 t \cdot h_2\overline{h_1} + \sin t \cos t \cdot |h_2|^2 \\ &\quad = -\cos t \sin t \cdot 1/2 + \cos^2 t \cdot h_1\overline{h_2} + \sin^2 t \cdot h_1\overline{h_2} + \sin t \cos t \cdot 1/2 = h_1\overline{h_2}, \end{aligned}$$

the curve $\{\pi_R((h_1^0(t), h_2^0(t)))\}$ is constant. □

By Propositions 7.5, 7.7 and the fact that the action R_g ($g \in Sp(1)$) leaves the sub-Riemannian metric invariant, the sub-bundle $\mathcal{H}_4$ defines a connection on the principal bundle $\pi_R : S^7 \backslash \mathcal{S} \longrightarrow P^1(\mathbb{H}) \backslash \pi_R(\mathcal{S})$ together with the Riemannian metric on $P^1(\mathbb{H}) \backslash \pi_R(\mathcal{S})$ in an obvious way. We denote the operator descended from the sub-Laplacian $\Delta^{\text{sub}}_{(4)}$ on S^4 by $\mathcal{D}$ and the one descended from Λ by $\overline{\Lambda}$. They can be identified with the sub-Laplacian $\Delta^{\text{sub}}_{(4)}$ and Λ, respectively, acting on functions invariant under the right-$Sp(1)$-action.

Proposition 7.8. *Since $d\pi_R(X_0) = 0$ on $\mathcal{S}$, the operator $\mathcal{D}$ is not elliptic, but hypo-elliptic and positive symmetric with respect to the volume form $(\pi_R)_*(dS(x))$, the fiber integral of the Riemannian volume form on S^7, which coincides with (the constant times) volume form on S^4 with respect to the standard Riemannian metric.*

The action of the group $\{\exp tA_0\}_{t\in\mathbb{R}}$ is descended to $P^1(\mathbb{H})$ and the resulting action is given by the transformation $\{{\phi^0}_t\}_{t\in\mathbb{R}}$,

$$\begin{aligned}{\phi^0}_t\colon S^4 \ni \Big(a_0, \sum y_i\mathbf{e}_i\Big) &\longmapsto \\ \big(\cos 2t\cdot a_0 + \sin 2t\cdot y_0, (\cos 2t\cdot y_0 - \sin 2t\cdot a_0)\mathbf{1} + y_1\mathbf{i} + y_2\mathbf{j} + y_3\mathbf{k}\big)& \\ \in S^4 \subset \mathbb{R}\times\mathbb{R}^4.&\end{aligned}$$

Hence the orbit space can be identified with the three-dimensional closed ball with radius $\frac{1}{2}$ through the map

$$\begin{aligned}P^1(\mathbb{H}) \cong \Big\{(a_0, \sum_{i=0}^3 y_i\mathbf{e}_i)\ \big|\ {a_0}^2 + |y|^2 = 1/2\Big\} \ni \Big(a_0, \sum_{i=0}^3 y_i\mathbf{e}_i\Big) \longmapsto& \\ (y_1, y_2, y_3) \in \overline{B^3(1/2)} = \Big\{(y_1,y_2,y_3)\ \big|\ \sum_{i=1}^3 {y_i}^2 \le 1/4\Big\} \subset \mathbb{R}^3.&\end{aligned}$$

Proposition 7.9. *The restriction of $\overline{\Lambda}$ to the open subspace $P^1(\mathcal{H})\setminus \pi_R(\mathcal{S})$ is invariant under the descended action $\{{\phi^0}_t\}$ of $\{\exp tA_0\}$ so that it can be still descended to the quotient space*

$$\{{\phi^0}_t\}\backslash\Big(P^1(\mathcal{H})\backslash\pi_R(\mathcal{S})\Big) \cong B^3(1/2),$$

and it is elliptic. It can be seen as an elliptic operator on the manifold $\overline{B^3(1/2)}$ with boundary S^3.

7.3. Singular metric on S^4 and a spherical Grushin operator

In this subsection we consider the *left* action of the group $Sp(1)$ on $\mathbb{H}^2$. Let $P^1(\mathbb{H})_L$ be the quaternion projective line with respect to the *left* action

$$L_g\colon S^7 \to S^7, \quad (h_1,h_2) \mapsto (gh_1, gh_2),\ g\in Sp(1).$$

The resulting Hopf bundle is denoted by

$$\pi_L\colon S^7 \longrightarrow P^1(\mathbb{H})_L \cong S^4, \tag{7.3}$$

$$\pi_L\colon S^7 \ni (h_1,h_2) \longmapsto \big(|h_1|^2 - 1/2, \overline{h_1}h_2\big) \in \mathbb{R}\times\mathbb{H}. \tag{7.4}$$

Since A_0, A_4, A_5 and A_6 commute with the left action L_g, $g\in Sp(1)$, the vector fields X_0, X_4, X_5 and X_6 are invariant under the action of L_g. So we can descend these vector fields to $P^1(\mathbb{H})_L$. Since the tangent bundle $T(P^1(\mathbb{H})_L) \cong T(S^4)$ is non-trivial, the vector fields

$$\big\{d\pi_L(X_0), d\pi_L(X_4), d\pi_L(X_5), d\pi_L(X_6)\big\}$$

are linearly dependent at some points. We describe them:

Proposition 7.10. *Let $\mathcal{E}$ be the sub-manifold in S^7 defined by*

$$\mathcal{E} = \big\{(h_1,h_2)\in S^7\ \big|\ |h_1|^2 = |h_2|^2 = 1/2\big\} \cong S^3\times S^3.$$

Then, the vector fields $\{d\pi_L(X_0), d\pi_L(X_4), d\pi_L(X_5), d\pi_L(X_6)\}$ *on* $P^1(\mathbb{H})_L$ *are linearly dependent on the subspace*

$$\pi_L(\mathcal{E}) = \Big\{(0, x_1, x_2, x_3, x_4) \mid \sum x_i^2 = 1/2\Big\} = S^3 \subset S^4.$$

The operator

$$-\big(d\pi_L(X_0)^2 + d\pi_L(X_4)^2 + d\pi_L(X_5)^2 + d\pi_L(X_6)^2\big)$$

is hypo-elliptic and symmetric with respect to the volume form $(d\pi_L)_*(dS(x))$ *and it is elliptic outside of* $\pi_L(\mathcal{E})$.

Remark 7.11. The operator

$$-\big(d\pi_L(X_0)^2 + d\pi_L(X_4)^2 + d\pi_L(X_5)^2 + d\pi_L(X_6)^2\big)$$

is called *a spherical Grushin operator* on $P^1(\mathbb{H})$ (cf. [BF1-08], [AB-08], [ABS-08]).

Proof. At each point $(h_1, h_2) \in S^7$ the tangent vectors in the fiber of the projection map π_L are linear combinations of the vectors $\{(h_1, h_2; \mathbf{e}_i h_1, \mathbf{e}_i h_2)\}_{i=1}^3$. So we consider the equation

$$a_0(h_2, -h_1) + \sum_{i=1}^{3} a_i(h_2\mathbf{e}_i, h_1\mathbf{e}_i) = \sum_{i=1}^{3} b_i(\mathbf{e}_i h_1, \mathbf{e}_i h_2),$$

where $a_0, a_1, a_2, a_3, b_1, b_2, b_3 \in \mathbb{R}$ and $h_1\overline{h}_1 + h_2\overline{h}_2 = 1$. Setting

$$\sum_{i=0}^{3} a_i\mathbf{e}_i = a_0\mathbf{e}_0 + a \quad \text{and} \quad b = \sum_{i=1}^{3} b_i\mathbf{e}_i,$$

then the above equation can be rewritten as

$$a_0h_2 + h_2a = bh_1 = h_2(a_0 + a) \quad \text{and} \quad -a_0h_1 + h_1a = bh_2 = -h_1(a_0 - a).$$

If we have a non-zero solution b at a point $(h_1, h_2) \in S^7$ of the above equation, then $|h_1|^2 = |h_2|^2 = 1/2$. Conversely, if (h_1, h_2) satisfies $|h_1|^2 = 1/2 = |h_2|^2$, we have the equality $\sum_{i=0}^{3} a_i\mathbf{e}_i = 2\overline{h_2}\, b\, h_1$ for arbitrary $b = \sum_{i=1}^{3} b_i\mathbf{e}_i$, and on such points it follows that $\dim \mathcal{H}_4 \cap \mathrm{Ker}(d\pi_L) = 3$. □

Now, we can install a Riemannian metric on $P^1(\mathbb{H})$ outside the subspace $\pi_L(\mathcal{E})$ such that the vector fields $d\pi_L(X)_0$, $d\pi_L(X)_4$, $d\pi_L(X)_5$ and $d\pi_L(X)_6$ are orthonormal at each point of $P^1(\mathbb{H})\backslash\pi_L(\mathcal{E})$. The one-parameter transformation groups $\{\exp tX_i\}$ generated by the vector field X_0, X_4, X_5, X_6 are given as follows:

$$\begin{aligned}
\exp tX_0(h_1, h_2) &= \big(\cos t\cdot h_1 + \sin t\cdot h_2, \cos t\cdot h_2 - \sin t\cdot h_1\big),\\
\exp tX_4(h_1, h_2) &= \big(\cos t\cdot h_1 + \sin t\cdot h_2\mathbf{i}, \cos t\cdot h_2 + \sin t\cdot h_1\mathbf{i}\big),\\
\exp tX_5(h_1, h_2) &= \big(\cos t\cdot h_1 + \sin t\cdot h_2\mathbf{j}, \cos t\cdot h_2 + \sin t\cdot h_1\mathbf{j}\big),\\
\exp tX_6(h_1, h_2) &= \big(\cos t\cdot h_1 + \sin t\cdot h_2\mathbf{k}, \cos t\cdot h_2 + \sin t\cdot h_1\mathbf{k}\big).
\end{aligned}$$

So the vector fields $d\pi_L(X_i)$ are expressed through the identification

$$T(P^1(\mathbb{H})) \cong T(S^4)$$
$$\cong \left\{(x_0, x; a_0, a) \in \mathbb{R} \times \mathbb{H} \times \mathbb{R} \times \mathbb{H} \;\middle|\; {x_0}^2 + |x|^2 = 1/2,\ x_0 a_0 + \frac{1}{2}(\overline{x}a + \overline{a}x) = 0\right\}$$

as follows:

Proposition 7.12.

$$\begin{aligned}
d\pi_L(X_0) &= \big(|h_1|^2 - 1/2, \overline{h_1}h_2; h_1\overline{h_2} + h_2\overline{h_1}, |h_2|^2 - |h_1|^2\big),\\
d\pi_L(X_4) &= \big(|h_1|^2 - 1/2, \overline{h_1}h_2; h_2\mathbf{i}\overline{h_1} - h_1\mathbf{i}\overline{h_2}, (|h_1|^2 - |h_2|^2)\mathbf{i}\big),\\
d\pi_L(X_5) &= \big(|h_1|^2 - 1/2, \overline{h_1}h_2; h_2\mathbf{j}\overline{h_1} - h_1\mathbf{j}\overline{h_2}, (|h_1|^2 - |h_2|^2)\mathbf{j}\big),\\
d\pi_L(X_6) &= \big(|h_1|^2 - 1/2, \overline{h_1}h_2; h_2\mathbf{k}\overline{h_1} - h_1\mathbf{k}\overline{h_2}, (|h_1|^2 - |h_2|^2)\mathbf{k}\big).
\end{aligned}$$

7.4. Sub-Riemannian structure on a hypersurface in S^7

In the preceding subsections §7.2 and §7.3 we have defined two operators, $\mathcal{D}$ which is similar to the horizontal Laplacian in the three-dimensional sphere case and a Grushin type operator on $P^1(\mathbb{H}) \cong S^4$ based on the Hopf bundle via the left action of $Sp(1)$ (also similar to the case of S^3, cf. [BF3-08]). However, the horizontal Laplacian is not elliptic in this case. In this subsection we show that if we restrict the sub-Riemannian structure to a hypersurface in S^7 we obtain an elliptic operator on S^3.

Let M be a hypersurface in S^7,

$$M = \left\{ (h_1, h_2) \in S^7 \;\middle|\; h_1\overline{h_2} + h_2\overline{h_1} = 0 \right\} \cong S^3 \times S^3.$$

Proposition 7.13.

1. *The vector fields X_4, X_5 and X_6 are tangent to the sub-manifold M.*
2. *The sub-manifold M is $Sp(1)$-invariant from both sides.*

Proof. 1. Since the one-parameter transformation group generated by the vector fields X_i $(i = 4, 5, 6)$ is given by

$$(h_1, h_2) \to \big(h_1 \cos t + h_2\mathbf{e}_i \sin t, h_1\mathbf{e}_i \sin t + h_2 \cos t\big),$$

we have in case of $h_1\overline{h_2} + h_2\overline{h_1} = 0$:

$$\begin{aligned}
&\big(h_1 \cos t + h_2\mathbf{e}_i \sin t\big)\big(\overline{h_1\mathbf{e}_i \sin t + h_2 \cos t}\big)\\
&\qquad\qquad + \big(h_1\mathbf{e}_i \sin t + h_2 \cos t\big)\big(\overline{h_1 \cos t + h_2\mathbf{e}_i \sin t}\big) = 0.
\end{aligned}$$

2. Direct calculation. □

According to Proposition 7.13 we consider the restriction of the Hopf bundle

$$\pi_R \colon M \longrightarrow \pi_R(M) = \left\{ (|h_1|^2 - 1/2, y_1\mathbf{i} + y_2\mathbf{j} + y_3\mathbf{k})\right\} = S^3.$$

The three commutators

$$[X_4, X_5],\ \ [X_4, X_6],\ \ [X_5, X_6]$$

form a basis of the canonical vector fields defined by the right action of the structure group $Sp(1)$. Together with Proposition 7.5 we have:

Proposition 7.14. *The sub-bundle spanned by the vector fields X_4, X_5 and X_6 defines a sub-Riemannian structure on M in the strong sense, i.e., trivial, step 2, and minimal. Moreover, this sub-bundle defines a connection on the principal bundle $\pi_R\colon M \to S^3 = \pi_R(M)$ and we can install a Riemannian metric on $\pi_R(M) = S^3$ in an obvious way, which coincides with the standard metric.*

Proof. We show that the installed metric on $\pi_R(M) = S^3$ coincides with the standard metric. It is enough to show that the vectors $d\pi_R(X_4)$, $d\pi_R(X_5)$ and $d\pi_R(X_6)$ are always orthonormal with respect to the Euclidean inner product in $\mathbb{R} \times \mathbb{H} \cong \mathbb{R}^5$.

For $i = 1, 2, 3$ and by differentiating the curves

$$\begin{aligned}&\pi_R\big(\exp tX_{i+3}\mathbf{e}_i\big)\\&\quad = \big(|h_1 \cos t + h_2\mathbf{e}_i \sin t|^2 - 1/2, (h_1 \cos t + h_2\mathbf{e}_i \sin t)(-\overline{h_1}\mathbf{e}_i \sin t + \overline{h_2} \cos t)\big)\end{aligned}$$

we have

$$\begin{aligned}&d\pi_R(X_i)\\&\quad = \big(|h_1|^2 - 1/2, h_1\overline{h_2}; h_2\mathbf{e}_i\overline{h_1} - h_1\mathbf{e}_i\overline{h_2}, h_2\mathbf{e}_i\overline{h_2} - h_1\mathbf{e}_i\overline{h_1}\big) \in \mathbb{R} \times \mathbb{H} \times \mathbb{R} \times \mathbb{H}.\end{aligned}$$

So, for $i = 1, 2, 3$,

$$\begin{aligned}&|d\pi_R(X_{i+3})|^2\\&= \big(h_2\mathbf{e}_i\overline{h_1} - h_1\mathbf{e}_i\overline{h_2}\big)^2 - \big(h_2\mathbf{e}_i\overline{h_2} - h_1\mathbf{e}_i\overline{h_1}\big)^2\\&= h_2\mathbf{e}_i\overline{h_1}h_2\mathbf{e}_i\overline{h_1} + 2|h_1|^2|h_2|^2 + h_1\mathbf{e}_i\overline{h_2}h_1\mathbf{e}_i\overline{h_2}\\&\qquad + h_2\mathbf{e}_i\overline{h_2}h_1\mathbf{e}_i\overline{h_1} + |h_1|^4 + |h_2|^4 + h_1\mathbf{e}_i\overline{h_1} + h_2\mathbf{e}_i\overline{h_2} = \big(|h_1|^2 + |h_2|^2\big)^2 = 1.\end{aligned}$$

Next, for $i \neq j$,

$$\begin{aligned}&\langle d\pi_R(X_{3+i}), d\pi(X_{3+j})\rangle_{\mathbb{R}}\\&\quad = \frac{1}{2}\big(h_2\mathbf{e}_i\overline{h_1}h_2\mathbf{e}_j\overline{h_1} - |h_1|^2h_2\mathbf{e}_i\mathbf{e}_j\overline{h_2} - |h_2|^2h_1\mathbf{e}_i\mathbf{e}_j\overline{h_1} + h_1\mathbf{e}_i\overline{h_2}h_1\mathbf{e}_j\overline{h_2}\\&\qquad\quad + h_2\mathbf{e}_j\overline{h_1}h_2\mathbf{e}_i\overline{h_1} - |h_1|^2h_2\mathbf{e}_i\mathbf{e}_i\overline{h_2} - |h_2|^2h_1\mathbf{e}_j\mathbf{e}_i\overline{h_1} + h_1\mathbf{e}_j\overline{h_2}h_1\mathbf{e}_i\overline{h_2}\big)\\&\qquad\quad + \frac{1}{2}\big(h_2\mathbf{e}_i\overline{h_2}h_1\mathbf{e}_j\overline{h_1} - |h_2|^2h_2\mathbf{e}_i\mathbf{e}_j\overline{h_2} - |h_1|^2h_1\mathbf{e}_i\mathbf{e}_j\overline{h_1}\\&\qquad\quad + h_1\mathbf{e}_i\overline{h_1}h_2\mathbf{e}_j\overline{h_2} + h_2\mathbf{e}_j\overline{h_2}h_1\mathbf{e}_i\overline{h_1} - |h_2|^2h_2\mathbf{e}_j\mathbf{e}_i\overline{h_2}\\&\qquad\quad - |h_1|^2h_1\mathbf{e}_j\mathbf{e}_i\overline{h_1} + h_1\mathbf{e}_j\overline{h_1}h_2\mathbf{e}_i\overline{h_2}\big) = 0,\end{aligned}$$

where we used the relation $h_1\overline{h_2} + h_2\overline{h_1} = 0 = \overline{h_1}h_2 + \overline{h_2}h_1$. □

We denote by $\mathcal{H}_M$ the sub-bundle spanned by X_4, X_5 and X_6. It is natural not only to define a metric on the sub-bundle $\mathcal{H}_M$, but also to define a Riemannian metric on M such that the sub-bundle $\mathcal{H}_M$ and the kernel $\mathrm{Ker}(d\pi_R)$ of the projection map π_R are orthogonal. We install a metric by assuming that the generators $1/2\,[X_4, X_5]$, $1/2\,[X_4, X_6]$ and $1/2\,[X_5, X_6]$ are orthonormal at each point.

Proposition 7.15. *This metric coincides with the induced metric from the standard metric on the sphere S^7.*

Proof. Let F_i $(i = 1, 2, 3)$ be the tangent vectors defined by the right multiplication of the generators **i**, **j**, **k** of the Lie algebra $\mathfrak{sp}(1)$. These are expressed as

$$F_i = (h_1, h_2; h_1\mathbf{e}_i, h_2\mathbf{e}_i),\quad |F_i| = 1 \text{ at any point in } S^7,\quad i = 1, 2, 3$$
$$F_1 = 1/2\,[X_5, X_6],\quad F_2 = 1/2\,[X_6, X_4],\quad F_3 = 1/2\,[X_4, X_5].$$

On the subspace M, these vectors and X_i $(i = 4, 5, 6)$ are orthogonal and each has length 1. More precisely, all X_i and F_j are orthogonal at any point on S^7 for $i \neq j$ and on M,

$$\langle X_{3+i}, F_i\rangle_{\mathbb{R}} = 2\left(h_1\overline{h_2} + h_2\overline{h_1}\right) = 0,\quad i = 1, 2, 3. \qquad \square$$

Then, with respect to the Riemannian volume form on M corresponding to this metric (which is denoted by dV_M), we have:

Proposition 7.16. *The sub-Laplacian Δ_M^{sub}*

$$\Delta_M^{\mathrm{sub}} = -\left({X_4}^2 + {X_5}^2 + {X_6}^2\right)$$

on M (which is the restriction of the operator Λ onto M) is positive, symmetric and hypo-elliptic. By Corollary 7.6, the operator Δ_M^{sub} restricted to the space consisting of functions invariant under the right action of $Sp(1)$ (we denote it by $\mathcal{L}$) can be considered as an elliptic operator on $\pi_R(M) \cong S^3$. It is positive and symmetric with respect to the volume form $(\pi_R)_*(dV_M)$.

Remark 7.17. To define a volume form on M it is not necessary to introduce a Riemannian metric on M. We also can use a method explained in [ABGR-09] (see also [Mo2-02, CCFI-10]). Let $\rho\colon \mathcal{H}_M \otimes \mathcal{H}_M \to T(M)/\mathcal{H}_M$ be the bundle map defined in an obvious way. Then ρ is surjective by assuming a sub-Riemannian structure. Now, we can introduce an inner product on $T(M)/\mathcal{H}_M$ by identifying it with the orthogonal complement of the kernel $\mathrm{Ker}(\rho)$. Then we have a well-defined volume form on M. This volume form is $\left(1/4\sqrt{2}\right)^3 dV_M$.

Let I_g $(g \in Sp(1))$ be the action of $Sp(1)$ on $\mathbb{H}^2$ defined by

$$I_g\colon (h_1, h_2) \longmapsto (gh_1g^{-1}, gh_2g^{-1}).$$

Then M is invariant under this action and this action can be descended to the base manifold $\pi_R(M)$. The descended action is given by

$$\overline{I_g} : S^3 \to S^3,\quad \overline{I_g}(a, y_1\mathbf{i} + y_2\mathbf{j} + y_3\mathbf{k}) = \left(a, g(y_1\mathbf{i} + y_2\mathbf{j} + y_3\mathbf{k})g^{-1}\right).$$

Proposition 7.18. *Let $g \in Sp(1)$. Then*

$$dI_g(X_4) = \big({g_0}^2 + {g_1}^2 - {g_2}^2 - {g_3}^2\big)X_4 + 2\big(g_0g_3 + g_1g_2\big)X_5 - 2\big(g_0g_2 - g_1g_3\big)X_6,$$
$$dI_g(X_5) = 2\big(g_1g_2 - g_0g_3\big)X_4 + \big({g_0}^2 - {g_1}^2 + {g_2}^2 - {g_3}^2\big)X_5 + 2\big(g_0g_1 + g_2g_3\big)X_6,$$
$$dI_g(X_6) = 2\big(g_0g_2 + g_1g_3\big)X_4 - 2\big(g_0g_1 - g_2g_3\big)X_5 + \big({g_0}^2 - g_1^2 - {g_2}^2 + {g_3}^2\big)X_6.$$

Proof. This is proved similarly to Proposition 7.5. □

Corollary 7.19. *Since the descended action $\overline{I_g}$ is in $SO(3)$, the operator $\mathcal{L}$ on $S^3 = \big\{(a, y) \in \mathbb{R} \times \mathbb{H} \,\big|\, y + \overline{y} = 0,\ |a|^2 + |y|^2 = 1/2\ \big\}$ is a-axis rotation invariant.*

8. Sub-Riemannian structure on nilpotent Lie groups

Let $\mathfrak{g}$ be a real nilpotent Lie algebra of step N. This means that the derived subalgebra $\mathfrak{g}_N = \{0\}$ at step $N > 1$. Here $\mathfrak{g}_0 = \mathfrak{g}$ and $\mathfrak{g}_k$ is defined inductively by $\mathfrak{g}_k = [\mathfrak{g}, \mathfrak{g}_{k-1}]$ ($N = 1$ means that $\mathfrak{g}$ is just a vector space). We denote by G the connected and simply connected nilpotent Lie group with the Lie algebra $\mathfrak{g}$. G can be identified with the algebra $\mathfrak{g}$ itself as a manifold through the exponential map

$$\exp\colon \mathfrak{g} \longrightarrow G.$$

Let $\{X_i\}_{i=1}^{\dim \mathfrak{g}/\mathfrak{g}_1}$ be linearly independent elements in a complement of the first derived algebra $\mathfrak{g}_1$ and denote by $\{\tilde{X}_i\}_{i=1}^{\dim \mathfrak{g}/\mathfrak{g}_1}$ the left-invariant vector fields defined by

$$\tilde{X}_i\big(f\big)(g) = \frac{d}{dt} f(g \cdot \exp tX_i)\Big|_{t=0}, \quad g \in G,\ f \in C^\infty(G).$$

Then the sub-bundle spanned by $\{\tilde{X}_i\}$ ($\cong G \times \mathbb{R}^{\dim \mathfrak{g} - \dim \mathfrak{g}_1}$) defines a left-invariant, minimal sub-Riemannian structure on the group G in the strong sense and of step N. For the rest of this article, our concern is a sub-Riemannian structure of this type on nilpotent Lie groups together with the induced sub-Riemannian structure on their quotient spaces. According to the classification of low-dimensional nilpotent Lie algebras ($\dim \mathfrak{g} \le 7$, see [Mag-86], [Se-93]), we have only a finite number of non-isomorphic nilpotent Lie algebras. So, one of our aims is to construct heat kernels in an explicit form for all such cases and with respect to the sub-Laplacian

$$\Delta_G^{\text{sub}} = - \sum_{i=1}^{\dim \mathfrak{g}/\mathfrak{g}_1} \tilde{X}_i^{\,2}$$

on G. We plan to determine the spectrum of Laplacians and sub-Laplacians and related spectral invariants on all their compact nilmanifolds ($= \Gamma\backslash G$, Γ is a lattice), in cases they have a lattice (= a uniform discrete subgroup). Unfortunately, unless the step is less than 3, no one has been successful constructing a heat kernel in an explicit integral form. It is even unknown in case of the so-called Engel group $\mathcal{E}_4$ which forms the 3-step nilpotent Lie group of minimal dimension 4.

However, for 2-step nilpotent Lie groups, the heat kernels of any (left) invariant sub-Laplacian and the Laplacian Δ_G ($= \Delta_G^{\text{sub}} - \sum \tilde{Z}_k^2$, $\{Z_k\}$ is a basis of $\mathfrak{g}_1$)

have been constructed in various ways ([Hu-76], [Ga-77], [BGG1-96], [BGG2-00], [BGG3-97], [Kl-97], etc). In particular, a method developed in [BGG1-96] (also [BGG2-00]), the so-called *complex Hamilton-Jacobi method*, enables us to express the heat kernels of sub-Laplacians and Laplacians for every two-step nilpotent Lie group in form of a fiber integration on the characteristic variety of the sub-Laplacian (understood as the dual of the center of the Lie algebra). According to this method heat kernels are expressed in the following form:

Let $n = \dim \mathfrak{g}/\mathfrak{g}_1$ and $d = \dim \mathfrak{g}_1$ and $\{X_i\}_{i=1}^n$ be linearly independent elements. Then the heat kernel of the sub-Laplacian $\Delta^{\mathrm{sub}} = -\sum \tilde{X}_i^2$ has the form

$$\frac{1}{(2\pi t)^{d+n/2}} \int_\Sigma e^{-\frac{A(g,\tau)}{t}} V(\tau)\, d\tau, \tag{8.1}$$

where Σ denotes the characteristic variety of the sub-Laplacian

$$\Sigma = \left\{\theta \in T^*(G) \;\middle|\; \theta(\tilde{X}_i) = 0,\ i = 1, \dots, n\right\}.$$

The function $A = A(g,\tau) \in C^\infty(\Sigma)$ is called a *complex action function* and $V = V(\tau)$ is called a *volume form*. The heat kernel of the Laplacian has a similar form including the same volume form and a complex action function including a quadratic term which comes from the center of the Lie algebra. In Sections §10, §12, §13 and based on this integral expression of the heat kernel for a five-dimensional and a six-dimensional 2-step nilpotent Lie group we determine the spectrum of their compact nilmanifolds with respect to a typical lattice.

It would be interesting to determine the lattice from the spectral data of the sub-Laplacian like the inverse spectral problem in the Riemannian cases.

9. Engel group and Grushin-type operators

In this section we describe Grushin-type operators defined by various subgroups of the Engel group. Then we construct an action function for a 3-step Grushin-type operator.

9.1. Engel group and their subgroups

Let $\mathfrak{e}_4$ be a nilpotent Lie algebra of dimension 4 with generators $\{X, Y, W, Z\}$ such that the bracket relations are given by

$$[X, Y] = W, \quad [X, W] = Z, \quad \text{all others are zero.}$$

Under the identification through the exponential map $\exp\colon \mathfrak{e}_4 \to \mathcal{E}_4$, the group law is given by

$$\mathcal{E}_4 \times \mathcal{E}_4 \ni \big((x,y,w,z), (\tilde{x},\tilde{y},\tilde{w},\tilde{z})\big) \longmapsto \left(x+\tilde{x}, y+\tilde{y}, w+\tilde{w}+\frac{x\tilde{y}-y\tilde{x}}{2}, z+\tilde{z}+\frac{x\tilde{w}-w\tilde{x}}{2}+\frac{1}{12}(x-\tilde{x})(x\tilde{y}-y\tilde{x})\right),$$

where we used the Campbell-Hausdorff formula for the three-step nilpotent Lie group case,

$$\exp A \cdot \exp B = \exp\left(A + B + \frac{1}{2}[A,B] + \frac{1}{12}[A-B,[A,B]]\right).$$

The left-invariant vector fields $\tilde{X}$ and $\tilde{Y}$ are given by

$$\tilde{X} = \frac{\partial}{\partial x} - \frac{y}{2}\frac{\partial}{\partial w} + \left(\frac{w}{2} - \frac{xy}{12}\right)\frac{\partial}{\partial z}, \quad \tilde{Y} = \frac{\partial}{\partial y} + \frac{x}{2}\frac{\partial}{\partial w} - \frac{x^2}{12}\frac{\partial}{\partial z}.$$

Obviously, these vector fields are skew-symmetric with respect to the Haar measure $dx \wedge dy \wedge dw \wedge dz$. We consider the three subgroups (i) $N_X = \{tX\}_{t\in\mathbb{R}}$, (ii) $N_Y = \{tY\}_{t\in\mathbb{R}}$ and (iii) $N_{Y,W} = \{sY + tW\}_{s,t\in\mathbb{R}}$, which give us higher-step Grushin-type operators.

(i) Let

$$\rho_0 \colon \mathcal{E}_4 \cong \mathbb{R}^4 \longrightarrow N_X\backslash\mathcal{E}_4 \cong \text{ left cosets space } \cong \mathbb{R}^3$$
$$\rho_0(x,y,w,z) = \left(y, w - \frac{xy}{2}, z - \frac{xw}{2} + \frac{x^2y}{6}\right) = (\alpha,\beta,\gamma).$$

Then this map ρ_0, together with a map $\mathcal{D}_0 \colon N_X \times N_X\backslash\mathcal{E}_4 \to \mathcal{E}_4$ such that

$$\mathcal{D}_0(t,\alpha,\beta,\gamma) = \left(t, \alpha, \beta + \frac{t\alpha}{2}, \gamma + \frac{t\beta}{2} + \frac{t^2\alpha}{12}\right),$$

gives us a trivialization of the bundle $\rho_0 \colon \mathcal{E}_4 \to N_X\backslash\mathcal{E}_4$. The Haar measure is decomposed into

$$dt \wedge \big(d\alpha \wedge d\beta \wedge d\gamma\big) = dx \wedge dy \wedge dw \wedge dz.$$

The vector fields descended by the maps $d\rho_0(\tilde{X})$ and $d\rho_0(\tilde{Y})$ are given by

$$d\rho_0(\tilde{X}) = -\alpha\frac{\partial}{\partial\beta} - \beta\frac{\partial}{\partial\gamma}, \quad d\rho_0(\tilde{Y}) = \frac{\partial}{\partial\alpha},$$

and one can check that these two vector fields are skew-symmetric with respect to the volume element $d\alpha \wedge d\beta \wedge d\gamma$ on the quotient space $N_X\backslash\mathcal{E}_4$. In this case the Grushin-type operator $\mathcal{G}_0$ is given by

$$\mathcal{G}_0 = -\frac{\partial^2}{\partial\alpha^2} - \left(\alpha\frac{\partial}{\partial\beta} + \beta\frac{\partial}{\partial\gamma}\right)^2,$$

and this is also step 2, i.e., we need the bracket operation twice to generate all the vector fields on $\mathbb{R}^3 \cong N_X\backslash\mathcal{E}_4$.

(ii) Let $\rho_1 \colon \mathcal{E}_4 \cong \mathbb{R}^4 \to \mathbb{R}^3 \cong N_Y\backslash\mathcal{E}_4$ be the map

$$\rho_1(x,y,w,z) = \left(x, w + \frac{xy}{2}, z - \frac{x^2y}{12}\right) = (\alpha,\beta,\gamma).$$

Then we have a trivialization of the principal bundle $\rho_1 \colon \mathcal{E}_4 \to N_Y \backslash \mathcal{E}_4$,

$$\mathcal{D}_1 \colon N_Y \times \mathbb{R}^3 \to \mathcal{E}_4,$$

$$\mathcal{D}_1(t,\alpha,\beta,\gamma) = \left(\alpha, t, \beta - \frac{t\alpha}{2}, \gamma + \frac{t\alpha^2}{12}\right).$$

The vector fields $d\rho_1(\tilde{X})$ and $d\rho_1(\tilde{Y})$ are given by

$$d\rho_1(\tilde{X}) = \frac{\partial}{\partial\alpha} - \frac{\beta}{2}\frac{\partial}{\partial\gamma}, \quad d\rho_1(\tilde{Y}) = \alpha\frac{\partial}{\partial\beta}.$$

The volume form $dx \wedge dy \wedge dw \wedge dz$ is decomposed as $dt \wedge \rho_1^* \left(d\alpha \wedge d\beta \wedge d\gamma\right)$ with a left N_Y-action-invariant one form dt. The descended vector fields $d\rho_1(\tilde{X})$ and $d\rho_1(\tilde{Y})$ are skew-symmetric with respect to the volume form $d\alpha \wedge d\beta \wedge d\gamma$ on $N_Y \backslash \mathcal{E}_4$. The Grushin-type operator is given by

$$-\alpha^2 \frac{\partial^2}{\partial\beta^2} - \left(\frac{\partial}{\partial\alpha} - \frac{\beta}{2}\frac{\partial}{\partial\gamma}\right)^2.$$

(iii) Let $\rho_3 \colon \mathcal{E}_4 \cong \mathbb{R}^4 \longrightarrow N_{\{Y,W\}} \backslash \mathcal{E}_4 \cong \mathbb{R}^2$ be

$$\rho_3(x,y,w,z) = \left(x, z + \frac{xw}{2} + \frac{yx^2}{6}\right).$$

Then together with the decomposition

$$\mathcal{D}_3 \colon N_{\{Y,W\}} \times \left(N_{\{Y,W\}} \backslash \mathcal{E}_4\right) \cong \mathbb{R}^2 \times \mathbb{R}^2 \longrightarrow \mathcal{E}_4 \cong \mathbb{R}^4,$$

$$\mathcal{D}_3(s,t,u,v) = \left(u, s, t - \frac{su}{2}, v - \frac{tu}{2} + \frac{su^2}{12}\right),$$

we have a trivialization of the principal bundle

$$\rho_3 \colon \mathcal{E}_4 \to N_{\{Y,W\}} \backslash \mathcal{E}_4.$$

The left-invariant vector fields $\tilde{X}$ and $\tilde{Y}$ can be descended to the base space $N_{\{Y,W\}} \backslash \mathcal{E}_4$ by the map ρ_3. The resulting vector fields are given by

$$d\rho_3(\tilde{X}) = \frac{\partial}{\partial u}, \quad d\rho_3(\tilde{Y}) = \frac{u^2}{2}\frac{\partial}{\partial v},$$

and the Grushin-type operator in this case is expressed as

$$-\frac{\partial^2}{\partial u^2} - \frac{u^4}{4}\frac{\partial^2}{\partial v^2}.$$

If we perform a Fourier transform with respect to the variable v, then this operator can be seen as the *quartic oscillator* with a parameter η which is the dual variable of v,

$$-\frac{d^2}{du^2} + \eta^2 \cdot u^4. \tag{9.1}$$

In the next subsection we construct a *real action function* (see §8) for the quartic oscillator (9.1).

9.2. Solution of a Hamilton-Jacobi equation

In the complex Hamilton-Jacobi theory (see [BGG1-96], [BGG2-00]), the action function is constructed by solving a Hamilton system with the Hamiltonian being the principal symbol of the sub-Laplacian under initial and mixed boundary conditions with complex parameter in the direction of the dual variables of the center.

Although even for the one-dimensional quartic oscillator we have no heat kernel in explicit form, in this subsection we show the unique existence of the real action function for a Grushin-type operator under the two-points boundary condition. The solutions are described in terms of elliptic functions (see [FI-06]).

Let $H^\eta = H^\eta(x,\xi) = \frac{1}{2}\left(\xi^2 - x^4\eta^2\right)$ be the Hamiltonian of the quartic oscillator

$$\mathcal{Q} = \frac{1}{2}\left(-\frac{d^2}{dx^2} + \eta^2 x^4\right)$$

($\eta \in \mathbb{R}$ is considered as a parameter) and consider the Hamiltonian system

$$\dot{x}(s) = \frac{\partial H^\eta(x,\xi)}{\partial \xi} = \xi, \quad \dot{\xi}(s) = -\frac{\partial H^\eta(x,\xi)}{\partial x} = 2x^3\eta^2$$

with the boundary condition

$$x(0) = x_0, \quad x(t) = x$$

(x_0, x and $t \neq 0$ are taken arbitrary). The system reduces to a single non-linear equation

$$\ddot{x} = 2x^3\eta^2 \tag{9.2}$$

with the boundary condition

$$x(0) = x_0, \quad x(t) = x.$$

It is enough to consider cases different from $x_0 = 0 = x$, since for the latter we have the trivial solution $x(s) \equiv 0$. Then, by the transformations $s \mapsto t - s$ and $x(s) \mapsto -x(s)$, it suffices to consider the following two cases for the boundary data with $t > 0$:

(I) $$x_0 \leq 0 < x,$$

(II) $$0 < x_0 \leq x.$$

We describe the solution.

(I) Let $x_0 \leq 0 < x$. Let $E > 0$ and the function $h(y,E)$ be

$$h(y,E) = \int_{x_0}^{y} \frac{du}{\sqrt{u^4\eta^2 + E}}.$$

Then, for each fixed y, the function $h(y,E)$ is monotone as a function of $E > 0$ and, for each fixed $x > 0 \geq x_0$, it takes values from 0 to ∞ when E moves from

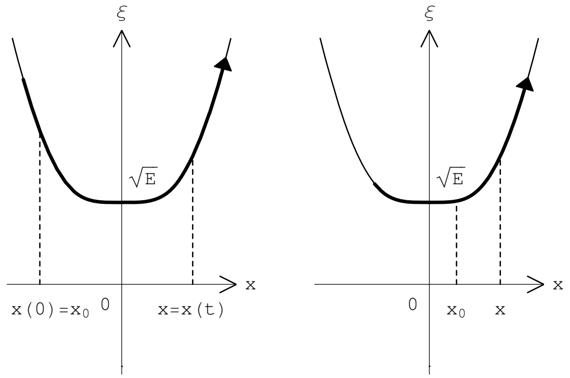

FIGURE 1. $\xi^2 = \eta^2 x^4 + E$ with $E > 0$. Cases (I) and (II-1).

∞ to 0. So let $E = E(x_0, x, t; \eta)$ be the unique constant such that

$$\int_{x_0}^{x} \frac{du}{\sqrt{u^4\eta^2 + E}} = t > 0$$

for the given value $t > 0$. Now, since the function $h(y, E(x_0, x, t; \eta))$ with $y \in \mathbb{R}$ is monotone, let $x(s; E(x_0, x, t; \eta))$ be its inverse function, i.e.,

$$\int_{x_0}^{x(s;E(x_0,x,t;\eta))} \frac{du}{\sqrt{u^4\eta^2 + E(x_0, x, t; \eta)}} = s.$$

Then $x(s; E(x_0, x, t; \eta))$ is the unique solution of the equation (9.2).

(II) Let $0 < x_0 \le x$. Then we need to distinguish three cases:

(II-1) Let $0 < t \le \frac{x_0^{-1} - x^{-1}}{|\eta|} = \int_{x_0}^{x} \frac{du}{\sqrt{u^4\eta^2}}$. Then, for such t and $x > x_0$, we have a unique value $E = E(x_0, x, t; \eta) \ge 0$ such that

$$\int_{x_0}^{x} \frac{du}{\sqrt{u^4\eta^2 + E}} = t.$$

The solution $x(s; E(x_0, x, t; \eta))$ of (9.2) is given by the integral

$$\int_{x_0}^{x(s,E(x_0,x,t;\eta))} \frac{du}{\sqrt{u^4\eta^2 + E(x_0, x, t; \eta)}} du = s.$$

(II-2) We assume that $\frac{x_0^{-1} - x^{-1}}{|\eta|} < t \le \int_{x_0}^{x} \frac{du}{\sqrt{u^4\eta^2 - x_0^4\eta^2}}$ and fix the unique value $E = E(x_0, x, t; \eta)$ $(0 > E \ge -x_0^4\eta^2)$ such that $\int_{x_0}^{x} \frac{du}{\sqrt{u^4\eta^2 + E(x_0,x,t;\eta)}} = t$. Then the solution of (9.2) is given by

$$\int_{x_0}^{x(s;E(x_0,x,t;\eta))} \frac{du}{\sqrt{u^4\eta^2 + E(x_0, x, t; \eta)}} = s.$$

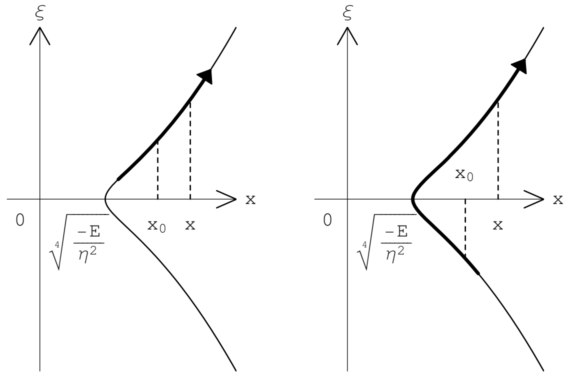

FIGURE 2. $\xi^2 = \eta^2 x^4 + E$ with $E < 0$. Cases (II-2) and (II-3).

(II-3) Let $t > \int_{x_0}^{x} \frac{du}{\sqrt{u^4\eta^2 - x_0^4\eta^2}}$. Then we take the unique value $a = a(x_0, x, t; \eta)$ ($a(x_0, x, t; \eta)$ can be chosen uniquely in $0 < a(x_0, x, t; \eta) < x_0$) such that

$$-\int_{x_0}^{a} \frac{du}{\sqrt{u^4\eta^2 - a^4\eta^2}} + \int_{a}^{x} \frac{du}{\sqrt{u^4\eta^2 - a^4\eta^2}} = t. \tag{9.3}$$

The monotonicity of the sum of integrals (9.3) with respect to the variable $a \in (0,\ x_0)$ can be seen by the coordinate change $u = va$ in the integral. If we set $E = E(x_0, x, t; \eta) = -a(x_0, x, t; \eta)^4\eta^2$, then the unique solution of (9.2) exists and is described as follows: Let

$$s_1 = -\int_{x_0}^{a(x_0,x,t;\eta)} \frac{du}{\sqrt{u^4\eta^2 - a(x_0, x, t; \eta)^4\eta^2}}.$$

Then, for $s < s_1$, the solution $x(s) = x(s; E(x_0, x, t; \eta))$ is defined by the integral

$$-\int_{x_0}^{x(s)} \frac{du}{\sqrt{u^4\eta^2 + E(x_0, x, t; \eta)}} = s$$

and, for $s_1 < s$, the solution $x(s) = x(s; E(x_0, x, t; \eta))$ is defined by

$$\int_{a}^{x(s)} \frac{du}{\sqrt{u^4\eta^2 + E(x_0, x, t; \eta)}} = s - s_1.$$

Note that $\lim_{s\to s_1 \pm 0} x(s) = a(x_0, x, t; \eta)$ and $\lim_{s\to s_1 \pm 0} \dot{x}(s) = 0$, and so this solution coincides with the solution of (9.2) under the initial condition $x(s_1) = a(x_0, x, t)$ and $\dot{x}(s_1) = 0$. The case $t \neq 0$, $0 < x_0 = x$ should be understood as being included in the case (II-3). The solution $x(s)$ satisfies the relations

$$x(st; E(x_0, x, t; \eta)) = x(s; E(x_0, x, 1; t\eta)) \ \text{and} \ E(x_0, x, 1; t\eta) = t^2 E(x_0, x, t; \eta).$$

Hence this implies the existence of the solution $x(s; E(x_0, x, t; \eta))$ of (9.2) for arbitrary boundary data $x(0) = x_0$, $x(t) = x$ (x_0, x, $t \neq 0$ can be taken arbitrary).

All these are expressed in terms of elliptic functions (sn-function, cn-function, and so on, cf. [WW-58], [La-89], [CC2-09]).

Based on the existence of the solution of (9.2), we can define the (classical) action integral A:

Theorem 9.1.

$$A(x_0,x,t;\eta)=\int_0^t \dot{x}(s)\xi(s)-H^{\eta}(x(s),\xi(s))\,ds. \tag{9.4}$$

By the relation $\dot{x}(s)^2=\eta^2x(s)^4+E(x_0,x,t;\eta)$, this integral equals

$$\begin{aligned}A(x_0,x,t;\eta)&=\eta^2\int_0^t x(s)^4ds\;+\;\frac{t}{2}\,E(x_0,x,t;\eta)\\&=\eta^2\int_{x_0}^{x}\frac{y^4}{\sqrt{y^4\eta^2+E(x_0,x,t;\eta)}}dy\;+\;\frac{t}{2}\,E(x_0,x,t;\eta)\\&=\pm\frac{1}{3}\{x\sqrt{x^4\eta^2+E(x_0,x,t;\eta)}-\\&\qquad -x_0\sqrt{{x_0}^4\eta^2+E(x_0,x,t;\eta)}\Big\}+\frac{t}{6}E(x_0,x,t;\eta)\end{aligned} \tag{9.5}$$

($\xi(s)=\dot{x}(s)=\pm\sqrt{x(s)^4\eta^2+E(x_0,x,t;\eta)}$). A is a solution of the Hamilton-Jacobi equation $\frac{\partial}{\partial t}A+H(x,\nabla A)=0$ and it also satisfies the *generalized Hamilton-Jacobi equation*

$$H(x,\nabla A)+\eta\frac{\partial}{\partial\eta}A(x_0,x,1;\eta)=A(x_0,x,1;\eta),$$

which is proved by making use of the relation $tA(x_0,x,t;\eta)=A(x_0,x,1;t\eta)$.

For fixed x_0, $t\neq 0$, $\eta\neq 0$, we consider $J_{(x_0,t;\eta)}\colon x\mapsto\dot{x}(0,E(x_0,x,t;\eta))=\xi(0)$ (note that $J_{(x_0,t;0)}=(x-x_0)/t$). The map $J_{(x_0,t;\eta)}$ has the derivative (for $t>0$)

$$\frac{dJ_{(x_0,t;\eta)}}{dx}(x)=\frac{1}{x_0^4\eta^2+E(x_0,x,t;\eta)}\left(\int_{x_0}^{x}\left(\frac{1}{u^4\eta^2+E(x_0,x,t;\eta)}\right)^{3/2}du\right)^{-1},$$

and $\frac{\partial}{\partial\eta}A(x_0,x,1;\eta)$ is highly related to the construction of the volume element.

We note that the function $\frac{\partial}{\partial\eta}A(x_0,x,1;\eta)\,\frac{dJ_{(x_0,1;\eta)}}{dx}(x)$ might be a candidate for the volume element we are looking for. The difficulty of proving this consists in the fact that the constant $E(x_0,x,t;\eta)$ is not given in explicit form. Also we remark that the above arguments can be used to show the existence of the solution for the Hamilton system (9.2) of the general higher-step Grushin operator

$$-\frac{d^2}{dx^2}+\eta^2x^{2k},$$

which reduces to solving the equation

$$\ddot{x}=kx^{2k-1}\eta^2$$

under the boundary condition $x(0)=x_0$ and $x(t)=x$ where t is also arbitrarily fixed. So, we will have an action integral similar to (9.5).

10. Free two-step nilpotent Lie algebra and group

Let $\{X_i\}_{i=1}^N$ be a basis of $\mathbb{R}^N$ and also, for $1 \leq i < j \leq N$, let $\{Z_{i\,j}\}$ be a basis of $\mathbb{R}^{{}_NC_2}$ $\left({}_NC_2 = \frac{N!}{2!(N-2)!}\right)$. We define Lie bracket relations by

$$[X_i, X_j] = -[X_j, X_i] = 2Z_{i\,j}, \text{ for } 1 \leq i < j \leq N,$$

and all others are zero (note that the factor 2 in front of the basis $Z_{i\,j}$ is just for avoiding unnecessary constants in describing a heat kernel). Then we can introduce a two-step nilpotent Lie algebra structure on $\mathbb{R}^{N(N+1)/2} = \mathbb{R}^N \oplus \mathbb{R}^{{}_NC_2}$ and also through the Campbell-Hausdorff formula a Lie group structure on $\mathbb{R}^{N(N+1)/2} = \mathbb{R}^N \oplus \mathbb{R}^{{}_NC_2}$ with the group multiplication $*$

$$\begin{aligned}&\left(\mathbb{R}^N \oplus \mathbb{R}^{{}_NC_2}\right) \times \left(\mathbb{R}^N \oplus \mathbb{R}^{{}_NC_2}\right) \ni \left(x \oplus z, \tilde{x} \oplus \tilde{z}\right)\\ &\qquad \mapsto (x, z) * (\tilde{x}, \tilde{z}) = (x + \tilde{x}) \oplus \Big(z + \tilde{z} + \sum_{1 \leq i < j \leq N} \left(x_i\tilde{x}_j - x_j\tilde{x}_i\right)\Big).\end{aligned}$$

This group is called a *free 2-step nilpotent Lie group*. We denote the Lie algebra by $\mathfrak{f}_{(N+N(N-1)/2)} \cong \mathbb{R}^{\frac{N(N+1)}{2}}$ and the connected and simply connected nilpotent Lie group with the Lie algebra $\mathfrak{f}_{(N+N(N-1)/2)}$ is denoted by $F_{(N+N(N-1)/2)}$ $(\cong \mathbb{R}^{\frac{N(N+1)}{2}})$. Under these identifications the exponential map can be seen as the identity map.

Remark 10.1. Let $\mathfrak{g}$ be a 2-step nilpotent Lie algebra. Let $\{X_i\}_{i=1}^N$ be a basis of a complement of the derived algebra $[\mathfrak{g}, \mathfrak{g}]$ and $\{Z_j\}_{j=1}^d$ a basis of $[\mathfrak{g}, \mathfrak{g}]$. Then we have structure constants $\{C_{i\,j}^{\,k}\}$ with the relations $[X_i, X_j] = \sum_k 2C_{i\,j}^{\,k} Z_k$.

Now, let $\mathfrak{f}_{(N+N(N-1)/2)}$ be the free 2-step nilpotent Lie algebra with the basis $\{X_i, Z_{i\,j}\}_{1\leq i<j\leq N}$ defined as above. We define a Lie algebra homomorphism ρ by

$$\rho\colon \mathfrak{f}_{(N+N(N-1)/2)} \to \mathfrak{g}$$

$$\rho\Big(\sum_i x_iX_i + \sum_{i\,j} z_{i\,j}Z_{i\,j}\Big) = \sum_i x_iX_i + \sum_{i\,j}\sum_k z_{i\,j}C_{i\,j}^{\,k}Z_k.$$

Then this defines the Lie group homomorphism between corresponding simply connected Lie groups. In this sense, any 2-step nilpotent Lie group (Lie algebra) is covered by a free 2-step nilpotent Lie group (Lie algebra).

Free nilpotent Lie algebras exist only in the dimensions $N +_N C_2 = \frac{N(N+1)}{2}$ for each integer $N \in \mathbb{N}$. For $N = 2$ the algebra $\mathfrak{f}_{(2+1)}$ is the three-dimensional Heisenberg algebra. Let $\tilde{X}_i$ be the left-invariant vector field defined by

$$\tilde{X}_i(f)(x, z) = \frac{d\,f(g \cdot \exp tX_i)}{dt}\Big|_{t=0} = \frac{\partial f(x, z)}{\partial x_i} + \sum_{j<i} \frac{\partial f(x, z)}{\partial z_{j\,i}} - \sum_{j>i} \frac{\partial f(x, z)}{\partial z_{i\,j}},$$

and we set

$$\tilde{Z}_{i\,j}(f)(g) = \frac{d\,f(g \cdot \exp tZ_{i\,j})}{dt}\Big|_{t=0} = \frac{\partial f(x, z)}{\partial z_{i\,j}}, \quad f \in C^\infty(F_N).$$

11. 2-step nilpotent Lie groups of dimension ≤ 6

If we only consider the nilpotent groups (of step 2) of indecomposable type of dimension less than 4 we have only one non-trivial case, which is three-dimensional Heisenberg group. We have two types in dimension five and there are three different types of nilpotent Lie algebras of dimension 6 and step 2. Indecomposability of the group implies that the first derived ideal $[\mathfrak{g},\mathfrak{g}]$ coincides with the center of the algebra (see [Eb-03]) and for six-dimensional Lie algebras, there are two possibilities of the dimension of the center. That is, $\dim[\mathfrak{g},\mathfrak{g}] = 2$ or 3. These three are characterized by the following brackets relations:

(I) The dimension of the center is 3. This is the case of the free nilpotent Lie algebra.

(II) The dimension of the center is 2.

Then we have two types. Let Z_1 and Z_2 be a basis of the center $[\mathfrak{g},\mathfrak{g}]$ and X_1, X_2, X_3, X_4 be a basis of a complement of the center.

(II-1)
$$\begin{aligned} &[X_1,X_2] = Z_1, \quad [X_1,X_3] = Z_2, \quad [X_2,X_3] = 0,\\ &[X_1,X_4] = 0, \quad [X_2,X_4] = 0, \quad [X_3,X_4] = Z_1. \end{aligned} \tag{11.1}$$

(II-2)
$$\begin{aligned} &[X_1,X_2] = Z_1, \quad [X_1,X_3] = Z_2, \quad [X_2,X_3] = 0,\\ &[X_1,X_4] = 0, \quad [X_2,X_4] = Z_2, \quad [X_3,X_4] = Z_1. \end{aligned} \tag{11.2}$$

These two cases (II-1) and (II-2) are covered by the ten-dimensional free nilpotent Lie group $\mathfrak{f}_{(4+6)}$. Let $\mathfrak{h}_3 \otimes \mathbb{C}$ be the complexification of the three-dimensional Heisenberg Lie algebra. Then the above case (II-2) is isomorphic to $\mathfrak{h}_3 \otimes \mathbb{C}$ if we consider it as a real Lie algebra.

11.1. Heat kernel of the free nilpotent Lie group of dimension 6

We consider a sub-Riemannian structure $\mathcal{H}$ on the free nilpotent Lie group $F_{(3+3)}$ of dimension 6 generated by the vector fields $\{\tilde{X}_i\}_{i=1}^3$. The sub-Laplacian $\Delta^{\text{sub}}_{F_{(3+3)}}$ is given by

$$\Delta^{\text{sub}}_{F_{(3+3)}} = -\sum_{i=1}^{3} \tilde{X}_i^2.$$

We write $[X_1,X_2] = 2Z_{1,2} = 2Z_1$, $[X_1,X_3] = 2Z_{1,3} = 2Z_2$ and $[X_2,X_3] = 2Z_{2\,3} = 2Z_3$.

According to a general formula, the heat kernel $K^{\text{sub}}_{F_{(3+3)}} = K^{\text{sub}}_{F_{(3+3)}}\big(t,(x,z),(\tilde{x},\tilde{z})\big) \in C^\infty(\mathbb{R}_+ \times F_{(3+3)} \times F_{(3+3)})$ of $\Delta^{\text{sub}}_{F_{(3+3)}}$ which is the kernel function of the operator $\big\{e^{-\frac{t}{2}\cdot\Delta^{\text{sub}}_{F_{(3+3)}}}\big\}_{t>0}$, has the form

$$K^{\text{sub}}_{F_{(3+3)}}\big(t,(x,z),(\tilde{x},\tilde{z})\big) = \frac{1}{(2\pi t)^{9/2}} \int_{\mathbb{R}^3} \exp\left\{-\frac{A\big((\tilde{x},\tilde{z})^{-1} * (x,z),\tau\big)}{t}\right\} W(\tau)\,d\tau, \tag{11.3}$$

where the function $A = A(x, z, \tau)$ is called action function and is given by the formula

$$A(x, z, \tau) = \sqrt{-1}\sum_{i=1}^{3}\tau_i z_i + \frac{1}{2}\left\langle \Omega(\sqrt{-1}\,\tau)\coth\Omega(\sqrt{-1}\,\tau)\cdot x,\, x\right\rangle .$$

From the above integral form (11.3) of the heat kernel, one sees that it satisfies the invariance

$$K^{\text{sub}}_{F_{(3+3)}}\big(t, g*(x,z), g*(\tilde{x},\tilde{z})\big) = K^{\text{sub}}_{F_{(3+3)}}\big(t, (x,z), (\tilde{x},\tilde{z})\big) \text{ for all } g \in F_{(3+3)}. \quad (11.4)$$

One also has

$$K^{\text{sub}}_{F_{(3+3)}}\big(t, (x,z), (\tilde{x},\tilde{z})\big) = K^{\text{sub}}_{F_{(3+3)}}\big(t, (\tilde{x},\tilde{z}), (x,z)\big). \quad (11.5)$$

In the above formula, the matrix $\Omega(\tau)$ is the most general 3×3 anti-symmetric matrix

$$\Omega(\tau) = \begin{pmatrix} 0 & \tau_1 & \tau_2 \\ -\tau_1 & 0 & \tau_3 \\ -\tau_2 & -\tau_3 & 0 \end{pmatrix},$$

with $\tau = (\tau_1, \tau_2, \tau_3) \in \mathbb{R}^3$ and we denote by $\langle\cdot,\cdot\rangle$ the standard inner product on $\mathbb{R}^3$. The matrix

$$\sqrt{-1}\,\Omega(\tau)\coth\sqrt{-1}\,\Omega(\tau)$$

is defined by the integral

$$\sqrt{-1}\,\Omega(\tau)\coth\sqrt{-1}\,\Omega(\tau) = \frac{1}{2\pi\sqrt{-1}}\int_C \frac{\lambda\cosh\lambda}{\sinh\lambda}\left(\lambda - \sqrt{-1}\,\Omega(\tau)\right)^{-1} d\lambda,$$

where the contour C is taken suitably in such a way that it encloses all eigenvalues of the matrix $\sqrt{-1}\,\Omega(\tau)$. The function $W(\tau)$ is given by the formula

$$W(\tau) = \left(\det\frac{\sqrt{-1}\,\Omega(\tau)}{\sinh\sqrt{-1}\,\Omega(\tau)}\right)^{1/2},$$

where

$$\frac{\sqrt{-1}\,\Omega(\tau)}{\sinh\sqrt{-1}\,\Omega(\tau)} = \frac{1}{2\pi\sqrt{-1}}\int_C \frac{\lambda}{\sinh\lambda}\left(\lambda - \sqrt{-1}\,\Omega(\tau)\right)^{-1} d\lambda,$$

and it is called the volume element. Since the eigenvalues of the matrix $\Omega(\sqrt{-1}\,\tau)$ are 0 and $\pm\sqrt{|\tau|}$, we can determine the volume element

$$W(\tau) = \left(\det\frac{\sqrt{-1}\,\Omega(\tau)}{\sinh\sqrt{-1}\,\Omega(\tau)}\right)^{1/2} = \frac{|\tau|}{\sinh|\tau|}.$$

The calculation of the matrix

$$\frac{1}{2\pi\sqrt{-1}}\int_C \frac{\lambda\cosh\lambda}{\sinh\lambda}\left(\lambda - \sqrt{-1}\,\Omega(\tau)\right)^{-1} d\lambda,$$

is reduced to the calculation of the power series of the matrix

$$\left(\mathrm{Id}+\frac{\left(\sqrt{-1}\,\Omega(\tau)\right)^2}{2!}+\frac{\left(\sqrt{-1}\,\Omega(\tau)\right)^4}{4!}+\cdots\right) \times\left(\mathrm{Id}+\frac{\left(\sqrt{-1}\,\Omega(\tau)\right)^2}{3!}+\frac{\left(\sqrt{-1}\,\Omega(\tau)\right)^4}{5!}+\cdots\right)^{-1}.$$

For that purpose we take a unitary matrix T

$$T=\begin{pmatrix} \frac{\tau_3}{|\tau|} & \sqrt{\frac{|\tau|^2\tau_1^2+\tau_2^2\tau_3^2}{2(\tau_1^2+\tau_2^2)|\tau|^2}}\frac{\tau_1^2+\tau_2^2}{\sqrt{-1}\,|\tau|\tau_1+\tau_2\tau_3} & \sqrt{\frac{|\tau|^2\tau_1^2+\tau_2^2\tau_3^2}{2(\tau_1^2+\tau_2^2)|\tau|^2}}\frac{\tau_1^2+\tau_2^2}{-\sqrt{-1}\,|\tau|\tau_1+\tau_2\tau_3} \\ \frac{-\tau_2}{|\tau|} & \sqrt{\frac{|\tau|^2\tau_1^2+\tau_2^2\tau_3^2}{2(\tau_1^2+\tau_2^2)|\tau|^2}} & \sqrt{\frac{|\tau|^2\tau_1^2+\tau_2^2\tau_3^2}{2(\tau_1^2+\tau_2^2)|\tau|^2}} \\ \frac{\tau_1}{|\tau|} & \sqrt{\frac{|\tau|^2\tau_1^2+\tau_2^2\tau_3^2}{2(\tau_1^2+\tau_2^2)|\tau|^2}}\frac{\sqrt{-1}\,|\tau|\tau_2-\tau_1\tau_3}{\sqrt{-1}\,|\tau|\tau_1+\tau_2\tau_3} & \sqrt{\frac{|\tau|^2\tau_1^2+\tau_2^2\tau_3^2}{2(\tau_1^2+\tau_2^2)|\tau|^2}}\frac{-\sqrt{-1}\,|\tau|\tau_2-\tau_1\tau_3}{-\sqrt{-1}\,|\tau|\tau_1+\tau_2\tau_3} \end{pmatrix},$$

which gives us

$$T^*\sqrt{-1}\,\Omega(\tau)T=\begin{pmatrix}0&0&0\\0&|\tau|&0\\0&0&-|\tau|\end{pmatrix},$$

for the case that $\tau_1\neq 0$. Then we have

$$\begin{aligned}
TT^*&\left(\mathrm{Id}+\sum_{k=1}^{\infty}\frac{\left(\sqrt{-1}\,\Omega(\tau)\right)^{2k}}{(2k)!}\right)\left(\mathrm{Id}+\sum_{k=1}^{\infty}\frac{\left(\sqrt{-1}\,\Omega(\tau)\right)^{2k}}{(2k+1)!}\right)^{-1}TT^*\\
&=T\begin{pmatrix}1&0&0\\0&|\tau|\coth|\tau|&0\\0&0&|\tau|\coth|\tau|\end{pmatrix}T^*\\
&=|\tau|\coth|\tau|\,\mathrm{Id}+\frac{1-|\tau|\coth|\tau|}{|\tau|^2}\begin{pmatrix}\tau_3^2&-\tau_2\tau_3&\tau_1\tau_3\\-\tau_2\tau_3&\tau_2^2&-\tau_1\tau_2\\\tau_1\tau_3&-\tau_1\tau_2&\tau_1^2\end{pmatrix}\\
&=\mathrm{Id}+\frac{|\tau|\coth|\tau|-1}{|\tau|^2}\left(\sqrt{-1}\,\Omega(\tau)\right)^2.
\end{aligned}$$

We can see that the resulting expression is valid also in the case $\tau_1=0$. Now the action function is

$$\begin{aligned}
&A(x_1,x_2,x_3,z_1,z_2,z_3,\tau_1,\tau_2,\tau_3)\\
&\quad=\sqrt{-1}\sum\tau_kz_k+\frac{1}{2}\left\langle TT^*\sqrt{-1}\,\Omega(\tau)\coth\sqrt{-1}\,\Omega(\tau)\,TT^*(x),x\right\rangle\\
&\quad=\sqrt{-1}\sum\tau_kz_k+\frac{1}{2}\Big\{|\tau|\coth|\tau|(x_1^2+x_2^2+x_3^2)\\
&\qquad+\frac{1-|\tau|\coth|\tau|}{|\tau|^2}\left(\tau_3^2x_1^2+\tau_2^2x_2^2+\tau_1^2x_3^2+(\tau_3x_1-\tau_2x_2+\tau_1x_3)^2\right)\Big\}.
\end{aligned}$$

The heat kernel $K^{\text{sub}}_{F_{(3+3)}}$ of the sub-Laplacian $\Delta^{\text{sub}}_{F_{(3+3)}}$ is given by the integral

$$K^{\text{sub}}_{F_{(3+3)}}\big(t,(x,z),(\tilde{x},\tilde{z})\big) = \frac{1}{(2\pi t)^{9/2}} \int_{\mathbb{R}^3} e^{-\frac{1}{t}\tilde{A}(x,z,\tilde{x},\tilde{z},\tau)} \frac{|\tau|}{\sinh|\tau|}\, d\tau$$

where the function $\tilde{A}(x,z,\tilde{x},\tilde{z},\tau)$ in the exponent is given by:

$$\tilde{A}(x,z,\tilde{x},\tilde{z},\tau) = \sqrt{-1}\Big[\tau_1(z_1 - \tilde{z}_1 + (\tilde{x}_2 x_1 - \tilde{x}_1 x_2)) + \tau_2(z_2 - \tilde{z}_2 \\ + (\tilde{x}_3 x_1 - \tilde{x}_1 x_3)) + \tau_3(z_3 - \tilde{z}_3 + (\tilde{x}_3 x_2 - \tilde{x}_2 x_3))\Big] + \frac{1}{2}\langle D(\tau)(x-\tilde{x}), x-\tilde{x}\rangle.$$

With $\tau = (\tau_1,\tau_2,\tau_3) \in \mathbb{R}^3$ the matrix $D(\tau)$ is defined by:

$$D(\tau) := |\tau|\coth|\tau| Id_3 + \frac{1-|\tau|\coth|\tau|}{|\tau|^2}\begin{pmatrix} \tau_3^2 & -\tau_2\tau_3 & \tau_1\tau_3 \\ -\tau_2\tau_3 & \tau_2^2 & -\tau_1\tau_2 \\ \tau_1\tau_3 & -\tau_1\tau_2 & \tau_1^2 \end{pmatrix} \in \mathbb{R}^{3\times 3}.$$

11.2. Heat kernel of Grushin-type operators

We consider four connected subgroups N_0, N_1, N_2 and N_3 in $F_{(3+3)}$ whose Lie algebras are generated by Z_3, X_1, $\{X_1, Z_1\}$ and $\{X_1, X_2, Z_1\}$, respectively.

We define the Grushin-type operators $\mathcal{G}_i$ on the left coset spaces $N_i\backslash F_{(3+3)}$, which all are hypo-elliptic and analogous to the Grushin operator

$$\frac{\partial^2}{\partial u^2} + u^2\frac{\partial^2}{\partial v^2}.$$

Note that the group N_3 is isomorphic to the three-dimensional Heisenberg group, the subgroup N_0 is normal and the quotient group $F_{(3+3)}/N_0$ (we denote this group by G_5) is one of the five-dimensional nilpotent Lie groups which is not isomorphic to the five-dimensional Heisenberg group and does not decompose into smaller-dimensional groups. (According to the classification of nilpotent Lie groups of low dimensions, this group is the non-trivial one other than the five-dimensional Heisenberg group among the non-isomorphic five-dimensional nilpotent Lie groups.)

(I) First we consider the subgroup N_1.

Let $\rho_1\colon F_{(3+3)} \to N_1\backslash F_{(3+3)}$ be the projection map. Then ρ_1 is realized as

$$\rho_1\colon F_{(3+3)} \cong \mathbb{R}^6 \to N_1\backslash F_{(3+3)} \cong \mathbb{R}^5,$$
$$(x_1,x_2,x_3,z_1,z_2,z_3) \mapsto (x_2,x_3,z_1 - x_1x_3, z_2 - x_1x_3, z_3) = (u_1,u_2,u_3,u_4,u_5),$$

and the principal bundle $\rho_1\colon F_{(3+3)} \to N_1\backslash F_{(3+3)}$ is trivialized as

$$\mathcal{D}_1\colon \mathbb{R}\times\mathbb{R}^5 \xrightarrow{\sim} \mathbb{R}^6 \cong F_{(3+3)}$$
$$\mathcal{D}_1(h,u_1,u_2,u_3,u_4,u_5) = (h,u_1,u_2,u_3+hu_1,u_4+hu_2,u_5).$$

The left-invariant vector fields $\tilde{X}_i$ $(i = 1,2,3)$ are descended to the quotient space $H_1 \backslash F_{(3+3)}$ by the map ρ_1 as

$$d\rho_1(\tilde{X}_1) = -2\left(u_1 \frac{\partial}{\partial u_3} + u_2 \frac{\partial}{\partial u_4}\right),$$
$$d\rho_1(\tilde{X}_2) = \frac{\partial}{\partial u_1} - u_2 \frac{\partial}{\partial u_5},$$
$$d\rho_1(\tilde{X}_3) = \frac{\partial}{\partial u_2} + u_1 \frac{\partial}{\partial u_5}.$$

From these expressions, we can see that on the space $\{u_1 = 0, u_2 = 0\}$ the vector fields $d\rho_1(\tilde{X}_i)$ $(i = 1,2,3)$ are not linearly independent. This means that at any point $(x_1, 0, 0, z_1, z_2, z_3) \in F_{(3+3)}$ the subspace spanned by three vector fields $\{\tilde{X}_i\}$ and the space tangent to the fiber of the map ρ_1 have one-dimensional intersection. In this case the Grushin-type operator $\mathcal{G}_1$ is

$$\mathcal{G}_1 = -4\left(u_1 \frac{\partial}{\partial u_3} + u_2 \frac{\partial}{\partial u_4}\right)^2 - \left(\frac{\partial}{\partial u_1} - u_2 \frac{\partial}{\partial u_5}\right)^2 - \left(\frac{\partial}{\partial u_2} + u_1 \frac{\partial}{\partial u_5}\right)^2.$$

By the commutativity of the diagram

$$\begin{array}{ccc} C_0^\infty(N_1 \backslash F_{(3+3)}) & \xrightarrow{\mathcal{G}_1} & C_0^\infty(N_1 \backslash F_{(3+3)}) \\ \rho_1^* \big\downarrow & & \big\downarrow \rho_1^* \\ C^\infty(F_{(3+3)}) & \xrightarrow{\Delta^{\mathrm{sub}}_{F(3+3)}} & C^\infty(F_{(3+3)}) \end{array}$$

and the decomposition of the volume element

$$dx_1 \wedge dx_2 \wedge dx_3 \wedge dz_1 \wedge dz_2 \wedge dz_3 = dh \wedge du_1 \wedge du_2 \wedge du_3 \wedge du_4 \wedge du_5$$

with respect to this volume form the vector fields $\tilde{X}_i$ are antisymmetric. We can express the heat kernel of the operator $\mathcal{G}_1$ in terms of the fiber integration of the heat kernel of the sub-Laplacian on $F_{(3+3)}$. More precisely, the heat kernel $K^{\mathrm{sub}}_{\mathcal{G}_1} \in C^\infty\big(\mathbb{R}_+ \times (N_1 \backslash F_{(3+3)}) \times (N_1 \backslash F_{(3+3)})\big)$ for the Grushin operator $\mathcal{G}_1$ is

$$\begin{aligned}(\rho_1)_*&\Big(K^{\mathrm{sub}}_{F_{(3+3)}}\big(t,(\cdot,\cdot,\cdot,\cdot,\cdot,\cdot),(\tilde{x},\tilde{z})\big)dh \wedge du_1 \wedge du_2 \wedge du_3 \wedge du_4 \wedge du_5\Big) \\ &= K^{\mathrm{sub}}_{\mathcal{G}_1}\big(t,(u_1,u_2,u_3,u_4,u_5),(\tilde{x},\tilde{z})\big)du_1 \wedge du_2 \wedge du_3 \wedge du_4 \wedge du_5. \qquad (11.6)\end{aligned}$$

Note that by the invariance (11.4) of $K^{\mathrm{sub}}_{F_{(3+3)}}$, the heat kernel $K^{\mathrm{sub}}_{\mathcal{G}_1}$ satisfies the invariance

$$K^{\mathrm{sub}}_{\mathcal{G}_1}\big(t,u,g*(\tilde{x},\tilde{z})\big) = K^{\mathrm{sub}}_{\mathcal{G}_1}\big(t,u,(\tilde{x},\tilde{z})\big), \quad \forall g \in N_1.$$

So it is a well-defined function on $\mathbb{R}_+ \times (N_1 \backslash F_{(3+3)}) \times (N_1 \backslash F_{(3+3)})$. Now, we calculate the integral (11.6) explicitly:

Theorem 11.1. *The heat kernel $K^{\mathrm{sub}}_{\mathcal{G}_1}$ of the operator $\mathcal{G}_1$, that is, the kernel distribution of the operator $\left\{e^{-\frac{t}{2}\cdot\mathcal{G}_1}\right\}_{t>0}$, is given by the integral* (11.7) *below.*

Proof. We change the variables from (x,z) to (h,u) and from $(\tilde{x},\tilde{z})$ to $(\tilde{h},\tilde{u})$. Then the imaginary part of the action function

$$A\big((\tilde{x},\tilde{z})^{-1}*(x,z),\tau\big) = A\big((\tilde{h},\tilde{u})^{-1}*(h,u),\tau\big)$$

is expressed as

$$\begin{aligned}
&\sqrt{-1}\,\big\{\tau_1(u_1+\tilde{x}_2)(h-\tilde{x}_1)+\tau_1(u_3-\tilde{z}_1+\tilde{x}_1\tilde{x}_2)\\
&\qquad \tau_2(u_2+\tilde{x}_3)(h-\tilde{x}_1)+\tau_2(u_4-\tilde{z}_2+\tilde{x}_1\tilde{x}_3)+\tau_3(u_5-\tilde{z}_3+\tilde{x}_3u_1-\tilde{x}_2u_2)\big\}\\
&=\sqrt{-1}\,\big\{\tau_1(u_1+\tilde{u}_1)(h-\tilde{h})+\tau_1(u_3-\tilde{u}_3)\\
&\qquad +\tau_2(u_2+\tilde{u}_2)(h-\tilde{h})+\tau_2(u_4-\tilde{u}_4)+\tau_3(u_5-\tilde{u}_5+\tilde{u}_2u_1-\tilde{u}_1u_2)\big\}\\
&=\sqrt{-1}\,\big\{\big(\tau_1(u_1+\tilde{u}_1)+\tau_2(u_2+\tilde{u}_2)\big)(h-\tilde{h})\\
&\qquad +\tau_1(u_3-\tilde{u}_3)+\tau_2(u_4-\tilde{u}_4)+\tau_3(u_5-\tilde{u}_5+\tilde{u}_2u_1-\tilde{u}_1u_2)\big\}.
\end{aligned}$$

By separating the variables h and $\tilde{h}$, the real part is given by

$$\begin{aligned}
&\frac{1}{2}\,|\tau|\coth|\tau|\,\Big((h-\tilde{h})^2+(u_1-\tilde{u}_1)^2+(u_2-\tilde{u}_2)^2\Big)\\
&\qquad\qquad +\frac{1-|\tau|\coth|\tau|}{2|\tau|^2}\big(\tau_3(h-\tilde{h})-\tau_2(u_1-\tilde{u}_1)+\tau_1(u_2-\tilde{u}_2)\big)^2\\
&=\frac{|\tau|\coth|\tau|(\tau_1^2+\tau_2^2)+\tau_3^2}{2|\tau|^2}\\
&\qquad \times\left(h-\tilde{h}+\frac{(1-|\tau|\coth|\tau|)\big(-\tau_2(u_1-\tilde{u}_1)+\tau_1(u_2-\tilde{u}_2)\big)\tau_3|\tau|^2}{|\tau|\coth|\tau|(\tau_1^2+\tau_2^2)+\tau_3^2}\right)^2\\
&\qquad +|\tau|\coth|\tau|\frac{1-|\tau|\coth|\tau|}{2|\tau|\coth|\tau|(\tau_1^2+\tau_2^2)+\tau_3^2}\big(-\tau_2(u_1-\tilde{u}_1)+\tau_1(u_2-\tilde{u}_2)\big)^2\\
&\qquad +\frac{1}{2}\,|\tau|\coth|\tau|\big((u_1-\tilde{u}_1)^2+(u_1-\tilde{u}_2)^2\big).
\end{aligned}$$

We integrate the heat kernel $K^{\mathrm{sub}}_{F_{(3+3)}}$ on each fiber of the map ρ_1 with respect to the variable h,

$$\begin{aligned}
&\frac{1}{(2\pi t)^{9/2}}\int_{\mathbb{R}}\int_{\mathbb{R}^3} e^{-\frac{A\left((\tilde{h},\tilde{u})^{-1}*(h,u),\tau\right)}{t}}\,\frac{|\tau|}{\sinh|\tau|}\,d\tau dh \qquad (11.7)\\
&=\frac{1}{(2\pi t)^4}\int_{\mathbb{R}^3} e^{\frac{\sqrt{-1}}{t}\left(\tau_1(u_1+\tilde{u}_1)+\tau_2(u_2+\tilde{u}_2)\right)\cdot\frac{|\tau|^2\tau_3^2\left(1-|\tau|\coth|\tau|\right)\left(-\tau_2(u_1-\tilde{u}_1)+\tau_1(u_2-\tilde{u}_2)\right)^2}{|\tau|\coth|\tau|(\tau_1^2+\tau_2^2)+\tau_3^2}}\\
&\qquad \times e^{-\frac{\sqrt{-1}}{t}\,\tau_1(u_3-\tilde{u}_3)+\tau_2(u_4-\tilde{u}_4)+\tau_3(u_5-\tilde{u}_5+\tilde{u}_2u_1-\tilde{u}_1u_2)}\cdot e^{-\frac{|\tau|^2\left(\tau_1(u_1+\tilde{u}_1)+\tau_2(u_2+\tilde{u}_2)\right)^2}{2t\left(|\tau|\coth|\tau|(\tau_1^2+\tau_2^2)+\tau_3^2\right)}}\\
&\qquad \times e^{-\frac{|\tau|\coth|\tau|}{2t}\cdot\left((u_1-\tilde{u}_1)^2+(u_2-\tilde{u}_2)^2+\frac{1-|\tau|\coth|\tau|}{|\tau|\coth|\tau|(\tau_1^2+\tau_2^2)+\tau_3^2}\left(-\tau_2(u_1-\tilde{u}_1)+\tau_2(u_2-\tilde{u}_2)\right)^2\right)}\\
&\qquad\quad \times\frac{|\tau|}{\sqrt{|\tau|\coth|\tau|(\tau_1^2+\tau_2^2)+\tau_3^2}}\,\frac{|\tau|}{\sinh|\tau|}\,d\tau_1d\tau_2d\tau_3.
\end{aligned}$$

□

(II) Next, we consider the subgroup N_2 and the left cosets space $N_2\backslash F_{(3+3)}$. We describe the projection map $\rho_2\colon F_{(3+3)} \to N_2\backslash F_{(3+3)} \cong \mathbb{R}^4$ and the trivialization $\mathcal{D}_2\colon N_2 \times \mathbb{R}^4 \overset{\sim}{\to} F_{(3+3)}$ of this principal bundle $\rho_2\colon F_{(3+3)} \to N_2\backslash F_{(3+3)}$:

$$\rho_2\colon F_{(3+3)} \cong \mathbb{R}^6 \ni (x_1,x_2,x_3,z_1,z_2,z_3) \mapsto (u_1,u_2,u_3,u_4) \in \mathbb{R}^4 \cong N_2\backslash F_{(3+3)},$$
$$\rho_2(x_1,x_2,x_3,z_1,z_2,z_3) = (u_1,u_2,u_3,u_4) = (x_2,x_3,z_2-x_1x_3,z_3),$$
$$\mathcal{D}_2\colon N_2\times\mathbb{R}^4 \overset{\sim}{\longrightarrow} F_{(3+3)},$$
$$\mathcal{D}_2(h_1,h_2,u_1,u_2,u_3,u_4) = (x_1,x_2,x_3,z_1,z_2,z_3) = (h_1,u_1,u_2,h_2,u_3+h_1u_2,u_4).$$

The vector fields $\tilde{X}_i$ $(i=1,2,3)$ are descended to $N_2\backslash F_{(3+3)}$ by the map ρ_2 with

$$d\rho_2(\tilde{X}_1) = -2u_2\frac{\partial}{\partial u_3},$$
$$d\rho_2(\tilde{X}_2) = \frac{\partial}{\partial u_1} - u_2\frac{\partial}{\partial u_4},$$
$$d\rho_2(\tilde{X}_3) = \frac{\partial}{\partial u_2} + u_1\frac{\partial}{\partial u_4}.$$

On the line $\{u_2=0\}$ these three vector fields are not linearly independent, but the sum of squares

$$\begin{aligned} -\mathcal{G}_2 &= d\rho_2(\tilde{X}_1)^2 + d\rho_2(\tilde{X}_2)^2 + d\rho_2(\tilde{X}_3)^2 \\ &= 4u_2^2\frac{\partial^2}{\partial u_3^2} + \left(\frac{\partial}{\partial u_1} - u_2\frac{\partial}{\partial u_4}\right)^2 + \left(\frac{\partial}{\partial u_2} + u_1\frac{\partial}{\partial u_4}\right)^2 \end{aligned}$$

is hypo-elliptic and $\mathcal{G}_2$ generalizes the Grushin operator to dimension 4. The kernel function $K^{\mathrm{sub}}_{\mathcal{G}_2}$ of the heat operator $\left\{e^{-\frac{t}{2}\cdot\mathcal{G}_2}\right\}_{t>0}$ is given by the fiber integral

$$\begin{aligned} &(\rho_2)_*\Big(K^{\mathrm{sub}}_{F_{(3+3)}}\big(t,(\cdot,\cdot),(\tilde{x},\tilde{z})\big)dx_1\wedge dx_2\wedge dx_3\wedge dz_1\wedge dz_2\wedge dz_3\Big) \\ &\qquad = K^{\mathrm{sub}}_{\mathcal{G}_2}\big(t,(u_1,u_2,u_3,u_4),(\tilde{x},\tilde{z})\big)du_1\wedge du_2\wedge du_3\wedge du_4. \end{aligned} \tag{11.8}$$

For the determination of the above integral (11.8) we change the coordinates (x,z) to the new coordinates $(h_1,h_2,u_1,u_2,u_3,u_4)$. Then we can express the action function $A = A\big((x,z),(\tilde{x},\tilde{z}),\tau\big)$ as

$$\begin{aligned} A\big((x,z),(\tilde{x},\tilde{z}),\tau\big) &= A\big((h,u),(\tilde{h},\tilde{u}),\tau\big) \\ &= \sqrt{-1}\,\tau_1\big(h_2-\tilde{h}_2+(h_1-\tilde{h}_1)(u_1+\tilde{u}_1)\big) \\ &\quad + \sqrt{-1}\tau_2\big(u_3-\tilde{u}_3+(h_1-\tilde{h}_1)(u_2+\tilde{u}_2)\big) \\ &\quad + \sqrt{-1}\tau_3\big(u_4-\tilde{u}_4+\tilde{u}_2u_1-\tilde{u}_1u_2\big) \\ &\quad + \frac{1}{2}\Big\{|\tau|\coth|\tau|\cdot\big((h_1-\tilde{h}_1)^2+(u_1-\tilde{u}_1)^2+(u_2-\tilde{u}_2)^2\big) \\ &\quad + \frac{1-|\tau|\coth|\tau|}{|\tau|^2}\cdot\big(\tau_3(h_1-\tilde{h}_1)-\tau_2(u_1-\tilde{u}_1)+\tau_1(u_2-\tilde{u}_2)\big)^2\Big\}. \end{aligned}$$

The integral (11.8) reduces to

$$\frac{2\pi\, t^3}{(2\pi\, t)^{9/2}} \int_{\mathbb{R}^3} e^{-\sqrt{-1}\left(\tau_2\left(u_3-\tilde{u}_3+(h_1-\tilde{h}_1)(u_2+\tilde{u}_2)\right)+\tau_3\left(u_4-\tilde{u}_4+\tilde{u}_2u_1-\tilde{u}_1u_2\right)\right)}$$
$$\times \exp\left\{-\frac{t|\tau|\coth t|\tau|}{2t}\cdot\left((h_1-\tilde{h}_1)^2+(u_1-\tilde{u}_1)^2+(u_2-\tilde{u}_2)^2\right)\right\}$$
$$\times \exp\left\{\frac{1}{2t}\cdot\frac{1-t|\tau|\cdot\coth t|\tau|}{|\tau|^2}\cdot\left(\tau_3(h_1-\tilde{h}_1)-\tau_2(u_1-\tilde{u}_1)\right)^2\right\}\frac{t|\tau|}{\sinh t|\tau|}\,dh_1d\tau_2d\tau_3,$$

where $|\tau|=\sqrt{\tau_2^2+\tau_3^2}$. Then we have:

Theorem 11.2.

$$\begin{aligned}
&K^{sub}_{\mathcal{G}_2}\left(t,u_1,u_2,u_3,u_4,\tilde{u}_1,\tilde{u}_2,\tilde{u}_3,\tilde{u}_4\right)\\
&=\frac{2\pi\, t^3}{(2\pi t)^{9/2}}\int_{\mathbb{R}^2}\exp\left\{-\sqrt{-1}\,\tau_2(u_3-\tilde{u}_3)-\sqrt{-1}\tau_3(u_4-\tilde{u_4}+\tilde{u}_2u_1-\tilde{u}_1u_2)\right\}\\
&\quad\times\exp\left\{-\sqrt{-1}\frac{\tau_2^2\tau_3(u_2+\tilde{u}_2)(u_1-\tilde{u}_1)(1-t|\tau|\coth t|\tau|)}{\tau_3^2+\tau_2^2\cdot t|\tau|\coth t|\tau|}\right\}\\
&\quad\times\exp\left\{-\frac{1}{2t}\cdot\frac{|\tau|^2\cdot t|\tau|\coth t|\tau|}{\tau_3^2+\tau_2^2\cdot t|\tau|\coth t|\tau|}\cdot(u_1-\tilde{u}_1)^2\right\}\\
&\quad\times\exp\left\{-\frac{(u_2-\tilde{u}_2)^2}{2t}\cdot t|\tau|\coth t|\tau|-\frac{t|\tau|^2\tau_2^2(u_2+\tilde{u}_2)^2}{2(\tau_3^2+\tau_2^2\cdot t|\tau|\coth t|\tau|)}\right\}\\
&\quad\times\exp\left\{-\sqrt{-1}\cdot\frac{\tau_2^2\tau_3(u_2+\tilde{u}_2)(u_1-\tilde{u}_1)(1-t|\tau|\coth t|\tau|)}{\tau_3^2+\tau_2^2\cdot t|\tau|\coth t|\tau|}\right\}\frac{t|\tau|}{\sinh t|\tau|}\,d\tau_2d\tau_3.
\end{aligned}$$

(III) We consider the left cosets space $N_3\backslash F_{(3+3)}$ and the principal bundle

$$\rho_3\colon F_{(3+3)}\longrightarrow N_3\backslash F_{(3+3)}\cong\mathbb{R}^3.$$

This is again a trivial bundle with the structure group N_3. We describe this explicitly. The projection map $\rho_3\colon F_{3+3}\cong\mathbb{R}^6\to N_3\backslash F_{(3+3)}\cong\mathbb{R}^3$ is realized as

$$\rho_3(x_1,x_2,x_3,z_1,z_2,z_3)=(u_1,u_2,u_3),$$
$$u_1=x_3,\ \ u_2=z_2-x_1x_3,\ \ u_3=z_3-x_2x_3,$$

and a trivialization of the bundle is given by

$$\begin{aligned}
\mathcal{D}_3\colon N_3\times\mathbb{R}^3\cong\mathbb{R}^3\times\mathbb{R}^3&\to\mathbb{R}^6\cong F_{(3+3)} \qquad (11.9)\\
(h_1,h_2,c,u_1,u_2,u_3)&\mapsto(x_1,x_2,x_3,z_1,z_2,z_3)\\
x_1=h_1,\ \ x_2=h_2,\ \ x_3=u_1,\ \ z_1=c,&\ \ z_2=u_2+h_1u_1,\ \ z_3+h_2u_1.
\end{aligned}$$

Then one sees that the left-invariant vector fields $\tilde{X}_i$ are descended to the quotient space $F_{(3+3)}\to N_3\backslash F_{(3+3)}$ by the projection map ρ_3 and the resulting vector fields are given as follows:

$$d\rho(\tilde{X}_1) = -2u_1\frac{\partial}{\partial u_2}, \quad d\rho(\tilde{X}_2) = -2u_1\frac{\partial}{\partial u_3}, \quad d\rho(\tilde{X}_3) = \frac{\partial}{\partial u_1}.$$

So, the operator

$$-\sum d\rho(\tilde{X}_i)^2 = -\left(\frac{\partial^2}{\partial u_1^2} + 4u_1^2\left(\frac{\partial^2}{\partial u_2^2} + \frac{\partial^2}{\partial u_3^2}\right)\right)$$

can be seen as a three-dimensional version of the Grushin operator.

We give the heat kernel of this operator by integrating along the fiber of the map ρ_3 which can be done explicitly by making use of the trivialization (11.9). First, by changing the variables from (x,z), $(\tilde{x},\tilde{z})$ to (h_1,h_2,u_1,c,u_2,u_3) and $(\tilde{h}_1,\tilde{h}_2,\tilde{u}_1,\tilde{c},\tilde{u}_2,\tilde{u}_3)$ we give the expression of the action function

$$f = \sqrt{-1}\,\mathrm{Im}(f) + \mathrm{Re}(f).$$

$$\begin{aligned}
\mathrm{Im}(f) &= \tau_1\big(z_1-\tilde{z}_1+\tilde{x}_2x_1-\tilde{x}_1x_2\big)+\tau_2\big(z_2-\tilde{z}_2+\tilde{x}_3x_1-\tilde{x}_1x_3\big)\\
&\qquad +\tau_3\big(z_1-\tilde{z}_1+\tilde{x}_3x_2-\tilde{x}_2x_3\big)\\
&= \tau_1\big(c-\tilde{c}+\tilde{h}_2(h_1-\tilde{h}_1)+\tilde{h}_1(h_2-\tilde{h}_2)\big)+\tau_2\big(u_2-\tilde{u}_2+(h_1-\tilde{h}_1)(u_1+\tilde{u}_1)\big)\\
&\qquad +\tau_3\big(u_3-\tilde{u}_3+(h_2-\tilde{h}_2)(u_1+\tilde{u}_1)\big),\\
2\mathrm{Re}(f) &= |\tau|\coth|\tau|\cdot\|x-\tilde{x}\|^2+\frac{1-|\tau|\coth|\tau|}{|\tau|^2}\cdot\big(\tau_3x_1-\tau_2x_2+\tau_1x_3\big)^2\\
&= |\tau|\coth|\tau|\cdot\big((h_1-\tilde{h}_1)^2+(h_2-\tilde{h}_2)^2+(u_1-\tilde{u}_1)^2\big)\\
&\qquad +\frac{1-|\tau|\coth|\tau|}{|\tau|^2}\cdot\big(\tau_3(h_1-\tilde{h}_1)-\tau_2(h_2-\tilde{h}_2)+\tau_1(u_1-\tilde{u}_1)\big)^2.
\end{aligned}$$

Then the integration along each fiber of the map ρ_3 is done in the following order:

(1) Take the Fourier transform with respect to the variable τ_1.

(2) Take the inverse Fourier transform with respect to the variable c.

(3) Calculate the Fourier transform with respect to the variables h_1 and h_2.

$$\begin{aligned}
&\frac{1}{(2\pi t)^{9/2}}\int_{\mathbb{R}^2}\left(\int_{\mathbb{R}^3} e^{-\frac{1}{t}A((\tilde{x},\tilde{z})^{-1}*(x,z),\tau)}\frac{|\tau|}{\sinh|\tau|}d\tau_1d\tau_2d\tau_3\right)dh_1dh_2dc\\
&= \frac{1}{(2\pi t)^{9/2}}\int_{\mathbb{R}^3}\left(\int_{\mathbb{R}^3} e^{-\frac{\sqrt{-1}}{t}\,\tau_1\left(c-\tilde{c}+\tilde{h}_2(h_1-\tilde{h}_1)+\tilde{h}_1(h_2-\tilde{h}_2)\right)}\right.\\
&\times\ e^{-\frac{\sqrt{-1}}{t}\,\left(\tau_2\left(u_2-\tilde{u}_2+(h_1-\tilde{h}_1)(u_1+\tilde{u}_1)\right)+\tau_3\left(u_3-\tilde{u}_3+(h_2-\tilde{h}_2)(u_1+\tilde{u}_1)\right)\right)}\\
&\times\ e^{-\frac{1}{2t}|\tau|\coth|\tau|\cdot\left((h_1-\tilde{h}_1)^2+(h_2-\tilde{h}_2)^2+(u_1-\tilde{u}_1)^2\right)}\\
&\times\ e^{-\frac{1-|\tau|\coth|\tau|}{2t|\tau|^2}\cdot\left(\tau_3(h_1-\tilde{h}_1)-\tau_2(h_2-\tilde{h}_2)+\tau_1(u_1-\tilde{u}_1)\right)^2}\left.\frac{|\tau|}{\sinh|\tau|}\,d\tau_1d\tau_2d\tau_3\right)dh_1dh_2dc
\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{(2\pi t)^{7/2}} \int_{\mathbb{R}^2} \Bigg(\int_{\mathbb{R}^2} e^{-\sqrt{-1}\, \frac{\tau_2\left(u_2-\tilde{u}_2+(h_1-\tilde{h}_1)(u_1+\tilde{u}_1)\right)+\tau_3\left(u_3-\tilde{u}_3+(h_2-\tilde{h}_2)(u_1+\tilde{u}_1)\right)}{t}} \\
&\quad \times e^{-\frac{1}{2t}|\tau|\coth|\tau|\left((h_1-\tilde{h}_1)^2+(h_2-\tilde{h}_2)^2+(u_1-\tilde{u}_1)^2\right)-\frac{1-|\tau|\coth|\tau|}{2t|\tau|^2}\left(\tau_3(h_1-\tilde{h}_1)-\tau_2(h_2-\tilde{h}_2)\right)^2} \\
&\quad \times \frac{|\tau|}{\sinh|\tau|}\, dh_1 dh_2 \Bigg) d\tau_2 d\tau_3 \\
&= \frac{1}{(2\pi t)^{7/2}} \int_{\mathbb{R}^2} e^{-\sqrt{-1}\frac{\tau_2(u_2-\tilde{u}_2)+\tau_3(u_3-\tilde{u}_3)}{t}-\frac{|\tau|\coth|\tau|\cdot(u_1-\tilde{u}_1)^2}{2t}} \cdot \frac{|\tau|}{\sinh|\tau|} \\
&\quad \times \Bigg(\int_{\mathbb{R}^2} e^{-\sqrt{-1}\, \frac{\tau_2(h_1-\tilde{h}_1)(u_1+\tilde{u}_1)+\tau_3(h_2-\tilde{h}_2)(u_1+\tilde{u}_1)}{t}} e^{-\frac{1}{2t}|\tau|\coth|\tau|\cdot\left((h_1-\tilde{h}_1)^2+(h_2-\tilde{h}_2)^2\right)} \\
&\quad \times e^{-\frac{1-|\tau|\coth|\tau|}{2t|\tau|^2}\cdot\left(\tau_3(h_1-\tilde{h}_1)-\tau_2(h_2-\tilde{h}_2)\right)^2}\, dh_1 dh_2 \Bigg) d\tau_2 d\tau_3 \\
&= \frac{1}{(2\pi t)^{7/2}} \int_{\mathbb{R}^2} e^{-\sqrt{-1}\frac{\tau_2(u_2-\tilde{u}_2)+\tau_3(u_3-\tilde{u}_3)}{t}-\frac{|\tau|\coth|\tau|\cdot(u_1-\tilde{u}_1)^2}{2t}} \cdot \frac{|\tau|}{\sinh|\tau|} \\
&\quad \times \left(e^{-\frac{\pi\tau\left(u_1+\tilde{u}_2\right)^2}{2t\coth|\tau|}} \frac{2\pi}{\sqrt{|\tau|\coth|\tau|}} \right) d\tau_2 d\tau_3 \\
&= \frac{2\pi}{(2\pi t)^{7/2}} \int_{\mathbb{R}^2} e^{-\sqrt{-1}\frac{\tau_2(u_2-\tilde{u}_2)+\tau_3(u_3-\tilde{u}_3)}{t}} \cdot e^{-\frac{|\tau|\coth|\tau|\cdot(u_1-\tilde{u}_1)^2}{2t}-\frac{\pi|\tau|(u_1+\tilde{u}_2)^2}{2t\coth|\tau|}} \\
&\quad \times \sqrt{\frac{|\tau|}{\sinh|\tau|\cosh|\tau|}}\, d\tau_2 d\tau_3,
\end{aligned}
$$

where $|\tau| = \sqrt{\tau_2^2+\tau_3^2}$. Now we have:

Theorem 11.3. *The kernel function of the operator* $\{e^{-\frac{t}{2}\mathcal{G}_3}\}_{t>0}$ *is given by the integral*

$$
\frac{2\pi}{(2\pi t)^{7/2}} \int_{\mathbb{R}^2} e^{-\sqrt{-1}\frac{\tau_2(u_2-\tilde{u}_2)+\tau_3(u_3-\tilde{u}_3)}{t}} \cdot e^{-\frac{|\tau|\coth|\tau|\cdot(u_1-\tilde{u}_1)^2}{2t}-\frac{\pi|\tau|(u_1+\tilde{u}_2)^2}{2t\coth|\tau|}} \times \sqrt{\frac{|\tau|}{\sinh|\tau|\cosh|\tau|}}\, d\tau_2 d\tau_3. \tag{11.10}
$$

(IV) We consider the case $N_0 = [\{Z_3\}]$. Since it is a normal subgroup, in fact it is a subgroup in the center, the quotient group is again a nilpotent Lie group of dimension 5 with the Lie brackets relations

$$[X_1, X_2] = 2Z_1, \quad [X_1, X_3] = 2Z_2$$

and all others are zero. We denote this group by G_5. The resulting Grushin-type operator coincides with the sub-Laplacian for this group defined by

$$\Delta^{\text{sub}}_{G_5} = -\tilde{X}_1^{\,2} - \tilde{X}_2^{\,2} - \tilde{X}_3^{\,2}.$$

So, for that group we can construct the kernel function of the heat semi-group $\left\{e^{-\frac{t}{2}\Delta^{\text{sub}}_{G_5}}\right\}_{t>0}$ by means of the complex Hamilton-Jacobi method (see [BGG1-96]). Here we construct it by the same method as above. It turns out that the kernel is obtained from the Fourier inversion formula, i.e., by integrating the heat kernel on $F_{(3+3)}$

$$K^{\text{sub}}_{F_{(3+3)}}\big(t,(x,z),(\tilde{x},\tilde{z})\big) = \frac{1}{(2\pi t)^{9/2}}\int_{\mathbb{R}^3} e^{-\frac{A((\tilde{x},\tilde{z})^{-1}*(x,z),\tau)}{t}}\frac{|\tau|}{\sinh|\tau|}\,d\tau_1 d\tau_2 d\tau_3,$$

first with respect to the variable τ_3 and then with respect to the variable z_3. We obtain:

Theorem 11.4.

$$\begin{aligned}
&\frac{1}{(2\pi t)^{9/2}}\int_{\mathbb{R}}\int_{\mathbb{R}^3} e^{-\sqrt{-1}\,\frac{A((\tilde{x},\tilde{z})^{-1}*(x,z),\tau)}{t}}\frac{|\tau|}{\sinh|\tau|}\,d\tau_1 d\tau_2 d\tau_3 dz_3\\
&= \frac{1}{(2\pi t)^{7/2}}\int_{\mathbb{R}^2} e^{-\frac{\sqrt{-1}}{t}(\tau_1(z_1-\tilde{z}_1+(\tilde{x}_2x_1-\tilde{x}_1x_2))+\tau_2(z_2-\tilde{z}_2+(\tilde{x}_3x_1-\tilde{x}_1x_3)))}\\
&\quad\times\ e^{-\frac{1}{2t}\left(\sqrt{\tau_1^2+\tau_2^2}\cdot\coth\sqrt{\tau_1^2+\tau_2^2}\cdot\left(x_1^{\,2}+x_2^{\,2}+x_3^{\,2}\right)+\frac{1-\sqrt{\tau_1^2+\tau_2^2}\cdot\coth\sqrt{\tau_1^2+\tau_2^2}}{\tau_1^2+\tau_2^2}\cdot\left(-\tau_2x_2+\tau_1x_3\right)^2\right)}\\
&\quad\times\ \frac{\sqrt{\tau_1^2+\tau_2^2}}{\sinh\sqrt{\tau_1^2+\tau_2^2}}\,d\tau_1 d\tau_2.
\end{aligned}$$

12. Spectrum of a five-dimensional compact nilmanifold

As we already explained in §11, in the dimension 5, there are only two non-isomorphic 2-step nilpotent Lie groups which are not of product type. One of them is the five-dimensional Heisenberg group and the other is G_5 explained in §11, the case (IV) (cf. [Mag-86], [Se-93]). In this section we calculate the heat kernel trace of a five-dimensional compact nilmanifold of G_5.

Although it is possible to deal with more general lattices, in this article we restrict the calculation to a typical lattice L in G_5,

$$L = \big\{(m_1,m_2,m_3,k_1,k_2)\;\big|\;m_i,\ k_i\ \in\mathbb{Z}\big\},$$

in order to present how the spectrum of a class of sub-Laplacians on such a compact nilmanifold $L\backslash G_5$, the left cosets space by the lattice L, looks like. The sub-Laplacian on G_5 is descended to the compact nilmanifold $L\backslash G_5$. Let $K^{\text{sub}}_{G_5} = K^{\text{sub}}_{G_5}\big(t,(\tilde{x},\tilde{z}),(x,z)\big)$ be the heat kernel on G_5 given in Theorem 11.4.

Then the heat kernel on $L\backslash G_5$ is given by the sum

$$\sum_{\gamma\in L} K^{\rm sub}_{G_5}\big(t,\gamma*(\tilde{x},\tilde{z}),(x,z)\big).$$

We denote a set of representatives of conjugacy classes of L by $[L]$ and for each element $\gamma\in L$ set $S_\gamma=\big\{(\mu^{-1}*\gamma*\mu\ \big|\ \mu\in L\big\}$, the set of conjugate elements to γ in L. The centralizer of $\gamma=(m_1,m_2,m_3,k_1,k_2)$ is denoted by

$$C_\gamma=\Big\{(a_1,a_2,a_3,c_1,c_2)\ \Big|\ (a_1,a_2,a_3,c_1,c_2)^{-1}*\gamma*(a_1,a_2,a_3,c_1,c_2)=\gamma,\\ (a_1,a_2,a_3,c_1,c_2)\in L\Big\}.$$

The set $[L]$ can be decomposed into eight components,

$$L=A_0\cup A_1\cup A_2\cup A_3\cup A_{1\,2}\cup A_{1\,3}\cup A_{2\,3}\cup A_{1\,2\,3},$$

given by

$$\begin{aligned}
A_0&=\big\{(0,0,0,k_1,k_2)\ \big|\ k_i\in\mathbb{Z}(i=1,2)\big\},\\
A_1&=\big\{(m_1,0,0,k_1,k_2)\ \big|\ m_1\neq 0,\ 0\le k_i\le 2|m_1|-1(i=1,2)\big\},\\
A_2&=\big\{(0,m_2,0,k_1,k_2)\ \big|\ m_2\neq 0,\ 0\le k_1\le 2|m_2|-1,\ k_2\in\mathbb{Z}\big\},\\
A_3&=\big\{(0,0,m_3,k_1,k_2)\ \big|\ m_3\neq 0,\ k_1\in\mathbb{Z},\ 0\le k_2\le 2|m_3|-1\big\},\\
A_{1\,2}&=\big\{(m_1,m_2,0,k_1,k_2)\ \big|\ m_1\neq 0,\ m_2\neq 0,\ 0\le k_1\le 2(|m_1|,|m_2|)-1,\\
&\qquad\qquad 0\le k_2\le 2|m_1|-1\big\},\\
A_{1\,3}&=\big\{(m_1,0,m_3,k_1,k_2)\ \big|\ m_1\neq 0,\ m_3\neq 0,\ 0\le k_1\le 2|m_1|-1,\\
&\qquad\qquad 0\le k_2\le 2(|m_1|,|m_3|)-1\big\},\\
A_{2\,3}&=\big\{(0,m_2,m_3,k_1,k_2)\ \big|\ m_2\neq 0,\ m_3\neq 0,\ 0\le k_1\le 2|m_2|-1,\ k_2\in\mathbb{Z}\big\},\\
A_{1\,2\,3}&=\big\{(m_1,m_2,m_3,k_1,k_2)\ \big|\ m_1\neq 0,\ m_2\neq 0,\ m_3\neq 0,\\
&\qquad 0\le k_1\le 2(|m_1|,|m_2|)-1,\ 0\le k_2\le 2\frac{|m_1|(|m_1|,|m_2|,|m_3|)}{(|m_1|,|m_2|)}-1\big\}.
\end{aligned}$$

Here we denote by (m,n) the greatest common divisor of $m,n\in\mathbb{N}$. We calculate the trace of the heat kernel on $L\backslash G_5$,

$$\sum_{\gamma\in L}\int_{\mathcal{F}_L} K^{\rm sub}_{G_5}\big(t,\gamma*(x,z),(x,z)\big)\,dxdz,$$

where $\mathcal{F}_L$ is a fundamental domain of the lattice L. Let $\mathcal{F}_\gamma$ be a fundamental domain of the centralizer (in L) of an element $\gamma\in L$. Then solving the integral reduces to the calculation of each integral for $\gamma \in [L]$,

$$\sum_{\gamma \in L} \int_{\mathcal{F}_L} K_{G_5}^{\mathrm{sub}}\big(t, \gamma * (x,z), (x,z)\big)\, dxdz = \sum_{\gamma \in [L]} \int_{\mathcal{F}_\gamma} K_{G_5}^{\mathrm{sub}}\big(t, \gamma * (x,z), (x,z)\big)\, dxdz.$$

So, we list the centralizer of each representative $\gamma \in [L]$ of the conjugacy classes and a fundamental domain $\mathcal{F}_\gamma$ for each $\gamma \in [L]$. Also we give expressions for the integrals

$$I_\gamma = \int_{\mathcal{F}_\gamma} K_{G_5}^{\mathrm{sub}}\big(t, \gamma * (x,z), (x,z)\big)\, dxdz$$

for $\gamma \in [L]$ and their sums

$$\begin{aligned} I_i(G_5) &= \sum_{\gamma \in A_i} I_\gamma, \qquad i = 0,1,2,3, \\ I_{i\,j}(G_5) &= \sum_{\gamma \in A_{i\,j}} I_\gamma, \qquad 1 \le i < j \le 3, \\ I_{1\,2\,3}(G_5) &= \sum_{\gamma \in A_{1\,2\,3}} I_\gamma. \end{aligned}$$

(0-0) $A_0 = \{\ (0,0,0,k_1,k_2)\ \big|\ k_i \in \mathbb{Z}\ \}$. The elements in A_0 are not mutually conjugate.

Let $\gamma = (0,0,0,k_1,k_2) \in A_0$. Then

$$C_{(0,0,0,k_1,k_2)} = L,$$

$$\mathcal{F}_{(0,0,0,k_1,k_2)} = \mathcal{F}_L = \Big\{(x_1,x_2,x_3,z_1,z_2)\ \Big|\ x_1,x_2,x_3,z_1,z_2 \in [0,1)\Big\},$$

$$\begin{aligned} I_0(G_5) &= \sum_{\gamma \in A_0} \int_{\mathcal{F}_\gamma} K_{G_5}^{\mathrm{sub}}\big(t, \gamma * (x,z), (x,z)\big)\, dxdz \\ &= \frac{1}{(2\pi t)^{7/2}} \sum_{k_1,k_2 \in \mathbb{Z}} \int_{[0,1)^5} \int_{\mathbb{R}^2} e^{-\sqrt{-1}\,\frac{\sum \tau_i k_i}{t}} \frac{|\tau|}{\sinh|\tau|}\, d\tau_1 d\tau_2 dx_1 dx_2 dx_3 dz_1 dz_2 \\ &= \frac{1}{(2\pi t)^{3/2}} \sum_{k_1,k_2 \in \mathbb{Z}} \frac{2\pi t\sqrt{k_1^2+k_2^2}}{\sinh 2\pi t\sqrt{k_1^2+k_2^2}}. \end{aligned}$$

(1-1) $A_1 = \big\{(m_1,0,0,k_1,k_2)\ \big|\ m_1 \ne 0,\ 0 \le k_1 \le 2|m_1|-1,\ 0 \le k_2 \le 2|m_1|-1\big\}$. Then

$$C_{(m_1,0,0,k_1,k_2)} = \big\{(a_1,0,0,c_1,c_2)\ \big|\ a_1,c_1,c_2 \in \mathbb{Z}\big\},$$

$$\mathcal{F}_{(m_1,0,0,k_1,k_2)} = \big\{(x_1,x_2,x_3,z_1,z_2)\ \big|\ x_2,x_3 \in \mathbb{R};\ x_1,z_1,z_2 \in [0,1)\big\}.$$

Let $\gamma = (m_1, 0, 0, k_1, k_2) \in A_1$. Then

$$\begin{aligned}
&\int_{\mathcal{F}_{(m_1,0,0,k_1,k_2)}} K_{G_5}^{\mathrm{sub}}\big(t, (m_1, 0, 0, k_1, k_2) * (x, z), (x, z)\big)\, dxdz \\
&\quad = \frac{1}{(2\pi t)^{7/2}} \int_0^1 \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{\mathbb{R}^2} e^{-\frac{\sqrt{-1}}{t}\left(\tau_1\left(k_1+2x_2m_1\right)+\tau_2\left(k_2+2x_3m_1\right)\right)} \\
&\qquad \times\ e^{-\frac{1}{2t}\left(\sqrt{\tau_1^2+\tau_2^2}\cdot\coth\sqrt{\tau_1^2+\tau_2^2}\cdot\left(m_1^2\right)\right)} \frac{\sqrt{\tau_1^2+\tau_2^2}}{\sinh\sqrt{\tau_1^2+\tau_2^2}}\, d\tau_1 d\tau_2 dx_2 dx_3 dx_1 \\
&\quad = \frac{t^2}{(2\pi t)^{7/2}} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} e^{-\sqrt{-1}\left(\tau_1\left(k_1+2x_2m_1\right)+\tau_2\left(k_2+2x_3m_1\right)\right)} \\
&\qquad \times\ e^{-\frac{1}{2t}\left(t\sqrt{\tau_1^2+\tau_2^2}\cdot\coth t\sqrt{\tau_1^2+\tau_2^2}\cdot\left(m_1^2\right)\right)} \frac{t\sqrt{\tau_1^2+\tau_2^2}}{\sinh t\sqrt{\tau_1^2+\tau_2^2}}\, d\tau_1 dx_2 d\tau_2 dx_3 \\
&\quad = \frac{1}{(2\pi t)^{3/2}} \frac{1}{(2m_1)^2}\, e^{-\frac{m_1^2}{2t}}.
\end{aligned}$$

Hence

$$\sum_{k_1=0}^{2|m_1|-1} \sum_{k_2=0}^{2|m_1|-1} \int_{\mathcal{F}_{(m_1,0,0,k_1,k_2)}} K_{G_5}^{\mathrm{sub}}\big(t, (m_1, 0, 0, k_1, k_2) * (x, z), (x, z)\big)\, dzdx = \frac{1}{(2\pi t)^{3/2}}\, e^{-\frac{m_1^2}{2t}}.$$

We define $I_1(G_5)$ by

$$I_1(G_5) = \sum_{\gamma\in A_1} \int_{\mathcal{F}_{(m_1,0,0,k_1,k_2)}} K_{G_5}^{\mathrm{sub}}\big(t, (m_1, 0, 0, k_1, k_2) * (x, z), (x, z)\big) dzdx.$$

Then by making use of the Jacobi identity we have

$$\begin{aligned}
I_1(G_5) &= \sum_{m_1\neq 0, m_1\in\mathbb{Z}} \frac{1}{(2\pi t)^{3/2}} e^{-\frac{m_1^2}{2t}} \\
&= \frac{1}{2\pi t} \sum_{\ell\in\mathbb{Z}} e^{-2\pi^2\,\ell^2\,t} - \frac{1}{(2\pi t)^{3/2}}.
\end{aligned}$$

(1-2) $A_2 = \left\{\ (0, m_2, 0, k_1, k_2)\ \middle|\ m_2 \neq 0,\ 0 \le k_1 \le 2|m_2| - 1,\ k_2 \in \mathbb{Z}\right\}$. Then

$$C_{(0,m_2,0,k_1,k_2)} = \left\{(0, a_2, a_3, c_1, c_2)\ \middle|\ a_2, a_3, c_1, c_2 \in \mathbb{Z}\right\},$$

$$\mathcal{F}_{(0,m_2,0,k_1,k_2)} = \left\{(x_1, x_2, x_3, z_1, z_2)\ \middle|\ x_1 \in \mathbb{R}; x_2, x_3, z_1, z_2 \in [0, 1)\right\}.$$

Let $\gamma = (0, m_2, 0, k_1, k_2) \in A_2$. Then

$$\begin{aligned}
&\int_{\mathcal{F}_{(0,m_2,0,k_1,k_2)}} K_{G_5}^{\mathrm{sub}}\big(t, (0, m_2, 0, k_1, k_2) * (x, z), (x, z)\big)\, dxdz \\
&\quad = \frac{1}{(2\pi t)^{7/2}} \int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_{-\infty}^{+\infty} \int_{\mathbb{R}^2} e^{-\frac{\sqrt{-1}}{t}\left(\tau_1\left(k_1 - 2x_1 m_2\right) + \tau_2 k_2\right)} \\
&\qquad \times e^{-\frac{1}{2t}\left(\sqrt{\tau_1^2+\tau_2^2}\cdot\coth\sqrt{\tau_1^2+\tau_2^2}\cdot\left(m_2^2\right) + \frac{1-\sqrt{\tau_1^2+\tau_2^2}\cdot\coth\sqrt{\tau_1^2+\tau_2^2}}{\tau_1^2+\tau_2^2}\cdot(\tau_2 m_2)^2\right)} \\
&\qquad \times \frac{\sqrt{\tau_1^2+\tau_2^2}}{\sinh\sqrt{\tau_1^2+\tau_2^2}}\, d\tau_1 d\tau_2 dx_1 dx_2 dx_3 dz_1 dz_2 \\
&\quad = \frac{t^2}{(2\pi t)^{7/2}} \int_{-\infty}^{+\infty} \int_{\mathbb{R}^2} e^{-\sqrt{-1}\left(\tau_1(k_1 - 2x_1 m_2) + \tau_2 k_2\right)} \\
&\qquad \times e^{-\frac{1}{2t}\left(t\sqrt{\tau_1^2+\tau_2^2}\cdot\coth t\sqrt{\tau_1^2+\tau_2^2}\cdot\left(m_2^2\right) + \frac{1-t\sqrt{\tau_1^2+\tau_2^2}\cdot\coth t\sqrt{\tau_1^2+\tau_2^2}}{\tau_1^2+\tau_2^2}\cdot\left(\tau_2 m_2\right)^2\right)} \\
&\qquad \times \frac{t\sqrt{\tau_1^2+\tau_2^2}}{\sinh t\sqrt{\tau_1^2+\tau_2^2}}\, d\tau_1 dx_1 d\tau_2 \\
&\quad = \frac{1}{2|m_2|} \frac{2\pi t^2}{(2\pi t)^{7/2}} e^{-\frac{m_2^2}{2t}} \int_{-\infty}^{+\infty} e^{-\sqrt{-1}\,\tau_2 k_2} \frac{t\tau_2}{\sinh t\tau_2} d\tau_2.
\end{aligned}$$

Hence by summing up with respect to $0 \le k_1 \le 2|m_2| - 1$ and $k_2 \in \mathbb{Z}$ and by applying the Poisson summation formula we have again

$$\begin{aligned}
&\sum_{k_1=0}^{2|m_2|-1} \sum_{k_2\in\mathbb{Z}} \int_{\mathcal{F}_{(0,m_2,0,k_1,k_2)}} K_{G_5}^{\mathrm{sub}}\big(t, (0, m_2, k_1, k_2) * (x, z), (x, z)\big)\, dxdz \\
&\qquad = \sum_{k_1=0}^{2|m_2|-1} \sum_{k_2\in\mathbb{Z}} \frac{1}{2|m_2|} \frac{2\pi t^2}{(2\pi t)^{7/2}} e^{-\frac{m_2^2}{2t}} \int_{-\infty}^{+\infty} e^{-\sqrt{-1}\,\tau_2 k_2} \frac{t\tau_2}{\sinh t\tau_2}\, d\tau_2 \\
&\qquad = \frac{1}{(2\pi t)^{3/2}} \sum_{k\in\mathbb{Z}} e^{-\frac{m_2^2}{2t}} \frac{2\pi t k}{\sinh 2\pi t k}.
\end{aligned}$$

We define $I_2(G_5)$ by

$$I_2(G_5) = \sum_{\gamma\in A_1} \int_{\mathcal{F}_\gamma} K_{G_5}^{\mathrm{sub}}\big(t, \gamma * (x, z), (x, z)\big)\, dxdz.$$

Then

$$I_2(G_5) = \sum_{m_2\neq 0, m_2\in\mathbb{Z}} \frac{1}{(2\pi t)^{3/2}} \sum_{k\in\mathbb{Z}} e^{-\frac{m_2^2}{2t}} \frac{2\pi t k}{\sinh 2\pi t k}.$$

Again by using Jacobi identity we have

$$I_2(G_5) = \frac{1}{(2\pi t)} \sum_{\ell\in\mathbb{Z}} \sum_{k\in\mathbb{Z}} e^{-2\pi^2\ell^2 t} \frac{2\pi kt}{\sinh 2\pi tk} - \frac{1}{(2\pi t)^{3/2}} \sum_{k\in\mathbb{Z}} \frac{2\pi kt}{\sinh 2\pi tk}$$
$$= 2\left(\sum_{\ell\in\mathbb{Z}} e^{-2\pi^2\,\ell^2\,t} \cdot \sum_{k=1}^{\infty} \frac{k}{\sinh 2\pi tk}\right) + \frac{1}{2\pi t}\sum_{\ell\in\mathbb{Z}} e^{-2\pi^2\,\ell^2\,t}$$
$$- \frac{1}{(2\pi t)^{3/2}} \sum_{k\in\mathbb{Z}} \frac{2\pi tk}{\sinh 2\pi tk}.$$

(1-3) $A_3 = \{(0,0,m_3,k_1,k_2) \mid m_3 \neq 0,\, k_1 \in \mathbb{Z},\, 0 \le k_2 \le 2|m_3|-1\}$. Then

$$C_{(0,0,m_3,k_1,k_2)} = \{(0,a_2,a_3,c_1,c_2) \mid a_2,a_3,c_1,c_2 \in \mathbb{Z}\},$$

$$\mathcal{F}_{(0,0,m_3,k_1,k_2)} = \{(x_1,x_2,x_3,z_1,z_2) \mid x_1 \in \mathbb{R}; x_2,x_3,z_1,z_2 \in [0,1)\}.$$

Let $\gamma \in A_3$. Then we have the same result as in the last case A_2 and

$$I_3(G_5) = \sum_{m_3\in\mathbb{Z},m_3\neq 0} \sum_{k_1\in\mathbb{Z}} \sum_{k_2=0}^{2|m_3|-1} \int_{\mathcal{F}_{(0,0,m_3,k_1,k_2)}} K^{\text{sub}}_{G_5}\big(t,(0,0,m_3,k_1,k_2)*(x,z),(x,z)\big)\,dxdz$$
$$= I_2(G_5).$$

(2-12) $A_{12} = \{(m_1,m_2,0,k_1,k_2) \mid m_1 \neq 0,\ m_2 \neq 0,\, 0 \le k_1 \le 2(|m_1|,|m_2|)-1,\, 0 \le k_2 \le 2|m_1|-1\}$. Then

$$C_{(m_1,m_2,0,k_1,k_2)} = \left\{\left(\ell\frac{m_1}{(|m_1|,|m_2|)}, \ell\frac{m_2}{(|m_1|,|m_2|)}, 0, c_1, c_2\right) \,\Big|\, \ell, c_1, c_2 \in \mathbb{Z}\right\},$$

where $(|m_1|,|m_2|)$ denotes the greatest common divisor of $|m_1|$ and $|m_2|$,

$$\mathcal{F}_{(m_1,m_2,0,k_1,k_2)} = \Big\{(x_1,x_2,x_3,z_1,z_2) \,\Big|\, 0 \le x_1 < \frac{m_1}{(|m_1|,|m_2|)}, x_2,x_3 \in \mathbb{R}, 0 \le z_1 < 1, 0 \le z_2 < 1\Big\}.$$

Further we have

$$\int_{\mathcal{F}_{(m_1,m_2,0,k_1,k_2)}} K^{\text{sub}}_{G_5}\big(t,(m_1,m_2,0,k_1,k_2)*(x,z),(x,z)\big)\,dxdz$$
$$= \frac{1}{(2\pi t)^{7/2}} \int_0^1 \int_0^1 \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_0^{\frac{m_1}{(|m_1|,|m_2|)}} \int_{\mathbb{R}^2} e^{-\sqrt{-1}\,\frac{\tau_1\left(k_1+2(x_2m_1-x_1m_2)\right)+\tau_2\left(k_2+2x_3m_1\right)}{t}}$$

$$\times\ e^{-\frac{1}{2t}\left(|\tau|\coth|\tau|\cdot\left(m_1^2+m_2^2\right)+\frac{1-|\tau|\coth|\tau|}{|\tau|^2}\cdot(\tau_2 m_2)^2\right)}$$

$$\times\ \frac{|\tau|}{\sinh|\tau|}\,d\tau_1 d\tau_2 dx_1 dx_2 dx_3 dz_1 dz_2$$

$$= \frac{t^2}{(2\pi t)^{7/2}} \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_0^{\frac{m_1}{(|m_1|,|m_2|)}}\int_{\mathbb{R}^2} e^{-\sqrt{-1}\left(\tau_1\left(k_1+2(x_2m_1-x_1m_2)\right)+\tau_2\left(k_2+2x_3m_1\right)\right)}$$

$$\times\ e^{-\frac{1}{2t}\left(t|\tau|\coth t|\tau|\cdot\left(m_1^2+m_2^2\right)+\frac{1-t|\tau|\coth t|\tau|}{|\tau|^2}\cdot(\tau_2 m_2)^2\right)}$$

$$\times\ \frac{t|\tau|}{\sinh t|\tau|}\,d\tau_1 d\tau_2 dx_1 dx_2 dx_3$$

$$= \frac{t^2}{(2\pi t)^{7/2}} \int_0^{\frac{m_1}{(|m_1|,|m_2|)}}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{\mathbb{R}^2} e^{-\sqrt{-1}\left(\tau_1\left(k_1+2(x_2m_1-x_1m_2)\right)+\tau_2\left(k_2+2x_3m_1\right)\right)}$$

$$\times\ e^{-\frac{1}{2t}\left(t|\tau|\coth t|\tau|\cdot\left(m_1^2+m_2^2\right)+\frac{1-t|\tau|\coth t|\tau|}{|\tau|^2}\cdot(\tau_2 m_2)^2\right)}$$

$$\times\ \frac{t|\tau|}{\sinh t|\tau|}\,d\tau_1 d\tau_2 dx_2 dx_3 dx_1$$

$$= \frac{(2\pi t)^2}{(2\pi t)^{7/2}}\frac{1}{(2m_1)^2}\int_0^{\frac{m_1}{(|m_1|,|m_2|)}} e^{-\frac{1}{2t}\left(m_1^2+m_2^2\right)}\,dx_1$$

$$= \frac{1}{(2\pi t)^{3/2}}\frac{|m_1|}{(|m_1|,|m_2|)(2m_1)^2}\ e^{-\frac{1}{2t}\left(m_1^2+m_2^2\right)}.$$

So we have $I_{12}(G_5)$ as

$$I_{12}(G_5) = \sum_{\gamma\in A_{1\,2}}\int_{\mathcal{F}_\gamma} K^{\mathrm{sub}}_{G_5}\big(t,\gamma*(x,z),(x,z)\big)\,dxdz.$$

Then

$$I_{12}(G_5) =$$

$$\frac{1}{(2\pi t)^{3/2}}\sum_{\substack{m_1,m_2\in\mathbb{Z}\\ m_1\cdot m_2\neq 0}}\ \sum_{k_1=0}^{2(|m_1|,|m_2|)-1}\ \sum_{k_2=0}^{2|m_1|-1}\frac{|m_1|}{(|m_1|,|m_2|)\cdot 2|m_1|\cdot 2|m_1|}\cdot e^{-\frac{1}{2t}\left(m_1^2+m_2^2\right)}$$

$$= \frac{1}{\sqrt{2\pi t}}\sum_{\ell_1,\ell_2\in\mathbb{Z}} e^{-2\pi^2\,t\left(\ell_1^2+\ell_2^2\right)} - \frac{2}{2\pi t}\sum_{\ell\in\mathbb{Z}} e^{-2\pi^2\,\ell^2\,t} + \frac{1}{(2\pi t)^{3/2}}.$$

(2-13) $A_{13} = \big\{(m_1,0,m_3,k_1,k_2)\ \big|\ m_1\neq 0,\ m_3\neq 0,\ 0\le k_1\le 2|m_1|-1,\ 0\le k_2\le 2(|m_1|,|m_3|)-1\big\}$. Then

$$C_{(m_1,0,m_3,k_1,k_2)} = \left\{\left(\ell\cdot\frac{|m_1|}{(|m_1|,|m_3|)},\ 0,\ \ell\cdot\frac{|m_3|}{(|m_1|,|m_3|)},c_1,c_2\right)\ \middle|\ \ell,c_1,c_2\in\mathbb{Z}\right\},$$

$$\mathcal{F}_{(m_1,0,m_3,k_1,k_2)} = \Big\{(x_1,x_2,x_3,z_1,z_2)\ \Big|\ 0 \le x_1 < \frac{|m_1|}{(|m_1|,|m_3|)},\, x_2,x_3\in\mathbb{R},\, 0\le z_1<1, 0\le z_2<1\Big\}.$$

By the symmetry between the variables x_2 and x_3 we have

$$I_{12}(G_5) = I_{13}(G_5),$$

i.e.,

$$\begin{aligned}
I_{13}(G_5) &= \sum_{\gamma=(m_1,0,m_3,k_1,k_2)\in A_{1\,3}} \int_{\mathcal{F}_\gamma} K^{\mathrm{sub}}_{G_5}\big(t,\gamma*(x,z),(x,z)\big)\,dxdz \\
&= \frac{1}{\sqrt{2\pi t}}\sum_{\ell_1,\ell_2\in\mathbb{Z}} e^{-2\pi^2 t\left(\ell_1^2+\ell_2^2\right)} - \frac{2}{2\pi t}\sum_{\ell\in\mathbb{Z}} e^{-2\pi^2\ell^2 t} + \frac{1}{(2\pi t)^{3/2}} = I_{12}(G_5).
\end{aligned}$$

(2-23) $A_{23} = \big\{(0,m_2,m_3,k_1,k_2)\ \big|\ m_2\neq 0,\, m_3\neq 0,\, 0\le k_1\le 2|m_2|-1,\, k_2\in\mathbb{Z}\big\}$. Then

$$C_{(0,m_2,m_3,k_1,k_2)} = \big\{(0,a_2,a_3,c_1,c_2)\ \big|\ a_2,a_3,c_1,c_2\in\mathbb{Z}\big\},$$

$$\mathcal{F}_{(0,m_2,m_3,k_1,k_2)} = \big\{(x_1,x_2,x_3,z_1,z_2)\ \big|\ x_1\in\mathbb{R}; x_2,x_3,z_1,z_2\in[0,1)\big\}.$$

Further we have

$$\begin{aligned}
&\int_{\mathcal{F}_{(0,m_2,m_3,k_1,k_2)}} K^{\mathrm{sub}}_{G_5}\big(t,(0,m_2,m_3,k_1,k_2)*(x,z),(x,z)\big)\,dxdz \\
&\quad= \frac{1}{(2\pi t)^{7/2}}\int_0^1\int_0^1\int_0^1\int_0^1\int_{-\infty}^{+\infty}\int_{\mathbb{R}^2} e^{-\sqrt{-1}\frac{\tau_1\left(k_1-2x_1m_2\right)+\tau_2\left(k_2-2x_1m_3\right)}{t}} \\
&\qquad\times\, e^{-\frac{1}{2t}\left(|\tau|\coth|\tau|\left(m_2^2+m_3^2\right)+\frac{1-|\tau|\coth|\tau|}{|\tau|^2}\left(-\tau_2m_2+\tau_1m_3\right)^2\right)} \\
&\qquad\times\,\frac{|\tau|}{\sinh|\tau|}\,d\tau_1d\tau_2dx_1dx_2dx_3dz_1dz_2 \\
&\quad= \frac{t^2}{(2\pi t)^{7/2}}\int_{-\infty}^{+\infty}\int_{\mathbb{R}^2} e^{-\sqrt{-1}\left(\tau_1(k_1-2x_1m_2)+\tau_2(k_2-2x_1m_3)\right)} \\
&\qquad\times\, e^{-\frac{1}{2t}\left(t|\tau|\coth t|\tau|\cdot\left(m_2^2+m_3^2\right)+\frac{1-t|\tau|\coth t|\tau|}{|\tau|^2}\left(-\tau_2m_2+\tau_1m_3\right)^2\right)} \\
&\qquad\times\,\frac{t|\tau|}{\sinh t|\tau|}\,d\tau_1d\tau_2dx_1 \\
&\quad= \frac{2\pi t^2}{(2\pi t)^{7/2}}\frac{1}{2|m_2|}\int_{-\infty}^{+\infty}\exp\left\{-\frac{\tau_2}{m_2}\big(k_2m_2-k_1m_3\big)\right\}
\end{aligned}$$

$$\times \exp\Big\{-\frac{1}{2t}\Big[t\tau_2\sqrt{1+\big(m_3/m_2\big)^2}\coth t\cdot\tau_2\sqrt{1+\big(m_3/m_2\big)^2}(m_2^2+m_3^2)$$

$$+\frac{1-t\tau_2\sqrt{1+(m_3/m_2)^2}\coth t\tau_2\sqrt{1+(m_3/m_2)^2}}{\big(1+(m_3/m_2)^2\big)\tau_2^2}\cdot\big(m_2+m_3^2/m_2\big)^2\tau_2^2\Big]\Big\}$$

$$\times\frac{t\tau_2\sqrt{1+(m_3/m_2)^2}}{\sinh t\tau_2\sqrt{1+(m_3/m_2)^2}}\,d\tau_2$$

$$=\frac{\pi t^2}{(2\pi t)^{7/2}}e^{-\frac{m_2^2+m_3^2}{2t}}\int_{-\infty}^{+\infty}e^{-\sqrt{-1}\,\tau_2(k_2m_2-k_1m_3)}\frac{t\tau_2\sqrt{m_2^2+m_3^2}}{\sinh t\tau_2\sqrt{m_2^2+m_3^2}}\,d\tau_2.$$

Hence the sum

$$I_{23}(G_5)=\sum_{\gamma\in A_{2\,3}}\int_{\mathcal{F}_\gamma}K^{\text{sub}}_{G_5}\big(t,\gamma*(x,z),(x,z)\big)\,dxdz$$

is equal to the following expression by making use of the Poisson summation formula:

$$I_{23}(G_5)=\frac{\pi t^2}{(2\pi t)^{7/2}}\sum_{\substack{m_2,m_3\in\mathbb{Z}\\ m_2\cdot m_3\neq 0}}\sum_{k_1=0}^{2|m_2|-1}\sum_{k_2\in\mathbb{Z}}e^{-\frac{m_2^2+m_3^2}{2t}}$$

$$\times\int_{-\infty}^{+\infty}e^{-\sqrt{-1}\,\tau_2(k_2m_2-k_1m_3)}\frac{t\tau_2\sqrt{m_2^2+m_3^2}}{\sinh t\tau_2\sqrt{m_2^2+m_3^2}}\,d\tau_2$$

$$=\frac{2\pi^2t^2}{(2\pi t)^{7/2}}\sum_{\substack{m_2,m_3\in\mathbb{Z}\\ m_2\cdot m_3\neq 0}}\sum_{k_1=0}^{2|m_2|-1}\sum_{\ell\in\mathbb{Z}}\frac{1}{|m_2|}e^{-\frac{m_2^2+m_3^2}{2t}}e^{2\pi\sqrt{-1}\,\frac{m_3}{m_2}\cdot\ell\cdot k_1}\frac{2\pi t\ell\frac{\sqrt{m_2^2+m_3^2}}{m_2}}{\sinh 2\pi t\ell\frac{\sqrt{m_2^2+m_3^2}}{m_2}}$$

$$=\frac{1}{(2\pi t)^{3/2}}\sum_{\substack{m_2,m_3\in\mathbb{Z}\\ m_2\cdot m_3\neq 0}}\sum_{\ell\in\mathbb{Z}}e^{-\frac{m_2^2+m_3^2}{2t}}\cdot\frac{2\pi t\ell\sqrt{\big(\frac{m_2}{(|m_2|,|m_3|)}\big)^2+\big(\frac{m_3}{(|m_2|,|m_3|)}\big)^2}}{\sinh 2\pi t\ell\sqrt{\big(\frac{m_2}{(|m_2|,|m_3|)}\big)^2+\big(\frac{m_3}{(|m_2|,|m_3|)}\big)^2}}.$$

(3-123)

$$A_{123}=\Big\{\,(m_1,m_2,m_3,k_1,k_2)\Big|m_1\neq 0,\ m_2\neq 0,\ m_3\neq 0,$$

$$0\leq k_1\leq 2(|m_1|,|m_2|)-1,\ 0\leq k_2\leq 2\left(\frac{|m_1|(|m_1|,|m_2|,|m_3|)}{(|m_1|,|m_2|)}\right)-1\Big\},$$

where $(|m_1|,|m_2|,|m_3|)$ is the greatest common divisor of $|m_1|$, $|m_2|$ and $|m_3|$. Then

$$C_{(m_1,m_2,m_3,k_1,k_2)}$$

$$=\Big\{\Big(\frac{\ell|m_1|}{(|m_1|,|m_2|,|m_3|)},\frac{\ell|m_2|}{(|m_1|,|m_2|,|m_3|)},\frac{\ell|m_3|}{(|m_1|,|m_2|,|m_3|)},c_1,c_2\Big)\,\Big|\,\ell,c_1,c_2\in\mathbb{Z}\Big\},$$

$$\mathcal{F}_{(m_1,m_2,m_3,k_1,k_2)} = \Big\{(x_1,x_2,x_3,z_1,z_2)\ \Big| \\ 0 \le x_1 < \frac{|m_1|}{(|m_1|,|m_2|,|m_3|)},\ x_2,x_3 \in \mathbb{R}, 0 \le z_1 < 1, 0 \le z_2 < 1\Big\}.$$

Further we have

$$\begin{aligned}
&\int_{\mathcal{F}_{(m_1,m_2,m_3,k_1,k_2)}} K^{\text{sub}}_{G_5}\big(t,(m_1,m_2,m_3,k_1,k_2)*(x,z),(x,z)\big)\,dxdz \\
&= \frac{1}{(2\pi t)^{7/2}} \int_0^1 \int_0^1 \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_0^{\frac{|m_1|}{(|m_1|,|m_2|,|m_3|)}} \\
&\qquad \int_{\mathbb{R}^2} e^{-\sqrt{-1}\,\frac{\tau_1(k_1+2(x_2m_1-x_1m_2))+\tau_2(k_2+2(x_3m_1-x_1m_3))}{t}} \\
&\quad \times\ e^{-\frac{1}{2t}\left(|\tau|\coth|\tau|\cdot(m_1^2+m_2^2+m_3^2)+\frac{1-|\tau|\coth|\tau|}{|\tau|^2}\cdot(-\tau_2m_2+\tau_1m_3)^2\right)} \\
&\quad \times\ \frac{|\tau|}{\sinh|\tau|}\,d\tau dx_1dx_2dx_3dz_1dz_2 \\
&= \frac{2\pi t^2}{(2\pi t)^{7/2}}\frac{1}{2|m_1|}\int_0^{\frac{|m_1|}{(|m_1|,|m_2|,|m_3|)}}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} e^{-\sqrt{-1}\,\tau_2(k_2+2(x_3m_1-x_1m_3)} \\
&\quad \times\ e^{-\frac{1}{2t}\left(t\tau_2\coth t\tau_2\cdot(m_1^2+m_2^2+m_3^2)+\frac{1-t\tau_2\coth t\tau_2}{\tau_2^2}\cdot\tau_2^2m_2^2\right)}\frac{t\tau_2}{\sinh t\tau_2}\,d\tau_2dx_3dx_1 \\
&= \frac{(2\pi t)^2}{(2\pi t)^{7/2}}\cdot\frac{|m_1|}{(|m_1|,|m_2|,|m_3|)}\cdot\frac{1}{2|m_1|\cdot 2|m_1|}e^{-\frac{1}{2t}\left(m_1^2+m_2^2+m_3^2\right)}.
\end{aligned}$$

Having the sum

$$\sum_{\gamma\in A_{1\,2\,3}}\int_{\mathcal{F}_\gamma} K^{\text{sub}}_{G_5}\big(t,\gamma*(x,z),(x,z)\big)dxdz$$

as $I_{123}(G_5)$, we then obtain

$$\begin{aligned}
I_{123}(G_5) &= \sum_{\substack{m_1,m_2,m_3\in\mathbb{Z}\\ m_1\cdot m_2\cdot m_3\neq 0}}\ \sum_{k_1=0}^{2(|m_1|,|m_2|)-1}\ \sum_{k_2=0}^{2\left(\frac{|m_1|(|m_1|,|m_2|,|m_3|)}{(|m_1|,|m_2|)}\right)-1} \\
&\qquad \int_{\mathcal{F}_{(m_1,m_2,m_3,k_1,k_2)}} K^{\text{sub}}_{G_5}\big(t,(m_1,m_2,m_3,k_1,k_2)*(x,z),(x,z)\big)\,dxdz \\
&= \frac{1}{(2\pi t)^{3/2}}\sum_{\substack{m_1,m_2,m_3\in\mathbb{Z}\\ m_1\cdot m_2\cdot m_3\neq 0}}\frac{|m_1|\cdot 2(|m_1|,|m_2|)}{(|m_1|,|m_2|,|m_3|)\cdot 2|m_1|\cdot 2|m_1|}\cdot 2\left(\frac{|m_1|}{(|m_1|,|m_2|)}\right) \\
&\quad \times\ e^{-\frac{1}{2t}\left(m_1^2+m_2^2+m_3^2\right)}
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{(2\pi t)^{3/2}} \sum_{\substack{m_1, m_2, m_3 \in \mathbb{Z} \\ m_1 \cdot m_2 \cdot m_3 \neq 0}} e^{-\frac{1}{2t}\left(m_1^2+m_2^2+m_3^2\right)} \\
&= \frac{1}{(2\pi t)^{3/2}} \left(\sum_{m \in \mathbb{Z}} e^{-\frac{m^2}{2t}} - 1 \right)^3 \\
&= \frac{1}{(2\pi t)^{3/2}} \left(\sqrt{2\pi t} \sum_{\ell \in \mathbb{Z}} e^{-2\pi^2 \ell^2 t} - 1 \right)^3 \\
&= \sum_{\ell_1, \ell_2, \ell_3 \in \mathbb{Z}} e^{-2\pi^2(\ell_1^2+\ell_2^2+\ell_3^2)t} \\
&\quad - \frac{3}{\sqrt{2\pi t}} \sum_{\ell_1, \ell_2 \in \mathbb{Z}} e^{-2\pi^2(\ell_1^2+\ell_2^2)t} + \frac{3}{2\pi t} \sum_{\ell \in \mathbb{Z}} e^{-2\pi^2 \ell^2 t} - \frac{1}{(2\pi t)^{3/2}}.
\end{aligned}$$

Here we list the expressions for $I_i(G_5)$, $I_{i\,j}(G_5)$ and $I_{123}(G_5)$:

$$\begin{aligned}
I_0(G_5) &= \frac{1}{(2\pi t)^{3/2}} \sum_{k_1, k_2 \in \mathbb{Z}} \frac{2\pi t \sqrt{k_1^2 + k_2^2}}{\sinh 2\pi t \sqrt{k_1^2 + k_2^2}} \\
&= \frac{1}{(2\pi t)^{1/2}} \sum_{\substack{k_1, k_2 \in \mathbb{Z} \\ k_1 \cdot k_2 \neq 0}} \frac{\sqrt{k_1^2 + k_2^2}}{\sinh 2\pi t \sqrt{k_1^2 + k_2^2}} \\
&\quad + \frac{2}{(2\pi t)^{1/2}} \sum_{\substack{k \in \mathbb{Z} \\ k \neq 0}} \frac{k}{\sinh 2\pi t k} + \frac{1}{(2\pi t)^{3/2}}, \\
I_1(G_5) &= \sum_{m_1 \neq 0, m_1 \in \mathbb{Z}} \frac{1}{(2\pi t)^{3/2}} e^{-\frac{m_1^2}{2t}} = \frac{1}{2\pi t} \sum_{\ell \in \mathbb{Z}} e^{-2\pi^2 \ell^2 t} - \frac{1}{(2\pi t)^{3/2}}, \\
I_2(G_5) &= \sum_{m_2 \neq 0, m_2 \in \mathbb{Z}} \frac{1}{(2\pi t)^{3/2}} \sum_{k \in \mathbb{Z}} e^{-\frac{m_2^2}{2t}} \frac{2\pi t k}{\sinh 2\pi t k} \\
&= \frac{1}{(2\pi t)} \sum_{\ell \in \mathbb{Z}} \sum_{k \in \mathbb{Z}} e^{-2\pi^2 \ell^2 t} \frac{2\pi k t}{\sinh 2\pi t k} - \frac{1}{(2\pi t)^{3/2}} \sum_{k \in \mathbb{Z}} \frac{2\pi k t}{\sinh 2\pi t k} \\
&= 2 \left(\sum_{\ell \in \mathbb{Z}} e^{-2\pi^2 \ell^2 t} \cdot \sum_{k=1}^{\infty} \frac{k}{\sinh 2\pi t k} \right) + \frac{1}{2\pi t} \sum_{\ell \in \mathbb{Z}} e^{-2\pi^2 \ell^2 t} \\
&\quad - \frac{1}{(2\pi t)^{1/2}} \sum_{\substack{k \in \mathbb{Z} \\ k \neq 0}} \frac{k}{\sinh 2\pi t k} - \frac{1}{(2\pi t)^{3/2}}, \\
I_3(G_5) &= I_2(G_5), \\
I_{12}(G_5) &= \frac{1}{(2\pi t)^{3/2}} \sum_{\substack{m_1, m_2 \in \mathbb{Z} \\ m_1 \cdot m_2 \neq 0}} e^{-\frac{1}{2t}\left(m_1^2+m_2^2\right)}
\end{aligned}$$

$$= \frac{1}{\sqrt{2\pi t}} \sum_{\ell_1,\ell_2\in\mathbb{Z}} e^{-2\pi^2\, t\left(\ell_1^2+\ell_2^2\right)} - \frac{2}{2\pi t}\sum_{\ell\in\mathbb{Z}} e^{-2\pi^2\,\ell^2\, t} + \frac{1}{(2\pi t)^{3/2}},$$

$$\begin{aligned}
I_{13}(G_5) &= I_{12}(G_5),\\
I_{23}(G_5) &= \frac{1}{(2\pi t)^{1/2}} \sum_{\substack{m_2,m_3\in\mathbb{Z}\\ m_2\cdot m_3\neq 0}} \sum_{\substack{\ell\in\mathbb{Z}\\ \ell\neq 0}} e^{-\frac{m_2^2+m_3^2}{2t}}\\
&\quad\times \frac{\ell\sqrt{\left(\frac{m_2}{(|m_2|,|m_3|)}\right)^2+\left(\frac{m_3}{(|m_2|,|m_3|)}\right)^2}}{\sinh 2\pi t\ell\sqrt{\left(\frac{m_2}{(|m_2|,|m_3|)}\right)^2+\left(\frac{m_3}{(|m_2|,|m_3|)}\right)^2}}\\
&\quad+\frac{1}{(2\pi t)^{1/2}}\sum_{\ell_1,\ell_2\in\mathbb{Z}} e^{-2\pi^2 t(\ell_1^2+\ell_2^2)} - \frac{2}{2\pi t}\sum_{\ell\in\mathbb{Z}} e^{-2\pi^2 t\ell^2} + \frac{1}{(2\pi t)^{3/2}},\\
I_{123}(G_5) &= \frac{1}{(2\pi t)^{3/2}} \sum_{\substack{m_1,m_2,m_3\in\mathbb{Z}\\ m_1\cdot m_2\cdot m_3\neq 0}} e^{-\frac{1}{2t}\left(m_1^2+m_2^2+m_3^2\right)}\\
&= \frac{1}{(2\pi t)^{3/2}}\left(\sum_{m\in\mathbb{Z}} e^{-\frac{m^2}{2t}} - 1\right)^3\\
&= \sum_{\ell_1,\,\ell_2,\,\ell_3\in\mathbb{Z}} e^{-2\pi^2(\ell_1^2+\ell_2^2+\ell_3^2)t} - \frac{3}{\sqrt{2\pi t}} \sum_{\ell_1,\,\ell_2\in\mathbb{Z}} e^{-2\pi^2(\ell_1^2+\ell_2^2)t}\\
&\quad+\frac{3}{2\pi t}\sum_{\ell\in\mathbb{Z}} e^{-2\pi^2\ell^2 t} - \frac{1}{(2\pi t)^{3/2}}.
\end{aligned}$$

The trace

$$\sum_{\gamma\in L}\int_{\mathcal{F}_L} K_{G_5}^{\mathrm{sub}}\big(t,\gamma*(x,z),(x,z)\big)dxdz$$

is the sum of all $I_0(G_5), I_1(G_5), \ldots, I_{123}(G_5)$ and we have:

Theorem 12.1. *Let* $0=\lambda_0<\lambda_1<\lambda_2<\cdots<\lambda_n<\cdots$ *be the distinct eigenvalues of the sub-Laplacian*

$$\Delta_{G_5}^{\mathrm{sub}} = -\left(\frac{\partial}{\partial x_1} - x_2\frac{\partial}{\partial z_1} - x_3\frac{\partial}{\partial z_2}\right)^2 - \left(\frac{\partial}{\partial x_2} + x_1\frac{\partial}{\partial z_2}\right)^2 - \left(\frac{\partial}{\partial x_3} + x_1\frac{\partial}{\partial z_2}\right)^2$$

on the space $L\backslash G_5$ *with multiplicities* $m_n>0$. *Then*

$$\sum_{\gamma\in L}\int_{L\backslash G_5} K_{G_5}^{\mathrm{sub}}\big(t,\gamma*(x,z),(x,z)\big)dxdz = \sum_{n=0}^{\infty} m_n^{-\lambda_n t}$$

$$= \sum_{\ell_1,\ell_2,\ell_3\in\mathbb{Z}} e^{-2\pi^2\, t(\ell_1^2+\ell_2^2+\ell_3^2)}$$
$$+ 2\sum_{\ell\in\mathbb{Z}}\sum_{k=1}^{+\infty} e^{-2\pi^2 t\ell^2}\frac{2k}{\sinh 2\pi kt}$$
$$+ \sum_{\substack{m_1,m_2\in\mathbb{Z},\, m_1\cdot m_2\neq 0\\ (|m_1|,|m_2|)=1}}\sum_{k=1}^{+\infty}\sum_{\ell\in\mathbb{Z}} e^{-2\pi^2\, t\,\frac{\ell^2}{m_1^2+m_2^2}}\frac{k}{\sinh 2\pi t\, k\sqrt{m_1^2+m_2^2}}.$$

Proof. By summing up all $I_*(G_5)$ with respect to the order of the time parameter t we have

$$\sum_{n=0}^{\infty} m_n^{-\lambda_n t} = I_0(G_5)+I_1(G_5)+I_2(G_5)+I_3(G_5)$$
$$+ I_{12}(G_5)+I_{13}(G_5)+I_{23}(G_5)+I_{123}(G_5)$$
$$= \sum_{\ell_1,\ell_2,\ell_3\in\mathbb{Z}} e^{-2\pi^2 t(\ell_1^2+\ell_2^2+\ell_3^2)}$$
$$+ 2\sum_{\ell\in\mathbb{Z}}\sum_{k=1}^{+\infty} e^{-2\pi^2 t\ell^2}\frac{2k}{\sinh 2\pi kt}$$
$$+ \frac{1}{(2\pi t)^{1/2}}\sum_{\substack{k_1,k_2\in\mathbb{Z}\\ k_1\cdot k_2\neq 0}}\frac{\sqrt{k_1^2+k_2^2}}{\sinh 2\pi t\sqrt{k_1^2+k_2^2}}$$
$$+ \frac{1}{(2\pi t)^{1/2}}\sum_{\substack{m,\,n\in\mathbb{Z}\\ m\cdot n\neq 0}}\sum_{\ell=1}^{+\infty} e^{-\frac{(m^2+n^2)}{2t}}\frac{2\ell\sqrt{\left(\frac{m}{(|m|,|n|)}\right)^2+\left(\frac{n}{(|m|,|n|)}\right)^2}}{\sinh 2\pi t\ell\sqrt{\left(\frac{m}{(|m|,|n|)}\right)^2+\left(\frac{m}{(|m|,|n|)}\right)^2}}$$
$$= \sum_{\ell_1,\ell_2,\ell_3\in\mathbb{Z}} e^{-2\pi^2 t(\ell_1^2+\ell_2^2+\ell_3^2)}$$
$$+ 2\sum_{\ell\in\mathbb{Z}}\sum_{k=1}^{+\infty} e^{-2\pi^2 t\ell^2}\frac{2k}{\sinh 2\pi kt}$$
$$+ \sum_{\substack{\ell_1,\ell_2\in\mathbb{Z}\\ \ell_1\cdot\ell_2\neq 0,(|\ell_1|,|\ell_2|)=1}}\sum_{k=1}^{+\infty}\sum_{\ell\in\mathbb{Z}} e^{-2\pi^2\, t\,\frac{\ell^2}{\ell_1^2+\ell_2^2}}\frac{k}{\sinh 2\pi t\, k\sqrt{\ell_1^2+\ell_2^2}}.$$

□

For convenience we provide another expression for the heat kernel trace which was initially given in Theorem 12.1.

Corollary 12.2.

$$\sum_{\gamma\in L}\int_{L\backslash G_5} K^{\text{sub}}_{G_5}\big(t,\gamma*(x,z),(x,z)\big)dxdz=\sum_{n=0}^{\infty} m_n^{-\lambda_n t}$$

$$=\sum_{\ell_1,\ell_2,\ell_3\in\mathbb{Z}} e^{-2\pi^2\, t(\ell_1^2+\ell_2^2+\ell_3^2)}+2\sum_{\ell\in\mathbb{Z}}\sum_{k=1}^{+\infty} e^{-2\pi^2 t\ell^2}\frac{2k}{\sinh 2\pi kt}$$

$$+\sum_{\substack{m_1,m_2\in\mathbb{Z}\\ m_1\cdot m_2\neq 0}}\sum_{\ell\in\mathbb{Z}} e^{-2\pi^2\, t\,\frac{\ell^2\cdot(|m_1|,|m_2|)^2}{m_1^2+m_2^2}}\frac{(|m_1|,|m_2|)}{\sinh 2\pi t\sqrt{m_1^2+m_2^2}}$$

$$=\sum_{\ell_1,\ell_2,\ell_3\in\mathbb{Z}} e^{-2\pi^2\, t(\ell_1^2+\ell_2^2+\ell_3^2)}+\sum_{\ell\in\mathbb{Z}}\sum_{k=1}^{+\infty}\sum_{j=0}^{+\infty} 8ke^{-t\left(2\pi^2\ell^2+2\pi\, k\,(2j+1)\right)}$$

$$+2\sum_{\substack{m_1,m_2\in\mathbb{Z}\\ m_1\cdot m_2\neq 0}}\sum_{\ell\in\mathbb{Z}}\sum_{j=0}^{+\infty}(|m_1|,|m_2|)\,e^{-t\left(\frac{2\pi^2\ell^2\cdot(|m_1|,|m_2|)^2}{m_1^2+m_2^2}+2\pi\sqrt{m_1^2+m_2^2}(2j+1)\right)}.$$

13. Spectrum of a six-dimensional compact nilmanifold

In this section, we provide the heat kernel trace on a six-dimensional compact nilmanifold $L\backslash F_{(3+3)}$ by a typical lattice L,

$$L=\big\{(m_1,m_2,m_3,k_1,k_2,k_3)\;\big|\;m_i,k_i\in\mathbb{Z}\big\}.$$

The method of calculating the trace is same as the one in the last section and so we do not repeat the details. We recall that the sub-Laplacian $\Delta^{\text{sub}}_{F_{(3+3)}}$ on the group $F_{(3+3)}$ is

$$-\Delta^{\text{sub}}_{F_{(3+3)}}=\left(\frac{\partial}{\partial x_1}-x_2\frac{\partial}{\partial z_1}-x_3\frac{\partial}{\partial z_2}\right)^2+\left(\frac{\partial}{\partial x_2}+x_1\frac{\partial}{\partial z_1}-x_3\frac{\partial}{\partial z_3}\right)^2$$
$$+\left(\frac{\partial}{\partial x_3}+x_1\frac{\partial}{\partial z_2}+x_2\frac{\partial}{\partial z_3}\right)^2.$$

The heat kernel on $L\backslash F_{(3+3)}$ has the form

$$\sum_{\gamma\in L} K^{\text{sub}}_{F_{(3+3)}}\big(t,\gamma\cdot(x,z),\ (\tilde{x},\tilde{z})\big)$$

and its trace is the integral

$$\sum_{\gamma\in L}\int_{\mathcal{F}_L} K^{\text{sub}}_{F_{(3+3)}}\big(t,\gamma\cdot(x,z),\ (x,z)\big)\,dxdz,$$

where $\mathcal{F}_L$ is a fundamental domain of the lattice L.

Theorem 13.1.

$$\sum_{\gamma\in L}\int_{\mathcal{F}_L} K^{\mathrm{sub}}_{F_{(3+3)}}\big(t,\gamma*(x,z),(x,z)\big)dxdz$$

$$= \sum_{\ell_1,\ell_2,\ell_3\in\mathbb{Z}} e^{-2\pi^2 t\left(\ell_1^2+\ell_2^2+\ell_3^2\right)} + 3\sum_{\ell\in\mathbb{Z}}\sum_{k=1}^{\infty} e^{-2\pi^2\ell^2 t}\frac{2k}{\sinh 2\pi tk}$$

$$+3\sum_{\substack{m_1,m_2\in\mathbb{Z},\ m_1\cdot m_2\neq 0\\ (|m_1|,|m_2|)=1}}\sum_{k=1}^{+\infty}\sum_{\ell\in\mathbb{Z}} e^{-2\pi^2 t\frac{\ell^2}{m_1^2+m_2^2}}\frac{k}{\sinh 2\pi tk\sqrt{m_1^2+m_2^2}}$$

$$+\sum_{\substack{m_1,m_2,m_3\in\mathbb{Z},\ m_1\cdot m_2\cdot m_3\neq 0\\ (|m_1|,|m_2|,|m_3|)=1}}\sum_{k=1}^{+\infty}\sum_{\ell\in\mathbb{Z}} e^{-2\pi^2 t\frac{\ell^2}{m_1^2+m_2^2+m_3^2}}\frac{k}{\sinh 2\pi tk\sqrt{m_1^2+m_2^2+m_3^2}}.$$

14. Heat trace asymptotics on compact nilmanifolds of the dimensions five and six

In the present section we calculate the short time expansion of the heat kernel trace for the sub-Laplacians $\Delta^{\mathrm{sub}}_{L\backslash G_5}$ and $\Delta^{\mathrm{sub}}_{L\backslash F_{(3+3)}}$ on a five- and six-dimensional compact nilmanifold, respectively. We make directly use of the integral forms of these kernels and as an application we show that the spectral zeta-functions corresponding to these sub-Laplacians admit a meromorphic extension to the complex plane with only one simple pole at $s=\frac{7}{2}$ and $s=\frac{9}{2}$ in the five- and six-dimensional cases, respectively. Moreover, we obtain the residues in these poles.

14.1. The six-dimensional case

According to a general formula it is known that the heat kernel $K^{\mathrm{sub}}_{F_{(3+3)}} = K^{\mathrm{sub}}_{F_{(3+3)}}\big(t,(x,z),(\tilde{x},\tilde{z})\big)\in C^\infty(\mathbb{R}_+\times F_{(3+3)}\times F_{(3+3)})$ for the sub-Laplacian $\Delta^{\mathrm{sub}}_{F_{(3+3)}}$, i.e., the kernel function of the operator $\big\{e^{-\frac{t}{2}\cdot\Delta^{\mathrm{sub}}_{F_{(3+3)}}}\big\}_{t>0}$ has the form

$$K^{\mathrm{sub}}_{F_{(3+3)}}\big(t,(x,z),(\tilde{x},\tilde{z})\big)=\frac{1}{(2\pi t)^{9/2}}\int_{\mathbb{R}^3}\exp\Big\{-\frac{A\big((\tilde{x},\tilde{z})^{-1}*(x,z),\tau\big)}{t}\Big\}W(\tau)\,d\tau,$$

where the function $A=A(x,z,\tau)$ is called action function and is given by the formula

$$A(x,z,\tau)=\sqrt{-1}\,\langle\tau,z\rangle+\frac{1}{2}\,\big\langle\Omega(\sqrt{-1}\,\tau)\coth\Omega(\sqrt{-1}\,\tau)\cdot x,\,x\big\rangle\,.$$

In the above formula, the matrix $\Omega(\tau)$ is the following 3×3 anti-symmetric matrix

$$\Omega(\tau)=\begin{pmatrix}0&\tau_1&\tau_2\\-\tau_1&0&\tau_3\\-\tau_2&-\tau_3&0\end{pmatrix}$$

with $\tau = (\tau_1, \tau_2, \tau_3) \in \mathbb{R}^3$ and we denote by $\langle \cdot, \cdot \rangle$ the standard inner product on $\mathbb{R}^3$. The function $W(\tau)$ is given by

$$W(\tau) = \left(\det \frac{\sqrt{-1}\,\Omega(\tau)}{\sinh \sqrt{-1}\,\Omega(\tau)} \right)^{1/2} = \frac{|\tau|}{\sinh |\tau|}$$

and with the definition $h(x) = x \coth x - 1$ we have

$$\sqrt{-1}\,\Omega(\tau) \coth \sqrt{-1}\,\Omega(\tau) = \mathrm{Id} + h(\sqrt{-1}\,\Omega(\tau)) = \mathrm{Id} + \frac{|\tau| \coth |\tau| - 1}{|\tau|^2} \left(\sqrt{-1}\,\Omega(\tau) \right)^2 .$$

We start with some preparations:

Theorem 14.1. *For any functions $f(x)$ in $\mathcal{S}(\mathbb{R}^n)$, we have*

$$\sum_{\ell \in \mathbb{Z}^n} \tilde{f}(\ell) = \sum_{k \in \mathbb{Z}^n} f(2\pi k),$$

where $\tilde{f}$ denotes the inverse Fourier transform of f. In particular, it follows that

$$\frac{1}{\sqrt{2\pi t}} \sum_{n \in \mathbb{Z}} e^{-\frac{n^2}{2t}} = \sum_{k \in \mathbb{Z}} e^{-2\pi^2 k^2 t}.$$

We also use the following estimate:

Theorem 14.2. *Let $f \in C^\infty(\mathbb{R})$ such that $\int_{\mathbb{R}} |\partial^\alpha f(x)|\, dx < \infty$ for any multi-index α. Then, for any integer $N \geq 2$, we have*

$$\left| \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}} e^{\sqrt{-1}\, \frac{n \cdot \zeta}{t}} f(\zeta)\, d\zeta - \int_{\mathbb{R}} f(\zeta)\, d\zeta \right| \leq t^N \zeta(N) \int_{\mathbb{R}} |\partial^N f(x)|\, dx.$$

Proof. For $n \neq 0$ we have

$$\begin{aligned} \int_{\mathbb{R}} e^{\sqrt{-1}\, \frac{n \cdot \zeta}{t}} f(\zeta)\, d\zeta &= \frac{t^N}{n^N} \int_{\mathbb{R}} \left((-\sqrt{-1}\, \partial_\zeta)^N e^{\sqrt{-1}\, \frac{n \cdot \zeta}{t}} \right) f(\zeta)\, d\zeta \\ &= \frac{t^N}{n^N} \int_{\mathbb{R}} e^{\sqrt{-1}\, \frac{n \cdot \zeta}{t}} (-\sqrt{-1}\, \partial_\zeta)^N f(\zeta) d\zeta. \end{aligned}$$

Therefore, it follows

$$\left| \sum_{n \in \mathbb{Z} \setminus \{0\}} \int_{\mathbb{R}} e^{\sqrt{-1}\, \frac{n \cdot \zeta}{t}} f(\zeta)\, d\zeta \right| \leq t^N \sum_{n=1}^{\infty} \frac{1}{n^N} \int_{\mathbb{R}} |\partial^N f(x)|\, dx$$

which proves the assertion. □

Corollary 14.3. *For any real constant k and all $N \in \mathbb{N}$, we have*

$$\sum_{n \in \mathbb{Z},\, n \neq 0} n^k e^{-\frac{n^2}{2t}} = O(t^N).$$

We need to evaluate the following integral:

Theorem 14.4. *It holds*

$$\int_{\mathbb{R}^d} \frac{|\tau|}{\sinh|\tau|}\, d\tau = 4\pi^{d/2} \frac{\Gamma(d+1)}{\Gamma(d/2)} \left(1 - 2^{-(d+1)}\right) \zeta(d+1).$$

In particular,

(i) $\int_{\mathbb{R}} \frac{|\tau|}{\sinh|\tau|}\, d\tau = \frac{\pi^2}{2}$,

(ii) $\int_{\mathbb{R}^2} \frac{|\tau|}{\sinh|\tau|}\, d\tau = 7\pi\zeta(3)$,

(iii) $\int_{\mathbb{R}^3} \frac{|\tau|}{\sinh|\tau|}\, d\tau = \frac{\pi^5}{2}$.

Proof. Since the integrand is a radial symmetric function, we have

$$\int_{\mathbb{R}^d} \frac{|\tau|}{\sinh|\tau|}\, d\tau = V_d \int_0^\infty \frac{r^d}{\sinh r}\, dr = 2V_d \int_0^\infty \frac{r^d e^{-r}}{1-e^{-2r}}\, dr,$$

where $V_d = 2\pi^{d/2}\,\Gamma(d/2)^{-1}$ is the surface volume of the unit sphere of dimension $d-1$. Further

$$\begin{aligned}\int_0^\infty & \frac{r^d e^{-r}}{1-e^{-2r}}\, dr \\ &= \sum_{j=0}^\infty \int_0^\infty r^d e^{-(1+2j)r}\, dr = \sum_{j=0}^\infty \frac{1}{(1+2j)^{d+1}} \int_0^\infty r^d e^{-r}\, dr \\ &= 2^{-(d+1)}\,\Gamma(d+1)\,\zeta\big(d+1, \frac{1}{2}\big) = \Gamma(d+1)\left(1-2^{-(d+1)}\right)\zeta(d+1).\end{aligned}$$

The results in (i)–(iii) are obtained by using $\zeta(2) = \frac{\pi^2}{6}$ and $\zeta(4) = \frac{\pi^4}{90}$. □

Now, we can calculate the short time asymptotics of the heat kernel trace for the sub-Laplacian $\Delta^{\mathrm{sub}}_{F_{(3+3)}}$. By fixing a lattice L in $F_{(3+3)}$,

$$L = \left\{(m_1, m_2, m_3, k_1, k_2, k_3) \;\middle|\; m_i,\, k_i \in \mathbb{Z}\right\}$$

we have the following result for the asymptotic behaviour as t goes to 0 for

$$\sum_{\gamma\in L} K^{\mathrm{sub}}_{F_{(3+3)}}\big(t, \gamma * (x,z), (x,z)\big)$$

and for the trace of the heat kernel on $L\backslash F_3$,

$$K_{L\backslash F_{(3+3)}}(t) = \sum_{\gamma\in L} \int_{\mathcal{F}_L} K^{\mathrm{sub}}_{F_3}\big(t, \gamma * (x,z), (x,z)\big) dxdz.$$

$\mathcal{F}_L$ is a fundamental domain of L, i.e., $\mathcal{F}_L = \left\{(x_1, x_2, x_3, z_1, z_2, z_3) \;\middle|\; 0 \le x_j < 1,\, 0 \le z_j < 1\right\}$.

Theorem 14.5. *For any* $(x,z)\in\mathcal{F}_L$*, it holds:*

$$\sum_{\gamma\in L} K^{\mathrm{sub}}_{F_{(3+3)}}\big(t,\gamma*(x,z),(x,z)\big)=\frac{1}{(2\pi)^{9/2}}\left(\int_{\mathbb{R}^3}\frac{|\tau|}{\sinh|\tau|}d\tau\right)t^{-9/2}+O(t^\infty)$$
$$=\frac{\sqrt{\pi}}{32\sqrt{2}}\,t^{-9/2}+O(t^\infty).$$

Proof. We have for $\gamma=(m,k)$

$$\gamma*(x,z)=\big(x+m,z_1+k_1+q_1(m,x),z_2+k_2+q_2(m,x),z_3+k_3+q_3(m,x)\big),$$
$$(x,z)^{-1}*\gamma*(x,z)=\big(m,k_1+2q_1(m,x),k_2+2q_2(m,x),k_3+2q_3(m,x)\big),$$

where

$$q_1(m,x)=m_1x_2-m_2x_1,\;\; q_2(m,x)=m_1x_3-m_3x_1,\;\; q_3(m,x)=m_2x_3-m_3x_2.$$

Hence it follows

$$A\big((x,z)^{-1}*\gamma*(x,z),\tau\big)$$
$$=\sqrt{-1}\,\big\langle\tau,k+2q(m,x)\big\rangle+\frac{1}{2}\,\big\langle\Omega(\sqrt{-1}\,\tau)\coth\Omega(\sqrt{-1}\,\tau)\cdot m,\,m\big\rangle,$$

and $K^{\mathrm{sub}}_{F_{(3+3)}}\big(t,\gamma*(x,z),(x,z)\big)$ is of the form

$$K^{\mathrm{sub}}_{F_{(3+3)}}\big(t,\gamma*(x,z),(x,z)\big)=\frac{1}{(2\pi t)^{9/2}}\int_{\mathbb{R}^3}\exp\left\{-\sqrt{-1}\,\frac{\sum_{j=1}^3(k_j+2q_j(m,x))\tau_j}{t}\right\}$$
$$\times\exp\Big\{-\frac{1}{2t}\,\big\langle\Omega(\sqrt{-1}\,\tau)\coth\Omega(\sqrt{-1}\,\tau)\cdot m,\,m\big\rangle\Big\}\,\frac{|\tau|}{\sinh|\tau|}\,d\tau.$$

Now, we distinguish the following four cases:

(I) Let $\gamma=(0,0)$. Then

$$K^{\mathrm{sub}}_{F_{(3+3)}}\big(t,\gamma*(x,z),(x,z)\big)=\frac{1}{(2\pi t)^{9/2}}\int_{\mathbb{R}^3}\frac{|\tau|}{\sinh|\tau|}d\tau.$$

(II) Let $\gamma=(0,k)$ with $k\in\mathbb{Z}^3\backslash\{0\}$. Then

$$K^{\mathrm{sub}}_{F_{(3+3)}}\big(t,\gamma*(x,z),(x,z)\big)=\frac{1}{(2\pi t)^{9/2}}\int_{\mathbb{R}^3}\exp\left\{-\frac{\sqrt{-1}}{t}\,\langle k,\tau\rangle\right\}\frac{|\tau|}{\sinh|\tau|}\,d\tau.$$

According to Theorem 14.2 we have

$$\sum_{k\in\mathbb{Z}^3\backslash\{0\}}K^{\mathrm{sub}}_{F_{(3+3)}}\big(t,(0,k)*(x,z),(x,z)\big)=O(t^\infty).$$

(III) Let $\gamma=(m,0)$ with $m\in\mathbb{Z}^3\backslash\{0\}$. Then

$$\exp\Big\{-\frac{1}{2t}\,\big\langle\Omega(\sqrt{-1}\,\tau)\coth\Omega(\sqrt{-1}\,\tau)\cdot m,\,m\big\rangle\Big\}$$
$$=\exp\Big\{-\frac{1}{2t}\,|m|^2-\frac{1}{2t}\,\big\langle h\big(\Omega(\sqrt{-1}\,\tau)\big)\cdot m,\,m\big\rangle\Big\}.$$

Noting that

$$\begin{aligned}&\big\langle h(\sqrt{-1}\,\Omega)\cdot m,\, m\big\rangle\\&\quad=\frac{|\tau|\coth|\tau|-1}{|\tau|^2}\Big\{(\tau_1m_2+\tau_2m_3)^2+(-\tau_1m_1+\tau_3m_3)^2+(\tau_2m_1+\tau_3m_2)^2\Big\}\end{aligned}$$

is nonnegative, we obtain

$$\Big|K^{\mathrm{sub}}_{F_{(3+3)}}\big(t,(m,0)*(x,z),(x,z)\big)\Big|\le\frac{1}{(2\pi t)^{9/2}}\,e^{-\frac{1}{2t}|m|^2}\int_{\mathbb{R}^3}\frac{|\tau|}{\sinh|\tau|}\,d\tau.$$

Therefore, this case is also negligible because

$$\begin{aligned}&\Big|\sum_{m\in\mathbb{Z}^3\backslash\{0\}}K^{\mathrm{sub}}_{F_3}\big(t,(m,0)*(x,z),(x,z)\big)\Big|\\&\qquad\le\frac{1}{(2\pi t)^{9/2}}\sum_{m\in\mathbb{Z}^3\backslash\{0\}}e^{-\frac{1}{2t}|m|^2}\int_{\mathbb{R}^3}\frac{|\tau|}{\sinh|\tau|}\,d\tau=O(t^\infty),\end{aligned}$$

where we have used Corollary 14.3.

(IV) Let $\gamma=(m,k)$ with $m\in\mathbb{Z}^3\backslash\{0\}$ and $k\in\mathbb{Z}^3\backslash\{0\}$. Then we can use the identity

$$\frac{t^2}{k_j^2}\left(\sqrt{-1}\,\frac{\partial}{\partial\tau_j}\right)^2e^{-\frac{\sqrt{-1}}{t}\langle k,\tau\rangle}=e^{-\frac{\sqrt{-1}}{t}\langle k,\tau\rangle}$$

for $k_j\neq 0$, and we can write

$$\begin{aligned}&K^{\mathrm{sub}}_{F_{(3+3)}}\big(t,\gamma*(x,z),(x,z)\big)\\&\quad=\frac{1}{(2\pi t)^{9/2}}\int_{\mathbb{R}^3}\frac{t^6}{\prod_{k_j\neq0}k_j^2}\,\exp\Big\{-\sqrt{-1}\,\frac{\langle k,\tau\rangle}{t}-\frac{|m|^2}{2t}\Big\}\prod_{\substack{j=1\\k_j\neq0}}^{3}\left(\sqrt{-1}\,\frac{\partial}{\partial\tau_j}\right)^2\\&\qquad\times\left[\exp\Big\{-\frac{\sqrt{-1}}{t}\,\langle 2q,\tau\rangle-\frac{1}{2t}\,\big\langle h(\sqrt{-1}\,\Omega)\cdot m,\,m\big\rangle\Big\}\frac{|\tau|}{\sinh|\tau|}\right]d\tau.\end{aligned}$$

Noting that $|q_j(m,x)|\le|m|$, we have

$$\begin{aligned}&\Big|K^{\mathrm{sub}}_{F_{(3+3)}}\big(t,\gamma*(x,z),(x,z)\big)\Big|=\frac{1}{(2\pi t)^{9/2}}\,\frac{t^6}{\prod_{k_j\neq0}k_j^2}\,\exp\Big\{-\frac{|m|^2}{2t}\Big\}\\&\qquad\times\int_{\mathbb{R}^3}\left\{1+\left(\frac{|m||\tau|}{t}\right)^6+\left(\frac{|m|^2}{t}\right)^3\right\}\max_{|\alpha|\le6}\left\{\frac{\partial^\alpha}{\partial\tau_\alpha}\left(\frac{|\tau|}{\sinh|\tau|}\right)\right\}d\tau\\&\qquad\qquad\le\frac{C(c_6+1)}{\prod_{k_j\neq0}k_j^2}\,\exp\left(-\frac{|m|^2}{4t}\right),\end{aligned}$$

where we have used

$$\left(\frac{|m|^2}{t}\right)^\ell\exp\left(-\frac{|m|^2}{2t}\right)\le c_\ell\exp\left(-\frac{|m|^2}{4t}\right)$$

with $c_\ell = \sup_{x>0}\{x^\ell e^{-\frac{x}{4}}\}$. Then

$$\Big| \sum_{m,k\in\mathbb{Z}^3\setminus\{0\}} K^{\text{sub}}_{F_{(3+3)}}\big(t, \gamma * (x,z), (x,z)\big)\Big| \leq C(c_6+1) \sum_{m\in\mathbb{Z}^3\setminus\{0\}} \exp\left(-\frac{|m|^2}{4t}\right) = O(t^\infty).$$

By Theorem 14.4 we obtain the second equality in Theorem 14.5. □

Corollary 14.6. *The heat kernel trace of* $\Delta^{\text{sub}}_{L\setminus F_{(3+3)}}$ *has the following short time asymptotic expansion*

$$K_{L\setminus F_{(3+3)}}(t) = \frac{\sqrt{\pi}}{32\sqrt{2}}\, t^{-9/2} + O(t^\infty).$$

Let $\Lambda_6 = \sigma(\Delta^{\text{sub}}_{L\setminus F_{(3+3)}})$ denote the spectrum of the sub-Laplacian $\Delta^{\text{sub}}_{L\setminus F_{(3+3)}}$. Then, the corresponding spectral zeta function is defined by

$$\zeta^{\text{sub}}_{L\setminus F_{(3+3)}}(s) = \sum_{0\neq\lambda\in\Lambda_6} \frac{1}{\lambda^s}. \tag{14.1}$$

Via Mellin transform we have the relation

$$\zeta^{\text{sub}}_{L\setminus F_{(3+3)}}(s) = \frac{1}{\Gamma(s)} \int_0^\infty \Big(K_{L\setminus F_{(3+3)}}(t) - 1\Big) t^{s-1}\, dt.$$

Now, the asymptotic expansion in Corollary 14.6 implies:

Theorem 14.7. *The function* (14.1) *is meromorphic on the complex plane with one simple pole in* $s = \frac{9}{2}$ *and residue*

$$Res_{s=9/2}\zeta^{\text{sub}}_{L\setminus F_{(3+3)}}(s) = \frac{\sqrt{\pi}}{32\sqrt{2}\,\Gamma(\frac{9}{2})} = \frac{1}{210\sqrt{2}}.$$

In particular, it follows that the spectral zeta-function is complex analytic in a neighbourhood of zero.

14.2. The five-dimensional case

We fix a lattice $L = \big\{(m_1, m_2, m_3, k_1, k_2) \,\big|\, m_i,\ k_i\ \in \mathbb{Z}\big\}$ in G_5. Then we have the following theorem for the asymptotic behaviour as t goes to 0 for

$$\sum_{\gamma\in L} K^{\text{sub}}_{G_5}\big(t, \gamma * (\tilde{x}, \tilde{z}), (x,z)\big)$$

and for the trace of the heat kernel on $L\setminus G_5$

$$K_{L\setminus G_5}(t) = \sum_{\gamma\in L} \int_{\mathcal{F}_L} K^{\text{sub}}_{G_5}\big(t, \gamma * (x,z), (x,z)\big)\, dxdz,$$

where $\mathcal{F}_L = \{(x_1, x_2, x_3.z_1, z_2) : 0 \leq x_j < 1, 0 \leq z_j < 1\}$ is a fundamental domain of the lattice L.

Theorem 14.8. *For any* $(x,z) \in \mathcal{F}_L$*, it holds that*

$$\sum_{\gamma \in L} K^{\mathrm{sub}}_{G_5}\big(t, \gamma * (x,z), (x,z)\big) = \frac{1}{(2\pi)^{7/2}} \left(\int_{\mathbb{R}^2} \frac{|\tau|}{\sinh |\tau|} d\tau \right) t^{-7/2} + O(t^\infty)$$
$$= \frac{7}{8\sqrt{2}} \frac{\zeta(3)}{\pi^{5/2}} t^{-7/2} + O(t^\infty).$$

Proof. In this case, $K^{\mathrm{sub}}_{G_5}\big(t, \gamma * (x,z), (x,z)\big)$ is of the form

$$K^{\mathrm{sub}}_{G_5}\big(t, \gamma * (x,z), (x,z)\big) = \frac{1}{(2\pi t)^{7/2}} \int_{\mathbb{R}^2} \exp\Big\{ -\sqrt{-1}\, \frac{\sum_{j=1}^2 (k_j + 2q_j(m,x))\tau_j}{t} \Big\}$$
$$\times \exp\Big\{ -\frac{1}{2t} \left\langle \Omega_0(\sqrt{-1}\,\tau) \coth \Omega_0(\sqrt{-1}\,\tau) \cdot m,\, m \right\rangle \Big\} \frac{|\tau|}{\sinh |\tau|}\, d\tau,$$

where the matrix $\Omega_0(\tau)$ is the following 3×3 anti-symmetric matrix:

$$\Omega(\tau) = \begin{pmatrix} 0 & \tau_1 & \tau_2 \\ -\tau_1 & 0 & 0 \\ -\tau_2 & 0 & 0 \end{pmatrix}$$

with $\tau = (\tau_1, \tau_2) \in \mathbb{R}^2$. Using arguments similar to those in the proof of the six-dimensional case, we get the assertion. □

Corollary 14.9. *The heat kernel trace of* $\Delta^{\mathrm{sub}}_{G_5}$ *has the following short time asymptotic expansion:*

$$K_{L \backslash G_5}(t) = \frac{7}{8\sqrt{2}} \frac{\zeta(3)}{\pi^{5/2}} t^{-7/2} + O(t^\infty).$$

Let $\Lambda_5 = \sigma(\Delta^{\mathrm{sub}}_{G_5})$ denote the spectrum of the sub-Laplace operator $\Delta^{\mathrm{sub}}_{G_5}$. As before we define the corresponding spectral zeta function by

$$\zeta^{\mathrm{sub}}_{L \backslash G_5}(s) = \sum_{0 \neq \lambda \in \Lambda_5} \frac{1}{\lambda^s}. \tag{14.2}$$

Theorem 14.10. *The function* (14.2) *is meromorphic on the complex plane with one simple pole at* $s = 7/2$ *and residue*

$$\mathrm{Res}_{s=7/2}\, \zeta^{\mathrm{sub}}_{L \backslash G_5}(s) = \frac{7\zeta(3)}{8\sqrt{2}\pi^{5/2}\,\Gamma(\frac{7}{2})} = \frac{7\zeta(3)}{15\sqrt{2}\pi^3}.$$

In particular, it follows that the spectral zeta function (14.2) *is complex analytic in a neighbourhood of zero.*

15. Concluding remarks

We end up with several remarks together with some of the future problems.

Remark 15.1. In both of the above cases and also for Heisenberg manifolds of any dimension, it turns out that the spectral zeta function has only one simple pole (see [BF4-10]). In the Riemannian case and even for three-dimensional Heisenberg manifolds, the spectral zeta function has infinitely many simple poles (see [FG-03]). It seems that the behaviour of the spectral zeta function of the sub-Laplacian on compact nilmanifolds is closer related to the flat torus case, since the compact nilmanifold is the total space of the fiber bundle. Both the base and the fiber spaces are flat tori. In the sense of the *Hörmander condition* the sub-Laplacian is dominated by the Laplacian on the base space (= torus). Note that the spectral zeta function of the flat torus is an *Epstein zeta function* which has only one simple pole at $s =$*half of the dimension of the torus*. So we may expect that for any compact 2-step nilmanifold the spectral zeta function of a sub-Laplacian can be extended to a meromorphic function and *that it has only one simple pole*.

Remark 15.2. According to the general construction of the heat kernel on 2-step nilpotent Lie groups given in [BGG1-96], we have an integral expression for the heat kernel. In the integrand hyperbolic functions of a skew-symmetric matrix $\Omega(\tau)$ defined by the structure constants of the group appear. The explicit expression of this matrix in terms of the components is used to determine the spectrum of the sub-Laplacian (and of the Laplacian) on their compact nilmanifolds. It seems to be difficult to accomplish the calculation purely from the matrix form of (11.3), since there are 2-step nilpotent Lie groups without any lattices, cf. [Rag-72], [Eb-03].

Remark 15.3. In the last two sections we only treated a typical lattice of the nilpotent Lie groups. Of course, it is possible to deal with general lattices. However, within the authors' knowledge we do not have a complete classification of lattices even for the general 2-step nilpotent Lie groups apart from the Heisenberg group cases. Though, if it is possible to parametrize a subclass of lattices, say in the free nilpotent Lie group in an obvious way, then we can develop the inverse spectral problem among such lattices similar to the results obtained in [GW-86].

Remark 15.4. By different methods, it is possible to calculate an integral form of the spectral zeta-functions given in the last section. This leads to an expression of its derivative at $s = 0$ and therefore gives the zeta-regularized determinant of the corresponding operators. The details will be given in a forthcoming paper [BFI] (see also [BF3-08]).

Appendix A. Basic theorems for pseudo-differential operators of Weyl symbols and heat kernel construction

Let $S^m_{\rho,\delta} \subset C^\infty(\mathbb{R}^n \times \mathbb{R}^n)$ be the symbol class as usual $(0 \le \delta \le \rho \le 1,\ \delta < 1)$,

$p(x,\xi) \in S^m_{\rho,\delta} \Longleftrightarrow \forall\alpha,\ \forall\beta$ (= multi-indices) $\exists$ constant $C = C_{\alpha,\beta} > 0$ such that

$$\left|\frac{\partial^{|\alpha|+|\beta|}p(x,\xi)}{\partial x^\alpha \partial \xi^\beta}\right| = \left|p^{(\beta)}_{(\alpha)}(x,\xi)\right| \le C_{\alpha,\beta}\,(1+|\xi|)^{m-\rho|\alpha|+\delta|\beta|},$$

where $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{Z}^n$, $\alpha_i \ge 0$, $|\alpha| = \sum \alpha_i$, $|\xi| = \sqrt{\sum {\xi_i}^2}$, and so on. For each integer $\ell \ge 0$ we denote by $|p|^{(m)}_\ell$ $(p \in S^m_{\rho,\,\delta})$ the semi-norm on the space $S^m_{\rho,\,\delta}$,

$$|p|^{(m)}_\ell = \sup_{|\alpha|+|\beta|\le\ell}\ \sup_{(x,\xi)\in\mathbb{R}^n\times\mathbb{R}^n} \left\{\left|p^{(\beta)}_{(\alpha)}(x,\xi)\right|(1+|\xi|)^{-m+\rho|\alpha|-\delta|\beta|}\right\}.$$

Equipped with these semi-norms $\{|\cdot|^{(m)}_\ell\}_{\ell\ge0}$, the space $S^m_{\rho,\,\delta}$ becomes a Fréchet space. We also use the notation $\langle\xi\rangle = \left(1+|\xi|^2\right)^{1/2}$ and $x\cdot\xi = \sum x_i\xi_i = \langle x,\xi\rangle$.

Definition A.1. A pseudo-differential operator P on $\mathbb{R}^n$ of Weyl symbol $p(x,\xi) \in S^m_{\rho,\delta}$ is defined in terms of the oscillatory integral $(Os-\int)$ by the following formula (see L. Hörmander [Hö2-79] and C. Iwasaki and N. Iwasaki [II1-79], [II2-81]):

$$\begin{aligned}Pu(x) &= p^w(x,D)u(x)\\ &= Os-(2\pi)^{-n}\int_{\mathbb{R}^n\times\mathbb{R}^n} e^{-\sqrt{-1}y\cdot\xi}p\left(x+\frac{y}{2},\xi\right)u(x+y)\,dyd\xi\\ &= Os-(2\pi)^{-n}\int_{\mathbb{R}^n\times\mathbb{R}^n} e^{\sqrt{-1}(x-y)\cdot\xi}p\left(\frac{x+y}{2},\xi\right)u(y)\,dyd\xi.\end{aligned}$$

For the rest of this chapter we use pseudo-differential operators of Weyl symbols.

The product of pseudo-differential operators of Weyl symbol $P = p^w(x,D)$ and $Q = q^w(x,D)$ is also a pseudo-differential operator of Weyl symbol $\sigma^w(p^w(x,D)q^w(x,D)) = p \circ_w q$, i.e.,

$$p^w(x,D)q^w(x,D) = (p\circ_w q)^w(x,D).$$

In fact, the Weyl symbol $p\circ_w q$ is given by the integral (A.1), which is proved in Theorem A.2:

$$\begin{aligned}(p\circ_w q)(x,\xi) &= Os-(2\pi)^{-2n}\int_{\mathbb{R}^n\times\mathbb{R}^n}\int_{\mathbb{R}^n\times\mathbb{R}^n} e^{-\sqrt{-1}(\mathbf{y}_1\cdot\mathbf{w}_1+\mathbf{y}_2\cdot\mathbf{w}_2)}\\ &\quad\times p\left(x-\frac{\mathbf{y}_2}{2},\xi+\mathbf{w}_1\right)q\left(x+\frac{\mathbf{y}_1}{2},\xi+\mathbf{w}_2\right)d\mathbf{y}_1d\mathbf{w}_1d\mathbf{y}_2d\mathbf{w}_2,\end{aligned}\tag{A.1}$$

where $\mathbf{y}_i = (y_{1,i},\dots,y_{n,i})$ and $\mathbf{w}_i = (w_{1,i},\dots,w_{n,i})$ $(i=1,2)$.

Theorem A.2. *Let $p \in S^{m_1}_{\rho,\delta}$ and $q \in S^{m_2}_{\rho,\delta}$. Then for any integer N we have an expansion*

$$p\circ_w q = \sum_{j=0}^{N-1}\left(\frac{1}{2\sqrt{-1}}\right)^j \sigma_j(p,q) + r^w_N(p,q),$$

where

$$\sigma_j(p,q) = \sum_{|\alpha|+|\beta|=j} \frac{(-1)^{|\beta|}}{\alpha!\beta!} p^{(\alpha)}_{(\beta)}(x,\xi) q^{(\beta)}_{(\alpha)}(x,\xi) \in S^{m-(\rho-\delta)j}_{\rho,\delta},$$

$$r^w_N(p,q) \in S^{m-(\rho-\delta)N}_{\rho,\delta}.$$

There exist constants ℓ_0 and C such that the following estimate holds for any ℓ:

$$|r^w_N|^{(m-(\rho-\delta)N)}_\ell \le C \sum_{|\alpha|+|\beta|=N} |p^{(\alpha)}_{(\beta)}|^{(m_1-\rho|\alpha|+\delta|\beta|)}_{\ell+\ell_0} |q^{(\beta)}_{(\alpha)}|^{(m_2+\delta|\alpha|-\rho|\beta|)}_{\ell+\ell_0}.$$

Remark A.3. Pseudo-differential operators of Weyl symbol are pseudo-differential operators in the usual sense. In fact, we have

$$p^w(x,D) = q(x,D)$$

if

$$q(x,\xi) = Os - (2\pi)^{-n} \int_{\mathbb{R}^n\times\mathbb{R}^n} e^{-\sqrt{-1}y\cdot\eta} p\left(x+\frac{y}{2}, \xi+\eta\right) dyd\eta$$

and

$$p(x,\xi) = Os - (2\pi)^{-n} \int_{\mathbb{R}^n\times\mathbb{R}^n} e^{\sqrt{-1}y\cdot\eta} q\left(x+\frac{y}{2}, \xi+\eta\right) dyd\eta.$$

This shows that the conditions $p(x,\xi) \in S^m_{\rho,\delta}$ and $q(x,\xi) \in S^m_{\rho,\delta}$ are equivalent.

Remark A.4. It is clear that

$$\sigma_j(p,q) = (-1)^j \sigma_j(q,p) \text{ for any } j,$$

so we have

$$\sigma_j(p,p) = 0 \text{ if } j \text{ is an odd integer.}$$

Remark A.5.

$$\sigma_1(p,q) = \langle J\nabla p, \nabla q\rangle,$$

$$\sigma_2(p,q) = -\frac{1}{2}\operatorname{tr}(JH_pJH_q),$$

where J is the $2n\times 2n$ matrix defined by

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

and $\nabla p = {}^t\left(\frac{\partial p}{\partial x_1}, \ldots, \frac{\partial p}{\partial x_n}, \frac{\partial p}{\partial \xi_1}, \ldots, \frac{\partial p}{\partial \xi_n}\right)$. The matrix H_p is called Hesse matrix and is given by

$$H_p = \begin{pmatrix} \frac{\partial^2 p}{\partial x_i \partial x_j} & \frac{\partial^2 p}{\partial x_i \partial \xi_j} \\ \\ \frac{\partial^2 p}{\partial \xi_i \partial x_j} & \frac{\partial^2 p}{\partial \xi_i \partial \xi_j} \end{pmatrix}.$$

The following holds for the multi-product of pseudo-differential operators of Weyl symbols.

Theorem A.6. *If p_j belongs to $S^{m(j)}_{\rho,\delta}$ $(j = 1,\dots,\nu)$, then the operator product $p^w_1(x,D)\dots\ p^w_\nu(x,D)$ is a pseudo-differential operator of Weyl symbol*

$$p(x,\xi) = \sigma^w(p^w_1(x,D)\dots p^w_\nu(x,D)) \in S^m_{\rho,\delta} \quad (m = \Sigma^\nu_{j=1} m(j))$$

again and p satisfies the following estimate: There exist constants C and ℓ_0 independent of ν such that for any ℓ:

$$|p|^{(m)}_\ell \le C^\nu \prod_{j=1}^{\nu} |p_j|^{(m(j))}_{\ell+\ell_0}.$$

In fact, $p(x,\xi)$ is given by

$$p(x,\xi) = Os - (2\pi)^{-n\nu} \overbrace{\int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\dots\int_{\mathbb{R}^n}}^{2\nu} \exp\left(-\sqrt{-1}\sum_{j=1}^{\nu} y_j\cdot w_j\right)$$
$$\times \prod_{j=1}^{\nu} p_j\left(x + \frac{1}{2}\sum_{k=1}^{j-1} y_k - \frac{1}{2}\sum_{k=j+1}^{\nu} y_k, \xi + w_j\right) dV,$$

where $dV = dy_1 dw_1 dy_2 dw_2 \dots dy_\nu dw_\nu$.

Let $p^w(x,D)$ be a pseudo-differential operator with $p(x,\xi) \in S^m_{\rho,\,\delta}$. We consider the heat operator

$$\frac{\partial}{\partial t} + p^w(x,D)$$

and construct the fundamental solution $E(t)$ as a pseudo-differential operator of a Weyl symbol $e(t;x,\xi)$,

$$\frac{d}{dt} e^w(t;x,D) + p^w(x,D)e^w(t;x,D) = 0 \quad \text{in } (0,T)\times\mathbb{R}^n,$$
$$e^w(0;x,D) = I,$$

where $p^w(x,D)$ is a pseudo-differential operator of Weyl symbol $p(x,\xi)$. We assume that the symbol $p(x,\xi)$ is in a classical symbol class, i.e., $p(x,\xi) \in S^m_{1,\,0}$ $(m \in \mathbb{N})$ and has an asymptotic expansion into homogeneous functions of the variables ξ.

In this section we consider a degenerate operator which has a sub-elliptic estimate and was characterized by A. Melin [Me-71]. We sketch the construction of the fundamental solution to the heat equation following the paper [II2-81].

Theorem A.7. *Let $p(x,\xi) \in S^m_{1,0}$ satisfies the following condition* (A):

$$\textbf{(A)} \begin{cases} \text{(a)} \;\; p_m(x,\xi) \ge 0, \\ \text{(b)} \;\; \mathrm{Re}(p_{m-1}) + \frac{1}{2}\,\mathrm{tr}^+(A) \ge c\,|\xi|^{m-1} \text{ for some positive constant } c \text{ on } \Sigma, \end{cases}$$

where $\Sigma = \{(x,\xi) \mid p_m(x,\xi) = 0\}$ is the characteristic set of $p_m(x,\xi)$, $A(x,\xi) = A = \sqrt{-1}JH_{p_m}$ and $\mathrm{tr}^+(A)$ is the sum of positive eigenvalues of A. Here H_{p_m} is the Hesse matrix of the principal symbol $p_m(x,\xi)$.

Then we can construct the symbol $e(t;x,\xi)$ *belonging to the symbol class* $S^0_{1/2,1/2}$ *and* $S^{-\infty}$ *for* $t>0$ *in the following form: For any integer* N *we have the expansion*

$$e(t;x,\xi)-\sum_{j=0}^{N-1}e_j(t;x,\xi)\in S^{-N/2}_{1/2,1/2},$$

$$e_0(t;x,\xi)=\exp\{\varphi(t;x,\xi)\}\quad\text{and}\quad e_j(t;x,\xi)\in S^{-j/2}_{1/2,1/2}$$

with the function

$$\begin{aligned}\varphi(t;x,\xi)&=-p_m(x,\xi)t-p_{m-1}(x,\xi)t\\&\quad-\frac{1}{2}\operatorname{tr}\left\{\log\left(\cosh\left(\frac{tA}{2}\right)\right)\right\}+\frac{\sqrt{-1}t^2}{4}\left\langle G\left(\frac{tA}{2}\right)J\nabla p_m,\ \nabla p_m\right\rangle\end{aligned}$$

and

$$G(x)=\frac{1-\frac{\tanh x}{x}}{x}.$$

Sketch of proof. Assume that the fundamental solution is a pseudo-differential operator of Weyl symbol $e(t;x,\xi)=e^{\varphi(t;x,\xi)}$. Then we have by Theorem 1.2

$$\frac{\partial}{\partial t}e(t)+\sum_{j=0}^{\infty}\left(\frac{1}{2\sqrt{-1}}\right)^j\sigma_j(p,e(t))=0,\quad e(0)=1.$$

Neglecting terms $\sigma_j(p,e(t))$ for $j\geq 3$, we get the following equation for φ with $\varphi(0)=0$

$$\frac{\partial}{\partial t}\varphi+p+\frac{1}{2\sqrt{-1}}\langle J\nabla p,\nabla\varphi\rangle+\frac{1}{8}\operatorname{tr}\big(JH_pJH_\varphi\big)-\frac{1}{8}\langle J\nabla\varphi,H_pJ\nabla\varphi\rangle=0.$$

It is hard to find the solution of the above equation. But neglecting the derivatives of p and φ of order greater than three, we can find a suitable solution as follows: The above equation means that $X=\sqrt{-1}JH_\varphi$ satisfies

$$\frac{\partial}{\partial t}X+A+\frac{1}{2}(AX-XA)-\frac{1}{4}XAX=0,\quad X|_{t=0}=0$$

with $A=\sqrt{-1}\,JH_p$. The unique solution of this equation is

$$X=-2\tanh(At/2).$$

Setting

$$y=J\nabla\varphi,\quad b=J\nabla p,$$

we have

$$\frac{\partial}{\partial t}y+b+\frac{1}{2}(Ay-Xb)-\frac{1}{4}XAy=0,\quad y|_{t=0}=0.$$

The unique solution of the above equation is given by

$$y=A^{-1}Xb.$$

We finally obtain

$$\varphi = -pt - \frac{1}{2}\,\mathrm{tr}\,[\log\{\cosh(At/2)\}] + \frac{\sqrt{-1}t^2}{4}\,\big\langle G(At/2)J\nabla p, \nabla p\big\rangle.$$

It is easy to show that

$$\left|\frac{1}{\sqrt{\det\{\cosh(At/2)\}}}\right| \le Ce^{-\mathrm{tr}^+ At/2}$$

and by the assumption on the characteristic set

$$\begin{aligned} \varphi(x,\xi) &\le -C\,\langle\xi\rangle^m\, t && \text{if } p_m(x,\xi) \ge c|\xi|^m, \\ \varphi(x,\xi) &\le -c\,\langle\xi\rangle^{m-1}\, t && \text{in } \Sigma. \end{aligned}$$

We need a precise argument to obtain an estimate for φ near the set Σ. According to [II2-81] we have

$$e^{\varphi} \in S^0_{1/2,1/2}.$$

We give some remarks on the construction of $e(t;x,\xi)$. If we have constructed $e_j(t;x,\xi)$ for $j = 1, 2, \ldots, N-1$ such that

$$\left(\frac{\partial}{\partial t} + p^w(x,D)\right)\left(\sum_{j=0}^{N-1} e_j^w(t;x,D)\right) = r_N^w(t;x,D),$$

with $r_N(t;x,\xi) \in S^{m-N/2}_{1/2,1/2}$, then we can construct the symbol of the fundamental solution of the form

$$e(t) = \sum_{j=0}^{N-1} e_j(t) + \int_0^t \sum_{j=0}^{N-1} e_j(t-s) \circ_w \psi(s)ds$$

with $\psi(t) \in S^{m-N/2}_{1/2,1/2}$ if $m - N/2 \le 0$. In fact, we can construct $\psi(t)$ as the unique solution of the following equation using the previous theorem:

$$r_N(t) + \psi(t) + \int_0^t r_N(t-s) \circ_w \psi(s)ds = 0.$$

In the case when $p(x,\xi)$ is a polynomial in (x,ξ) of degree at most 2 the fundamental solution $E(t)$ is obtained as a pseudo-differential operator of Weyl symbol $e(t;x,\xi) = \exp\{\varphi(t,x,\xi)\}$, where

$$\varphi(t;x,\xi) = -pt - \frac{1}{2}\,\mathrm{tr}\left\{\log\left(\cosh\left(\frac{At}{2}\right)\right)\right\} + \frac{\sqrt{-1}t^2}{4}\,\big\langle G(At/2)J\nabla p, \nabla p\big\rangle,$$

because $\varphi(t;x,\xi)$ is the exact solution of the equation

$$\frac{d\varphi}{dt} + p + \frac{1}{2\sqrt{-1}}\,\sigma_1(p,\varphi) - \frac{1}{4}\,\sigma_2(p,\varphi) - \frac{1}{8}\,\big\langle J\nabla\varphi, H_p J\nabla\varphi\big\rangle = 0.$$

More precisely, we have the following Theorem A.8. It is a key theorem if we study the construction of the fundamental solution for the heat equation of polynomial coefficients.

Theorem A.8. *Let $p(x,\xi)$ be a quadratic polynomial with respect to the variable $X=(x,\xi)^t \in \mathbb{R}^d \times \mathbb{R}^d$,*

$$p(x,\xi)=\frac{1}{2}\langle X, HX\rangle.$$

Then $E(t)=e^w(t;x,D)$ is given as a pseudo-differential operator with symbol

$$e(t;x,\xi)=\frac{1}{\sqrt{\det\cosh(At/2)}}\exp\Big[-\sqrt{-1}\,\langle J\tanh(At/2)X, X\,\rangle\Big],$$

and with the $2d\times 2d$-matrix $A=\sqrt{-1}\,JH$.

Appendix B. Heat kernel of the sub-Laplacian on 2-step nilpotent groups

We apply the previous construction of the fundamental solution to a degenerate operator, i.e., to the case of the sub-Laplacian on a 2-step free nilpotent Lie group.

So, let $F_{(N+N(N-1)/2)} \cong \mathbb{R}^N \oplus \mathbb{R}^{N(N-1)/2}$ be a connected and simply connected free 2-step nilpotent Lie group with the Lie algebra $\mathfrak{f}_{(N+N(N-1)/2)}$ (which is also identified with $\mathbb{R}^N \oplus \mathbb{R}^{N(N-1)/2}$). We fix a basis $\big\{X_i,\, Z_{i,j} \;\big|\; 1\le i,\, j\le N,\, i<j\big\}$ of the Lie algebra $\mathfrak{f}_{(N+N(N-1)/2)}$. Their bracket relation are assumed to be

$$[X_i, X_j]=2Z_{ij}$$

for $1\le i<j\le N$ and the group multiplication

$$*\colon F_{(N+N(N-1)/2)}\times F_{(N+N(N-1)/2)}\to F_{(N+N(N-1)/2)}$$

is given as follows: let

$$\Big(\sum x_iX_i\oplus\sum z_{ij}Z_{ij}, \sum \tilde{x}_iX_i\oplus\sum\tilde{z}_{ij}Z_{ij}\Big)\in \mathbb{R}^N\oplus\mathbb{R}^{\frac{N(N-1)}{2}}\times\mathbb{R}^N\oplus\mathbb{R}^{\frac{N(N-1)}{2}},$$

then we have

$$\begin{aligned}\Big(\sum x_iX_i\oplus\sum z_{ij}Z_{ij}\Big) * \Big(\sum \tilde{x}_i)X_i\oplus\sum\tilde{z}_{ij}Z_{ij}\Big)\\ =\sum\big(x_i+\tilde{x}_i\big)X_i\oplus\sum\big(z_{ij}+\tilde{z}_{ij}+x_i\tilde{x}_j-x_j\tilde{x}_i\big)Z_{ij}.\end{aligned}$$

Let $\tilde{X}_i$ be the left-invariant vector field on $F_{(N+(N-1)/2)}$ corresponding to X_i,

$$\begin{aligned}\tilde{X}_i(f)g&=\frac{d}{dt}f(g*e^{tX_i})|_{t=0}\\ &=\frac{\partial f}{\partial x_i}+\sum_{j<i}x_j\frac{\partial f}{\partial z_{ji}}-\sum_{j>i}x_j\frac{\partial f}{\partial z_{ij}},\end{aligned}$$

where $g=(x,z)\in\mathbb{R}^N\oplus\mathbb{R}^{N(N-1)/2}\cong F_{(N+N(N-1)/2)}$. Let

$$\begin{aligned}(x,z;\xi,\zeta)&=(x_i,z_{ij};\xi_i,\zeta_{ij})\\ &\in T^*(F_{(N+N(N-1)/2)})\cong\mathbb{R}^N\oplus\mathbb{R}^{N(N-1)/2}\times\mathbb{R}^N\oplus\mathbb{R}^{N(N-1)/2}\end{aligned}$$

be the dual coordinates on the cotangent bundle. Then we understand the symbol of vector fields $\tilde{X}_i$ and their Weyl symbols as

$$\sigma^w(\tilde{X}_i) = \sigma(\tilde{X}_i) = \sqrt{-1}\left(\xi_i + \sum_{j<i} x_j \zeta_{ji} - \sum_{j>i} x_j \zeta_{ij}\right)$$
$$= \sqrt{-1}\left(\xi - \Omega(\zeta)x\right)_i,$$

where $\Omega = \Omega(\zeta)$ is a $N \times N$ skew symmetric matrix defined by

$$\Big(\Omega(\zeta)\Big)_{ij} = \zeta_{ij} \quad (1 \leq i < j \leq N).$$

Let P be the sub-Laplacian

$$P = -\frac{1}{2}\sum_{i=1}^{N} \tilde{X}_i^2.$$

Its Weyl symbol is given by

$$\sigma^w(P) = -\frac{1}{2}\sum_{i=1}^{N} \sigma^w(\tilde{X}_i)^2 = \frac{1}{2}\langle X, HX\rangle, \quad X = {}^t(x,\xi)$$

with a $2N \times 2N$-matrix H defined by

$$H = \begin{pmatrix} -(\Omega(\zeta))^2 & \Omega(\zeta) \\ -\Omega(\zeta) & I \end{pmatrix}.$$

We consider the pseudo-differential operator $p^w(x,z,D_x,D_z)$ with the Weyl symbol $\sigma^w(P)$ and construct the following fundamental solution $E(t)$ as a pseudo-differential operator of Weyl symbol $e(t;x,z,\xi,\zeta)$,

$$\frac{d}{dt} e^w(t;x,z,D_x,D_z) + p^w(x,z,D_x,D_z)e^w(t;x,z,D_x,D_z) = 0 \text{ in } (0,T)\times\mathbb{R}^n,$$
$$e^w(0;x,z,D_x,D_z) = I.$$

Theorem B.1. *The symbol $e(t;x,z,\xi,\zeta)$ of the fundamental solution is given by*

$$e(t;x,z,\xi,\zeta) = \frac{1}{\sqrt{\det\cosh\big(\sqrt{-1}\,t\Omega(\zeta)\big)}}\exp\left[-\frac{t}{2}\left\langle \frac{\tanh\sqrt{-1}\,t\Omega_0}{\sqrt{-1}\,t\Omega_0}\,H\,X,\,X\right\rangle\right],$$

where

$$\Omega_0 = \begin{pmatrix} \Omega(\zeta) & 0 \\ 0 & \Omega(\zeta) \end{pmatrix}.$$

Then

$$E(t)u(x,z) = e^w(t;x,z,D_x,D_z)u(x,z)$$
$$= (2\pi)^{-N-N(N-1)/2}\int_{\mathbb{R}^N\times\mathbb{R}^N}\int_{\mathbb{R}^{N(N-1)/2}\times\mathbb{R}^{N(N-1)/2}} e^{i\langle x-\tilde{x},\xi\rangle + i\langle z-\tilde{z},\zeta\rangle}$$
$$\times\; e(t;(x+\tilde{x})/2,\ (z+\tilde{z})/2,\ \xi,\ \zeta)\,u(\tilde{x},\ \tilde{z})\,d\zeta d\tilde{z} d\xi d\tilde{x}.$$

Corollary B.2. *The kernel function $K(t;x,z,\tilde{x},\tilde{z})$ of the above fundamental solution is given by*

$$K(t;x,z,\tilde{x},\tilde{z}) = (2\pi t)^{-N/2-N(N-1)/2} \int_{\mathbb{R}^{N(N-1)/2}} e^{\sqrt{-1}\,\langle x,\Omega(\zeta)\tilde{x}\rangle/t+\sqrt{-1}\,\langle z-\tilde{z},\zeta\rangle/t}$$

$$\times \exp\left\{-\frac{1}{2t}\left\langle x-\tilde{x}, \frac{\sqrt{-1}\Omega(\zeta)}{\tanh(\sqrt{-1}\Omega(\zeta))}(x-\tilde{x})\right\rangle\right\} \sqrt{\det\left\{\frac{\sqrt{-1}\,\Omega(\zeta)}{\sinh(\sqrt{-1}\,\Omega(\zeta))}\right\}}\, d\zeta,$$

where $< z,\zeta > = \sum_{1\le i<j\le N} z_{ij}\zeta_{ij}$.

From the above expression of the kernel function $K(t;x,z,\tilde{x},\tilde{z})$, we conclude that it values on the diagonal are given by:

Corollary B.3.

$$K(t;x,z,x,z) = (2\pi t)^{-N/2-N(N-1)/2} \int_{\mathbb{R}^{N(N-1)/2}} \sqrt{\det\left\{\frac{\sqrt{-1}\,\Omega(\zeta)}{\sinh(\sqrt{-1}\,\Omega(\zeta))}\right\}}\, d\zeta.$$

Proof of Theorem B.1. Let $A = \sqrt{-1}\,JH$ be a $2N \times 2N$-matrix. Then the nth power of the matrix A is given by

$$A^n = A(-2\sqrt{-1}\,\Omega_0)^{n-1} = (-2\sqrt{-1}\,\Omega_0)^{n-1}A. \tag{B.1}$$

Since

$$A = \sqrt{-1}\begin{pmatrix} -\Omega(\zeta) & I \\ \Omega(\zeta)^2 & -\Omega(\zeta)\end{pmatrix},$$

the formula (B.1) is proved by the induction with respect to n if we note that

$$A^2 = -2\begin{pmatrix} \Omega(\zeta)^2 & -\Omega(\zeta) \\ -\Omega(\zeta)^3 & \Omega(\zeta)^2\end{pmatrix} = -2\sqrt{-1}\,\Omega_0 A.$$

Lemma B.4. *Let $h_0(x)$ be an entire function. Then for the entire function $h(x) = xh_0(x)$ we have*

$$h\left(\frac{tA}{2}\right) = \frac{t}{2}\,A\,h_0(-\sqrt{-1}\,t\Omega_0). \tag{B.2}$$

Moreover, it holds

$$\det\left(\cosh\left(\frac{t\,A}{2}\right)\right) = \det\left(\cosh(\sqrt{-1}\,t\Omega)\right). \tag{B.3}$$

Proof. The formula (B.2) is clear by the previous formula (B.1). Also the formula

$$\cosh(t\,A/2) = \frac{t}{2}A\,h(-\sqrt{-1}\,t\Omega_0) + I_{2N},$$

is derived from (B.1), where

$$I_{2N} = \text{the identity matrix of size } (2N)\times(2N)$$

and $h(x) = (\cosh x - 1)/x$. By the formula,

$$\begin{aligned}
\cosh(tA/2) &= \frac{t}{2} A\, h\big(-\sqrt{-1} t\,\Omega_0\big) + I_{2N} = -\frac{t}{2} A h\big(\sqrt{-1} t\,\Omega_0\big) + I_{2N} \\
&= \sqrt{-1} \begin{pmatrix} \frac{t}{2}\,\Omega(\zeta) h\big(\sqrt{-1} t\,\Omega(\zeta)\big) & -\frac{t}{2}\, h\big(\sqrt{-1} t\,\Omega(\zeta)\big) \\ -\frac{t}{2}\,(\Omega(\zeta))^2 h\big(\sqrt{-1} t\,\Omega(\zeta)\big) & \frac{t}{2}\,\Omega(\zeta) h\big(\sqrt{-1} t\,\Omega(\zeta)\big) \end{pmatrix} + I_{2N} \\
&= \begin{pmatrix} \frac{\sqrt{-1}t}{2}\,\Omega(\zeta) h\big(\sqrt{-1} t\,\Omega(\zeta)\big) + I & -\frac{\sqrt{-1}t}{2}\, h\big(\sqrt{-1} t\Omega(\zeta)\big) \\ -\frac{\sqrt{-1}t}{2}\,(\Omega(\zeta))^2 h\big(\sqrt{-1} t\,\Omega(\zeta)\big) & \frac{\sqrt{-1}t}{2}\,\Omega(\zeta) h\big(\sqrt{-1} t\,\Omega(\zeta)\big) + I \end{pmatrix},
\end{aligned}$$

we have

$$\begin{aligned}
&\det\big(\cosh(tA/2)\big) \\
&\quad= \det \begin{pmatrix} \frac{\sqrt{-1}t}{2}\Omega(\zeta) h\big(\sqrt{-1} t\,\Omega(\zeta)\big) + I & -\frac{\sqrt{-1}t}{2} h\big(\sqrt{-1} t\,\Omega(\zeta)\big) \\ -\frac{\sqrt{-1}t}{2}(\Omega(\zeta))^2 h\big(\sqrt{-1} t\,\Omega(\zeta)\big) & \frac{\sqrt{-1}t}{2}\Omega(\zeta) h\big(\sqrt{-1} t\,\Omega(\zeta)\big) + I \end{pmatrix} \\
&\quad= \det \begin{pmatrix} I & -\frac{\sqrt{-1}t}{2} h\big(\sqrt{-1} t\,\Omega(\zeta)\big) \\ \Omega(\zeta) & \frac{\sqrt{-1}t}{2}\Omega(\zeta) h\big(\sqrt{-1} t\,\Omega(\zeta)\big) + I \end{pmatrix} \\
&\quad= \det \begin{pmatrix} I & -\frac{\sqrt{-1}t}{2} h\big(\sqrt{-1} t\,\Omega(\zeta)\big) \\ 0 & \sqrt{-1} t\,\Omega(\zeta) h\big(\sqrt{-1} t\,\Omega(\zeta)\big) + I \end{pmatrix} \\
&\quad= \det\big(\sqrt{-1} t\,\Omega(\zeta) h\big(\sqrt{-1} t\,\Omega(\zeta)\big) + I\big) \\
&\quad= \det\cosh\big(\sqrt{-1} t\,\Omega(\zeta)\big). \qquad \square
\end{aligned}$$

Theorem B.1 is obtained from the lemma above and Theorem A.8. The kernel is given by

$$\begin{aligned}
K(t; x, z, \tilde{x}, \tilde{z}) = (2\pi)^{-N-N(N-1)/2} &\int_{\mathbb{R}^N} \int_{\mathbb{R}^{N(N-1)/2}} e^{i\langle x-\tilde{x}, \xi\rangle + i\langle z-\tilde{z}, \zeta\rangle} \\
&\times\ e\big(t\ ;\ (x+\tilde{x})/2,\ (z+\tilde{z})/2,\ \xi,\ \zeta\big)\, d\zeta d\xi.
\end{aligned}$$

By applying the formula

$$\begin{aligned}
&\int_{\mathbb{R}^N} \exp\big(-\langle M\xi, \xi\rangle + \sqrt{-1}\,\langle a, \xi\rangle\big)\, d\xi \\
&\qquad\qquad = \big(\det M\big)^{-1/2} \pi^{N/2} \exp\big(-\big\langle a, M^{-1} a\big\rangle/4\big)
\end{aligned}$$

with

$$M = \frac{t}{2} \frac{\tanh(\sqrt{-1} t\,\Omega(\zeta))}{\sqrt{-1} t\,\Omega(\zeta)} \quad \text{and} \quad a = (x - \tilde{x}) - \tanh\big(\sqrt{-1} t\,\Omega(\zeta)\big)(x + \tilde{x})/2$$

we get the assertion of Corollary B.2.

Appendix C. The trace of the fundamental solution

In this appendix we consider a heat equation on a closed manifold under the condition (A) and an additional condition (B).

(B) The principal symbol $p_m(x,\xi)$ vanishes exactly to the second order on the characteristic set

$$\Sigma = \big\{(x,\xi) \;\big|\; p_m(x,\xi) = 0, \xi \neq 0\big\},$$

i.e., there exists a coordinate system $(\mathcal{U}\times\mathcal{V}; u, v)$ about each point in Σ with the property that

$$\Sigma \cap \big(\mathcal{U}\times\mathcal{V}\big) = \{(u,0)\},$$

and

$$p_m(x,\xi) = \sum a_{i\,j}(u)\, v_i v_j + O(|v|^3) \text{ near } v = 0 \tag{C.1}$$

with $\det\big(a_{i\,j}(u)\big) > 0$. With this property we have an invariantly defined volume form $d\Sigma$ on Σ in such a way that

$$d\Sigma = \frac{1}{\sqrt{\det\big(a_{i\,j}(u)\big)}}\, G(u)\, du,$$

where $G\, du \wedge dv$ is the local expression of the Liouville volume form.

Definition C.1. Under condition (B) the characteristic set Σ is the disjoint union $\Sigma = \bigsqcup \Sigma^j$ of connected components Σ^j. Then we call the minimum codimension,

$$d := \min\big\{\text{codimension of } \Sigma^j\big\}$$

the codimension of the characteristic set Σ. By Σ^0 we denote the union of all components Σ^j having codimension d.

Theorem C.2. *Let M be a closed manifold. If $p(x,\xi) \in S^m_{1,0}(M)$ satisfies conditions* (A) *and* (B)*. Then the trace of the fundamental solution $E(t)$ has the following asymptotic behaviour as t goes to 0:*

$$\operatorname{tr} E(t) = \begin{cases} (C_1 + o(1))\, t^{-n/m} & \text{if } n - md/2 < 0, \\ \big(C_2 \log(t^{-1}) + O(1)\big)\, t^{-n/m} & \text{if } n - md/2 = 0, \\ (C_3 + o(1))\, t^{-(n-d/2)/(m-1)} & \text{if } n - md/2 > 0, \end{cases}$$

where

$$C_1 = (2\pi)^{-n} \int_{T^*M} \exp(-p_m(x,\xi))\, dx d\xi,$$

$$C_2 = m^{-1}(2\pi)^{-n+d/2} \int_{\Sigma^0} (p_{m-1} + \operatorname{tr}^+(A)/2) \exp(-p_{m-1} - \operatorname{tr}^+(A)/2)\, d\Sigma^0,$$

$$C_3 = (2\pi)^{-n+d/2} \int_{\Sigma^0} \Big[\det\big\{(A/2 \sinh(A/2)\big\}\Big]^{1/2} \exp(-p_{m-1})\, d\Sigma^0.$$

Remark C.3. In the case where $n - md/2 = 0$, $p_{m-1} + \frac{1}{2}\operatorname{tr}^+(A)$ can be replaced by any positive function homogeneous of order $m-1$. So the constant C_2 depends only on $d\Sigma^0$.

Sketch of proof. Assume that the codimension of Σ is d. Let V be a local chart of M. Set

$$\Omega_1 = T^*V \cap \big\{X = (x,\xi) \bigm| p_m(X) \le \langle\xi\rangle^{m-1+2\varepsilon},\ t\langle\xi\rangle^{m-1} \le \langle\xi\rangle^{\delta}\big\},$$
$$\Omega_2 = T^*V \cap \big\{X = (x,\xi) \bigm| p_m(X) \ge \langle\xi\rangle^{m-1+2\varepsilon}\big\}$$

for suitable positive constants ε and δ. Then we have

$$\int_V \operatorname{tr}E(t)dx = (2\pi)^{-n}\int_V\int_{\mathbb{R}^n} e(t;x,\xi)\,d\xi dx$$
$$= (1+o(1))\,(2\pi)^{-n}\left(\int_{\Omega_1}\exp\varphi(t)dxd\xi + \int_{\Omega_2}\exp\phi_0(t)\,dxd\xi\right),$$

where

$$\phi_0(t) = -tp_m(X).$$

Choose a point $X = (x,\xi)$ near the characteristic set and choose a conical neighbourhood Ω of X. By condition (B) we can construct a smooth function $a = a(X)$ defined in Ω such that

$$|d(X,a(X)) - d(X,\Sigma)| \le d(X,\Sigma)^2.$$

Instead of $\varphi(t)$ we can use

$$\phi_3(t) = -p_{m-1}(a)t$$
$$-\frac{1}{2}\operatorname{tr}\left(\log[\cosh(A(a)t/2)]\right) - \left\langle\, a-X, \sqrt{-1}J\tanh(A(a)t/2)(a-X)\,\right\rangle,$$

where $a = a(X)$. Set

$$I(W) = \int_W \chi_1\exp\phi_3(t,x,\xi)\,dxd\xi,$$
$$J(W) = \int_W \chi_2\exp\phi_0(t,x,\xi)\,dxd\xi,$$

where χ_1 and χ_2 are characteristic functions of Ω_1 and Ω_2, respectively. We introduce a local coordinate system (ω,r,y) as follows: There exists an open set U of $\mathbb{R}^{2n-1-d}$ and a smooth map $\tau(\omega,r,y)$ from $U\times\mathbb{R}_+\times\mathbb{R}^d$ to $T^*(\mathbb{R}^n)$ such that τ is a local diffeomorphism from $U\times\mathbb{R}_+\times Y$ with $Y = \{|y| < L\}$ onto Ω that satisfies the following conditions:

(1) $\tau(\omega,r,y) = \tau_0(\omega,r) + \tau_1(\omega,r)y = (x,\xi)$,
(2) $\tau_0(\omega,r)$ is a diffeomorphism from $U\times\mathbb{R}_+$ onto Σ, especially $\tau_0(\omega,1)$ is a diffeomorphism from U onto the intersection Σ_1 of Σ and $S^*(\mathbb{R}^n) = \big\{(x,\xi)\in\mathbb{R}^n\times\mathbb{R}^n \bigm| |\xi| = 1\big\}$,
(3) if $X = \tau(\omega,r,y)$, then $a(X) = \tau_0(\omega,r)$.

Introduce a function $\Phi(\omega,y)$ by

$$dxd\xi = \Phi r^{n-1}\,drd\omega dy.$$

Ω is divided into

$$\Omega_a = \{(x,\xi) \in \Omega \mid r^{m-1}t > 1,\, r > 1\},$$
$$\Omega_b = \{(x,\xi) \in \Omega \mid r^{m-1}t \le 1,\, r > 1\},$$
$$\Omega_c = \{(x,\xi) \in \Omega \mid r \le 1\}.$$

It is clear that

$$I(\Omega_c) = O(1), \quad J(\Omega_c) = O(1).$$

(I) If $2n - md < 0$, then we have

$$I(\Omega_a) = O(t^{-(n-d/2)/(m-1)}) \quad \text{and} \quad I(\Omega_b) = o(t^{-n/m})$$

and

$$\begin{aligned} J(\Omega_a \cup \Omega_b) &= \int_U \int_{r>1} \int_Y \chi_2 \exp \phi_0(t)\, dx d\xi \\ &= \left(\int_U \int_Y \int_{t^{1/m}}^{\infty} \exp(\phi_0(1)) \Phi r^{n-1}\, dr dy d\omega + o(1) \right) t^{-n/m} \\ &= \left(\int_\Omega \exp(\phi_0(1))\, dx d\xi + o(1) \right) t^{-n/m}. \end{aligned}$$

Note that the above integral is finite by the inequality $\phi_0(t) \le -C|y|^2 r^m t$.

(II) If $2n - md = 0$, then we have

$$I(\Omega_a) = O(t^{-n/m}) \quad \text{and} \quad \mathrm{J}(\Omega_a) = O(t^{-n/m}).$$

Set

$$\phi_1(t) = -\frac{1}{2} \left\langle \tau_1(\omega) y, \nabla^2 p_m(\omega) \tau_1(\omega) y \right\rangle r^m t,$$

where $\tau_1(\omega) = \tau(\omega, 1)$. Then we have

$$I(\Omega_b) = \int_{\Omega_b} \chi_1 \exp \phi_1(t)\, dx d\xi + O(t^{-n/m}),$$
$$J(\Omega_b) = \int_{\Omega_b} \chi_2 \exp \phi_1(t)\, dx d\xi + O(t^{-n/m}).$$

So it holds that

$$I(\Omega_b) + J(\Omega_b) = \int_{\Omega_b} \exp \phi_1(t)\, dx d\xi + O(t^{-n/m}).$$

Set $\Omega_b = D_1 \cup D_2$, where

$$D_1 = \Omega_b \cap \{1 \le \tilde{r} \le t^{-1/m(m-1)}\}, \quad D_2 = \Omega_b \cap \{t^{1/m} \le \tilde{r} < 1\}$$

and $\tilde{r} = r t^{1/m}$. Then we have

(i) $$\begin{aligned} \int_{D_2} \exp \phi_1(t)\, dx d\xi &= \int_U \int_Y \int_{t^{1/m}}^{1} \exp(\phi_1(1)) \Phi \tilde{r}^{n-1}\, d\tilde{r} dy d\omega\, t^{-n/m} \\ &= O(t^{-n/m}), \end{aligned}$$

$$\text{(ii)}\quad \int_U\int_Y\int_1^{t^{1/m(m-1)}} \exp(\phi_1(1))(\Phi-\Phi|_{y=0})\tilde{r}^{n-1}\,d\tilde{r}dyd\omega\,t^{-n/m}=O(t^{-n/m}),$$

$$\begin{aligned}\text{(iii)}\quad &\int_U\int_Y\int_1^{t^{-1/m(m-1)}} \exp(\phi_1(1))(\Phi|_{y=0})\tilde{r}^{n-1}\,d\tilde{r}dyd\omega\,t^{-n/m}\\
&=\int_U\int_{\mathbb{R}^d}\int_1^{t^{-1/m(m-1)}} \exp(\phi_1(1))(\Phi|_{y=0})\tilde{r}^{n-1}\,d\tilde{r}dyd\omega\,t^{-n/m}\\
&=\int_U\int_1^{t^{-1/m(m-1)}} \pi^{d/2}(\Phi|_{y=0})\tilde{r}^{n-1-\frac{md}{2}}\,d\tilde{r}\\
&\qquad\times\left(\frac{\det H^+(\omega)}{2}\right)^{-1/2}(\det T_1)^{-1/2}\,d\omega\,t^{-n/m}+O(t^{-n/m})\\
&=\frac{(2\pi)^{d/2}}{m(m-1)}\log\left(\frac{1}{t}\right)\left(\int_U\left\{\det H^+(\omega)\right\}^{-1/2}d\Sigma_1\right)t^{-n/m}+O(t^{-n/m})\\
&=\frac{(2\pi)^{d/2}}{m(m-1)}\log\left(\frac{1}{t}\right)\left(\int_U d\Sigma_s\right)t^{-n/m}+o(t^{-n/m}),\end{aligned}$$

where we have used that

$$d\Sigma_1=(\Phi|_{y=0})(\det T_1)^{-1/2}\,d\omega$$

and the notations

$$T_1={}^t\tau_1(\omega)\tau_1(\omega),\quad d\Sigma_s=d\Sigma^0\big|_{|\xi|=1}.$$

Finally, we have that

$$I(\Omega_b)+J(\Omega_b)=\frac{(2\pi)^{d/2}}{m(m-1)}\log\left(\frac{1}{t}\right)\left(\int_U d\Sigma_s\right)t^{-n/m}+O(t^{-n/m}).$$

(III) If $2n-md>0$, then

$$J(\Omega_a\cup\Omega_b)=o(t^{-(n-d/2)/(m-1)}).$$

By the change of variables

$$rt^{1/(m-1)}=\tilde{r},\quad yt^{-1/2(m-1)}=\tilde{y},$$

we have

$$\begin{aligned}I(\Omega_a\cup\Omega_b)&=\int_U\int_{r>1}\int_Y\chi_1\exp\phi_3(t)\,dxd\xi\\
&=t^{-(n-d/2)/(m-1)}\cdot\left(\int_U\int_{\mathbb{R}_+}\int_{\mathbb{R}^d}\exp\phi_3(1)(\det T_1)^{1/2}\,d\tilde{y}\tilde{r}^{n-1}d\tilde{r}d\Sigma_1+o(1)\right).\end{aligned}$$

Set

$$\phi_3(1)=\phi_4-p_{m-1}(\tau_0(\omega,\tilde{r}))-\frac{1}{2}\operatorname{tr}\left(\log\left[\cosh(A(\tau_0(\omega,\tilde{r}))/2)\right]\right),$$

with

$$\phi_4=-\left\langle\tau_1(\omega)\tilde{y},\sqrt{-1}\,J\tanh(A(\tau_0(\omega,\tilde{r})/2)\tau_1(\omega)\tilde{y}\right\rangle\tilde{r}.$$

By

$$\int_{\mathbb{R}^d} \exp \phi_4 \, d\tilde{y}$$
$$= (\pi/\tilde{r})^{d/2}\{\det H^+(\tau_0(\omega,\tilde{r}))/2\}^{-1/2}(\det T_1)^{-1/2}\left[\det\left(\frac{A(\tau_0(\omega,\tilde{r}))/2}{\tanh(A(\tau_0(\omega,\tilde{r}))/2)}\right)\right]^{1/2}$$

it holds that

$$\int_{\mathbb{R}^d} \exp \phi_3(1)\, d\tilde{y}\, (\det\, T_1)^{1/2} = (\pi/\tilde{r})^{d/2}\{\det H^+(\tau_0(\omega,\tilde{r}))/2\}^{-1/2}$$
$$\times \exp\{-p_{m-1}(\tau_0(\omega,\tilde{r}))\}\left[\det\left(\frac{A(\tau_0(\omega,\tilde{r}))/2}{\sinh(A(\tau_0(\omega,\tilde{r}))/2)}\right)\right]^{1/2}.$$

Finally, we have

$$\int_U \int_{\mathbb{R}_+} \int_{\mathbb{R}^d} \exp \phi_3(1)(\det T_1)^{1/2} d\tilde{y}\tilde{r}^{n-1}\, d\tilde{r} d\Sigma_1$$
$$= (2\pi)^{d/2} \int_U \int_{\mathbb{R}_+} \{\det H^+(\tau_0(\omega,\tilde{r}))\}^{-1/2} \exp\{-p_{m-1}(\tau_0(\omega,\tilde{r}))\}$$
$$\times \left[\det\left(\frac{A(\tau_0(\omega,\tilde{r}))/2}{\sinh(A(\tau_0(\omega,\tilde{r}))/2)}\right)\right]^{1/2} \tilde{r}^{n-d/2-1} d\tilde{r} d\Sigma_1$$
$$= (2\pi)^{d/2} \int_U \int_{\mathbb{R}_+} \exp\{-p_{m-1}(\tau_0(\omega,\tilde{r}))\}\left[\det\left(\frac{A(\tau_0(\omega,\tilde{r}))/2}{\sinh(A(\tau_0(\omega,\tilde{r}))/2)}\right)\right]^{1/2} d\Sigma^0.$$

Appendix D. Selberg trace formula

In this appendix we sum up algebraic and geometric arguments of the Selberg trace formula calculation. Convergences of sum and integrals are always assumed.

Let Γ be a discrete group which acts on a space M freely and properly discontinuously with the (compact) quotient space $\Gamma\backslash M$,

$$\Gamma \times M \to M.$$

Also we assume that there is a measure $dV = dV(x)$ on M invariant under the action of Γ,

$$\gamma^*(dV) = dV, \quad \forall\gamma \in \Gamma.$$

So we have a measure on the quotient space $\Gamma\backslash M$ which we denote by dV, as well.

Let $K = K(x,y)$ be a function on $M \times M$ satisfying the invariance property

$$K(\gamma \cdot x, \gamma \cdot y) = K(x,\, y), \quad \forall x,\, y \in M \text{ and } \forall \gamma \in \Gamma.$$

Then the sum

$$\overline{K}(x,y) = \sum_{\gamma\in\Gamma} K(\gamma \cdot x, y)$$

is a well-defined function on $(\Gamma\backslash M)\times(\Gamma\backslash M)$, since for $\mu,\nu\in\Gamma$

$$\begin{aligned}\overline{K}(\mu\cdot x,\nu\cdot y)&=\sum_{\gamma\in\Gamma}K(\gamma\cdot(\mu\cdot x),\nu\cdot y)=\sum_{\gamma\in\Gamma}K((\nu^{-1}\gamma\mu)\cdot x,y)\\&=\sum_{\nu^{-1}\gamma\mu\in\Gamma}K((\nu^{-1}\gamma\mu)\cdot x,y)=\sum_{\gamma\in\Gamma}K(\gamma\cdot x,y)=\overline{K}(x,y).\end{aligned}$$

Let us denote a fundamental domain of the action of Γ by F and consider the integral

$$T=\int_{\Gamma\backslash M}\overline{K}(x,y)\,dV(x)=\sum_{\gamma\in\Gamma}\int_F K(\gamma\cdot x,x)\,dV(x).$$

We denote a complete set of representatives of the conjugacy classes of Γ by $[\Gamma]$. Let S_γ be the set of conjugate elements (in Γ) to γ, i.e.,

$$S_\gamma=\left\{\mu^{-1}\gamma\mu\;\middle|\;\mu\in\Gamma\right\}.$$

The integral T can be rewritten as

$$T=\sum_{\gamma\in[\Gamma]}\sum_{\tau\in S_\gamma}\int_F K(\tau\cdot x,x)\,dV(x)=\sum_{\gamma\in[\Gamma]}\sum_{\mu^{-1}\gamma\mu\in S_\gamma}\int_F K(\gamma\mu\cdot x,\mu\cdot x)\,dV(x),$$

since $\Gamma=\bigcup_{\gamma\in[\Gamma]}S_\gamma$.

Let us pick a $\gamma\in[\Gamma]$ and consider the integral

$$I_\gamma=\sum_{\mu^{-1}\gamma\mu\in S_\gamma}\int_F K(\gamma\mu\cdot x,\mu\cdot x)\,dV(x).$$

Let C_γ be the centralizer of the element γ,

$$C_\gamma=\left\{h\in\Gamma\;\middle|\;h\gamma=\gamma h\right\},$$

and choose a complete set $\{\mu_i\}$ (which we denote by $[C_\gamma]$) of representatives of the quotient set Γ/C_γ. Then $S_\gamma=\{\mu_i^{-1}\gamma\mu_i|\mu_i\in[C_\gamma]\}$. Now the sum of integrals I_γ is expressed as

$$I_\gamma=\int_{\bigcup_{\mu_i\in[C_\gamma]}\mu_i\cdot F}K(\gamma\cdot x,x)\,dV(x).$$

Since

$$F_\gamma=\bigcup_{\mu_i\in[C_\gamma]}\mu_i\cdot F$$

is a fundamental domain of the group action by C_γ, the integral T reduces to the sum of integrals

$$T=\sum_{\gamma\in[\Gamma]}I_\gamma=\sum_{\gamma\in[\Gamma]}\int_{F_\gamma}K(\gamma\cdot x,x)\,dV(x).$$

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Zeta Functions of Elliptic Cone Operators

Gerardo A. Mendoza

Abstract. This paper is an overview of aspects of the singularities of the zeta function, equivalently, of the small time asymptotics of the trace of the heat semigroup, of elliptic cone operators. It begins with a brief description of classical results for regular differential operators on smooth manifolds, and includes a concise introduction to the theory of cone differential operators. The later sections describe recent joint work of the author with J. Gil and T. Krainer on the existence of the resolvent of elliptic cone operators and the structure of its asymptotic behavior as the modulus of the spectral parameter tends to infinity within a sector in $\mathbb{C}$ on which natural ray conditions on the symbol of the operator are assumed. These ideas are illustrated with examples.

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1. Introduction

The principal aim of these notes is to give an overview of certain interesting structural properties of the zeta function of an elliptic cone operator on a compact manifold. We begin, in Section 2, with an account of the zeta function of elliptic operators in the classical settings, and continue in Section 3 with a description of a number of results mostly concerning the equivalent problem of the structure of the small time asymptotics of the trace of the heat semigroup of elliptic operators on manifolds with conical singularities (assuming of course some appropriate positivity conditions).

A reader wishing to go somewhat further into the details of the theory and the meaning of some terms used in the statements in Section 3 may benefit from the material in Sections 4 and 5, which go into some of the details of the theory of cone operators. Some aspects of the spectral theory of elliptic cone operators are

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presented in Section 6. Sections 4, 5, and 6 are needed for Sections 7 and 8. The first of these last two sections presents results concerning rays of minimal growth, while the last is intended to give an idea of the origin of the complicated structure of the singularities of the zeta function.

The expositions in Sections 4 to 8 are based on joint work with Juan B. Gil and Thomas Krainer contained in the papers [14, 15, 16, 17, 18].

2. Classical results

Leaving aside the *a posteriori* observation about the relation between the classical Riemann (or the Epstein) zeta function and the zeta function of the Laplacian on a circle (or torus), it is fair to say that the zeta function of a differential operator appeared first in a paper of T. Carleman [6]. There he proves Weyl's estimate for the eigenvalues of the Dirichlet Laplacian on a planar region $\mathcal{M}$ with piecewise C^2 boundary ("continuous curvature") using the Ikehara-Wiener Tauberian theorem (Ikehara [22], see Korevaar [27]). In Carleman's paper, the zeta function appears in the form

$$\frac{1}{2\pi i}\int_\gamma \sum_{k=1}^\infty \frac{\lambda \phi_k(p)^2}{\lambda_k(\lambda_k-\lambda)}\lambda^{-s}\,d\lambda$$

where the ϕ_k form a complete orthonormal system of eigenfunctions, $\Delta\phi_k = \lambda_k\phi_k$ with the λ_k forming a nondecreasing sequence, and γ is a line $\Im\lambda = a$, $0 < a < \lambda_1$ (throughout this note the convention will be to take the positive Laplacian). Of course this is the zeta function after integration over $\mathcal{M}$. The fact that $s = 1$ is a simple pole allows the use of Ikehara's theorem, and gives a first direct link between the residues of the zeta function and what one may term the classical spectral information.

Carleman's work not withstanding, the explicit study of zeta functions, and related objects, of elliptic differential operators, began with work of S. Minakshisundaram in the late 1940's, in particular his work with Å. Pleijel [33] in which one finds, among other things, the following:

Theorem 2.1 (Minakshisundaram and Pleijel [33]). *Let Δ the Laplacian on a compact orientable Riemannian manifold $\mathcal{M}$ without boundary, or with smooth boundary and either Dirichlet or Neumann boundary condition. Let λ_k be the eigenvalues repeated with multiplicity. Then the corresponding zeta function has a meromorphic extension to $\mathbb{C}$ with simple poles contained in*

$$\{(n-\ell)/m : \ell \in \mathbb{N}_0\}\backslash(-\mathbb{N}_0) \tag{2.2}$$

where $n = \dim\mathcal{M}$, $m = 2$ is the order of Δ, and $\mathbb{N}_0$ is the set of non-negative integers.

Minakshisundaram and Pleijel proved their theorems in [33] by first constructing the Schwartz kernel of a parametrix for the initial value problem for the heat equation. From this they constructed (using a Laplace transform) the

Schwartz kernel of a parametrix for the resolvent of Δ, which they then exploited using Cauchy's integral formula to write expressions for the zeta function from which the meromorphic continuation and other properties were read off.

The idea of going directly from the heat kernel to the zeta function via Mellin transform to establish the fundamental analytic properties of zeta functions appears in a paper of Minakshisundaram [31] (submitted only 4 days after the paper with Pleijel cited above) where he discusses the behavior of the zeta function associated with the flat Laplacian with Dirichlet or Neumann conditions on a domain with smooth boundary. A few years later Minakshisundaram [32] used this to give more direct proofs of his results with Pleijel. See [12] for a perspective on Minakshisundaram's conceptual contribution to spectral analysis.

Incidentally, the relation between the ζ function and the trace of the heat kernel is the following. Suppose that A is an unbounded selfadjoint operator on some Hilbert space with discrete spectrum $\{\lambda_k\}_{k=0}^{\infty}$ (assumed to lie in $(0,\infty)$ and to satisfy a Weyl-type estimate, $\lambda_k \sim ck^\alpha$ for some $c, \alpha > 0$). Then e^{-tA} is trace-class for $t > 0$,

$$\operatorname{Tr} e^{-tA} = \sum_{k=0}^{\infty} e^{-\lambda_k t}$$

and one has

$$\zeta(s) = \frac{1}{\Gamma(s)} \int_0^\infty \operatorname{Tr} e^{-tA} t^s \, \frac{dt}{t} \tag{2.3}$$

for every s with sufficiently large real part.

The proofs of Minakshisundaram and Pleijel in [33] become at some point what amounts to an analysis of the Schwartz kernel of the complex powers of the Laplacian. This analysis was made explicit by R.T. Seeley, who gave far reaching extensions of these theorems, to general elliptic differential operators on compact manifolds without boundary acting on sections of a vector bundle [34], and to elliptic boundary value problems [35, 36], in both cases assuming that a ray condition if satisfied. Seeley showed, among other things, that for selfadjoint problems, the zeta function of a differential operator of order m on an n-dimensional manifold has a meromorphic continuation to all of $\mathbb{C}$ with simple poles contained in the set (2.2).

Greiner [21] obtained an expansion of the heat trace for small time for elliptic partial differential operators of even order acting on sections of a vector bundle (essentially constructing a parametrix for the heat operator via an anisotropic pseudodifferential calculus), again both for closed manifolds and for compact manifold with boundary and suitable boundary conditions. In Greiner's work, the principal symbol of the operator is assumed to have the property that the real part of its eigenvalues is bounded below uniformly by a positive number on the cosphere bundle of the manifold.

There is a direct, explicit relation by way of (2.3) between the coefficients of the small time asymptotics of $\operatorname{Tr} e^{-tA}$ (to the extent that such expansion exists) and the residues of the zeta function of A. Therefore the analysis of the residues of the zeta function and that of the coefficients of the expansion of $\operatorname{Tr} e^{-tA}$ at $t = 0$ are equivalent problems. There is by now a wealth of information gathered through, and about, the heat kernel, see [20] and [23] for instance, with many implications and applications in a number of areas beyond zeta functions; describing these would take us far away in a direction which is not the subject here, so in the rest of these notes we focus on manifolds with conical singularities.

3. Conical singularities

The simple meromorphic structure (location and order of the poles) of the zeta function, even its meromorphic extendability, begins to disappear when considering differential operators with singularities. This showed up first in the from of a logarithmic term in the short time expansion of the heat trace in J. Cheeger's analysis [8] of spectral properties of compact manifolds with conical singularities with straight cone metrics near the conical points. The latter means, in effect, that $\mathcal{M}$ is a compact manifold with boundary with a metric which is Riemannian in $\overset{\circ}{\mathcal{M}}$ and of the form

$$g_c = dx \otimes dx + x^2 \pi^* g \tag{3.1}$$

in a tubular neighborhood U of $\partial\mathcal{M}$; the map $\pi : U \to \partial\mathcal{M}$ is the projection, x is a defining function of $\partial\mathcal{M}$ (positive in the interior of $\mathcal{M}$), and g is a Riemannian metric on $\partial\mathcal{M}$. The structure of the metric (3.1) is that of the Euclidean metric g_e in polar coordinates. More generally, if $\mathcal{N}$ is a closed submanifold of S^{N-1} and

$$\mathcal{M} = [0,\infty) \times \mathcal{N},\ \wp : \mathcal{M} \to \mathbb{R}^N,\ \mathcal{M} \ni (x,y) \mapsto \wp(x,y) = xy \in \mathbb{R}^N,$$

then $\wp^* g_e$ has the structure of the metric in (3.1)

Cheeger's primary concern in [8] and various other of his papers at the time such as [9] (which considerably extends [8]) lies with various spectral invariants associated with the Laplacian for such metrics on forms of any degree. He observes that one can obtain a parametrix for the heat equation on $\mathcal{M}$ by gluing together parametrices for the problem in the interior of $\mathcal{M}$ and an exact parametrix near the boundary (this is the same general scheme as that in the first step of the paper of Minakshisundaram and Pleijel), from which the asymptotics of the trace of heat kernel can be obtained with arbitrary precision by a recursive process. The exact parametrix near the boundary is obtained using separation of variables. The end result is the validity of an expansion of the form

$$\operatorname{Tr} e^{-t\Delta_F} \sim \sum_{k=0}^{\infty} a_k t^{(k-n)/2} + a_0' \log t$$

where Δ_F means the Friedrichs extension, in which the novelty is the appearance of the logarithmic term; as before, $n = \dim\mathcal{M}$. Following Minakshisundaram [32] one obtains that the zeta function, computed using (2.3), extends as a meromorphic function to all of $\mathbb{C}$ with simple poles in the set (2.2) ($m = 2$ and $n = \dim\mathcal{M}$) and possibly also at 0.

Around the same time, Callias and Taubes [5] also found logarithmic singularities in the short time asymptotics of the heat trace of certain selfadjoint operators related to the Dirac operator with singular potential (where such a logarithmic term appears in a relative trace formula). An explicit calculation by Callias [4] shows that if A is the closure of

$$D_x^2 + \kappa/x^2 : C_c^\infty(\mathbb{R}_+) \subset L^2(\mathbb{R}_+) \to L^2(\mathbb{R}_+) \tag{3.2}$$

with Lebesgue measure and $\kappa \geq 3/4$ (which implies that (3.2) has exactly one selfadjoint extension, namely its Friedrichs extension) then (see *ibid.*, Theorem (5.κ))

$$\langle \operatorname{tr} e^{-tA}, \varphi\rangle \sim \sum_{k=0}^\infty \langle c_k, \varphi\rangle t^{(k-1)/2} + \sum_{k=1}^\infty \langle c_k', \varphi\rangle t^{k-1/2} \log t, \qquad \varphi \in C_c^\infty(\overline{\mathbb{R}}_+)$$

as $t \to 0^+$. Here $\operatorname{tr} e^{-tA}$ is the restriction of the Schwartz kernel of e^{-tA} for fixed $t > 0$ to the diagonal and the c_k and c_k' are certain distributions. As a consequence, the "zeta" function of A, computed via (2.3) has, at least in principle, double poles on the set (2.2) with $n = 1$ and $m = 2$.

Several questions on regions with conical singularities were studied by Kondrati'ev in the 1960's, see for example [26]. But it was the work of Cheeger cited above that generated the impetus for intense subsequent work by many authors, including Brüning, Melrose, Schulze, and Seeley, eventually also Lesch, Mazzeo, and many others, on various aspects of analysis on manifolds with conical singularities or cylindrical ends and other variants of the problem.

To go further we need some terminology (more will be given in subsequent sections). Analysis on a manifold with conical singularities or cylindrical ends really means analysis of a partial differential operator of a special type on a manifold $\mathcal{M}$ with boundary together with, explicitly or implicitly, a cone metric or a b-metric (see Section 4 for the general definitions; the metric g_c in (3.1) is an example of a cone metric, see (4.2), and $g_b = x^{-2}g_c$ is the prototype of a b-metric). The Laplacian with respect to a general cone metric serves as the model for elliptic cone operators, sometimes also called a Fuchs-type operator. For example, the Laplacian with respect to the product metric (3.1), easily computed, has the form

$$\frac{1}{x^2}\big((xD_x)^2 - i(n-2)xD_x + \Delta_g\big).$$

Here a neighborhood of $\partial\mathcal{M}$ in $\mathcal{M}$ is thought of as $\partial\mathcal{M} \times [0,\varepsilon)$, $\varepsilon > 0$, and Δ_g is the Laplacian on $\partial\mathcal{M}$ with respect to g. In general, a b-differential operator is a differential operator on $\mathcal{M}$ which near any point of the boundary has the form

$$P = \sum_{k+|\alpha|\leq m} a_{k,\alpha}(x,y)(xD_x)^k D_y^\alpha$$

with smooth coefficients $a_{k,\alpha}$, where (x,y) are coordinates near the point with x a defining function for $\partial\mathcal{M}$. The class of b-operators of order m mapping sections of a vector bundle E to sections of a vector bundle F is denoted $\operatorname{Diff}_b^m(\mathcal{M}; E, F)$, or just $\mathrm{Diff}_b^m(\mathcal{M};E)$ if $F = E$, or $\mathrm{Diff}_b^m(\mathcal{M})$ in the case of scalar operators. A general cone differential operator of order m is an operator A such that $x^m A$ is a b-operator. As indicted above, more details will be given in Section 4.

In the specific case of interest to us here, namely operators on manifolds with conical singularities, there were a number of results proved in fair generality in connection with the asymptotic of the trace of the heat kernel in the 1990's. Among these we single out the following two theorems, the first of which is a general result.

Theorem 3.3 (Lesch [28], Theorem 2.4.1). *Let $A \in x^{-\nu}\,\mathrm{Diff}_b^m(\mathcal{M};E)$ be a positive differential operator on a compact manifold with boundary, assume $x^\nu A$ is b-elliptic. Let $\mathcal{D}$ be the domain of a positive selfadjoint extension of A. Then $e^{-tA_\mathcal{D}}$ is a trace class operator and*

$$\mathrm{Tr}(e^{-tA_\mathcal{D}}) \sim \sum_{k=0}^{n-1} a_k t^{(k-n)/m} + \mathcal{O}(\log t) \qquad \text{as } t \to 0^+.$$

It is interesting to pass along Lesch's observation that the coefficients a_k are independent of the extension, since they are local invariants determined by A. The effect of the domain is hidden in the $\mathcal{O}(\log t)$ term.

A complete expansion was obtained by Brüning and Seeley [2] for certain second-order operators which near the boundary of $\mathcal{M}$ are of the form $D_x^2 + x^{-1}A(x)$ where $A(x)$ is an unbounded selfadjoint operator satisfying certain lower bound estimates. The statement about $A(x)$ incorporates the choice of a domain for the operator. This is generally a necessary step since cone operators, initially defined on compactly supported smooth functions or sections in the interior of $\mathcal{M}$ may have many selfadjoint extensions.

Another complete expansion, this time for operators of arbitrary order but with special assumptions on its structure near the boundary (leading to the property essentially that separation of variables works) and on the domain is the following:

Theorem 3.4 (Lesch [28], Theorem 2.4.6). *Let $A = x^{-\nu}P$ with $P \in \mathrm{Diff}_b^m(\mathcal{M};E)$ b-elliptic. Suppose A is symmetric positive on its minimal domain. Suppose further that A has constant coefficients near $\partial\mathcal{M}$, and let $\mathcal{D}$ be the domain of a positive selfadjoint extension of A. Assume further that $\mathcal{D}$ is stationary (see (5.9)). Then $\mathrm{Tr}(e^{-tA_\mathcal{D}})$ has a full asymptotic expansion,*

$$\mathrm{Tr}(e^{-tA_\mathcal{D}}) \sim \sum_{k=0}^{\infty} a_k t^{(k-n)/m} + b\log t \qquad \text{as } t \to 0^+. \tag{3.5}$$

Constant coefficients means that there is a tubular neighborhood $\pi : U \to \partial\mathcal{M}$, a defining function x, and a connection ∇ on E, such that with $P = x^\nu A$ (an element of $\mathrm{Diff}_b^m(\mathcal{M};E)$) one has that $[x\nabla_{D_x}, A] = 0$ near $\partial\mathcal{M}$. Here $D_x = -i\partial_x$ and ∂_x means the vector field tangent to the fibers of π such that $\partial_x x = 1$.

A complete asymptotic expansion was also obtained by Gil [13] for a general elliptic cone operator, with the hypothesis of selfadjointness replaced by a sector property and with the assumption that the operator has only one closed extension:

Theorem 3.6 (Gil, [13], Theorem 4.9). *Let $\Lambda \subset \mathbb{C}$ be the complement of a closed sector in contained in $\Re\lambda > 0$. Let $A \in x^{-m}\operatorname{Diff}_b^m(\mathcal{M})$, $m > 0$, be such that $A - \lambda$ is parameter-elliptic with respect to some $\gamma \in \mathbb{R}$ on Λ (see* [13, Definition 3.1]*). Suppose further that*

$$A : C_c^\infty(\mathring{\mathcal{M}}) \subset x^{\gamma-n/2-m}L_b^2(\mathcal{M}) \to x^{\gamma-n/2-m}L_b^2(\mathcal{M})$$

has only one closed extension. Then the heat trace admits the asymptotic expansion

$$\operatorname{Tr} e^{-tA} \sim \sum_{k=0}^{\infty} a_k t^{(k-n)/m} + \sum_{k=0}^{\infty} a_k' t^{k/m} \log t \qquad \text{as } t \to 0^+,$$

where a_k and a_k' are constants depending on the symbolic structure of A.

Gil proves his theorem by first constructing the resolvent of A on the sector Λ and then using a Dunford integral to obtain the heat semigroup. A similar result can be deduced from the work of Loya [29] on the structure of the resolvent of a cone operator (in which the underlying assumptions are similar to those of Gil, *op. cit.*). Incidentally, the asymptotic structure of the resolvent for elliptic pseudodifferential operators on a closed manifold was obtained by Agranovich [1].

Returning to the specific topic of the structure of the zeta function itself, Falomir, Pisani, and Wipf [10] discovered an example (an ordinary differential operator) showing that the location of the poles of the zeta function need not be the set (2.2). This work was followed by investigations of a similar nature by Falomir, Muschietti, Pisani, and Seeley [11] and then by work by Kirsten, Loya, and Park [24] for second-order Laplace-like cone operators with constant coefficients near the boundary (see the definition of this concept above after Theorem 3.4) showing that the zeta function may not have a meromorphic extension at all due to the presence of logarithmic terms. These same authors showed in a more extensive analysis [25] (still in the very important case of Laplace-like operators, with constant coefficients near the boundary) that the poles of the zeta function may occur at arbitrary places in $\mathbb{C}$, and that the singularities may be logarithmic.

The most general result on the asymptotic expansion of the resolvent of a general cone operator as the modulus of spectral parameter tends to infinity within a sector, with no other assumption than the correct ellipticity and ray (or sector) conditions was obtained by Gil, Krainer, and the author of the present note in [18], see Theorem 8.2 below. The implications of the complicated asymptotics on the zeta function are similar to those obtained by Kirsten, Loya, and Park in [24].

4. Cone differential operators

Cone differential operators are a generalization of the kind of operators one obtains when writing regular differential operators with smooth coefficients in spherical coordinates. The underlying manifold is a manifold with boundary (interpreted as the spherical blowup of a manifold with conical [isolated] singularities).

Explicitly, let $\mathcal{M}$ be a manifold with boundary and $E, F \to \mathcal{M}$ be complex vector bundles over $\mathcal{M}$, then a cone differential operator of order m is an element of $x^{-m} \operatorname{Diff}^m_b(\mathcal{M}; E, F)$, where x is a defining function for $\partial\mathcal{M}$, $x > 0$ in $\overset{\circ}{\mathcal{M}}$ and $\operatorname{Diff}^m_b(\mathcal{M}; E, F)$ is the class of totally characteristic operators, or b-differential operators, of Melrose (see [30]); this is a subspace of the space $\operatorname{Diff}^m(\mathcal{M}; E, F)$ of linear differential operators

$$P : C^\infty(\mathcal{M}; E) \to C^\infty(\mathcal{M}; F).$$

Thus the elements of $\operatorname{Diff}^m_b(\mathcal{M}; E, F)$ are linear differential operators with smooth coefficients up to the boundary that can be represented locally near the boundary as matrices of linear combinations with smooth coefficients of products of up to m vector fields which are tangential to the boundary. Equivalently, using conjugation with the multiplication operator x^k,

$$\begin{aligned}&\operatorname{Diff}^m_b(\mathcal{M}; E, F)\\ &\qquad = \{P \in \operatorname{Diff}^m(\mathcal{M}; E, F) : x^{-k} P x^k \in \operatorname{Diff}^m(\mathcal{M}; E, F)\ \forall k \in \mathbb{N}_0\}. \qquad (4.1)\end{aligned}$$

Because of their definition, the natural primary structure bundle when dealing with b-differential operators is the b-tangent bundle, ${}^b\pi : {}^bT\mathcal{M} \to \mathcal{M}$, the vector bundle over $\mathcal{M}$ whose smooth sections are in one-to-one correspondence with the submodule $C^\infty_{\tan}(\mathcal{M}; T\mathcal{M})$ of the $C^\infty(\mathcal{M}; \mathbb{R})$-module $C^\infty(\mathcal{M}; T\mathcal{M})$ whose elements are vector fields which are tangential to the boundary. Since $C^\infty_{\tan}(\mathcal{M}; T\mathcal{M})$ is locally free finitely generated over $C^\infty(\mathcal{M}; \mathbb{R})$, there are indeed a vector bundle ${}^bT\mathcal{M}$ and bundle homomorphism ${}^b\mathrm{ev} : {}^bT\mathcal{M} \to T\mathcal{M}$ inducing an isomorphism ${}^b\mathrm{ev}_* : C^\infty(\mathcal{M}; {}^bT\mathcal{M}) \to C^\infty_{\tan}(\mathcal{M}; T\mathcal{M})$.

A b-differential operator $P \in \operatorname{Diff}^m_b(\mathcal{M}; E, F)$ has a well-defined principal symbol, a smooth section ${}^b\boldsymbol{\sigma}(P)$ of ${}^b\pi^* \operatorname{Hom}(E, F)$ over ${}^bT^*\mathcal{M}\backslash 0$, related to the standard principal symbol of P through the commutative diagram

$$\begin{array}{ccc} \pi^* \operatorname{Hom}(E, F) & \xrightarrow{({}^b\mathrm{ev}^*)^*} & {}^b\pi^* \operatorname{Hom}(E, F) \\ {\scriptstyle \boldsymbol{\sigma}(P)}\big\uparrow & & \big\uparrow{\scriptstyle {}^b\boldsymbol{\sigma}(P)} \\ T^*\mathcal{M}\backslash 0 & \xrightarrow[{}^b\mathrm{ev}^*]{} & {}^bT^*\mathcal{M}\backslash 0 \end{array}$$

in which the bottom map is the dual of ${}^b\mathrm{ev}$ (off of the zero section) and the top map is the natural map.

There is a vector bundle over $\mathcal{M}$ whose smooth sections (up to the boundary) are in one-to one correspondence with the elements of $x^{-1}C^\infty_{\tan}(\mathcal{M}; T\mathcal{M})$, and which we may denote by $x^{-1}\,{}^bT\mathcal{M}$. One can make the case that the principal symbols of elements of cone operators live on the dual of this bundle, denoted $x\,{}^bT^*\mathcal{M}$. But the definition appears to depend on the defining function x. Following a more natural path, define first (see [15]) $C^\infty_{\mathrm{cn}}(\mathcal{M}, T^*\mathcal{M})$ as the $C^\infty(\mathcal{M}; \mathbb{R})$-submodule of $C^\infty(\mathcal{M}; T^*\mathcal{M})$ whose sections are conormal to $\partial\mathcal{M}$, that is, the elements $\alpha \in C^\infty(\mathcal{M}; T^*\mathcal{M})$ such that $\iota^*\alpha = 0$ (where $\iota : \partial\mathcal{M} \to \mathcal{M}$ is the inclusion map). Then again $C^\infty_{\mathrm{cn}}(\mathcal{M}, T^*\mathcal{M})$ is a locally free finitely generated module over $C^\infty(\mathcal{M}; \mathbb{R})$, so it is $C^\infty(\mathcal{M}; \mathbb{R})$-isomorphic to the space of smooth sections of a vector bundle ${}^c\pi : {}^cT^*\mathcal{M} \to \mathcal{M}$. It is not hard to see that ${}^cT^*\mathcal{M}$ is isomorphic to $x\,{}^bT^*\mathcal{M}$. We can now make a precise definition:

A cone metric is a smooth metric on ${}^cT^*\mathcal{M}$, that is, a smooth section of the symmetric tensor product $S^2\,{}^cT^*\mathcal{M}$ which is pointwise strictly positive. (4.2)

The map $C^\infty(\mathcal{M}; {}^cT^*\mathcal{M}) \to C^\infty(\mathcal{M}; T^*\mathcal{M})$ induces a vector bundle homomorphism

$$ {}^c\mathrm{ev} : {}^cT^*\mathcal{M} \to T^*\mathcal{M} $$

The bundle ${}^cT^*\mathcal{M}$ together with the map ${}^c\mathrm{ev}$ is the natural structure bundle in the context of cone operators. A cone operator $A \in x^{-m}\,\mathrm{Diff}(\mathcal{M}; E, F)$ has as principal symbol a smooth section ${}^c\boldsymbol{\sigma}(A)$ of ${}^c\pi^*\,\mathrm{Hom}(E, F)$. This principal symbol is related to the standard principal symbol of A over $\mathring{\mathcal{M}}$ (there A is a standard differential operator) by

$$ {}^c\boldsymbol{\sigma}(A)(\eta) = \boldsymbol{\sigma}(A)({}^c\mathrm{ev}(\eta)). $$

Ellipticity of $A \in x^{-m}\,\mathrm{Diff}^m_b(\mathcal{M}; E, F)$ (c-ellipticity) is defined as invertibility of ${}^c\boldsymbol{\sigma}(A)$. Writing $P = x^m A$ one verifies that c-ellipticity of A is equivalent to b-ellipticity of P.

Associated with A there is another symbol, the "wedge" symbol. This is a differential operator on the inward pointing normal bundle $N_+\partial\mathcal{M}$ of $\partial\mathcal{M}$ in $\mathcal{M}$ (with the zero section, its boundary, included), which we define in the next few paragraphs.

Any $P \in \mathrm{Diff}^m_b(\mathcal{M}; E, F)$ determines an operator

$$ P_b \in \mathrm{Diff}^m_b(\partial\mathcal{M}; E_{\partial\mathcal{M}}, F_{\partial\mathcal{M}}) $$

(where $E_{\partial\mathcal{M}}$ means the part of E over $\partial\mathcal{M}$, as a vector bundle over $\partial\mathcal{M}$) by way of the following procedure. Let ϕ be a smooth section of E along $\partial\mathcal{M}$, let $\tilde\phi$ be a smooth extension to a neighborhood of $\partial\mathcal{M}$. The characterization (4.1) implies that $(P\tilde\phi)|_{\partial\mathcal{M}}$ is independent of the extension $\tilde\phi$. Define

$$ P_b\phi = (P\tilde\phi)|_{\partial\mathcal{M}}. $$

Noting that $x^{-i\sigma}Px^{i\sigma} \in \mathrm{Diff}^m_b(\mathcal{M}; E, F)$ one may define the indicial family of P as the family

$$ \mathbb{C} \ni \sigma \mapsto \widehat{P}(\sigma) = (x^{-i\sigma}Px^{i\sigma})_b \in \mathrm{Diff}^m(\partial\mathcal{M}, E_{\partial\mathcal{M}}, F_{\partial\mathcal{M}}) $$

and the indicial operator

$$ P_\wedge \in \mathrm{Diff}^m(N_+\partial\mathcal{M}; E_\wedge, F_\wedge) $$

with the aid of the Mellin inversion formula, as

$$ P_\wedge u = \frac{1}{2\pi}\int_{\mathbb{R}}\int_0^\infty (x_\wedge/x'_\wedge)^{i\sigma}\widehat{P}(\sigma)u(x'_\wedge, y)\,\frac{dx'_\wedge}{x'_\wedge}\,d\sigma, \quad u \in C^\infty_c(\mathring{N}_+\partial\mathcal{M}; E_\wedge). $$

Here $E_\wedge$ is the pullback of E to $N_+\partial\mathcal{M}$ by the projection map and $x_\wedge$ is the function $dx : N_+\partial\mathcal{M} \to \mathbb{R}$ determined by x; this function is linear on the fibers. The definition of $P_\wedge$ appears to depend on the defining function x, but in fact it does not.

Finally if $A \in x^{-m}\operatorname{Diff}_b^m(N_+\partial\mathcal{M}; E, F)$, define

$$A_\wedge = x_\wedge^{-m} P_\wedge$$

using $P = x^m A$. Again $A_\wedge$ is independent of the defining function x.

If A is c-elliptic, then so is $A_\wedge$, and if P is b-elliptic, then $\widehat{P}(\sigma)$ is elliptic for every σ, $P_\wedge$ is b-elliptic, and the set

$$\operatorname{spec}_b(P) = \{\sigma \in \mathbb{C} : \widehat{P}(\sigma) \text{ is not invertible}\},$$

the boundary spectrum of P (or $A = x^{-m}P$), is a discrete set with the property that $\operatorname{spec}_b(P) \cap \{\sigma \in \mathbb{C} : a < \Im\sigma < b\}$ is finite for every a and $b \in \mathbb{R}$ (see Melrose [30]).

The operator $A_\wedge$ has an important homogeneity property inherited from that of $P_\wedge$. For $\varrho > 0$ let

$$\chi_\varrho : E_\wedge \to E_\wedge$$

denote parallel transport from $p \in N_+\partial\mathcal{M}$ to ϱp. In terms of the definition of $E_\wedge$ as the pull back of the bundle $\pi_E : E \to \mathcal{M}$ by the projection map $\pi : N_+\partial\mathcal{M} \to \partial\mathcal{M}$, we have

$$E_\wedge = \{(p,\eta) : p \in N_+\partial\mathcal{M},\ \eta \in E,\ \pi_{\partial\mathcal{M}}(p) = \pi_E(\eta)\}$$

and $\chi_\varrho(p,\eta) = (\varrho p, \eta)$. This parallel transport was implicitly used above, in the formula defining $P_\wedge$. Define

$$\kappa_\varrho \phi = \varrho^{-\mu}\chi_\varrho^* \phi \quad \text{for sections } \phi : N_{\partial\mathcal{M}} \to E_\wedge \tag{4.3}$$

Using this it is very easy to see that $P_\wedge \kappa_\varrho = \kappa_\varrho P_\wedge$ and from this, that

$$\kappa_\varrho^{-1} A_\wedge \kappa_\varrho = \varrho^m A_\wedge. \tag{4.4}$$

The factor $\varrho^{-\mu}$ in (4.3), correctly chosen, will end up giving that κ_ϱ is unitary. This property is not too important because the formulas in which κ_ϱ appears it does so either as a conjugating operator, as it already did, or as the image by it of some space.

Example 4.5. Let $\mathcal{M}_0$ be a smooth closed orientable Riemannian 2-manifold, let Δ be the positive Laplacian, let $p_0 \in \mathcal{M}_0$. Let $\mathcal{M}$ be the spherical blowup of $\mathcal{M}_0$ at p_0 and $\wp : \mathcal{M} \to \mathcal{M}_0$ the blowdown map. Thus (i) $\mathcal{M}$ is diffeomorphic to $\mathcal{M}_0 \backslash D$ where $D \subset \mathcal{M}_0$ is a (small) metric open disc centered at p_0 in which we have normal coordinates (y_1, y_2) and (ii) $\wp$ gives a diffeomorphism from $\mathring{\mathcal{M}} = \mathcal{M}\backslash\partial\mathcal{M}$ to $\mathcal{M}_0\backslash\{p_0\}$ and sends a suitable tubular neighborhood U of the circle $\partial\mathcal{M}$ to D by way of the map $(x,\theta) \mapsto (y_1, y_2) = (x\cos\theta, x\sin\theta)$.

Let A be the operator determined by Δ on $\mathring{\mathcal{M}}$. Then $A_\wedge$ is just the Euclidean Laplacian of $\mathbb{R}^2$ in polar coordinates (an operator on $\mathring{N}_+(\partial\mathcal{M}) = S^1 \times (0,\infty)$).

5. Domains

The L^2 theory of elliptic cone operators on a compact manifold with boundary is very much like that of elliptic differential operators on a closed manifold. Indeed, suppose given a smooth b-measure on $\mathcal{M}$ (a Borel measure $\mathfrak{m}_b$ such that $x\mathfrak{m}_b$ is a smooth positive measure on $\mathcal{M}$) and hermitian metrics on E and F with which the spaces $x^\mu L^2_b(\mathcal{M};E) = L^2(\mathcal{M};E;x^{-2\mu}\mathfrak{m}_b)$, likewise $x^\mu L^2_b(\mathcal{M};F)$ are defined. Basing the analysis on these Hilbert spaces, any c-elliptic operator $A \in x^{-m}\operatorname{Diff}^m_b(\mathcal{M};E,F)$ is, on its natural maximal domain,

$$\mathcal{D}_{\max}(A) = \{u \in x^\mu L^2_b(\mathcal{M};E) : Au \in x^\mu L^2_b(\mathcal{M};F)\},$$

a Fredholm operator (Lesch [28, Proposition 1.3.16]).

But the theory is also like that of regular elliptic operators on manifolds with boundary, with boundary conditions. This is because if $A \in x^{-m}\operatorname{Diff}^m_b(\mathcal{M};E,F)$ is c-elliptic, then the closure of

$$A : C^\infty_c(\mathring{\mathcal{M}};E) \subset x^\mu L^2_b(\mathcal{M};E) \to x^\mu L^2_b(\mathcal{M};F) \tag{5.1}$$

is again a Fredholm operator (Lesch *op. cit.*). The domain of the closure, $\mathcal{D}_{\min}(A)$, is often a proper subspace of $\mathcal{D}_{\max}(A)$. In this case a condition needs to be imposed to determine which domain is being used to study the operator.

For a proof of the Fredholm properties of A on its minimal and maximal domains (and many other facts concerning elliptic cone operators) the reader may consult, as already indicated, Lesch [28]. Alternatively, the reader may fill in the details of the following outline in which parts of Chapters 4 through 6 of Melrose [30] are assumed.

Let $P = x^m A$. Since P is b-elliptic, the set

$$\{\Im\sigma : \sigma \in \operatorname{spec}_b(P)\}$$

is a discrete subset of $\mathbb{R}$ without points of accumulation. The closure of

$$P : C^\infty_c(\mathcal{M};E) \subset x^{\mu'} L^2_b(\mathcal{M};E) \to x^{\mu'} L^2_b(\mathcal{M};F)$$

is Fredholm if and only if $\mu' \notin -\Im\operatorname{spec}_b(P)$ ([30, Theorem 5.40]), in fact in this case there are operators

$$\begin{aligned} Q &: x^{\mu'} L^2_b(\mathcal{M};F) \to x^{\mu'} H^m_b(\mathcal{M};E),\\ R_{\mathfrak{l}} &: x^{\mu'} L^2_b(\mathcal{M};E) \to x^{\mu'+\varepsilon} H^\infty_b(\mathcal{M};E),\\ R_{\mathfrak{r}} &: x^{\mu'} L^2_b(\mathcal{M};F) \to x^{\mu'+1} H^\infty_b(\mathcal{M};F) \end{aligned} \tag{5.2}$$

(ε is positive and smaller than $\min\{-\mu'-\rho : \rho \in \Im\operatorname{spec}_b(P),\ \rho < -\mu'\}$) such that

$$QP = I - R_{\mathfrak{l}}, \qquad PQ = I - R_{\mathfrak{r}}. \tag{5.3}$$

For nonnegative integers m the Sobolev spaces H^m_b are defined inductively as follows. First $H^0_b = L^2_b$. Next if $m > 0$ is an integer, then $u \in H^m_b$ iff $Yu \in H^{m-1}_b$ for all $Y \in C^\infty_{\tan}(\mathcal{M};T\mathcal{M})$. The space H^{-m}_b is the dual of H^m_b, and for noninteger s, H^s_b is defined by interpolation; see [30] for a more detailed description. A fundamental property of these Sobolev spaces is that the inclusion $x^{\mu''}H_b^{s''} \hookrightarrow x^{\mu'}H_b^{s'}$ is compact if $\mu'' > \mu'$ and $s'' > s'$; this uses that $\mathcal{M}$ is compact. Thus $R_{\mathfrak{l}}$ and $R_{\mathfrak{r}}$ are compact as operators $x^{\mu'}L_b^2 \to x^{\mu'}L_b^2$.

Suppose $\delta > 0$ is such that $(-\mu - m, -\mu - m + \delta] \cap \Im \operatorname{spec}_b(P) = \emptyset$, pick $\mu' = \mu + m - \delta$ above and let Q and $R_{\mathfrak{r}}$ be as stated. So

$$Q : x^{\mu+m-\delta}L_b^2(\mathcal{M}; F) \to x^{\mu+m-\delta}H_b^m(\mathcal{M}; E)$$

and

$$R_{\mathfrak{r}} : x^{\mu+m-\delta}L_b^2(\mathcal{M}; F) \to x^{\mu+m-\delta+1}H_b^\infty(\mathcal{M}; F).$$

If $f \in x^\mu L_b^2$, then $x^m f \in x^{\mu+m}L_b^2$. Since the latter space is a subspace of $x^{\mu+m-\delta}L_b^2$, $Qx^m f \in x^{\mu+m-\delta}H_b^m$. The inclusion $x^{\mu+m-\delta}H_b^m \subset x^\mu H_b^m$ gives in particular $Qx^m f \in x^\mu L_b^2$. Note that $Qx^m : x^\mu L_b^2 \to x^\mu L_b^2$ is compact. Further,

$$AQx^m f = x^{-m}(PQx^m f) = f - x^{-m}R_{\mathfrak{r}}x^m f.$$

Since

$$x^{-m}R_{\mathfrak{r}}x^m f \in x^{\mu+m-\delta+1}H_b^\infty(\mathcal{M}; F) \subset x^\mu L_b^2,$$

Qx^m maps $x^\mu L_b^2$ into the maximal domain of A. The inclusion in the last displayed equation is compact, so $B = Qx^m$ is a compact parametrix for A with compact error. One can show that B maps into the minimal domain, and with some more work (see [19]), that

$$\mathcal{D}_{\min}(A) = \mathcal{D}_{\max}(A) \cap \bigcap_{\delta>0} x^{\mu+m-\delta}H_b^m(\mathcal{M}; E). \tag{5.4}$$

It is easy to see that $x^{\mu+m}H_b^m(\mathcal{M}; E) \subset \mathcal{D}_{\min}(A)$. If $-\mu - m \in \Im \operatorname{spec}_b(P)$, then (5.4) is the best statement one can make about the minimal domain. On the other hand, if $-\mu - m \notin \Im \operatorname{spec}_b(P)$, then we may repeat the argument above with $\delta = 0$ and conclude that $\mathcal{D}_{\min}(A) = x^{\mu+m}H_b^m(\mathcal{M}; E)$. In either case we see that A as an operator on its minimal domain is Fredholm. The argument also gives that $A^\star$, the formal adjoint of A, is Fredholm on its minimal domain. But the Hilbert space adjoint of $A^\star$ with its minimal domain is A with its maximal domain, so A with its maximal domain is also Fredholm.

Since A with either the minimal or the maximal domain is Fredholm, every closed extension of (5.1) is Fredholm. The domain $\mathcal{D}$ of any such extension contains $\mathcal{D}_{\min}$ and is contained in $\mathcal{D}_{\max}$. It also follows that $\mathcal{D}_{\max}(A)/\mathcal{D}_{\min}(A)$ is finite dimensional. So we may parametrize the closed extensions of (5.1) by the set of subspaces of $\mathcal{D}_{\max}/\mathcal{D}_{\min}$.

Define

$$(u, v)_A = (Au, Av) + (u, v), \quad u, v \in \mathcal{D}_{\max}(A)$$

where the inner products on the right are those of $x^\mu L^2(\mathcal{M}; F)$ and $x^\mu L^2(\mathcal{M}; E)$, respectively. This defines an inner product on $\mathcal{D}_{\max}(A)$, and the latter space is complete with respect to the induced norm, which of course is equivalent to the graph norm. Note that the space $\mathcal{D}_{\min}(A)$ is the closure of $C_c^\infty(\mathcal{M}; E)$ in $\mathcal{D}_{\max}(A)$ with respect to the graph norm. We always view $\mathcal{D}_{\max}(A)$ as a Hilbert space with the inner product just defined. The arguments just presented show that the inclusion

$$\mathcal{D}_{\max}(A) \hookrightarrow x^{\mu} L^2_b(\mathcal{M}; E) \tag{5.5}$$

is compact.

The space $\mathcal{D}_{\max}(A)/\mathcal{D}_{\min}(A)$ is isomorphic to the orthogonal $\mathcal{E}(A) = \mathcal{D}_{\min}(A)^{\perp}$ of $\mathcal{D}_{\min}(A)$ in $\mathcal{D}_{\max}(A)$. One can prove (see [15]) that

$$\mathcal{E}(A) = \ker(A^{\star}A + I) \cap \mathcal{D}_{\max}(A).$$

Here $\ker(A^{\star}A + I)$ is the kernel of $A^{\star}A + I$ acting on the space of E-valued distributions on $\mathring{\mathcal{M}}$. We may now write the domain of any closed extension of (5.1) as $\mathcal{D} = D + \mathcal{D}_{\min}$ where D is a subspace of $\mathcal{E}(A)$. This is a particularly useful description when discussing selfadjoint extensions of symmetric elliptic cone operators. Define

$$\mathrm{Gr}(\mathcal{E}(A)) = \{D : D \text{ is a subspace of } \mathcal{E}(A)\}.$$

Thus $\mathrm{Gr}(\mathcal{E}(A)) = \bigcup_k \mathrm{Gr}_k(\mathcal{E}(A))$ is the disjoint union of the various Grassmannian varieties associated with $\mathcal{E}(A)$.

All aspects of this section have counterparts associated with the operator $A_{\wedge}$, except for the Fredholm property of the extensions of

$$A_{\wedge} : C_c^{\infty}(N_+\partial\mathcal{M}; E_{\wedge}) \subset x_{\wedge}^{\mu} L^2_b(N_+\partial\mathcal{M}; E_{\wedge}) \to x_{\wedge}^{\mu} L^2_b(N_+\partial\mathcal{M}; F_{\wedge}).$$

It remains true that $\mathcal{D}_{\wedge,\min}$ has finite codimension in $\mathcal{D}_{\wedge,\max}$, hence the domain of any closed extension is of the form $D_{\wedge} + \mathcal{D}_{\wedge,\min}$. Additionally, because of (4.4), we have that κ_{ϱ} acts on $\mathcal{D}_{\wedge,\max}$ albeit not as a unitary map, only as an isomorphism of Banach spaces. It is easy to see, again using (4.4), that κ_{ϱ} preserves $\mathcal{D}_{\wedge,\min}$. It follows that $\pi_{\wedge,\max}\kappa_{\varrho} = \pi_{\wedge,\max}\kappa_{\varrho}\pi_{\wedge,\max}$ and that we also have an action

$$\boldsymbol{\kappa}_{\varrho} : \mathcal{E}_{\wedge} \to \mathcal{E}_{\wedge}, \quad \boldsymbol{\kappa}_{\varrho} v = \pi_{\wedge,\max}\kappa_{\varrho} v. \tag{5.6}$$

Letting $\pi_{\wedge,\max} : \mathcal{D}_{\wedge,\max} \to \mathcal{D}_{\wedge,\max}$ be the orthogonal projection, we get diffeomorphisms

$$\mathrm{Gr}_k(\mathcal{E}(A_{\wedge})) \ni D_{\wedge} \mapsto \boldsymbol{\kappa}_{\varrho} D_{\wedge} \in \mathrm{Gr}_k(\mathcal{E}(A_{\wedge})). \tag{5.7}$$

The infinitesimal generator of the one-parameter family of diffeomorphisms $\boldsymbol{\kappa}_{e^t}$,

$$\mathcal{T}(D_{\wedge}) = \frac{d}{dt}\bigg|_{t=0} \boldsymbol{\kappa}_{e^t} D_{\wedge}$$

is a smooth (in fact real-analytic) vector field.

There is a natural isomorphism (see [15])

$$\theta : \mathcal{E}(A) \to \mathcal{E}(A_{\wedge}) \tag{5.8}$$

that allows passage from domains for closed extensions of A to domains of closed extensions of $A_{\wedge}$. This map and the action (5.7) are fundamental in the analysis of the resolvent of A with a given domain.

An element $D_{\wedge} \in \mathrm{Gr}_k(\mathcal{E}(A_{\wedge}))$ is said to be stationary if it is a fixed point of the action $\boldsymbol{\kappa}$. A domain $\mathcal{D} = D + \mathcal{D}_{\min}$ (or $\mathcal{D}_{\wedge} = D_{\wedge} + \mathcal{D}_{\min}$) is said to be stationary if $\theta(D)$ (or $D_{\wedge}$) is so. (5.9)

Stationary domains always exist because the Euler characteristic of $\mathrm{Gr}_k(\mathcal{E}_\wedge)$ is not zero, so the vector field $\mathcal{T}$ must vanish somewhere.

In the following sections we drop the argument A from objects whenever there is no ambiguity ($\mathcal{D}_{\min}$, $\mathcal{D}_{\max}$, $\mathcal{E}$, etc.), and add $\wedge$ as a subscript for objects associated with $A_\wedge$ ($\mathcal{D}_{\wedge,\min}$, $\mathcal{D}_{\wedge,\max}$, $\mathcal{E}_\wedge$, etc.).

Example 5.10. Continuing with the setup of Example 4.5, the L^2 spaces are those defined by the measure associated with the metric. Using that $\mathring{\mathcal{M}}$ is diffeomorphic to $\mathcal{M}_0\backslash\{p_0\}$ we see that $\mathcal{D}_{\min}$ is naturally isomorphic to the domain of the closure of

$$\Delta : C_c^\infty(\mathcal{M}_0\backslash\{p_0\}) \subset L^2(\mathcal{M}_0) \to L^2(\mathcal{M}_0).$$

It is immediate that $\{u \in H^2(\mathcal{M}_0) : u(p_0) = 0\}$ contains $\mathcal{D}_{\min}(A)$; in fact equality holds,

$$\mathcal{D}_{\min} = \{u \in H^2(\mathcal{M}_0) : u(p_0) = 0\},$$

as the reader may easily verify.

The maximal domain contains $H^2(\mathcal{M}_0)$ (more properly, $\wp^* H^2(\mathcal{M}_0)$). But it contains more elements. Namely, let $g^2 : \mathcal{M}_0 \to \mathbb{R}$ be a smooth function such that $g^2(p) = \mathrm{dist}(p, p_0)^2$ if p is near p_0. Then $\log g \in L^2(\mathcal{M})$. Since

$$\Delta \log g = \delta_{p_0} + h = \text{the Dirac } \delta \text{ at } p_0 \text{ plus a smooth function on } \mathcal{M}_0,$$

$A \log g = h$ (because A only "sees" what happens in $\mathcal{M}_0\backslash\{p_0\}$). Thus $A \log g \in L^2$, hence $\log g \in \mathcal{D}_{\max}(A)$. One can show that

$$\mathcal{D}_{\max}(A) = H^2(\mathcal{M}_0) \oplus \mathrm{span} \log g.$$

Similarly, for $A_\wedge$, which we may treat as the Euclidean Laplacian restricted to $\mathbb{R}^2\backslash 0$, we have that $\mathcal{D}_{\wedge,\min} = \{u \in H^2(\mathbb{R}^2) : u(0) = 0\}$ and

$$\mathcal{D}_{\wedge,\max} = H^2(R^2) \oplus \mathrm{span} \log g_\wedge.$$

where $g_\wedge$ is any compactly supported function on $\mathbb{R}^2$ which is smooth outside 0 and satisfies $g_\wedge(p) = \|p\|$ (the Euclidean norm of $p \in \mathbb{R}^2$) near 0. Thus if χ is an arbitrary compactly supported function on $\mathbb{R}^2$ with $\chi(0) \neq 0$, then

$$\mathcal{D}_{\wedge,\max} = \mathcal{D}_{\wedge,\min} \oplus \mathrm{span}\{\chi, \log g_\wedge\}.$$

The space $\mathcal{E}_\wedge$ is two-dimensional, spanned by the functions

$$\pi_{\wedge,\max}\chi \quad \text{and} \quad \pi_{\wedge,\max} \log g_\wedge.$$

It is also equal to $\ker(A_\wedge^2 + I) \cap \mathcal{D}_{\wedge,\max}$ (we are using that $A_\wedge$ is symmetric on $C_c^\infty(\mathbb{R}^2\backslash 0)$). The statement that $u \in L^2(\mathbb{R}^2)$ satisfies $A_\wedge^2 u + u = 0$ is equivalent to the statement that $\Delta^2 u + u$ is supported at 0. Passing to Fourier transform we see that $\widehat{u}(\xi) = p(\xi)/(1 + \|\xi\|^4)$ where p is a polynomial. Using that $\widehat{u}(\xi)$ is also in $L^2(\mathbb{R}^2)$ and that $A_\wedge u \in L^2(\mathbb{R}^2\backslash 0)$ (that is, $\Delta u = c\delta_0 + f$, $c \in \mathbb{C}$, $f \in L^2(\mathbb{R}^2)$) we get conditions on p from which one concludes that u must be a linear combination of the functions

$$u_1(x) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} e^{ix\cdot\xi} \frac{1}{1 + \|\xi\|^4}\, d\xi, \qquad u_2(x) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} e^{ix\cdot\xi} \frac{\|\xi\|^2}{1 + \|\xi\|^4}\, d\xi.$$

Clearly $u_1 \in H^2(\mathbb{R}^2)$. As for u_2, note that

$$\Delta u_2(x) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} e^{ix\cdot\xi} \frac{\|\xi\|^4}{1+\|\xi\|^4}\, d\xi = \delta_0 - u_1(x).$$

Restricting to $\mathbb{R}^2\backslash 0$ we have $\Delta u_2 = -u_1$, that is, $A_\wedge u_2 = -u_1$. Also $A_\wedge u_1 = u_2$, so these two functions do belong to $\ker(A_\wedge^2 + I)$. Note that $(u_1, u_2)_{A_\wedge} = 0$, so $\{u_1, u_2\}$ is an $A_\wedge$-orthogonal basis of $\mathcal{E}_\wedge$. Finally, note that $\|u_1\|^2_{A_\wedge} = \|u_2\|^2_{A_\wedge}$; let μ denote this number ($\mu = 1/8$). The formulas

$$\pi_{\wedge,\max}\kappa_\varrho u_j = \frac{1}{\mu}\big((\kappa_\varrho u_j, u_1)_{A_\wedge} u_1 + (\kappa_\varrho u_j, u_2)_{A_\wedge} u_2\big), \quad j = 1, 2$$

give

$$\pi_{\wedge,\max}\kappa_\varrho u_1 = u_1, \quad \pi_{\wedge,\max}\kappa_\varrho u_2 = -\frac{2}{\pi}\log\varrho^2\, u_1 + u_2.$$

The integrals leading to these formulas can be evaluated by elementary means using polar coordinates.

Since $\mathcal{E}_\wedge$ is two-dimensional, the only interesting Grassmannian variety based on it is $\mathrm{Gr}_1(\mathcal{E}_\wedge)$, the one-dimensional complex projective space, in other words, the Riemann sphere. The action of $\boldsymbol{\kappa}_\varrho$ on elements of $\mathrm{Gr}_1(\mathcal{E}_\wedge)$ is easily described using the formulas for $\pi_{\wedge,\max}\kappa_\varrho u_j$. If $D \in \mathrm{Gr}_1(\mathcal{E}_\wedge)$ is spanned by $\alpha u_1 + \beta u_2$, $(\alpha, \beta) \neq 0$, then of course

$$\boldsymbol{\kappa}_\varrho D = \mathrm{span}\left\{\left(\alpha - \frac{2\beta}{\pi}\log\varrho^2\right) u_1 + \beta u_2\right\}. \tag{5.11}$$

The curve $\varrho \mapsto \boldsymbol{\kappa}_\varrho D$ has a limit as $\varrho \to 0$ or ∞. Namely, if $\beta = 0$, then $\boldsymbol{\kappa}_\varrho D = D_{\wedge,F} = \mathrm{span}\{u_1\}$ and if $\beta \neq 0$, then (once $\log\varrho \neq \alpha\pi/4\beta$)

$$\mathrm{span}\left\{\left(\alpha - \frac{2\beta}{\pi}\log\varrho^2\right) u_1 + \beta u_2\right\} = \mathrm{span}\left\{u_1 + \frac{\pi\beta}{\pi\alpha - 2\beta\log\varrho^2} u_2\right\}$$

also tends to $D_{\wedge,F}$, regardless of whether ϱ tends to 0 or ∞.

Also the infinitesimal generator of the one-parameter group $t \mapsto \boldsymbol{\kappa}_{e^t}$ can easily be described in terms of the homogenous coordinates on S^2. Writing either $u_1 + \zeta u_2$ or $z u_1 + u_2$ as basis for elements of $\mathrm{Gr}_1(\mathcal{E}_\wedge)$, the formulas above give, if $D = \mathrm{span}\{z_0 u_1 + u_2\}$, that the curve $\varrho \mapsto \boldsymbol{\kappa}_\varrho D$ is

$$\varrho \mapsto z(\varrho) = z_0 - \frac{2}{\pi}\log\varrho^2$$

in terms of the ζ coordinate. The derivative of $\zeta(\varrho)$ is

$$\frac{dz}{d\varrho}\frac{\partial}{\partial z}\bigg|_{\zeta(\varrho)} + \frac{d\overline{z}}{d\varrho}\frac{\partial}{\partial\overline{z}}\bigg|_{z(\varrho)} = -\frac{4}{\varrho\pi}\left(\frac{\partial}{\partial z}\bigg|_{z(\varrho)} + \frac{\partial}{\partial\overline{z}}\bigg|_{z(\varrho)}\right).$$

Evaluating at $\varrho = 1$ gives $\mathcal{T}$ at D. Thus if $z = x + iy$, then

$$\mathcal{T} = -\frac{4}{\pi}\frac{\partial}{\partial x}.$$

In terms of the coordinate $\zeta = \xi + i\eta$ we have

$$\mathcal{T} = -\frac{4}{\pi}\left((\eta^2 - \xi^2)\frac{\partial}{\partial\xi} + 2\xi\eta\frac{\partial}{\partial y}\right)$$

which has a zero at $\zeta = 0$ (which corresponds to $D_{\wedge,F}$).

6. Spectra

We assume now that $F = E$. Write $A_{\mathcal{D}}$ for the operator $A \in x^{-m}\operatorname{Diff}^m_b(\mathcal{M}; E)$ with domain $\mathcal{D}$; we continue to assume that A is c-elliptic and $\mathcal{M}$ is compact. Since $\operatorname{Ind}(A_{\mathcal{D}}) \neq 0$ implies $\operatorname{spec}(A_{\mathcal{D}}) = \mathbb{C}$, having index 0 is necessary in order for $A_{\mathcal{D}}$ to have nonempty resolvent set. It was pointed out by Lesch, *op. cit.* that the index of A with domain $\mathcal{D}$ ($A_{\mathcal{D}}$ for short) is given by the formula

$$\operatorname{Ind}(A_{\mathcal{D}}) = \operatorname{Ind}(A_{\mathcal{D}_{\min}}) + \dim D.$$

Since $\dim \mathcal{D} \geq 0$, a necessary condition for A to admit a closed extension with nonempty resolvent set is that $\operatorname{Ind}(A_{\mathcal{D}_{\min}}) \leq 0$. Since $\dim D \leq \dim \mathcal{E}$, also the condition $\operatorname{Ind}(A_{\mathcal{D}_{\max}}) \geq 0$ is necessary. Of course these two conditions together imply that there is a subspace $D \subset \mathcal{E}$ such that with $\mathcal{D} = D + \mathcal{D}_{\min}$ we have $\operatorname{Ind}(A_{\mathcal{D}}) = 0$. For this reason we assume henceforth that

$$\operatorname{Ind}(A_{\mathcal{D}_{\min}}) \leq 0 \leq \operatorname{Ind}(A_{\mathcal{D}_{\max}}). \tag{6.1}$$

Thus generally we will be interested in the extensions of (5.1) with domain $\mathcal{D} = D + \mathcal{D}_{\min}$ where $D \in \operatorname{Gr}_{d''}(\mathcal{E})$, $d'' = -\operatorname{Ind}(A_{\mathcal{D}_{\min}})$.

Suppose $A_{\mathcal{D}} - \lambda_0$ is invertible. Then, since the inclusion $\mathcal{D} \hookrightarrow x^\mu L^2_b(\mathcal{M}; E)$ is compact (because of (5.5)), the spectrum of A is a discrete subset of $\mathbb{C}$. It is convenient to classify the spectrum as follows (see [15]). Let

$$\text{bg-spec}(A) = \bigcap_{\mathcal{D}=D+\mathcal{D}_{\min}} \operatorname{spec}(A_{\mathcal{D}})$$

where D runs over all elements of $\operatorname{Gr}(\mathcal{E})$. The set bg-spec$(A)$ is the background spectrum of A; it is the subset of $\mathbb{C}$ present in all closed extensions of (5.1). It is easy to verify that $\lambda \in \text{bg-spec}(A)$ if and only if $A_{\mathcal{D}_{\min}} - \lambda$ is not injective or $A_{\mathcal{D}_{\max}} - \lambda$ is not surjective. We also define

$$\text{bg-res}(A) = \mathbb{C} \setminus \text{bg-spec}(A).$$

With this we can split spec$(A_{\mathcal{D}})$ as

$$\operatorname{spec}(A_{\mathcal{D}}) = \text{bg-spec}(A) \cup \big(\text{bg-res}(A) \cap \operatorname{spec}(A_{\mathcal{D}})\big).$$

The part of the spectrum of $A_{\mathcal{D}}$ in bg-res(A) can be analyzed further.

For $\lambda \in \text{bg-res}(A)$ define

$$\mathcal{K}_\lambda = \ker(A_{\mathcal{D}_{\max}} - \lambda).$$

The dimension of $\mathcal{K}_\lambda$ is independent of λ, equal to $d' = \operatorname{Ind}(A_{\mathcal{D}_{\max}})$. These vector spaces form a complex vector bundle over bg-res(A).

Let $\mathcal{D} = D + \mathcal{D}_{\min}$ be some domain. If $\lambda \in \text{bg-res}(A)$, then $\lambda \in \operatorname{spec}(A_{\mathcal{D}})$ if and only if $A_{\mathcal{D}} - \lambda$ has nontrivial kernel K. Of course $K = \mathcal{K}_\lambda \cap \mathcal{D}$, so

$$\text{bg-res}(A) \cap \operatorname{spec}(A_{\mathcal{D}}) = \{\lambda \in \text{bg-res}(A) : \mathcal{D} \cap \mathcal{K}_\lambda \neq 0\}.$$

Let $\pi_{\max} : \mathcal{D}_{\max} \to \mathcal{D}_{\max}$ be the orthogonal projection on $\mathcal{E}$. The restriction of $\pi_{\max}$ to $\mathcal{K}_\lambda$ is injective. This is elementary: if $\phi \in \mathcal{K}_\lambda$ and $\pi_{\max}(\phi) = 0$, then $\phi \in \mathcal{D}_{\min}$; since $A_{\mathcal{D}_{\min}} - \lambda$ is injective (because $\lambda \in \text{bg-res}(A)$), $\phi = 0$. Letting $K_\lambda = \pi_{\max}\mathcal{K}_\lambda$ one gets from this that

$$\lambda \in \text{bg-res}(A) \cap \operatorname{spec}(A_{\mathcal{D}}) \iff K_\lambda \cap D \neq 0. \tag{6.2}$$

Note that $K_\lambda \cap D = 0$ implies $K_\lambda \oplus D = \mathcal{E}$ because $d' + d'' = \dim \mathcal{E}$.

Given $D \in \operatorname{Gr}_{d''}(\mathcal{E})$, let

$$\mathscr{V}_D = \{K \in \operatorname{Gr}_{d'}(\mathcal{E}) : D \cap K \neq 0\}. \tag{6.3}$$

The set $\operatorname{Gr}_{d'}(\mathcal{E})$ is a compact complex manifold and $\mathscr{V}_D$ is a complex subvariety of complex codimension 1 (locally given as the set of zeros of a determinant). Of course we also have the reverse variety: if $K \in \operatorname{Gr}_{d'}(\mathcal{E})$, then there is an associated variety $\mathscr{V}_K \subset \operatorname{Gr}_{d''}(\mathcal{E})$. Using this terminology we may rephrase (6.2) as

$$\text{bg-res}(A) \cap \operatorname{spec}(A_{\mathcal{D}}) = \{\lambda : K_\lambda \in \mathscr{V}_D\}. \tag{6.4}$$

In other words, in terms of the map

$$\text{bg-res}(A) \ni \lambda \xrightarrow{K} K_\lambda \in \operatorname{Gr}_{d'}(\mathcal{E}),$$

a holomorphic map, we have $\text{bg-res}(A) \cap \operatorname{spec}(A_{\mathcal{D}}) = K^{-1}(\mathscr{V}_D)$.

Again all objects described so far have their counterparts in the case of $A_\wedge$, for example $\mathcal{K}_{\wedge,\lambda} = \ker(A_{\mathcal{D}_{\wedge,\max}} - \lambda)$ when $\lambda \in \text{bg-res}(A_\wedge)$. The homogeneity property (4.4) implies that $\text{bg-spec}(A_\wedge)$ consists of a union of closed rays and sectors issuing from the origin. Namely, if $\lambda_0 \in \mathbb{C}\backslash 0$ and $A_\wedge - \lambda_0$ is not injective on $\mathcal{D}_{\wedge,\min}$ or not surjective on $\mathcal{D}_{\wedge,\max}$, then the same is true for $\kappa_\varrho^{-1}(A - \lambda_0)\kappa_\varrho$ since

$$\kappa_\varrho^{-1}(A - \lambda_0)\kappa_\varrho = \varrho^m(A_\wedge - \varrho^{-m}\lambda_0). \tag{6.5}$$

Thus $\text{bg-res}(A_\wedge)$ is a union of open sectors with vertex at the origin. It is immediate that

$\forall D_\wedge \in \mathcal{E}_\wedge$: $A_\wedge - \lambda$ with domain $\mathcal{D}_\wedge = D_\wedge + \mathcal{D}_{\wedge,\min}$ is Fredholm and $\operatorname{Ind}(A_{\wedge,\mathcal{D}_\wedge} - \lambda)$ is constant on each component of $\text{bg-res}(A_\wedge)$. (6.6)

Note also that (6.5) implies

$$\kappa_\varrho \mathcal{K}_{\wedge,\lambda} = \mathcal{K}_{\wedge,\varrho^m\lambda} \tag{6.7}$$

Example 6.8. Continuing with Example 5.10, we have

$$\text{bg-spec}(A) = \{\lambda \in \mathbb{C} : \exists u \in C^\infty(\mathcal{M}_0),\ u \neq 0, u(p_0) = 0,\ \Delta u = \lambda u\}.$$

This is a subset of spectrum of Δ on $\mathcal{M}_0$. An interesting description of this set is as the set of eigenvalues of Δ for which there is a mode with p_0 in its nodal set.

And since $A_\wedge$ is the positive Euclidean Laplacian on $\mathbb{R}^2\backslash 0$,

$$\text{bg-spec}(A_\wedge) = [0,\infty) \subset \mathbb{C}$$

Namely, if λ is real and nonnegative, then $A_\wedge - \lambda$, while injective on $\mathcal{D}_{\wedge,\min}$, is not surjective on $\mathcal{D}_{\wedge,\max}$, in fact its range is dense but not closed.

7. Rays of minimal growth for elliptic cone operators

Following Seeley's program [34], the first step in determining the meromorphic structure of the zeta function of an elliptic cone operator is to determine the existence of rays of minimal growth.

Theorem 7.1 ([14, Theorem 6.36]). *Let $A \in x^{-m}\operatorname{Diff}^m_b(\mathcal{M},E)$, let $\Lambda \subset \mathbb{C}$ be a closed sector, and let $\mathcal{D} = D + \mathcal{D}_{\min}$ be the domain of a closed extension of* (5.1). *Suppose that ${}^c\!\boldsymbol{\sigma}(A) - \lambda$ is invertible on $({}^cT^*\mathcal{M}\backslash 0)\times\Lambda$ and that Λ is a sector of minimal growth for $A_\wedge$ with domain $\theta(D) + \mathcal{D}_{\wedge,\min}$. Then Λ is a sector of minimal growth for $A_{\mathcal{D}}$.*

The proof in [14], relies on constructing first a left inverse for $A-\lambda$ on the minimal domain of A (always $\lambda\in\Lambda$, $|\lambda|$ large), and then correcting additively to get an inverse for $A_{\mathcal{D}} - \lambda$. We will describe some aspects of this in the case of $A_{\wedge,\mathcal{D}_\wedge} - \lambda$. In particular, we will discuss the issue of exactly when is Λ a sector of minimal growth for $A_\wedge$ with domain $\mathcal{D}_\wedge = \theta(D) + \mathcal{D}_{\wedge,\min}$.

Suppose for the time being that Λ is a closed sector such that $\Lambda\backslash 0$ is contained in bg-res$(A_\wedge)$. For example, if Λ is a sector of minimal growth for $A_{\wedge,\mathcal{D}_\wedge}$, then there is $R \geq 0$ such that $A_{\wedge,\mathcal{D}_\wedge} - \lambda$ is invertible for $\lambda \in \Lambda_R = \{\lambda\in\Lambda : |\lambda| > R\}$. This implies that $\Lambda_R \subset$ bg-res$(A_\wedge)$, therefore that

$$\Lambda\backslash 0 \subset \text{bg-res}(A_\wedge), \tag{7.2}$$

because the latter set is a union of open sectors.

Because of (6.6), $A_\wedge - \lambda$ has a left inverse on $\mathcal{D}_{\wedge,\min}$ for every $\lambda\in\Lambda\backslash 0$. In fact there is a left inverse with range $\mathcal{D}_{\wedge,\min}$ and kernel equal to the orthogonal space (in L^2_b) of $(A_\wedge - \lambda)(\mathcal{D}_{\wedge,\min})$ which we will denote $B_{\wedge,\min}(\lambda)$. Note that

$$B_{\wedge,\min}(\lambda)(A_\wedge - \lambda) : \mathcal{D}_{\wedge,\max} \to \mathcal{D}_{\wedge,\max} \text{ is a projection onto } \mathcal{D}_{\wedge,\min}. \tag{7.3}$$

Also due to (6.6), we have that $A_\wedge - \lambda$ with domain $\mathcal{D}_{\wedge,\max}$ has a right inverse for each $\lambda\in\Lambda_0$ with range equal to $\mathcal{K}^\perp_{\wedge,\lambda}\cap\mathcal{D}_{\wedge,\max}$. Here $\mathcal{K}^\perp_{\wedge,\lambda}$ is the orthogonal space, also in L^2_b of $\mathcal{K}_{\wedge,\lambda}$. We will denote this specific right inverse by $B_{\wedge,\max}(\lambda)$.

The homogeneity property (4.4) of $A_\wedge$ and the fact that κ_ϱ preserves L^2 orthogonality of spaces (unitarity is not the relevant reason) imply that

$$\kappa_\varrho^{-1}B_{\wedge,\min}(\varrho^m\lambda)\kappa_\varrho = \varrho^{-m}B_{\wedge,\min}(\lambda),\ \kappa_\varrho^{-1}B_{\wedge,\max}(\varrho^m\lambda)\kappa_\varrho = \varrho^{-m}B_{\wedge,\max}(\lambda). \tag{7.4}$$

It is automatic that

$$B_{\wedge,\min}(\lambda), B_{\wedge,\max}(\lambda) : x^\mu L^2_b(\mathcal{M};E) \to \mathcal{D}_{\wedge,\max}$$

are continuous maps depending smoothly on λ. Further, their homogeneity implies decay of their norm as operators $x^\mu L^2_b(\mathcal{M};E) \to x^\mu L^2_b(\mathcal{M};E)$. For instance,

$$\begin{aligned}\|B_{\wedge,\min}(\varrho^m\lambda)u\| = \|\varrho^{-m}\kappa_\varrho B_{\wedge,\min}(\lambda)\kappa_\varrho^{-1}u\| = \varrho^{-m}\|B_{\wedge,\min}(\lambda)\kappa_\varrho^{-1}u\| \\ \leq \varrho^{-m}\|B_{\wedge,\min}(\lambda)\|\,\|\kappa_\varrho^{-1}(\lambda)u\| = \varrho^{-m}\|B_{\wedge,\min}(\lambda)\|\,\|u\|,\end{aligned}$$

so $\|B_{\wedge,\min}(\lambda)\| \leq |\lambda|^{-1}\|B_{\wedge,\min}(\lambda/|\lambda|)\|$ when $\lambda \in \Lambda\backslash 0$.

Now pick a domain $\mathcal{D}_\wedge = D_\wedge + \mathcal{D}_{\wedge,\min}$. Assume that for $\lambda \in \Lambda\backslash 0$ we have $\operatorname{Ind}(A_{\mathcal{D}_\wedge} - \lambda) = 0$; this is the case if we already know that Λ is a sector of minimal growth for $A_{\wedge,\mathcal{D}_\wedge}$. Then, as discussed in the previous section in the case of A, and keeping in mind (7.2), the part of the resolvent set of $A_{\wedge,\mathcal{D}_\wedge}$ in $\Lambda\backslash 0$ is

$$\mathscr{R} = \operatorname{res}(A_{\wedge,\mathcal{D}_\wedge}) \cap (\Lambda\backslash 0) = \{\lambda \in \Lambda\backslash 0 : \mathcal{K}_{\wedge,\lambda} \cap \mathcal{D}_\wedge = 0\}. \tag{7.5}$$

Recall that $\mathcal{K}_{\wedge,\lambda} = \ker(A_{\wedge,\mathcal{D}_{\wedge,\max}} - \lambda)$. Because of the analyticity in the parameter λ of $(A_{\wedge,\mathcal{D}_{\wedge,\max}} - \lambda)$, the set $\mathscr{R}$ is the complement of a closed discrete set in $\Lambda\backslash 0$.

If $\lambda \in \mathscr{R}$, then

$$\mathcal{K}_{\wedge,\lambda} + \mathcal{D}_\wedge = \mathcal{D}_{\wedge,\max}$$

as a direct sum. For such λ define

$$\pi_{\mathcal{K}_{\wedge,\lambda},\mathcal{D}_\wedge} = \text{projection on } \mathcal{K}_{\wedge,\lambda} \text{ along } \mathcal{D}_\wedge.$$

Now,

$$(A_\wedge - \lambda)B_{\wedge,\max}(\lambda) = I$$

and of course

$$(A_\wedge - \lambda)\pi_{\mathcal{K}_{\wedge,\lambda},\mathcal{D}_\wedge}B_{\wedge,\max}(\lambda) = 0$$

so

$$(A_\wedge - \lambda)(I - \pi_{\mathcal{K}_{\wedge,\lambda},\mathcal{D}_\wedge})B_{\wedge,\max}(\lambda) = I.$$

The operator

$$B_{\mathcal{D}_\wedge}(\lambda) = (I - \pi_{\mathcal{K}_{\wedge,\lambda},\mathcal{D}_\wedge})B_{\wedge,\max}(\lambda) \tag{7.6}$$

obviously maps into $\mathcal{D}_\wedge$ an thus

$$B_{\mathcal{D}_\wedge}(\lambda) : x^\mu L^2_b(N_+\partial\mathcal{M};E_\wedge) \to \mathcal{D}_\wedge$$

is a right inverse for

$$(A_\wedge - \lambda) : \mathcal{D}_\wedge \to x^\mu L^2_b(N_+\partial\mathcal{M};E_\wedge).$$

We will let the reader show that $B_{\mathcal{D}_\wedge}(\lambda)$ is also surjective, so that we may conclude that $B_{\mathcal{D}_\wedge}(\lambda)$ is the resolvent (in $\mathscr{R}$) of the unbounded operator

$$A_\wedge : \mathcal{D}_\wedge \subset x^\mu L^2_b(N_+\partial\mathcal{M};E_\wedge) \to x^\mu L^2_b(N_+\partial\mathcal{M};E_\wedge).$$

Another tautological formula for $B_{\mathcal{D}_\wedge}(\lambda)$ is

$$B_{\mathcal{D}_\wedge}(\lambda) = B_{\wedge,\min}(\lambda) + \big(I - B_{\wedge,\min}(\lambda)(A_\wedge - \lambda)\big)B_{\mathcal{D}_\wedge}(\lambda)$$

(just expand the right-hand side and use that $(A_\wedge - \lambda)B_{\mathcal{D}_\wedge}(\lambda)$ is the identity on $x^\mu L^2_b(N_+\partial\mathcal{M};E_\wedge)$). Replacing (7.6) in the right-hand side of this formula and some more elementary algebraic manipulations (this time exploiting the fact that

$(A_\wedge - \lambda)B_{\wedge,\max}(\lambda)$ is the identity on $x^\mu L^2_b(N_+\partial\mathcal{M}; E_\wedge))$ leads to

$$B_{\mathcal{D}_\wedge}(\lambda) = B_{\wedge,\max}(\lambda) - \big(I - B_{\wedge,\min}(\lambda)(A_\wedge - \lambda)\big)\pi_{\mathcal{K}_{\wedge,\lambda},\mathcal{D}_\wedge} B_{\wedge,\max}(\lambda).$$

Because of (7.3), the operator $I - B_{\wedge,\min}(\lambda)(A_\wedge - \lambda)$ is a projection with kernel $\mathcal{D}_{\wedge,\min}$. Using that $I - \pi_{\wedge,\max}$ is a projection on $\mathcal{D}_{\wedge,\min}$ we thus get

$$I - B_{\wedge,\min}(\lambda)(A_\wedge - \lambda) = \big(I - B_{\wedge,\min}(\lambda)(A_\wedge - \lambda)\big)\pi_{\wedge,\max}$$

The projection $\pi_{\mathcal{K}_{\wedge,\lambda},\mathcal{D}_\wedge}$ also vanishes on $\mathcal{D}_{\wedge,\min}$, so

$$\pi_{\mathcal{K}_{\wedge,\lambda},\mathcal{D}_\wedge} = \pi_{\mathcal{K}_{\wedge,\lambda},\mathcal{D}_\wedge}\pi_{\wedge,\max}$$

Therefore

$$B_{\mathcal{D}_\wedge}(\lambda) = B_{\wedge,\max}(\lambda) - \big(I - B_{\wedge,\min}(\lambda)(A_\wedge - \lambda)\big)\pi_{\wedge,\max}\pi_{\mathcal{K}_{\wedge,\lambda},\mathcal{D}_\wedge}\pi_{\wedge,\max}B_{\wedge,\max}(\lambda).$$

We will now rewrite $\pi_{\wedge,\max}\pi_{\mathcal{K}_{\wedge,\lambda},\mathcal{D}_\wedge}\pi_{\wedge,\max}$.

The subspace $K_{\wedge,\lambda} = \pi_{\wedge,\max}\mathcal{K}_{\wedge,\lambda}$ of $\mathcal{E}_\wedge$ is isomorphic to $\mathcal{K}_{\wedge,\lambda}$. The characterization (7.5) of $\mathscr{R}$ can also be given in terms of $K_{\wedge,\lambda}$ and $D_\wedge$, as

$$\mathscr{R} = \{\lambda \in \Lambda\backslash 0 : K_{\wedge,\lambda} \cap D_\wedge = 0\}. \tag{7.7}$$

Thus whenever $\lambda \in \mathscr{R}$, $\mathcal{E}_\wedge = K_{\wedge,\lambda} \oplus D_\wedge$. Let then $\pi_{K_\lambda,D_\lambda} : \mathcal{E}_\wedge \to \mathcal{E}_\wedge$ be the projection on K_λ along $D_\wedge$. Then

$$\pi_{\wedge,\max}\pi_{\mathcal{K}_{\wedge,\lambda},\mathcal{D}_\wedge}\pi_{\wedge,\max} = \pi_{K_{\wedge,\lambda},D_\wedge}\pi_{\wedge,\max}.$$

Indeed, suppose $u \in \mathcal{E}_\wedge$. Then

$$u = \phi + v, \quad \phi = \pi_{\mathcal{K}_{\wedge,\lambda},\mathcal{D}_\wedge} u \in \mathcal{K}_{\wedge,\lambda}, \quad v \in \mathcal{D}_\wedge.$$

Let $\phi_0 = \pi_{\wedge,\max}\phi$, $v_0 = \pi_{\wedge,\max}v$. both $\phi_1 = \phi - \phi_0$ and $v_1 = v - v_0$ belong to $\mathcal{D}_{\wedge,\min}$. Since $u \in \mathcal{E}_\wedge$, the formula $u = (\phi_0 + v_0) + (\phi_1 + v_1)$ gives $\phi_1 + v_1 = 0$. So

$$\pi_{\wedge\,\max}\pi_{\mathcal{K}_{\wedge,\lambda},\mathcal{D}_\wedge} u = \phi_0 = \pi_{K_{\wedge,\lambda},D_\wedge} u.$$

Thus

$$B_{\mathcal{D}_\wedge}(\lambda) = B_{\wedge,\max}(\lambda) - \big(I - B_{\wedge,\min}(\lambda)(A_\wedge - \lambda)\big)\pi_{K_{\wedge,\lambda},D_\wedge}\pi_{\wedge,\max}B_{\wedge,\max}(\lambda). \tag{7.8}$$

We now discuss necessary and sufficient conditions for Λ to be sector of minimal growth for $A_\wedge$ with domain $D_\wedge$. This pertains to two issues: existence of the resolvent for all sufficiently large $\lambda \in \Lambda$, and decay estimates for the norm of the resolvent. To get a hold on these issues, we fix $\lambda_0 \in \Lambda\backslash 0$ and analyze $B_{\mathcal{D}_\wedge}(\lambda)$ as λ moves to ∞ along the ray through λ_0. We do this by setting $\lambda = \varrho^m\lambda_0$ in (7.8) and analyzing the expressions that result from using (7.4) as $\varrho \to \infty$.

The issue of existence of the inverse of $A_{\wedge,\mathcal{D}_\wedge} - \lambda$ for $\lambda = \varrho^m\lambda_0$ for ϱ large is by now easily understood. The condition $K_{\wedge,\varrho^m\lambda_0} \cap D = 0$ is both necessary and sufficient in order for $A_{\wedge,\mathcal{D}_\wedge} - \varrho^m\lambda_0$ to be invertible. Since $\boldsymbol{\kappa}_\varrho : \mathcal{E}_\wedge \to \mathcal{E}_\wedge$ is an isomorphism, this condition is equivalent to $\boldsymbol{\kappa}_\varrho^{-1}K_{\wedge,\varrho^m\lambda_0} \cap \boldsymbol{\kappa}_\varrho^{-1}D = 0$, that is, $K_{\wedge,\lambda_0} \cap \boldsymbol{\kappa}_\varrho^{-1}D = 0$ (see (6.7)). Therefore, the requirement is

$$\boldsymbol{\kappa}_\varrho^{-1}D_\wedge \notin \mathscr{V}_{K_{\wedge,\lambda_0}} \text{ for all sufficiently large } \varrho.$$

We assume this henceforth.

As for the issue of decay, straight from (7.4) we get

$$B_{\wedge,\max}(\varrho^m\lambda_0) = \varrho^{-m}\kappa_\varrho B_{\wedge,\max}(\lambda_0)\kappa_\varrho^{-1}.$$

Further,

$$\begin{aligned} I - B_{\wedge,\min}(\varrho^m\lambda_0)(A_\wedge - \varrho^m\lambda_0) &= I - \varrho^{-m}\kappa_\varrho B_{\wedge,\min}(\lambda_0)\kappa_\varrho^{-1}(A_\wedge - \varrho^m\lambda_0) \\ &= I - \varrho^{-m}\kappa_\varrho B_{\wedge,\min}(\lambda_0)(A_\wedge - \lambda_0)\kappa_\varrho^{-1} \\ &= \kappa_\varrho\big(I - B_{\wedge,\min}(\lambda_0)(A_\wedge - \lambda_0)\big)\kappa_\varrho^{-1} \end{aligned}$$

in which (6.5) was used in the second equality. Altogether this gives

$$\begin{aligned} B_{\mathcal{D}_\wedge}(\varrho^m\lambda_0) &= \varrho^{-m}\kappa_\varrho\big\{B_{\wedge,\max}(\lambda_0) \\ &\quad - \big(I - B_{\wedge,\min}(\lambda_0)(A_\wedge - \lambda_0)\big)\kappa_\varrho^{-1}\pi_{K_{\wedge,\varrho^m\lambda_0},D_\wedge}\pi_{\wedge,\max}\kappa_\varrho B_{\wedge,\max}(\lambda_0)\big\}\kappa_\varrho^{-1}. \end{aligned}$$

In the second term we replace the factor

$$\kappa_\varrho^{-1}\pi_{K_{\wedge,\varrho^m\lambda_0},D_\wedge}\pi_{\wedge,\max}\kappa_\varrho$$

by

$$\pi_{\wedge,\max}\kappa_\varrho^{-1}\pi_{K_{\wedge,\varrho^m\lambda_0},D_\wedge}\pi_{\wedge,\max}\kappa_\varrho\pi_{\wedge,\max}$$

taking advantage again of the fact that $I - B_{\wedge,\min}(\lambda_0)(A_\wedge - \lambda_0)$ vanishes on $\mathcal{D}_{\wedge,\min}$, and also that $\pi_{\wedge,\max}\kappa_\varrho = \pi_{\wedge,\max}\kappa_\varrho\pi_{\wedge,\max}$ because κ_ϱ preserves $\mathcal{D}_{\wedge,\min}$. With the notation of (5.6),

$$\pi_{\wedge,\max}\kappa_\varrho^{-1}\pi_{K_{\wedge,\varrho^m\lambda_0},D_\wedge}\pi_{\wedge,\max}\kappa_\varrho|_{\mathcal{E}_\wedge} = \boldsymbol{\kappa}_\varrho^{-1}\pi_{K_{\wedge,\varrho^m\lambda_0},D_\wedge}\boldsymbol{\kappa}_\varrho$$

Using (6.7) one easily obtains $\boldsymbol{\kappa}_\varrho^{-1}\pi_{K_{\wedge,\varrho^m\lambda_0},D_\wedge}\boldsymbol{\kappa}_\varrho = \pi_{K_{\wedge,\lambda_0},\boldsymbol{\kappa}_\varrho^{-1}D_\wedge}$. So, finally we arrive at

$$\begin{aligned} B_{\mathcal{D}_\wedge}(\varrho^m\lambda_0) &= \varrho^{-m}\kappa_\varrho\big\{B_{\wedge,\max}(\lambda_0) \\ &\quad - \big(I - B_{\wedge,\min}(\lambda_0)(A_\wedge - \lambda_0)\big)\pi_{K_{\wedge,\lambda_0},\boldsymbol{\kappa}_\varrho^{-1}D_\wedge}\pi_{\wedge,\max}B_{\wedge,\max}(\lambda_0)\big\}\kappa_\varrho^{-1}. \end{aligned} \tag{7.9}$$

Note that the norm of $B_{\mathcal{D}_\wedge}(\varrho^m\lambda_0) : x^\mu L^2(N_+\partial\mathcal{M}, E_\wedge) \to L^2(N_+\partial\mathcal{M}, E_\wedge)$ is bounded by ϱ^{-m} times the norm of

$$B_{\wedge,\max}(\lambda_0) - \big(I - B_{\wedge,\min}(\lambda_0)(A_\wedge - \lambda_0)\big)\pi_{K_{\wedge,\lambda_0},\boldsymbol{\kappa}_\varrho^{-1}D_\wedge}\pi_{\wedge,\max}B_{\wedge,\max}(\lambda_0)$$

The fact that the only dependence of ϱ is in $\pi_{K_{\wedge,\lambda_0},\boldsymbol{\kappa}_\varrho^{-1}D_\wedge}$ lends credence to what we showed in [15, Theorem 8.3], namely that the ray through λ_0 is a ray of minimal growth for $A_{\wedge,\mathcal{D}_\wedge}$ if and only if the norm of $\pi_{K_{\wedge,\lambda_0},\boldsymbol{\kappa}_\varrho^{-1}D_\wedge}$ is bounded as $\varrho \to \infty$, and that this norm is bounded if

> there is a neighborhood U of $\mathscr{V}_{K_{\lambda_0}}$ and $\varrho_0 > 0$ such that $\varrho > \varrho_0 \implies \boldsymbol{\kappa}_\varrho^{-1}D_\wedge \notin U$.

Completing this, we showed in [16, Theorem 4.3] that this last displayed condition is also sufficient for the boundedness of $\|\pi_{K_{\wedge,\lambda_0},\boldsymbol{\kappa}_\varrho^{-1}D_\wedge}\|$ as $\varrho \to \infty$. This condition is equivalent to the statement that the limit set

$$\Omega^-(D_\wedge) = \{D'_\wedge \in \mathrm{Gr}_{d''}(\mathcal{E}_\wedge) : \exists\{\varrho_k\}_{k=1}^\infty,\ \lim_{k\to\infty}\varrho_k = \infty,\ \lim_{k\to\infty}\boldsymbol{\kappa}_{\varrho_k}^{-1}D_\wedge = D'_\wedge\}$$

is disjoint from $\mathscr{V}_{K_{\wedge,\lambda_0}}$; this is how the condition is stated in the theorem just cited. The number d'' is the negative of the index of $A_{\wedge,\min} - \lambda$ for $\lambda \in \Lambda_0$ (see (6.6)).

If one insists on having a condition on the sector Λ, one can take the arc $C = \{\lambda \in \Lambda : |\lambda| = |\lambda_0|\}$ and define

$$\mathscr{V}_{K_{\wedge,C}} = \bigcup_{\lambda \in C} \mathscr{V}_{K_{\wedge,\lambda}}.$$

Then $\mathscr{V}_{K_{\wedge,C}}$ is a closed subset of $\mathrm{Gr}_{d''}(\mathscr{E}_\wedge)$, and Λ is a sector of minimal growth if and only if

$$\Omega^-(D_\wedge) \cap \mathscr{V}_{K_{\wedge,C}} = \emptyset. \tag{7.10}$$

The set $\Omega^-(D_\wedge)$ is in some sense the principal symbol of $\mathcal{D}_\wedge$ (or of $\mathcal{D} = D + \mathcal{D}_{\min}$ if $D_\wedge = \theta(D)$), and the condition (7.10) is like an ellipticity condition.

Obviously:

if $\mathcal{D}_\wedge$ is stationary (see (5.9)) then $\pi_{K_{\wedge,\lambda_0}, \boldsymbol{\kappa}_\varrho^{-1} D_\wedge}$ is independent of ϱ. (7.11)

This property results in a considerable simplification of the analysis of the asymptotics of the resolvent of $A_{\mathcal{D}} - \lambda$.

Example 7.12. Continuing with Example 5.10 (see also Example 6.8), assume in all formulas that follow that $\lambda \notin [0,\infty)$. Recall that $\text{bg-spec}(A_\wedge) = [0,\infty) \subset \mathbb{C}$.

Let

$$\phi(\lambda) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{e^{ix\cdot\xi}}{|\xi|^2 - \lambda}\, d\xi, \quad \lambda \notin [0,\infty).$$

Then $\phi(\lambda) \in L^2(\mathbb{R}^2)$. Also

$$(\Delta\phi(\lambda))\widehat{\ }(\xi) = 1 + \frac{\lambda}{|\xi|^2 - \lambda},$$

which means that

$$\Delta\phi(\lambda) = \delta_0 + \lambda\phi(\lambda).$$

so by restriction to $\mathbb{R}^2 \backslash 0$,

$$A_\wedge \phi(\lambda) = \lambda\phi(\lambda)$$

Thus $\phi(\lambda) \in \mathcal{D}_{\wedge,\max}$ and spans $\mathcal{K}_{\wedge,\lambda}$.

Let $\mathfrak{p}_\lambda : L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2)$ be the orthogonal projection on $\mathcal{K}_{\wedge,\lambda}$:

$$\mathfrak{p}(f) = 4\pi|\lambda|(f, \phi(\lambda))\phi(\lambda).$$

Let $B_F(\lambda)$ be the inverse of $(\Delta - \lambda) : H^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2)$. The reason for the subindex F is that the space $\mathcal{D}_{\wedge,F} = H^2(\mathbb{R}^2)$ is the domain of the Friedrichs extension of

$$\Delta : C_c^\infty(\mathbb{R}^2\backslash 0) \subset L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2),$$

so $B_F(\lambda)$ is actually the resolvent of $A_{\wedge,\mathcal{D}_{\wedge,F}}$. We have

$$B_{\wedge,\max}(\lambda) = (1 - \mathfrak{p}_\lambda) B_F(\lambda).$$

Indeed, this $B_{\wedge,\max}(\lambda)$ is the right inverse of $(A_\wedge - \lambda)$ with range orthogonal (in L^2) to $\mathcal{K}_{\wedge,\lambda}$.

The Hilbert space adjoint of $A_{\wedge,\mathcal{D}_{\wedge,\min}}$ is $A_{\wedge,\mathcal{D}_{\wedge,\max}}$ so the range of $A_{\wedge,\mathcal{D}_{\wedge,\min}} - \lambda$ is the orthogonal space (in L^2) of $\ker(A_{\wedge,\mathcal{D}_{\wedge,\max}} - \lambda)$ which of course is $\mathcal{K}_{\wedge,\lambda}$. So

$$B_{\wedge,\min}(\lambda) = B_F(\lambda)(I - \mathfrak{p}_\lambda).$$

Let $D_\wedge = \operatorname{span}\{\alpha u_1 + \beta u_2\}$ with fixed $(\alpha,\beta) \neq 0$, and let $\mathcal{D}_\wedge = D_\wedge + \mathcal{D}_{\wedge,\min}$. To compute the spectrum of $A_{\wedge,\mathcal{D}_\wedge}$ we need to compute the spaces $K_{\wedge,\lambda}$, which here just means to compute $\pi_{\wedge,\max}\phi(\lambda)$. In terms of the basis u_1, u_2 of $\mathcal{E}_\wedge$ discussed in Example 5.10,

$$\pi_{\wedge,\max}\phi(\lambda) = -\frac{2}{\pi}\log(-\lambda)u_1 + u_2. \tag{7.13}$$

The log is the principal branch of the logarithm with cut $(-\infty,0]$. The part of the spectrum of $A_{\wedge,\mathcal{D}_\wedge}$ in $\text{bg-res}(A_\wedge)$ is

$$\left\{\lambda \in \text{bg-res}(A_\wedge) : \alpha u_1 + \beta u_2 \text{ and } -\frac{2}{\pi}\log(-\lambda)u_1 + u_2 \text{ are linearly dependent}\right\}.$$

In other words, $\lambda \in \operatorname{spec}(A_{\wedge,\mathcal{D}_\wedge}) \cap \text{bg-res}(A_\wedge)$ if and only if the determinant, $f(\lambda,\alpha,\beta) = \alpha + (2\beta/\pi)\log(-\lambda)$, of

$$\begin{bmatrix} \alpha & -\frac{2}{\pi}\log(-\lambda) \\ \beta & 1 \end{bmatrix}$$

is zero. If $\beta = 0$ then $f(\lambda,\alpha,\beta)$ has no zeros, corresponding to the fact that the spectrum of the Friedrichs extension is exactly $[0,\infty)$. If $\beta \neq 0$ and $\Im(\alpha/\beta) \notin 2 + 4\mathbb{Z}$, then there is exactly one zero, at

$$\lambda = -e^{-\pi\alpha/2\beta}.$$

It follows that in any closed sector Λ with $\Lambda\backslash 0 \subset \text{bg-res}(A_\wedge)$ there is at most one eigenvalue of $A_{\wedge,\mathcal{D}_\wedge}$.

We have already shown that $\boldsymbol{\kappa}_\varrho D_\wedge \to D_{\wedge,F}$ as ϱ tends to 0, equivalently,

$$\boldsymbol{\kappa}_\varrho^{-1} D_\wedge \to D_\wedge \quad \text{as } \varrho \to \infty.$$

So $\Omega^-(D_\wedge) = D_{\wedge,F}$ and thus, for any $\lambda_0 \in \text{bg-res}(A_\wedge)$,

$$\Omega^-(D_\wedge) \cap \mathcal{K}_{\wedge,\lambda_0} = \emptyset$$

since $\pi_{\wedge,\max}\phi(\lambda)$ is never an element of $D_{\wedge,F}$.

8. Asymptotics

Suppose that it has been determined by way of [14, Theorem 6.36] (quoted above as Theorem 7.1) that the closed $\Lambda \subset \mathbb{C}$ is a sector of minimal growth for a given extension $A_\mathcal{D}$ of our elliptic cone operator. In [17] we discussed the asymptotics in the case of a stationary domain, and in [18] we were able to complete our results to general general domains. We will discuss some aspects of the latter result below.

In the case of stationary domains (see (5.9)) we have:

Theorem 8.1. [17, Theorem 1.1] *Suppose $\mathcal{D}$ is stationary in the sense of* (5.9). *Then, for any $\varphi \in C^\infty(\mathcal{M};\operatorname{End}(E))$ and $\ell \in \mathbb{N}$ with $m\ell > n = \dim \mathcal{M}$,*

$$\operatorname{Tr}\big(\varphi(A_{\mathcal{D}}-\lambda)^{-\ell}\big) \sim \sum_{j=0}^{\infty}\sum_{k=0}^{m_j} \alpha_{jk}\lambda^{\frac{n-j}{m}-\ell}\log^k\lambda \quad \text{as } |\lambda|\to\infty,$$

with a suitable branch of the logarithm, with constants $\alpha_{jk}\in\mathbb{C}$. The numbers m_j vanish for $j<n$, and $m_n\le 1$. In general, the α_{jk} depend on φ, A, $\mathcal{D}$, and ℓ, but the coefficients α_{jk} for $j<n$ and $\alpha_{n,1}$ do not depend on $\mathcal{D}$. If both A and φ have coefficients independent of x near $\partial\mathcal{M}$, then $m_j=0$ for all $j>n$.

The asymptotics of the trace of the resolvent, which ultimately determines the behavior of the ζ function, depends fundamentally on the asymptotics of the resolvent of $A_{\wedge,\mathcal{D}_\wedge}$, which by virtue of (7.9) depends in an essential manner on the asymptotics of $\pi_{\mathcal{K}_{\wedge,\lambda_0},\boldsymbol{\kappa}_\varrho^{-1}D_\wedge}$. If the domain is stationary then $\pi_{\mathcal{K}_{\wedge,\lambda_0},\boldsymbol{\kappa}_\varrho^{-1}D_\wedge}$ has a simple asymptotics (indeed, it is homogeneous of degree 0 in ϱ, see (7.11)). On the other hand, if $\mathcal{D}$ is not stationary, its asymptotics, therefore that of the resolvent, can be rather complicated:

Theorem 8.2. [18, Theorem 1.4] *For any $\varphi\in C^\infty(\mathcal{M};\operatorname{End}(E))$ and $\ell\in\mathbb{N}$ with $m\ell>n$,*

$$\operatorname{Tr}\big(\varphi(A_{\mathcal{D}}-\lambda)^{-\ell}\big) \sim \sum_{j=0}^{\infty} r_j(\lambda^{i\mu_1},\dots,\lambda^{i\mu_N},\log\lambda)\lambda^{\nu_j/m} \quad \text{as } |\lambda|\to\infty,$$

where each r_j is a rational function in $N+1$ variables, $N\in\mathbb{N}_0$, with real numbers μ_k, $k=1,\dots,N$, and $\nu_j>\nu_{j+1}\to-\infty$ as $j\to\infty$. We have $r_j=p_j/q_j$ with p_j, $q_j\in\mathbb{C}[z_1,\dots,z_{N+1}]$ such that $q_j(\lambda^{i\mu_1},\dots,\lambda^{i\mu_N},\log\lambda)$ is uniformly bounded away from zero for large λ.

The asymptotic behavior of $\pi_{\mathcal{K}_{\wedge,\lambda_0},\boldsymbol{\kappa}_\varrho^{-1}D_\wedge}$ is rooted in the behavior of the curve $\varrho\mapsto\boldsymbol{\kappa}_\varrho^{-1}D_\wedge$ in $\operatorname{Gr}_{d''}(\mathcal{E}_\wedge)$. We gain an understanding of this by analyzing the infinitesimal generator of the action

$$\varrho\mapsto\boldsymbol{\kappa}_\varrho:\mathcal{E}_\wedge\to\mathcal{E}_\wedge.$$

Since this is a one-parameter group of isomorphisms, there is a linear operator $\mathfrak{a}:\mathcal{E}_\wedge\to\mathcal{E}_\wedge$ such that $\boldsymbol{\kappa}_\varrho=e^{-\log\varrho\,\mathfrak{a}}$ (the choice of sign for $\mathfrak{a}$ is a matter of convenience; we are interested in letting ϱ tend to ∞ in $\boldsymbol{\kappa}_\varrho^{-1}D_\wedge$, so in fact we are looking at $e^{\log\varrho\mathfrak{a}}$). The precise determination of $\mathfrak{a}$ is best done using the Mellin transform.

Fix some defining function for $\partial\mathcal{M}$, let $P_\wedge=x_\wedge^m A_\wedge$ (an elliptic b-operator with respect to the boundary of $N_+\partial\mathcal{M}$; the latter is trivialized by the choice of x as $\partial\mathcal{M}\times[0,\infty)$). Let $\widehat{P}_\wedge(\sigma)$ be the indicial family of $P_\wedge$. Let

$$\Sigma=\{\sigma\in\operatorname{spec}_b(P_\wedge):-\mu-m<\Im\sigma<-\mu\},$$

let $\mathfrak{Mero}_\Sigma$ be the space of meromorphic functions on $\mathbb{C}$ with poles in Σ to the space of smooth sections of $E_{\partial\mathcal{M}} \to \partial\mathcal{M}$ and let $\mathfrak{Holo}$ be the subspace consisting of entire functions. Then $\widehat{P}$ induces maps

$$\widehat{P} : \mathfrak{Mero}_\Sigma \to \mathfrak{Mero}_\Sigma, \quad \widehat{P} : \mathfrak{Holo} \to \mathfrak{Holo}$$

which in turn give a map

$$\widehat{P} : \mathfrak{Mero}_\Sigma/\mathfrak{Holo} \to \mathfrak{Mero}_\Sigma/\mathfrak{Holo}.$$

Then $\mathcal{E}_\wedge$ is canonically isomorphic to the kernel, $\widehat{\mathcal{E}}_\wedge$, of this map. Namely, if $u \in \mathcal{E}_\wedge$ and $\omega : N_+\partial\mathcal{M} \to \mathbb{R}$ is smooth compactly supported, equal 1 in a neighborhood of the zero section, then

$$\mathscr{M}(u)(y,\sigma) = \int_0^\infty x_\wedge^{-i\sigma} u(x_\wedge, y)\omega(x_\wedge, y)\frac{dx_\wedge}{x_\wedge}$$

is holomorphic for $\Im\sigma \geq -\mu$, meromorphic in $\Im\sigma > -\mu - m$ with poles in Σ, and $\widehat{P}\mathscr{M}(u)$ is holomorphic in $\Im\sigma > -m-\mu$. Taking the singular parts of $\mathscr{M}(u)$ at the points of Σ gives an element $\mathrm{s}_\Sigma\mathscr{M}(u) \in \mathfrak{Mero}_\Sigma$ such that $\widehat{P}\mathrm{s}_\Sigma\mathscr{M}(u)$ is entire. This gives a map

$$\mathcal{E}_\wedge \ni u \mapsto [\mathrm{s}_\Sigma\mathscr{M}(u)] \in \widehat{\mathcal{E}}_\wedge,$$

where [ ] means class in $\mathfrak{Mero}_\Sigma$ modulo $\mathfrak{Holo}$. This map is the isomorphism mentioned above.

Now, $u \mapsto \mathscr{M}(u)$ conjugates κ_ϱ with multiplication by $\varrho^{i\sigma}$:

$$\begin{aligned}\mathscr{M}(\kappa_\varrho u)(y,\sigma) &= \int_0^\infty x_\wedge^{-i\sigma}\varrho^{-\mu}u(\varrho x_\wedge, y)\omega(x_\wedge, y)\frac{dx_\wedge}{x_\wedge}\\ &= \varrho^{i\sigma-\mu}\int_0^\infty x_\wedge^{-i\sigma}u(x_\wedge, y)\omega(x_\wedge/\varrho, y)\frac{dx_\wedge}{x_\wedge}\\ &\equiv \varrho^{i\sigma-\mu}\mathscr{M}(u) \mod \mathfrak{Holo}.\end{aligned}$$

Associated with each $\sigma_j \in \Sigma$, $j = 1,\dots,N$, there is the subspace $\widehat{\mathcal{E}}_{\wedge,\sigma_j} \subset \widehat{\mathcal{E}}_\wedge$ whose elements have representatives in $\mathfrak{Mero}_\Sigma$ with pole only at σ_j. We may view $\widehat{\mathcal{E}}_{\wedge,\sigma_j}$ directly as a space of singular parts of elements of $\mathfrak{Mero}_\Sigma$ with pole only at σ_j. If

$$\sum_{k=1}^{\nu}\frac{\phi_j}{(\sigma-\sigma_j)^k}$$

is an element of $\widehat{\mathcal{E}}_{\wedge,\sigma_j}$, then (using $\varrho^{i\sigma} = \varrho^{i\sigma_j}\varrho^{i(\sigma-\sigma_j)}$)

$$\varrho^{i\sigma-\mu}\sum_{k=1}^{\nu}\frac{\phi_k}{(\sigma-\sigma_j)^k} \equiv \varrho^{i\sigma_j-\mu}\sum_{\vartheta=1}^{\nu}\frac{1}{(\sigma-\sigma_j)^\vartheta}\sum_{k-\ell=\vartheta}\frac{i^\ell\log^\ell\varrho}{\ell!}\phi_k \mod \mathfrak{Holo}$$

Thus $\mathfrak{a}$, viewed on the Mellin transform side, has eigenvalues $-i\sigma_j + \mu$, $\sigma_j \in \Sigma$, and the generalized eigenspace corresponding to $-i\sigma_j + \mu$ is $\widehat{\mathcal{E}}_{\wedge,\sigma_j}$.

Each space $\widehat{\mathcal{E}}_{\wedge,\sigma_j}$ corresponds to a subspace $\mathcal{E}_{\wedge,\sigma_j} \subset \mathcal{E}_\wedge$. These spaces are, as we saw, the generalized eigenspaces of $\mathfrak{a}$. We may write $\mathfrak{a} = \mathfrak{a}_0 + N$ where $\mathfrak{a}_0$

is diagonal and N is nilpotent. Let $\mathfrak{a}' : \mathcal{E}_\wedge \to \mathcal{E}_\wedge$ be the operator which acts on each $\mathcal{E}_{\wedge,\sigma_j}$ by multiplication by $-i\Re\sigma_j$. The eigenvalues of $\mathfrak{a}_0 - \mathfrak{a}'$ are the numbers $\Im\sigma_j + \mu$. Order the set of these numbers as $\mu_0 > \mu_1 > \dots$ (i.e., no repetitions). Since $\sigma_j \in \Sigma$, $-m < \mu_k < 0$. Let

$$\tilde{\mathcal{E}}_{\wedge,\mu_k} = \bigoplus_{\substack{\sigma_j\in\Sigma\\ \Im\sigma_j+\mu=\mu_k}} \mathcal{E}_{\wedge,\sigma_j}.$$

Also let π_{σ_j} be the projection on $\mathcal{E}_{\wedge,\sigma_j}$ and N_{σ_j} the restriction of N to this space.

In [18, Sections 3 and 4] we showed the following. Given any subspace $D_\wedge \subset \mathcal{E}_\wedge$, there are functions $v_k : \mathbb{R} \to \mathcal{E}_\wedge$, $k = 1, \dots, d'' = \dim D_\wedge$, (perhaps not defined at $t = 0$) such that

$$e^{t\mathfrak{a}} D_\wedge = \operatorname{span}\{v_k(t) : k = 1, \dots, d''\}, \quad t \gg 0,$$

is of the form

$$v_k(t) = e^{t\mathfrak{a}'} g_k(t) + \sum_{\substack{\sigma\in\Sigma\\ \Im\sigma+\mu<\mu_k}} e^{t(-i\sigma+\mu-\mu_k)} \hat{p}_{k,\sigma}(t). \tag{8.3}$$

The $g_k(t)$ are polynomials in $1/t$ with values in $\tilde{\mathcal{E}}_{\wedge,\mu_k}$ and the collection of vectors

$$g_{\infty,k} = \lim_{t\to\infty} g_k(t)$$

is an independent set spanning a subspace $D_{\wedge,\infty}$, and

$$\hat{p}_{k,\sigma}(t) = e^{tN_\sigma} \pi_\sigma p_{k,\sigma}(t), \quad \sigma \in \Sigma,$$

where the $p_{k,\sigma}(t)$ are polynomials in t and $1/t$ with values in $\mathcal{E}_\wedge$.

The numbers $-i\sigma + \mu - \mu_k$ appearing in the exponents in the sum in (8.3) all have negative real part. It follows that $\|v_k(t) - e^{t\mathfrak{a}'} g_k(t)\| \to 0$ as $t \to \infty$. From this one concludes that the distance in $\mathrm{Gr}_{d''}(\mathcal{E}_\wedge)$ between $\boldsymbol{\kappa}_\varrho^{-1} D_\wedge = e^{\log\varrho\mathfrak{a}} D_\wedge$ and $e^{\log\varrho\mathfrak{a}'} D_{\wedge,\infty}$ tends to 0 as $t \to \infty$. Separately one can show (consult the details in [18]) that the closure of

$$\{e^{t\mathfrak{a}'} D_{\wedge,\infty} : t \in \mathbb{R}\}$$

is an embedded torus, which immediately proves that $\Omega^-(D_\wedge)$ is a subset of this torus, and in fact is equal to it. The dimension of the torus may be zero (a point) in which case the statement is that the limit $\lim_{\varrho\to\infty} e^{\log\varrho\mathfrak{a}} D_\wedge$ exists. This will be the case for any $D_\wedge$ if no two distinct elements of Σ have the same imaginary part.

The term $e^{t\mathfrak{a}'} g_k(t)$ in (8.3) is

$$\sum_{\substack{\sigma\in\Sigma\\ \Im\sigma+\mu=\mu_k}} e^{t(-i\Im\sigma+\mu-\mu_k)} \hat{p}_{k,\sigma}(t).$$

So all the numbers $-i\sigma + \mu - \mu_k$ appearing in the exponents of the right-hand side in (8.3) are of the form $-i\sigma + \mu - \Re(-i\sigma_j + \mu)$ with $\sigma, \sigma' \in \Sigma$ and $\Re(-i\sigma + \mu) < \Re(-i\sigma_j + \mu)$. The collection of these numbers is thus

$$\{-i\sigma - \Im\sigma' : \sigma, \sigma' \in \Sigma,\ \Re(-i\sigma) < \Re(-i\sigma')\},$$

The additive semigroup $\mathfrak{G} \subset \mathbb{C}$ generated by this set is a subset of $\{\vartheta \in \mathbb{C} : \Re\vartheta \leq 0\}$ with the property that $\{\vartheta \in \mathfrak{G} : \Re\vartheta > \mu\}$ is finite for every $\mu \in \mathbb{R}$.

All this information comes together to produce, after some more work, the following theorem slightly adapted from Theorem 7.4 of [18] (see the proof there):

Theorem 8.4. *If Λ is a sector of minimal growth for $A_{\wedge,\mathcal{D}_\wedge}$, $\mathcal{D}_\wedge = D_\wedge + \mathcal{D}_{\wedge,\min}$, and $\lambda_0 \in \Lambda\backslash 0$, then there are polynomials $p_\vartheta(z^1,\dots,z^N,t)$ with values in $\mathrm{End}(\mathcal{E}_\wedge)$ and $\mathbb{C}$-valued polynomials $q_\vartheta(z^1,\dots,z^N,t)$ such that*

$$\exists\, C,\ R > 0 \text{ such that } |q_\vartheta(\varrho^{i\Re\sigma_1},\dots,\varrho^{i\Re\sigma_N},t)| > C \text{ if } \ \varrho > R \tag{8.5}$$

and such that

$$\pi_{K_{\wedge,\lambda_0},\boldsymbol{\kappa}_\varrho^{-1}D_\wedge} = \sum_{\vartheta\in\mathfrak{G}} \frac{\varrho^\vartheta p_\vartheta(\varrho^{i\Re\sigma_1},\dots,\varrho^{i\Re\sigma_N},\log\varrho)}{q_\vartheta(\varrho^{i\Re\sigma_1},\dots,\varrho^{i\Re\sigma_N},\log\varrho)},\ \ \varrho > R \tag{8.6}$$

with uniform convergence in norm in $\varrho > R$. The σ_j are an enumeration of Σ.

Note that the exponents ϑ of the factors ϱ^ϑ have real parts tending to $-\infty$. The parameter ϱ can be complexified (while keeping it in a sector around the positive real axis) and then replaced by $\zeta^{1/m}$ where $\zeta = \lambda/\lambda_0$ using the principal branch of m-th root). This is how Theorem 7.4 of [18] is stated.

Replacing $\lambda = \varrho^m e^{i\theta}\lambda_0$ in (7.8) and following through to (7.9) one obtains

$$\begin{aligned} B_{\mathcal{D}_\wedge}(\lambda) &= (\lambda_0/\lambda)\kappa_{(\lambda/\lambda_0)^{1/m}}\big\{B_{\wedge,\max}(\lambda_0) \\ &- \big(I - B_{\wedge,\min}(\lambda_0)(A_\wedge-\lambda_0)\big)\pi_{K_{\wedge,\lambda_0},\boldsymbol{\kappa}^{-1}_{(\lambda/\lambda_0)^{1/m}}D_\wedge}\pi_{\wedge,\max}B_{\wedge,\max}(\lambda_0)\big\}\kappa^{-1}_{(\lambda/\lambda_0)^{1/m}}. \end{aligned} \tag{8.7}$$

Of course we need to verify that (7.9) remains true after complexifying ϱ, but that is indeed the case since all elements of (7.9) depend real-analytically on ϱ. The fact that $B_{\wedge\,\min}(\lambda)$ and $B_{\wedge,\max}(\lambda)$ as they appear in (7.8) do not depend analytically on λ is immaterial because the formula we are extending analytically is (7.9).

The final step in obtaining the asymptotics of $B_{\mathcal{D}_\wedge}(\lambda)$ in $\lambda\in\Lambda$ as $|\lambda|\to\infty$ is to replace $\pi_{K_{\wedge,\lambda_0},\boldsymbol{\kappa}_\varrho^{-1}D_\wedge}$ in the formula for $B_{\mathcal{D}_\wedge}(\lambda)$.

It is the complicated structure of the expansion of $\pi_{K_{\wedge,\lambda_0},\boldsymbol{\kappa}_\varrho^{-1}D_\wedge}$ in (8.6) that is responsible for the unusual behavior of the zeta function of a cone operator. Indeed, if the domain is stationary, then (obviously) $\pi_{K_{\wedge,\lambda_0},\boldsymbol{\kappa}_\varrho^{-1}D_\wedge}$ is independent of ϱ.

Example 8.8. The indicial family of $A_\wedge$ of Example 5.10, the Laplacian on the blowup of $\mathbb{R}^2$ at 0, is

$$\sigma^2 + D_\theta^2.$$

Thus the boundary spectrum of A (or $A_\wedge$) is $i\mathbb{Z}$. We have been viewing $A_\wedge$ as an unbounded operator on subspaces of

$$L^2(\mathbb{R}^2) = r^{-1}L^2_b\left(S^1\times[0,\infty);\frac{dr}{r}\,d\theta\right)$$

so $\Sigma = \{\sigma \in \operatorname{spec}_b(A_\wedge) : -1 < \Im\sigma < -2\} = \{0\}$. So we expect a rather simple structure for the asymptotics of $\pi_{K_{\wedge,\lambda_0},D_\wedge}$ for any one-dimensional subspace $D_\wedge \subset \mathcal{E}_\wedge$.

We know from Example 7.12 that for any $\lambda_0 \notin [0,\infty)$, the ray through λ_0 is a ray of minimal growth for $A_{\mathcal{D}_\wedge}$, for any $\mathcal{D}_\wedge = D_\wedge + \mathcal{D}_{\wedge,\min}$. The space $K_{\wedge,\lambda_0}$ is spanned by

$$\pi_{\wedge,\max}\phi(\lambda_0) = -\frac{2}{\pi}\log(-\lambda_0)u_1 + u_2,$$

see (7.13). If $D_\wedge$ is the space spanned by $\psi = \alpha u_1 + \beta u_2$, $(\alpha,\beta) \neq 0$, then $\boldsymbol{\kappa}_\varrho^{-1} D_\wedge$ is spanned by

$$\boldsymbol{\kappa}_\varrho^{-1}\psi = \left(\alpha + \frac{2\beta}{\pi}\log\varrho^2\right)u_1 + \beta u_2,$$

see (5.11). The pair $\{\pi_{\wedge,\max}\phi(\lambda_0), \boldsymbol{\kappa}_\varrho^{-1}\psi\}$ is a basis of $\mathcal{E}_\wedge$ when $\varrho^2\lambda_0$ is not in the spectrum of $A_{\wedge,\mathcal{D}_\wedge}$, in which case we may express an arbitrary element $v = v_1u_1 + v_2u_2 \in \mathcal{E}_\wedge$ in terms of $\pi_{\wedge,\max}\phi(\lambda_0)$ and $\boldsymbol{\kappa}_\varrho^{-1}\psi$:

$$v = \frac{-\pi\beta\, v_1 + \pi(\alpha + 2\beta\log\varrho^2)\, v_2}{\pi\alpha + 2\beta\log(-\varrho^2\lambda_0)}\pi_{\wedge,\max}\phi(\lambda_0) + \frac{\pi\, v_1 + 2\log(-\lambda_0)\, v_2}{\pi\alpha + 2\beta\log(-\varrho^2\lambda_0)}\boldsymbol{\kappa}_\varrho^{-1}\psi$$

Consequently,

$$\pi_{K_{\wedge,\lambda_0},D_\wedge} v = \frac{-\pi\beta\, v_1 + \pi(\alpha + 4\beta\log\varrho)\, v_2}{\pi\alpha + 4\beta\log\varrho\,\log(-\lambda_0)}\,\pi_{\wedge,\max}\phi(\lambda_0).$$

Note that $D_\wedge$ is stationary if and only if $\beta = 0$, which corresponds to the Friedrichs extension.

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Pseudodifferential Operators on Manifolds: A Coordinate-free Approach

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Abstract. The main aim of the paper is to demonstrate the advantage of a coordinate-free approach to the theory of pseudodifferential operators. We explain how one can define symbols and construct a symbolic calculus without using local coordinates, briefly review some known definitions and results, and discuss possible applications and further developments.

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1. Introduction

The theory of pseudodifferential operators (PDOs) is a powerful technique, which has many applications in analysis and mathematical physics. In the framework of this theory, one can effectively construct the inverse of an elliptic differential operator L on a closed manifold, its non-integer powers and even some more general functions of L. For operators with constant coefficients in $\mathbb{R}^n$, this can be easily done by applying the Fourier transform. In a sense, the theory of PDOs extends the Fourier transform method to operators with variable coefficients and operators on manifolds at the expense of losing infinitely smooth contributions. This is normally acceptable for theoretical purposes and is useful for numerical analysis, since numerical methods for the determination of the smooth part are usually more stable.

Traditionally, PDOs on manifolds are defined with the use of local coordinates. This leads to certain restrictions on operators under consideration, as all the definitions and results must be invariant with respect to transformations of coordinates. The main aim of this paper is to introduce the reader to a little known approach to the theory of PDOs that allows one to avoid this problem.

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The paper is constructed as follows. In Section 2 we recall some basic definitions and results of the classical theory of PDOs. Their detailed proofs (as well as other relevant statements and definitions) can be found, for instance, in [H2, Shu, Ta, Tr]. Section 3 gives a brief overview of some elementary concepts of differential geometry (see [KN] or any other textbook for details). In Sections 4 and 5 we explain how to define PDOs without using local coordinates and quote some results from the paper [Sa1] and the conference article [Sa2]. Section 6 contains new results on approximate spectral projections of the Laplacian obtained in the Ph.D. thesis [McK]. Finally, in Section 7 we give a review of other related results and discuss possible developments in the field.

Throughout the paper C_0^∞ denotes the space of infinitely differentiable functions with compact supports, and $\mathcal{D}'$ is the dual space of Schwartz distributions. Recall that, by the Schwartz theorem, for each operator $A : C_0^\infty \mapsto \mathcal{D}'$ there exists a distribution $\mathcal{A}(x,y) \in \mathcal{D}'$ such that $\langle Au, v\rangle = \langle \mathcal{A}(x,y)\,,\, u(y)v(x)\rangle$ for all $u, v \in C_0^\infty$. The distribution $\mathcal{A}(x,y)$ is called the *Schwartz kernel* of A.

2. PDOs: local definition and basic properties

Let $a(x,y,\xi)$ be a C^∞-function defined on $U \times U \times \mathbb{R}^n$, where U is an open subset of $\mathbb{R}^n$.

Definition 2.1. The function a belongs to the class $S^m_{\rho,\delta}$ with $\rho, \delta \in [0,1]$ and $m \in \mathbb{R}$ if

$$\sup_{(x,y)\in K} |\partial_x^\alpha \partial_y^\beta \partial_\xi^\gamma a(x,y,\xi)| \;\le\; C_{K;\alpha,\beta,\gamma}\,(1+|\xi|)^{m+\delta(|\alpha|+|\beta|)-\rho|\gamma|} \tag{2.1}$$

for each compact set $K \subset U \times U$ and all multi-indices α, β, γ, where $C_{K;\alpha,\beta,\gamma}$ are some positive constants.

Definition 2.2. An operator $A : C_0^\infty(U) \mapsto \mathcal{D}'(U)$ is said to be a *pseudodifferential* operator of class $\Psi^m_{\rho,\delta}$ if

- **(c)** its Schwartz kernel $\mathcal{A}(x,y)$ is infinitely differentiable outside the diagonal $\{x = y\}$,
- **(c$_1$)** $\mathcal{A}(x,y) = (2\pi)^{-n} \int e^{i(x-y)\cdot\xi} a(x,y,\xi)\,\mathrm{d}\xi$ with some $a \in S^m_{\rho,\delta}$ in a neighbourhood of the diagonal.

The function a in **(c$_1$)** is called an *amplitude*, and the number m is said to be the *order* of the amplitude a and the corresponding PDO A. Note that for amplitudes of order $m > -n$ the integral in **(c$_1$)** does not converge in the usual sense. However, it is well defined as a distribution in x and y.

Let $S^{-\infty} := \bigcap_{m\in\mathbb{R}} S^m_{\rho,\delta}$, and let $\Psi^{-\infty}$ be the class of operators with infinitely differentiable Schwartz kernels. If $a \in S^{-\infty}$ (that is, if a and all its derivatives vanish faster than any power of $|\xi|$ as $|\xi| \to \infty$) then the corresponding PDO A belongs to $\Psi^{-\infty}$. The classical theory of PDOs is used to study singularities. Therefore one usually assumes that a is defined modulo $S^{-\infty}$ and that x is close to y.

Let $a \in S^m_{\rho,\delta}$ and $a_j \in S^{m_j}_{\rho,\delta}$ for some $\rho, \delta \in [0,1]$, where $m_j \to -\infty$ as $j \to \infty$. We shall write

$$a \sim \sum_j a_j\,, \quad |\xi| \to \infty\,, \tag{2.2}$$

if $a - \sum\limits_{j<k} a_j \in S^{n_k}_{\rho,\delta}$ where $n_k \to -\infty$ as $k \to \infty$. Such series $\sum_j a_j$ are called asymptotic. If $m_j \to -\infty$ then for every collection of amplitudes $a_j \in S^{m_j}_{\rho,\delta}$ there exists an amplitude a satisfying (2.2). Obviously, if a' is another amplitude satisfying (2.2) then $a - a' \in S^{-\infty}$ (or, in other words, (2.2) defines a modulo $S^{-\infty}$).

Lemma 2.3. *Let $z_\tau := x + \tau(y-x)$ where $\tau \in [0,1]$. If $\delta < \rho$ and $a \in S^m_{\rho,\delta}$ then*

$$\int e^{i(x-y)\cdot\xi} a(x,y,\xi)\,\mathrm{d}\xi \;=\; \int e^{i(x-y)\cdot\xi} \sigma_{A,\tau}(z_\tau,\xi)\,\mathrm{d}\xi$$

modulo an infinitely differentiable function, where $\sigma_{A,\tau}(z,\xi)$ is an amplitude of class $S^m_{\rho,\delta}$ given by the asymptotic expansion

$$\sigma_{A,\tau}(z,\xi) \sim \sum_{\alpha,\beta} \frac{(-i)^{|\alpha|+|\beta|}\,\tau^{|\alpha|}(1-\tau)^{|\beta|}}{\alpha!\,\beta!}\;\partial_x^\alpha \partial_y^\beta \partial_\xi^{\alpha+\beta} a(x,y,\xi)\Big|_{y=x=z}\,, \quad |\xi| \to \infty\,. \tag{2.3}$$

Sketch of proof. Expand the amplitude a by Taylor's formula at the point $(x,y) = (z_\tau, z_\tau)$, replace $(y-x)e^{i(x-y)\cdot\xi}$ with $i\nabla_\xi e^{i(x-y)\cdot\xi}$ and integrate by parts with respect to ξ. □

The amplitude $\sigma_{A,\tau}(x,\xi)$ is called the *τ-symbol* of the PDO A. It is uniquely defined by the operator A modulo $S^{-\infty}$. The 0-symbol is usually called just the symbol and is denoted σ_A. The $\frac{1}{2}$-symbol and 1-symbol are said to be the Weyl and the dual symbol respectively.

In the theory of PDOs, properties of operators are usually described and results are stated in terms of their symbols. The following composition formula plays a key role in the symbolic calculus.

Theorem 2.4. *Let $A \in \Psi^{m_1}_{\rho,\delta}$ and $B \in \Psi^{m_2}_{\rho,\delta}$. If $\delta < \rho$ then the composition AB is a PDO of class $\Psi^{m_1+m_2}_{\rho,\delta}$ whose symbol admits the asymptotic expansion*

$$\sigma_{AB}(x,\xi) \;\sim\; \sum_\alpha \frac{(-i)^{|\alpha|}}{\alpha!}\,\partial_\xi^\alpha \sigma_A(x,\xi)\,\partial_x^\alpha \sigma_B(x,\xi)\,, \quad |\xi| \to \infty\,. \tag{2.4}$$

Sketch of proof. From the inversion formula for the Fourier transform it follows that the Schwartz kernel of AB is given by $(\mathbf{c}_1)$ with the amplitude $a(x,y,\xi) = \sigma_A(x,\xi)\sigma_{B,1}(y,\xi)$. Applying Lemma 2.3 with $\tau = 0$ to a, we obtain (2.4). □

Remark 2.5. Theorem 2.4 implies, in particular, that the resolvent of an elliptic differential operator is a PDO. Using (2.4), one can also show that a PDO of order m maps $W_2^s \bigcap C_0^\infty$ into W_2^{s-m}, where W_2^r are the Sobolev spaces.

Note that in the above lemmas the condition $\delta < \rho$ is of crucial importance; if it is not fulfilled then the terms in the right-hand sides of (2.3) and (2.4) do not form asymptotic series.

Clearly, the phase function $(x-y)\cdot\xi$ in $(\mathbf{c}_1)$ depends on the choice of coordinates on U. Passing to new coordinates $\tilde{x}$ and $\tilde{y}$, we obtain

$$\mathcal{A}(\tilde{x},\tilde{y}) \;=\; (2\pi)^{-n}\int e^{i(x(\tilde{x})-y(\tilde{y}))\cdot\xi}a(x(\tilde{x}),y(\tilde{y}),\xi)\,\mathrm{d}\xi\,.$$

In a sufficiently small neighbourhood of the diagonal $\{\tilde{x}=\tilde{y}\}$, the new phase function $\varphi(\tilde{x},\tilde{y},\xi)=(x(\tilde{x})-y(\tilde{y}))\cdot\xi$ can be written in the form

$$\varphi(\tilde{x},\tilde{y},\xi) \;=\; (\tilde{x}-\tilde{y})\cdot\Phi(\tilde{x},\tilde{y})\,\xi,$$

where $\Phi(\tilde{x},\tilde{y})$ is a smooth $n\times n$-matrix function such that $\det\Phi(\tilde{x},\tilde{y})\neq 0$. Changing variables $\eta=\Phi(\tilde{x},\tilde{y})\,\xi$, we see that

$$\mathcal{A}(\tilde{x},\tilde{y}) \;=\; (2\pi)^{-n}\int e^{i(\tilde{x}-\tilde{y})\cdot\xi}\tilde{a}(\tilde{x},\tilde{y},\eta)\,\mathrm{d}\eta\,,$$

where

$$\tilde{a}(\tilde{x},\tilde{y},\eta) \;=\; |\det\Phi(\tilde{x},\tilde{y})|^{-1}\,a(x(\tilde{x}),y(\tilde{y}),\Phi^{-1}(\tilde{x},\tilde{y})\eta)$$

is a new amplitude. Thus Definition 2.2 does not depend on the choice of coordinates. However, there are two obvious problems.

Problem 2.6. If $a\in S^m_{\rho,\delta}$ then, generally speaking, the new amplitude $\tilde{a}$ belongs only to the class $S^m_{\rho,\delta'}$ with $\delta':=\max\{\delta,1-\rho\}$. If $\rho<\frac12$ then $\delta'>\rho$ and the above lemmas fail. Thus for $\delta<\rho<\frac12$ it is impossible to define PDOs of class $S^m_{\rho,\delta}$ on a manifold and to develop a symbolic calculus using local coordinates.

Problem 2.7. If $\max\{\delta,1-\rho\}<\rho$ then the "main part" of the symbol σ_A (called the *principal* symbol of A) behaves as a function on the cotangent bundle under change of coordinates. However, lower-order terms in (2.3) do not have a clear geometric meaning. Therefore, the coordinate approach does not allow one to study the subtle properties of PDOs, which depend on the lower-order terms.

3. Linear connections

The above problems do not arise if we define the phase function $(x-y)\cdot\xi$ in an invariant way, without using local coordinates. It is possible, in particular, when the manifold is equipped with a linear connection. In this section we shall briefly recall some relevant definitions and results from differential geometry.

Let M be an n-dimensional C^∞-manifold. Further on we shall denote the points of M by x, y or z. The same letters will be used for local coordinates on M. Similarly, ξ, η and ζ will denote points of (or the dual coordinates) on the fibres T^*_xM, T^*_yM and T^*_zM of the cotangent bundle T^*M.

We are going to consider operators acting in the spaces of κ-densities on M, $\kappa\in\mathbb{R}$. Recall that a complex-valued "function" u on M is said to be a κ-density if it behaves under change of coordinates in the following way

$$u(y) \;=\; |\det\{\partial x^i/\partial y^j\}|^\kappa\, u\big(x(y)\big)\,.$$

The usual functions on M are 0-densities. The κ-densities are sections of some complex linear bundle Ω^κ over M. We denote by $C^\infty(M;\Omega^\kappa)$ and $C_0^\infty(M;\Omega^\kappa)$ the spaces of smooth κ-densities and smooth κ-densities with compact supports respectively. If $u\in C_0^\infty(M;\Omega^\kappa)$ and $v\in C^\infty(M;\Omega^{1-\kappa})$ then the product uv is a density and the integral $\int_M u\,v\,dx$ is independent of the choice of coordinates. This allows one to define the inner product $(u,v)=\int_M u\,\bar v\,dx$ on the space of half-densities $C_0^\infty(M;\Omega^{1/2})$ and to introduce the Hilbert space $L_2(M;\Omega^{1/2})$ in the standard way.

In this and the next sections we shall be assuming that the manifold M is provided with a linear connection Γ (which may be non-complete). This means that, for each local coordinate system, we have fixed a set of smooth "functions" $\Gamma^i_{jk}(x)$, $i,j,k=1,\dots,n$, which behave under change of coordinates in the following way,

$$\sum_l \frac{\partial y^i}{\partial x^l}\,\Gamma^l_{pq}(x) \;=\; \sum_{p,q} \frac{\partial y^j}{\partial x^p}\,\Gamma^i_{jk}\big(y(x)\big)\,\frac{\partial y^k}{\partial x^q} \;+\; \frac{\partial^2 y^i}{\partial x^p\,\partial x^q}\,. \tag{3.1}$$

The "functions" $\Gamma^i_{jk}(x)$ are called the *Christoffel symbols*. They can be chosen in an arbitrary way (provided that (3.1) holds), and every set of Christoffel symbols determines a linear connection of M.

A linear connection Γ is uniquely characterized by the torsion tensor $T^i_{jk}:=\Gamma^i_{jk}-\Gamma^i_{kj}$ and the curvature tensor

$$R^i_{jkl} \;:=\; \partial_{y^k}\Gamma^i_{lj} \;-\; \partial_{y^l}\Gamma^i_{kj} \;+\; \sum_p \Gamma^i_{kp}\Gamma^p_{lj} \;-\; \sum_p \Gamma^i_{lp}\,\Gamma^p_{kj}\,.$$

If both these tensors vanish on an open set $U\subset M$ then one can choose local coordinates on a neighbourhood of each point $x\in U$ in such a way that $\Gamma^i_{jk}=0$. Such connections are called *flat*. A connection Γ is called *symmetric* if $T^i_{jk}=0$.

Let $\nu=\sum \nu^k(y)\,\partial_{y^k}$ be a vector field on M. The equality (3.1) implies that

$$\nabla_\nu \;:=\; \sum_k \nu^k(y)\,\partial_{y^k} \;+\; \sum_{i,j,k} \Gamma^i_{kj}(y)\,\nu^k(y)\eta_i\,\partial_{\eta_j} \tag{3.2}$$

is a correctly defined vector field on T^*M. The vector field (3.2) is called the *horizontal lift* of ν. The horizontal lifts generate a n-dimensional subbundle HT^*M of the tangent bundle TT^*M over T^*M, which is called the *horizontal distribution*. The vertical vector fields $\partial_{\eta_1},\dots,\partial_{\eta_n}$ generate another n-dimensional subbundle $VT^*M\subset TT^*M$ which is called the *vertical distribution*. Since $HT^*M\cap VT^*M=\{0\}$, the tangent space $T_{(y,\eta)}T^*M$ at each point $(y,\eta)\in T^*M$ coincides with the sum of its horizontal and vertical subspaces. Obviously, the horizontal subspaces depend on the choice of Γ whereas the vertical subspaces do not.

A curve in the cotangent bundle T^*M is said to be horizontal (or vertical) if its tangent vectors belong to HT^*M (or VT^*M). For any given curve $y(t)\subset M$

and covector $\eta_0 \in T^*_{y(0)}M$ there exists a unique horizontal curve $\big(y(t),\eta(t)\big) \subset T^*M$ starting at the point $(y(0),\eta_0)$, whose projection onto M coincides with $y(t)$. It is defined in local coordinates y by the equations

$$\frac{d}{dt}\,\eta_j(t) \;-\; \sum_{i,k} \Gamma^i_{kj}\big(y(t)\big)\,\dot y^k(t)\,\eta_i(t) \;=\; 0\,, \quad \forall j=1,\dots,n\,,$$

and is called the *horizontal lift* of $y(t)$. The corresponding linear transformation $\eta_0 \to \eta(t)$ is said to be the *parallel displacement* along the curve $y(t)$. By duality, horizontal curves and parallel displacements are defined in the tangent bundle TM (and then in all the tensor bundles over M).

A curve $y(t) \subset M$ is said to be a geodesic if the curve $\big(y(t),\dot y(t)\big) \subset TM$ is horizontal or, equivalently, if

$$\ddot y^k(t) \;+\; \sum_{i,j} \Gamma^k_{ij}\big(y(t)\big)\,\dot y^i(t)\,\dot y^j(t) \;=\; 0\,, \quad \forall k=1,\dots,n\,.$$

in any local coordinate system. If U_x is a sufficiently small neighbourhood of x then for every $y \in U_x$ there exists a unique geodesic $\gamma_{y,x}(t)$ such that $\gamma_{y,x}(0)=x$ and $\gamma_{y,x}(1)=y$. The mapping $U_x \ni y \mapsto \dot\gamma_{y,x}(0) \in T_xM$ is a bijection between U_x and a neighbourhood of the origin in T_xM, and the corresponding coordinates on U_x are called the *normal coordinates*. In the normal coordinates y centred at x we have $\gamma_{y,x}(t) = x + t(y-x)$, so that $\dot\gamma_{y,x}(t) = y - x$ for all $t \in [0,1]$.

Let $\Phi_{y,x} : T^*_xM \to T^*_yM$ be the parallel displacement along the geodesic $\gamma_{y,x}$, and let $\Upsilon_{y,x} = |\det \Phi_{y,x}|$. One can easily check that $\Upsilon_{y,x}$ is a density in y and a (-1)-density in x (the map $w_x \to \Upsilon_{y,x}w_x$ is the parallel displacement along $\gamma_{y,x}$ between the fibres of the bundle Ω). Note that $\Phi_{y,x}$ and $\Upsilon_{y,x}$ depend on the torsion tensor, whereas the geodesics are determined only by the symmetric part of Γ.

Given local coordinates $x = \{x^1,\dots,x^n\}$, let us denote by ∇_i the horizontal lifts of vector fields ∂_{x^i}. For a multi-index α with $|\alpha| = q$, let $\nabla^\alpha_x = \frac{1}{q!}\sum \nabla_{i_1}\dots\nabla_{i_q}$ where the sum is taken over all ordered collections of indices $i_1,\dots,i_q$ corresponding to the multi-index α. The following simple lemma can be found, for instance, in [Sa2, Section 3].

Lemma 3.1. *If $a \in C^\infty(T^*M)$ then $a(y,\Phi_{y,x}\xi)$ admits the following asymptotic expansion,*

$$a(y,\Phi_{y,x}\xi) \;\sim\; \sum_\alpha \frac{1}{\alpha!}\,\dot\gamma^\alpha_{y,x}\,\nabla^\alpha_x a(x,\xi)\,, \quad y \to x\,. \tag{3.3}$$

Sketch of proof. Write down the left-hand side in normal coordinates y centred at x and apply Taylor's formula. □

Remark 3.2. If a is a function on T^*M then the "hypermatrix" $\{\partial^\beta_\xi \nabla^\alpha_x a(x,\xi)\}_{\substack{|\alpha|=q\\|\beta|=p}}$ behaves as a (p,q)-tensor under change of coordinates. Therefore all the formulae in the next section have an invariant meaning and do not depend on the choice of coordinates.

4. PDOs: a coordinate-free approach

Definition 4.1. We shall say that an amplitude a defined on $M \times T^*M$ belongs to the class $S^m_{\rho,\delta}(\Gamma)$ with $\rho,\delta \in [0,1]$ and $m \in \mathbb{R}$ if

$$\sup_{(x,z)\in K} |\partial_x^\alpha \partial_\zeta^\beta \nabla_{i_1}\nabla_{i_2}\dots\nabla_{i_q} a(x,z,\zeta)| \;\le\; C_{K;\alpha,\beta,q}\,(1+|\xi|)^{m+\delta(|\alpha|+q)-\rho|\beta|} \quad (4.1)$$

for each compact set $K \subset M \times M$, all multi-indices α,β and all sets of indices $i_1,\dots,i_q$, where ∇_k are horizontal lifts of the vector fields ∂_{z_k} and $C_{K;\alpha,\beta,\gamma}$ are some positive constants.

From the definition of the horizontal lifts it follows that $a \in S^m_{\rho,\delta}(\Gamma)$ with $\delta \ge 1-\rho$ if and only if a satisfies (2.1) in any local coordinate system. In this case the class $S^m_{\rho,\delta}(\Gamma)$ is the same for all linear connections Γ. If $\delta < 1-\rho$ then $S^m_{\rho,\delta}(\Gamma)$ depends on the choice of Γ. Note that (2.1) is a particular case of (4.1), in which the connection Γ is flat.

Let us fix a sufficiently small neighbourhood V of the diagonal in $M \times M$ and define $z_\tau = z_\tau(x,y) = \gamma_{y,x}(\tau)$, where $\tau \in [0,1]$ is regarded as a parameter. Consider the phase function

$$\varphi_\tau(x,\zeta,y) \;=\; -\langle \dot\gamma_{y,x}(\tau),\zeta\rangle\,, \quad (x,y)\in V\,, \quad \zeta \in T^*_{z_\tau}M\,, \quad (4.2)$$

where $\langle\cdot,\cdot\rangle$ denotes the standard pairing between vectors and covectors. The function φ_τ is invariantly defined and, by the above, coincides with $(x-y)\cdot\zeta$ in normal coordinates y centred at x.

Definition 4.2. An operator A acting in the space of κ-densities on M is said to be a PDO of class $\Psi^m_{\rho,\delta}(\Omega^\kappa,\Gamma)$ if

(c) its Schwartz kernel $\mathcal{A}(x,y)$ is infinitely differentiable outside the diagonal $\{x=y\}$,

(c$_2$) $\mathcal{A}(x,y) \;=\; (2\pi)^{-n}\,p_{\kappa,\tau}(x,y)\int_{T^*_{z_\tau}M} e^{i\varphi_\tau(x,\zeta,y)} a(z_s;z_\tau,\zeta)\,\mathrm{d}\zeta$ in a neighbourhood of the diagonal, where $a \in S^m_{\rho,\delta}(\Gamma)$, $p_{\kappa,\tau} := \Upsilon^{1-\kappa}_{y,z_\tau}\Upsilon^{-\kappa}_{z_\tau,x}$ and $s,\tau \in [0,1]$ are some fixed numbers.

Remark 4.3. If y are normal coordinates centred at x then $\varphi_\tau(x,\zeta,y) = (x-y)\cdot\zeta$ and the integral **(c$_2$)** takes the form **(c$_1$)**. However, Definition 2.2 assumes that x and y are the same local coordinates on U, whereas the above identity holds if we choose coordinates y depending on the point x.

Remark 4.4. The weight factor $p_{\kappa,\tau}$ is introduced for the following two reasons.

(1) It makes the definition independent of the choice of coordinates ζ in the cotangent space $T^*_{z_\tau}M$.

(2) Because of this factor, the Schwartz kernel behaves as a $(1-\kappa)$-density in y and κ-density in x, that is, **(c$_2$)** defines an operator in the space of κ-densities for all $\kappa \in \mathbb{R}$ and all $s,\tau \in [0,1]$. In particular, this allows us to consider PDOs in the Hilbert space $L_2(M,\Omega^{1/2})$ and to introduce Weyl symbols (corresponding to $\tau = \frac{1}{2}$).

One can replace $p_{\kappa,\tau}$ in Definition 4.2 with any other smooth weight factor $p(x,y)$ which behaves in a similar way under change of coordinates. The precise choice of the weight factor seems to be of little importance, since all formulae in the symbolic calculi corresponding to different weight factors p and $\tilde p$ can easily be deduced from each other by expanding the function $p^{-1}\tilde p$ into an asymptotic series of the form (3.3), replacing $\dot\gamma_{y,x}(z_\tau)\, e^{i\varphi_\tau(x,\zeta,y)}$ with $i\nabla_\zeta\, e^{i\varphi_\tau(x,\zeta,y)}$ and integrating by parts with respect to ζ.

Lemma 4.5. *If $\delta<\rho$ and $a\in S^m_{\rho,\delta}(\Gamma)$ then for all $s,\tau\in[0,1]$*

$$p_{\kappa,\tau}\int_{T^*_{z_\tau}M} e^{i\varphi_\tau(x,\zeta,y)}a(z_s;z_\tau,\zeta)\,\mathrm{d}\zeta \;=\; p_{\kappa,\tau}\int_{T^*_{z_\tau}M} e^{i\varphi_\tau(x,\zeta,y)}\sigma_{A,\tau}(z_\tau,\zeta)\,\mathrm{d}\zeta$$

and

$$p_{\kappa,\tau}\int_{T^*_{z_\tau}M} e^{i\varphi_\tau(x,\zeta,y)}\sigma_{A,\tau}(z_\tau,\zeta)\,\mathrm{d}\zeta \;=\; p_{\kappa,s}\int_{T^*_{z_s}M} e^{i\varphi_s(x,\zeta,y)}\sigma_{A,s}(z_s,\zeta)\,\mathrm{d}\zeta$$

modulo C^∞-densities, where $\sigma_{A,\tau}$ and $\sigma_{A,s}$ are amplitudes of class $S^m_{\rho,\delta}(\Gamma)$ given by the asymptotic expansions

$$\sigma_{A,\tau}(x,\xi)\;\sim\;\sum_\alpha \frac{(-i)^{|\alpha|}\,(s-\tau)^{|\alpha|}}{\alpha!}\;\partial_\xi^\alpha\nabla_y^\alpha a(y;x,\xi)\big|_{y=x},\quad |\xi|\to\infty\,,$$

$$\sigma_{A,s}(x,\xi)\;\sim\;\sum_\alpha \frac{(-i)^{|\alpha|}\,(\tau-s)^{|\alpha|}}{\alpha!}\;\partial_\xi^\alpha\nabla_x^\alpha \sigma_{A,\tau}(x,\xi),\qquad |\xi|\to\infty\,.$$

Sketch of proof. The first identity is proved by applying (3.3) with $x=z_\tau$ and $y=z_s$ to the function $a(\cdot;z_\tau,\zeta)$ with fixed (z_τ,ζ), substituting $\dot\gamma_{z_s,z_\tau}\,e^{i\varphi_\tau}=(\tau-s)\,\nabla_\zeta e^{i\varphi_\tau}$ and integrating by parts. The second is obtained in a similar way, after changing variables $\zeta=\Phi_{z_s,z_\tau}\zeta'$. □

Lemma 4.5 shows that Definition 4.2 does not depend on the choice of τ and s, and that every PDO A is defined modulo $\Psi^{-\infty}$ by its τ-symbol $\sigma_{A,\tau}$. The other way round, for each linear connection Γ, the τ-symbol $\sigma_{A,\tau}$ is determined by the operator A modulo $S^{-\infty}$.

If $A\in\Psi^m_{\rho,\delta}(\Omega^\kappa,\Gamma)$ then, in a similar way, one can show that

$$\sigma_{A^*,\tau}(x,\xi)\;\sim\;\sum_\alpha \frac{(-i)^{|\alpha|}\,(1-2\tau)^{|\alpha|}}{\alpha!}\;\partial_\xi^\alpha\nabla_x^\alpha\overline{\sigma_{A,\tau}(x,\xi)},\quad |\xi|\to\infty\,, \tag{4.3}$$

where A^* is the adjoint operator acting in the space of $(1-\kappa)$-densities. In particular, for the Weyl symbols we have $\sigma_{A^*,1/2}-\overline{\sigma_{A,1/2}}\in S^\infty$ for all $\kappa\in\mathbb{R}$.

Remark 4.6. The full τ-symbol $\sigma_{A,\tau}$ depends on Γ and τ. If $\max\{\delta,1-\rho\}<\rho$ then all the τ-symbols $\sigma_{A,\tau}$ corresponding to different connections Γ coincide with the principal symbol of A modulo a lower-order term. However, in the general case it seems to be impossible to define a principal symbol of A without introducing an additional structure on the manifold M or a global phase function (see Subsection 7.8).

Let

$$\Upsilon_\kappa(x,y,z) := \Upsilon_{y,z}^{1-\kappa}\,\Upsilon_{z,x}^{2-\kappa}\,\Upsilon_{x,y}^{1-\kappa},$$
$$\psi(x,\xi;y,z) := \langle\dot\gamma_{y,x},\xi\rangle - \langle\dot\gamma_{z,x},\xi\rangle - \langle\dot\gamma_{y,z},\Phi_{z,x}\xi\rangle$$

and

$$P_{\beta,\gamma}^{(\kappa)}(x,\xi) \;=\; \Big((\partial_y+\partial_z)^\beta\partial_y^\gamma \sum_{|\beta'|\le|\beta|} \frac{1}{\beta'!} D_\xi^{\beta'}\partial_y^{\beta'}(e^{i\psi}\Upsilon_\kappa)\Big)\Big|_{y=z=x},$$

where y and z are normal coordinates centred at x. The functions $P_{\beta,\gamma}^{(\kappa)} \in C^\infty(T^*M)$ are polynomials in ξ; we shall denote their degrees by $d_{\beta,\gamma}^{(\kappa)}$.

One can easily show that $P_{0,\gamma}^{(\kappa)} \equiv 0$, $P_{\beta,0}^{(\kappa)} \equiv 0$ and $d_{\beta,\gamma}^{(\kappa)} \le \min\{\,|\beta|,|\gamma|\,\}$ for any connection Γ. Moreover, if Γ is symmetric then $d_{\beta,\gamma}^{(\kappa)} \le \min\{\,|\beta|,|\gamma|,(|\beta|+|\gamma|)/3\,\}$ [Sa2, Lemma 8.1].

Theorem 4.7. *Let* $A \in \Psi_{\rho,\delta}^{m_1}(\Omega^\kappa,\Gamma)$ *and* $B \in \Psi_{\rho,\delta}^{m_2}(\Omega^\kappa,\Gamma)$, *where* $\rho > \delta$. *Assume, in addition, that*

(1) *either* $\rho > 1/2$,
(2) *or the connection* Γ *is symmetric and* $\rho > 1/3$,
(3) *or at least one of the PDOs A and B belongs to* $\Psi_{1,0}^m(\Omega^\kappa,\Gamma)$.

Then $AB \in \Psi_{\rho,\delta}^{m_1+m_2}(\Omega^\kappa,\Gamma)$ *and*

$$\sigma_{AB}(x,\xi) \sim \sum_{\alpha,\beta,\gamma} \frac{1}{\alpha!}\frac{1}{\beta!}\frac{1}{\gamma!}\; P_{\beta,\gamma}^{(\kappa)}(x,\xi)\; D_\xi^{\alpha+\beta}\sigma_A(x,\xi)\; D_\xi^\gamma\nabla_x^\alpha\sigma_B(x,\xi)\,,\qquad |\xi|\to\infty. \tag{4.4}$$

The proof of Theorem 4.7 is similar to that of Theorem 2.4 (see [Sa2, Sec. 8]). In particular, if the connection Γ is flat then $P_{\beta,\gamma}^{(\kappa)} \equiv 0$ as $|\beta|+|\gamma|\ge 1$ and (4.4) turns into (2.4).

Remark 4.8. The conditions on ρ and the estimates for $d_{\beta,\gamma}^{(\kappa)}$ imply that the terms in the right-hand side of (4.4) form an asymptotic series. It is plausible that the composition formula (4.4) holds whenever the orders of the terms in the right-hand side tend to $-\infty$ as $|\alpha|+|\beta|+|\gamma|\to\infty$. However, it is not clear how this can be proved.

Remark 4.9. Coefficients of the polynomials $P_{\beta,\gamma}^{(\kappa)}$ are components of some tensors, which are polynomials in the curvature and torsion tensors and their symmetric covariant differentials.

In the same way as in the local theory of PDOs, Theorem 4.7 implies standard results on the boundedness of PDOs in the Sobolev spaces and allows one to construct the resolvent of an elliptic operator in the form of a PDO.

5. Functions of the Laplacian

In this section we assume that M is a compact Riemannian manifold without boundary and denote $|\xi|_x := \sqrt{\sum_{i,j} g^{ij}(x)\,\xi_i\xi_j}$ where $\xi \in T_x^*M$ and $\{g^{ij}\}$ is the metric tensor. It is well known that there exist a unique symmetric connection $\Gamma_{\mathbf{g}}$ on M, called the Levi–Civita connection, such that the function $|\xi|_x$ is constant along every horizontal curve in T^*M.

Denote by Δ the Laplace operator acting in the space of half-densities; in local coordinates

$$\Delta u(x) \;=\; g^{\kappa-1}(x) \sum_{i,j} \partial_{x^i} \left(g(x)\, g^{ij}(x)\, \partial_{x^j} \left(g^{-\kappa}(x) u(x)\right)\right),$$

where $g := |\det g^{ij}|^{-1/2}$ is the canonical Riemannian density. Let ν be a self-adjoint first-order PDO such that $-\Delta + \nu > 0$, and let $A_\nu := \sqrt{-\Delta+\nu}$. The operator A_ν is a PDO of class $\Psi^1_{1,0}$ whose symbol coincides with $|\xi|_x$ modulo S^0 in any local coordinate system. Thus we have $A_\nu \in \Psi^1_{1,0}(\Omega^{1/2},\Gamma)$ for any linear connection Γ.

Definition 5.1. If $\rho \in (0,1]$, let S^m_ρ be the class of infinitely differentiable functions ω on $\mathbb{R}$ such that

$$|\partial_s^j \omega(s)| \;\le\; C_j\,(1+|s|)^{m-j\rho}\,, \quad \forall j = 0,1,\dots, \tag{5.1}$$

where C_k are some constants.

A natural conjecture is that the operator $\omega(A_\nu)$ is a PDO whenever $\omega \in S^m_\rho$. If it is true then the symbol of $\omega(A_\nu)$ should coincide with $\omega(|\xi|_x)$ modulo lower-order terms. If $\rho < 1/2$ then, generally speaking, this function does not belong to the class $S^m_{\rho,\delta}$ with $\rho > \delta$ in any local coordinate system. However, since its horizontal derivatives corresponding to the Levi–Civita connection are equal to zero, we have $\omega(|\xi|_x) \in S^m_{\rho,\delta}(\Gamma_{\mathbf{g}})$ for all $\omega \in S^m_\rho$. In particular, this implies the following

Lemma 5.2. *Let $\tau \in [0,1)$ and $U_\tau(t) := \exp(itA_\nu^\tau)$. Then $U_\tau(t) \in \Psi^m_{1-\tau,0}(\Omega^{1/2},\Gamma_{\mathbf{g}})$ for all $t \in \mathbb{R}$ and $\sigma_{U_\tau(t)}(x,\xi) = e^{it|\xi|_x^\tau}\, b^{(\tau)}(t,x,\xi)$, where $b^{(\tau)} \in C^\infty(\mathbb{R}\times T^*M)$ and $\partial_t^k b^{(\tau)} \in S^0_{1,0}$ for all $k = 0,1,\dots$ and each fixed t.*

Sketch of proof. Write down $U_\tau(t)$ formally as an integral $(\mathbf{c}_2)$ with an unknown symbol of the form $e^{it|\xi|_x^\tau}\, b^{(\tau)}(t,x,\xi)$, substitute the integral into the equation $\partial_t U_\tau(t) = iA_\nu^\tau U_\tau(t)$, apply the composition formula (4.4) to $A_\nu^\tau U_\tau(t)$ and equate terms of the same order in the right- and left-hand sides. □

Using Lemma 5.2, one can construct other functions of the operator A_ν.

Theorem 5.3. *If $\omega \in S^m_\rho$ then $\omega(A_\nu) \in \Psi^m_{\rho,0}(\Omega^{1/2},\Gamma_{\mathbf{g}})$ and*

$$\sigma_{\omega(A_\nu)} \;\sim\; \omega(|\xi|_x) + \sum_{j=1}^{\infty} c_{j,\nu}(x,\xi)\,\omega^{(j)}(|\xi|_x)\,, \quad |\xi| \to \infty, \tag{5.2}$$

where $\omega^{(j)} := \partial_s^j \omega$ *and* $c_{j,\nu}(x,\xi) \in S^0_{1,0}$. *The functions* $c_{j,\nu}$ *are determined recursively by the equations*

$$\sigma_{A_\nu^k}(x,\xi) = |\xi|_x^k + \sum_{j=1}^{k} \frac{k!}{(k-j)!} |\xi|_x^{k-j}\, c_{j,\nu}(x,\xi). \tag{5.3}$$

Sketch of proof. Define $\omega_\tau(s) = \omega(s^{1/\tau})$, and let $\widehat{\omega_\tau}(t)$ be the Fourier transform of ω_τ. Then

$$\omega(A_\nu) = (2\pi)^{-1} \int \widehat{\omega_\tau}(t)\, e^{itA_\nu^\tau}\, \mathrm{d}t.$$

Let $\varsigma \in C_0^\infty(\mathbb{R})$ be equal to 1 in a neighbourhood of the origin and have support contained in a small neighbourhood of the origin. Consider the operators

$$\omega_1(A_\nu) = (2\pi)^{-1} \int \varsigma(t)\, \widehat{\omega_\tau}(t)\, e^{itA_\nu^\tau}\, \mathrm{d}t,$$
$$\omega_2(A_\nu) = (2\pi)^{-1} \int (1-\varsigma(t))\, \widehat{\omega_\tau}(t)\, e^{itA_\nu^\tau}\, \mathrm{d}t.$$

By integration by parts, the operator $\omega_2(A_\nu)$ can be written as

$$\omega_2(A_\nu) = (2\pi)^{-1} A_\nu^{-k} \int D_t^k \left((1-\varsigma(t))\, \widehat{\omega_\tau}(t)\right) e^{itA_\nu^\tau}\, \mathrm{d}t.$$

Since k may be chosen arbitrarily large, this shows that $\omega_2(A_\nu)$ has an infinitely smooth kernel. By Lemma 5.2, the operator $\omega_1(A_\nu)$ is a PDO whose symbol coincides with

$$(2\pi)^{-1} \int_{-\infty}^{\infty} \varsigma(t)\, \widehat{\omega_\tau}(t)\, e^{it|\xi|_x^\tau}\, b^{(\tau)}(t,x,\xi)\, \mathrm{d}t\,.$$

Expanding $\varsigma(t) b^{(\tau)}(t,x,\xi)$ by Taylor's formula at $t=0$, we see that the symbol of $\omega_1(A_\nu)$ admits an asymptotic expansion of the form (5.2) with some functions $c_{j,\nu}$. These functions do not depend on ω and can be found by substituting $\omega(s) = s^k$ with $k = 1,2,\dots$ This leads to (5.3). □

Definition 5.4. If $\rho \in (0,1]$, let $S_\rho^m(\mathbf{g})$ be the class of C^∞-functions on T^*M which admit asymptotic expansions of the form

$$a(x,\xi) \;\sim\; \sum_{j=0}^{\infty} c_j(x,\xi)\, \omega_j(|\xi|_x)\,, \quad |\xi| \to \infty, \tag{5.4}$$

where $c_j \in S^0_{1,0}$, $\omega_j \in S_\rho^{m_j}$ with $m_0 = m$ and $m_j \to -\infty$. Denote by $\Psi_\rho^m(\Omega^{1/2},\mathbf{g})$ the class of PDOs acting in the space of half-densities whose $\Gamma_{\mathbf{g}}$-symbols belong to $S_\rho^m(\mathbf{g})$.

Theorem 5.3 immediately implies that $\omega(A_\nu) \in \Psi_\rho^m(\Omega^{1/2},\mathbf{g})$ whenever $\omega \in S_\rho^m$. The other way round, any PDOs of class $\Psi_\rho^m(\Omega^{1/2},\mathbf{g})$ can be represented in terms of functions of the operator A_ν.

Lemma 5.5. *For each $A \in \Psi_\rho^m(\Omega^{1/2}, \mathbf{g})$ there exist PDOs $C_{j,\nu} \in \Psi_{1,0}^0$ and functions $\tilde\omega_j \in S_\rho^{l_j}$ such that $l_0 = m$, $l_j \to -\infty$ and*

$$A \sim \sum_{j=0}^{\infty} C_{j,\nu}\, \tilde\omega_j(A_\nu)\,, \tag{5.5}$$

where $\sim$ means that the Schwartz kernel of the difference $A - \sum_{j=0}^{k} C_{j,\nu}\, \tilde\omega_j(A_\nu)$ becomes smoother and smoother as $k \to \infty$.

Sketch of proof. Assume that (5.4) holds and denote by C_0 the PDO with symbol $c_0(x,\xi)$. Theorems 4.7 and 5.3 imply that $A = C_0\, \omega_0(A_\nu) + A_\nu^{(1)}$ where $A_\nu^{(1)} \in \Psi_\rho^{l_1}(\Omega^{1/2}, \mathbf{g})$ with $l_1 \le \max\{m_1, m_0 - \rho\}$. The same arguments show that $A_\nu^{(1)} = C_{1,\nu}\, \tilde\omega_1(A_\nu) + A_\nu^{(2)}$ where $C_{1,\nu} \in \Psi_{1,0}^0$, $\tilde\omega_1 \in S_\rho^{l_1}$ and $A_\nu^{(2)} \in \Psi_\rho^{l_2}(\Omega^{1/2}, \mathbf{g})$ where $l_2 \le \max\{m_2, l_1 - \rho\}$. Repeatedly applying this procedure, we obtain a sequence of operators $A_\nu^{(k)} \in \Psi_\rho^{l_k}(\Omega^{1/2}, \mathbf{g})$ such that $A - A_\nu^{(k)} = \sum_{j=0}^{k-1} C_{j,\nu}\, \tilde\omega_j(A_\nu)$, where $C_{j,\nu}$ and $\tilde\omega_j$ satisfy the required conditions and $l_k \to -\infty$ as $k \to \infty$. □

Since $\omega_1(A_\nu)\, \omega_2(A_\nu) = \omega_1\omega_2\,(A_\nu)$ for any two functions ω_1 and ω_2, combining Theorem 4.7 and Lemma 5.5, we obtain

Corollary 5.6. *If $A \in \Psi_\rho^{m_1}(\Omega^{1/2}, \mathbf{g})$ and $B \in \Psi_\rho^{m_2}(\Omega^{1/2}, \mathbf{g})$ then the composition AB is a PDO of class $\Psi_\rho^{m_1+m_2}(\Omega^{1/2}, \mathbf{g})$ whose symbol admits the asymptotic expansion* (4.4).

Remark 5.7. Under the conditions of Corollary 5.6, the estimates on $d_{\beta,\gamma}^{(\kappa)}$ obtained in Section 4 do not directly imply that (4.4) is an asymptotic series, as it seems to contain terms of growing orders. However, these "bad" terms cancel out due to the symmetries of the curvature tensor. It would be interesting to find a direct proof of Corollary 5.6, which does not use Lemma 5.5 (a relevant problem was mentioned in Remark 4.8).

From the above results it follows that the restriction of the operator $\omega(A_\nu)$ to an open subset of M is determined modulo $\Psi^{-\infty}$ by the restrictions of the metric $\mathbf{g}$ and the operator ν to this subset. More precisely, we have the following

Corollary 5.8. *Let $\upsilon \in C_0^\infty(M)$, and let $\{\upsilon\}$ be the corresponding multiplication operator. Consider the operator $\tilde A_{\tilde\nu}$ generated by another metric $\tilde{\mathbf{g}}$ and another first-order PDO $\tilde\nu$. If $\tilde{\mathbf{g}} = \mathbf{g}$ on the support of the function υ and $\tilde\nu\,\{\upsilon\} = \nu\,\{\upsilon\}$ then*

$$\{\upsilon\}\big(\omega(A_\nu) - \omega(\tilde A_{\tilde\nu})\big) \in \Psi^{-\infty} \quad \textit{and} \quad \big(\omega(A_\nu) - \omega(\tilde A_{\tilde\nu})\big)\{\upsilon\} \in \Psi^{-\infty}$$

for every $\omega \in S_\rho^m$.

Sketch of proof. The multiplication operator $\{\upsilon\}$ is a PDO with symbol $\upsilon(x)$, which belongs to $\Psi_\rho^0(\Omega^{1/2}, \mathbf{g})$. Applying Lemma 5.5 and Corollary 5.6, we see that $\{\upsilon\}\big(\omega(A_\nu) - \omega(\tilde A_{\tilde\nu})\big)$ and $\big(\omega(A_\nu) - \omega(\tilde A_{\tilde\nu})\big)\{\upsilon\}$ are PDOs whose full symbols are identically equal to zero. □

Remark 5.9. In a similar way, it is possible to define the classes $\Psi^m_\rho(\Omega^\kappa, \mathbf{g})$ which consist of PDOs acting in the space of κ-densities. Theorem 4.7 implies that $A \in \Psi^m_\rho(\Omega^\kappa, \mathbf{g})$ if and only if $g^{1/2-\kappa} A g^{\kappa-1/2} \in \Psi^m_\rho(\Omega^{1/2}, \mathbf{g})$. Using this observation, one can easily reformulate all results of this section for operators $A \in \Psi^m_\rho(\Omega^\kappa, \mathbf{g})$.

6. An approximate spectral projection

In applications, one often has to deal with functions of an operator which depend on additional parameters. It is more or less clear that the results of the previous section can be extended to parameter-dependent functions ω under the assumption that the estimates (5.1) hold uniformly with respect to the parameters. Therefore, instead of formulating general statements, we shall consider an example which is of particular interest for spectral theory.

Further on we assume that $\lambda > 0$ and denote by $\Psi^{-\infty}(\lambda)$ the class of parameter-dependent operators with infinitely smooth Schwartz kernels $\mathcal{A}_\lambda(x,y)$ such that

$$\lim_{\lambda\to\infty} \lambda^p \, |\partial_x^\alpha \partial_y^\beta \mathcal{A}_\lambda(x,y)| \;=\; 0$$

for all multi-indices α, β and all $p = 1, 2, \ldots$ Similarly, let $S^{-\infty}(\lambda)$ be the class of parameter-dependent amplitudes a_λ such that

$$(\lambda + |\xi|)^p \sup_{(x,y)\in M} |\partial_\xi^\alpha \nabla_x^\beta \nabla_y^\gamma a_\lambda(y;x,\xi)| \;\to\; 0 \quad \text{as } \lambda + |\xi| \to \infty$$

for all multi-indices α, β, γ and all $p = 1, 2, \ldots$

Let us fix a small $\varepsilon > 0$ and a nonincreasing function $f \in C^\infty(\mathbb{R})$ such that

$$f(s) = \begin{cases} 1 & \text{if } s \le 0; \\ 0 & \text{if } s \ge \varepsilon, \end{cases}$$

and $0 \le f(s) \le 1$ for all $s \in \mathbb{R}$. If $\rho \in (0,1]$ and $\lambda > 0$, let

$$\chi_\rho(\lambda, s) \;:=\; f(\lambda^{-\rho}(s - \lambda)) .$$

For each fixed $\lambda > 0$, the function χ_ρ vanishes on the interval $[\lambda + \varepsilon\lambda^\rho, \infty)$, is identically equal to 1 on the interval $(-\infty, \lambda]$ and smoothly descends from 1 to 0 on the interval $[\lambda, \lambda + \varepsilon\lambda^\rho]$. Since this functions differs from the characteristic function of the interval $[-\infty, \lambda]$ only on the relatively small interval $(\lambda, \lambda + \varepsilon\lambda^\rho)$, the operator $\chi(\lambda, A_\nu)$ can be thought of as an approximate spectral projection of A_ν corresponding to $(-\infty, \lambda]$. The standard elliptic regularity theorem implies that the operator $\chi(\lambda, A_\nu)$ has an infinitely differentiable Schwartz kernel for each fixed λ.

The derivatives $\partial_s^j \chi_\rho(\lambda, s)$ are equal to zero outside the interval $(\lambda, \lambda + \varepsilon\lambda^\rho)$. Therefore

$$|\partial_s^j \chi_\rho(\lambda, s)| \;\le\; \tilde{C}_j \, (|s| + \lambda)^{-j\rho} , \quad \forall j = 0, 1, \ldots, \tag{6.1}$$

for all $s \in \mathbb{R}$ and all $\lambda > 1$, where $\tilde{C}_j$ are some constants independent of λ and s. The same arguments as in the proof of Theorem 5.3 show that $\chi(\lambda, A_\nu)$ is a parameter-dependent PDO whose symbol admits the asymptotic expansion

$$\sigma_{\chi(\lambda,A_\nu)} \sim \chi(\lambda,|\xi|_x) + \sum_{j=1}^{\infty} c_{j,\nu}(x,\xi)\,\chi^{(j)}(\lambda,|\xi|_x)\,, \quad \lambda + |\xi| \to \infty, \tag{6.2}$$

where $c_{j,\nu}(x,\xi)$ are the same functions as in (5.3) and $\chi^{(j)}$ denotes jth s-derivative of the function χ.

Note that the functions $\chi^{(j)}(\lambda,|\xi|_x)$ belong to $S^{-\infty}$ for each fixed λ. However, their rate of decay depends on λ. The asymptotic expansion (6.2) is uniform with respect to λ; it defines $\sigma_{\chi(\lambda,A_\nu)}$ modulo $S^{-\infty}(\lambda)$. Substituting the terms from (6.2) into the integral **(c$_2$)**, we obtain an asymptotic expansion of the Schwartz kernel of $\chi(\lambda, A_\nu)$ into a series of infinitely smooth half-densities, which decay more and more rapidly as $\lambda \to \infty$. This expansion defines $\chi(\lambda, A_\nu)$ modulo $\Psi^{-\infty}(\lambda)$.

Straightforward analysis of the proof of Theorem 4.7 shows that it remains valid in the case where one of the operators belongs to $\Psi^0_{1,0}$ and the other is a parameter-dependent PDO whose symbol admits an asymptotic expansion of the form (6.2). In this case (4.4) gives an expansion of σ_{AB} as $\lambda + |\xi| \to \infty$ and defines the symbol modulo $S^{-\infty}(\lambda)$.

Now, in the same way as in Section 5, one can show that the composition of parameter-dependent PDOs whose symbols admit asymptotic expansions of the form

$$\sigma(x,\xi) \sim \sum_{j=0}^{\infty} c_j(x,\xi)\,\chi^{(j)}(\lambda,|\xi|_x)\,, \quad \lambda + |\xi| \to \infty, \quad c_j \in \Psi^0_{1,0} \tag{6.3}$$

is also a parameter-dependent PDO whose symbol is given by (4.4) modulo $S^{-\infty}(\lambda)$.

Let $\Pi_\nu(\lambda)$ be the spectral projection of the operator A_ν corresponding to the interval $(-\infty, \lambda)$. The above results imply the following

Theorem 6.1. *Let $\upsilon \in C_0^\infty(M)$, and let $\{\upsilon\}$ be the corresponding multiplication operator. Consider the spectral projections $\Pi_\nu(\lambda)$ and $\tilde{\Pi}_{\tilde\nu}(\lambda)$ generated by different metrics $\mathbf{g}$, $\tilde{\mathbf{g}}$ and different first-order PDOs ν, $\tilde\nu$ satisfying the conditions of Section 5. If $\tilde{\mathbf{g}} = \mathbf{g}$ on the support of the function υ then*

$$\Pi_\nu(\lambda)\,\{\upsilon\}\,\big(I - \tilde{\Pi}_{\tilde\nu}(\lambda + c\lambda^\rho)\big) \in \Psi^{-\infty}(\lambda)\,, \quad \forall\, c, \rho > 0. \tag{6.4}$$

Sketch of proof. Assume that $\rho \in (0,1]$, and let $\chi(\lambda, s)$ be defined as above with some $\varepsilon < c/3$. Then $\chi(\lambda, s) \equiv 1$ for $s \geq \lambda$ and $\chi(\lambda, s - \varepsilon\lambda^\rho) \equiv 0$ for $s \geq \lambda + c\lambda^\rho$. It follows that

$$\Pi_\nu(\lambda)\,\chi(\lambda, A_\nu) = \Pi_\nu(\lambda) \quad \text{and} \quad \chi(\lambda, A_{\tilde\nu} - \varepsilon\lambda^\rho I)\,\big(I - \Pi_{\tilde\nu}(\lambda + c\lambda^\rho)\big) = 0\,.$$

Consequently, we have

$$\begin{aligned}\Pi_\nu(\lambda))\,\{\upsilon\}\,\big(I - \Pi_{\tilde\nu}(\lambda + c\lambda^\rho)\big) \\ = \Pi_\nu(\lambda)\,\chi(\lambda, A_\nu))\,\{\upsilon\}\,\big(I - \chi(\lambda, A_{\tilde\nu} - \varepsilon\lambda^\rho I)\big)\,\big(I - \Pi_{\tilde\nu}(\lambda + c\lambda^\rho)\big)\end{aligned} \tag{6.5}$$

Since $\chi(\lambda,s)=\chi(\lambda,s)\,\chi(\lambda,s-\varepsilon\lambda^\rho)$, the composition formula implies that

$$\chi(\lambda,A_\nu))\,\{\upsilon\}\,\big(I-\chi(\lambda,A_{\tilde\nu}-\varepsilon\lambda^\rho I)\big)\ \in\ \Psi^{-\infty}(\lambda)\,.$$

Now the required result follows from (6.5) and the fact that the Schwartz kernel of the spectral projection is polynomially bounded in λ with all its derivatives (see, for instance, [SV, Section 1.8]). □

Remark 6.2. It is not surprising that the operator in the left-hand side of (6.4) has a lower order than the spectral projections themselves as $\lambda\to\infty$. However, one would expect its norm to decay as a fixed negative power of λ, since the perturbation $A_\nu - A_{\tilde\nu}$ is a more or less arbitrary PDO of order zero. We do not know whether (6.4) can be obtained by other techniques (including that of Fourier integral operators).

Remark 6.3. All results of this section can easily be extended to a noncompact closed manifold M. In this case all the asymptotic expansions are unform on compact subsets of M and $M\times M$.

7. Other known results and possible developments

7.1. Other definitions for scalar PDOs

If Γ is a linear connection, then the corresponding symbol of a PDO A can easily be recovered from the asymptotic expansion of $A(e^{i\varphi_\tau(x,\zeta,y)}\chi(x,y))$ as $\zeta\to\infty$, where φ_τ is defined by (4.2) and χ is a smooth cut-off function or κ-density (we suppose that x is fixed and that the operator acts in the variable y). After that, all the standard formulae of the local theory of PDOs can be rewritten in terms of their Γ-symbols. Moreover, making appropriate assumptions about the asymptotic behaviour of $A(e^{i\varphi_\tau(x,\zeta,\cdot)}\chi(x,y))$, one can try to define various classes of PDOs associated with the linear connection Γ.

This approach was introduced and developed by Harold Widom and Lance Drager (see [Wi1], [Wi2] and [Dr]). Its main disadvantage is the absence of an explicit formula representing the Schwartz kernel of a PDO via its symbol. As a consequence, one has to assume that PDOs and the corresponding classes of amplitudes are defined in local coordinates, which makes it impossible to extend the definition to $\rho<\max\{\delta,1-\rho\}$.

In [Pf1], Markus Pflaum defined a PDO in the space of functions by the formula

$$Au(x)\ =\ (2\pi)^{-n}\int_{T_x^*M}\int_{T_xM}\chi(x,y)\,e^{i\varphi_0(x,\xi,y)}\,a(x,\xi)\,u(y)\,\mathrm{d}y\,\mathrm{d}\xi\,, \tag{7.1}$$

where $a(x,\xi)$ is a function on T^*M of class $S^m_{\rho,\delta}$, y are normal coordinates centred at x and χ is a smooth cut-off function vanishing outside a neighbourhood of the diagonal. He obtained asymptotic expansions for the symbols of the adjoint operator and the composition of PDOs and, in the later paper [Pf2], extended them to

τ-symbols. However, the results in [Pf1, Pf2] are stated and proved with the use of local coordinates and, therefore, the author had to assume that $\max\{\delta, 1-\rho\} < \rho$.

Recall that under this condition the standard results of the local theory of PDOs hold, and the only advantage of a coordinate-free calculus is that it helps to fight Problem 2.7. A typical example, considered in [Pf1], is the PDO with a symbol of the form $(1+|\xi|^2)^{b(x)}$ where $b(x)$ is a smooth function on M. Formally speaking, this PDO belongs only to the class $S^m_{1,\delta}$ with $m = \sup_x b(x)$ and any $\delta \in (0,1)$. But its properties are determined by the values of the function b at all points $x \in M$; in a sense, this operator has a variable order depending on $x \in M$. In such a situation, it is not sufficient to consider only the principal symbol. One has to define a full symbol which can be done with the use of a linear connection.

It is clear that (7.1) differs from Definition 4.2 only by the choice of the weight factor $p_{\kappa,\tau}$. Applying the procedure described in Remark 4.4, one can easily show that

$$\sigma_A(x,\xi) \sim \sum_\alpha P_\alpha(x)\, \partial_\xi^\alpha a(x,\xi)\,, \quad |\xi| \to \infty\,, \tag{7.2}$$

where $a(x,\xi)$ is the symbol appearing in (7.1) and P_α are components of some tensor fields. Using (7.2), one can rewrite all the results obtained in [Sa2] in terms of symbols defined by (7.1). This shows that Pflaum's formulae can be reformulated in terms of the horizontal derivatives ∇_x^α and thus extended to the classes $\Psi^m_{\rho,\delta}(\Omega^\kappa, \Gamma)$ and τ-symbols.

In particular, Pflaum's composition formula can be written in the form (4.4) with some other polynomials $\tilde{P}^{(\kappa)}_{\beta,\gamma}$. For operators acting in the space of functions and $\tau = 0$, this result was established by Vladimir Sharafutdinov in [S1]. He chose to give a direct proof instead of deducing the formula from (4.4) and (7.2) and, for some reason, considered only the classes $\Psi^m_{1,0}$. Sharafutdinov gave an alternative description of the polynomials $\tilde{P}^{(0)}_{\beta,\gamma}$ which may be useful for obtaining more explicit composition formulae (this investigation was continued in [Ga]). He also proved an analogue of (4.3) in the case $\kappa = 1/2$ and $\tau = 0$ [S1, Theorem 6.1].

Remark 7.1. From (7.2) it easily follows that the degrees of the polynomials $\tilde{P}^{(\kappa)}_{\beta,\gamma}$ admit the same estimates as $d^{(\kappa)}_{\beta,\gamma}$ (see Section 4).

7.2. Operators on sections of vector bundles

In [FK, Pf2, S2, Wi2] the authors considered PDOs acting between spaces of sections of vector bundles over M. In this case, in order to construct a global symbolic calculus, it is sufficient to define parallel displacement and horizontal curves in the induced bundles over T^*M. This can be achieved by introducing linear connections on M and the vector bundles over M. After that the results are stated and proved in the same way as in the scalar case (further details and references can be found in the above papers).

A more radical approach was proposed by Cyril Levy in [Le]. He noticed that in order to develop an intrinsic calculus of PDOs one actually needs only an exponential map, which does not have to be associated with a linear connection. In his paper Levy assumed that the manifold M is noncompact and is provided with a global exponential map (that is, M is a manifold with linearization in the sense of [Bo]). He then defined associated maps in the induced vectors bundles and constructed a global coordinate-free symbolic calculus.

Remark 7.2. All the papers mentioned in this subsection dealt only with symbols whose restriction to compact subsets of M belong to $S^m_{\rho,\delta}$ with $\rho > \max\{\delta, 1-\rho\}$. It should be possible to extend their results to $\rho < 1/2$, using the technique outlined in Section 4.

7.3. Noncompact manifolds

In order to study global properties of PDOs on a noncompact manifold M, one has to assume that all estimates for symbols and their derivatives hold uniformly for all $x \in M$ (rather than only on compact subsets of M, as in Definitions 2.1 and 4.1). In [Ba], Frank Baldus defined classes of symbols and developed an intrinsic calculus of PDOs on a noncompact manifold M under the assumption that M has an atlas satisfying certain global conditions. The statements and proofs in [Ba] were given in terms of local coordinates, and global results were obtained by considering the transition maps between coordinates charts. It is quite possible that these results can be simplified or/and improved under the assumption that M has a global exponential map (as in [Le]).

7.4. Other symbol classes

The paper [Ba] dealt with the more general classes of symbols $S(m,g)$ instead of $S^m_{\rho,\delta}$. The classes $S(m,g)$ were introduced by L. Hörmander in [H1] (see also [H2]). They are defined with the use of coordinates, and in each coordinate system $S^m_{\rho,\delta}$ is a particular case of $S(m,g)$. It would be interesting to construct similar classes $S(m,g)$ associated with a linear connection (or an exponential map) and to study the corresponding classes of symbols and PDOs.

Remark 7.3. Note that the introduction of "coordinate" classes $S(m,g)$ does not help to resolve Problem 2.6. The relation between these "coordinate" classes and the classes $S^m_{\rho,\delta}(\Gamma)$ was discussed in [Sa2, Remark 3.5].

7.5. Operators generated by vector fields

Let $\nu := \{\nu_1, \nu_2, \ldots, \nu_n\}$ be a family of smooth vector fields ν_j on M which span T_xM at every point $x \in M$. Consider the corresponding first-order differential operators ∂_{ν_j} and denote

$$\partial_\nu^\alpha := \frac{1}{q!} \sum_{j_1,\ldots,j_q} \partial_{\nu_{j_1}} \partial_{\nu_{j_2}} \ldots \partial_{\nu_{j_q}}$$

where $q = |\alpha|$ and the sum is taken over all ordered sets of indices $j_1, \ldots, j_q$ corresponding to the multi-index $\alpha = (\alpha_1, \ldots, \alpha_n)$. In other words, ∂_ν^α can be thought of as the symmetrized composition of $\partial_{\nu_{j_k}}$.

The family ν generates a unique curvature-free connection Γ_ν, with respect to which all covariant derivatives of the vector fields ν_j are identically equal to zero. The Γ_ν-symbol of ∂_ν^α coincides with $\sigma_1^{\alpha_1}\dots\sigma_n^{\alpha_n}$, where $\sigma_k = \sigma_k(x,\xi) := \langle \nu_k, \xi\rangle$ (see [Sa2, Example 5.4]). Since the functions σ_k are constant along horizontal curves in T^*M generated by the connection Γ_ν, the operators ∂_ν^α and their linear combinations can be regarded as constant coefficient operators relative to the connection Γ_ν (or to the family of the vector fields ν).

This observation was used by Eugene Shargorodsky in [Sha], where he developed a complete theory of pseudodifferential operators generated by a family of vector fields ν. He introduced anisotropic analogues of classes $S^m_{\rho,\delta}$, proved the composition formula for the corresponding classes of PDOs, defined semi-elliptic operators associated with the family ν, and constructed their resolvents. All the results in [Sha] were obtained for operators acting on sections of vector bundles equipped with linear connections (see Section 7.2).

7.6. Operators on Lie groups

In [RT], the authors defined full symbols of scalar PDOs on a compact Lie group M in terms of its irreducible representations and developed a calculus for such symbols. It would be interesting to compare their formulae with those obtained by introducing an invariant linear connection Γ on M and applying the methods of [Sa2] or [Sha].

7.7. Geometric aspects and physical applications

The importance of intrinsic approach in the theory of PDOs for quantum mechanics is explained in the excellent review [Fu] by Stephen Fulling. Further discussions can be found in the Ph.D. thesis [Gu]. Various geometric applications are considered in [BNPW] and [Vo]. We refer the interested reader to the above papers and references therein.

7.8. Global phase functions

It is worth noticing that one does not need a linear connection or even an exponential map to define PDOs on a manifold in a coordinate-free manner. It is sufficient to fix a globally defined phase function satisfying certain conditions.

Namely, let $\varphi(x;y,\eta)$ be an infinitely differentiable function on $M\times T^*M$ such that

$$\operatorname{Im}\varphi(x;y,\eta)\ge 0\,,\quad \varphi(x;y,\lambda\eta)=\lambda\,\varphi(x;y,\eta)$$

for all $x\in M$, $(y,\eta)\in T^*M$ and $\lambda>0$, and

$$\varphi(x;y,\eta) \;=\; (x-y)\cdot\eta \;+\; O(|x-y|^2|\eta|)\,,\quad x\to y\,,$$

in any local coordinate system. If $a(x;y,\eta)$ is a smooth function on $M\times T^*M$ such that $a\in S^m_{1,0}$ in any local coordinate system then

$$\mathcal{A}(x,y) \;:=\; \int e^{i\varphi(x;y,\eta)}\,a(x;y,\eta)\,\mathrm{d}\eta$$

is the Schwartz kernel of a PDO $A \in \Psi^m_{1,0}$ acting in the space of functions. Moreover, there exists an amplitude $a_\varphi(y,\eta)$ independent of x such that

$$\mathcal{A}(x,y) \;-\; \int e^{i\varphi(x;y,\eta)}\, a_\varphi(y,\eta)\,\mathrm{d}\eta \;\in\; C^\infty(M\times M)\,,$$

and this amplitude a_φ is uniquely defined by A modulo $S^{-\infty}$. The operator A belongs to $\Psi^m_{1,0}$ if and only if $a_\varphi \in S^m_{1,0}$ in any local coordinate system.

Remark 7.4. For a real-valued phase function φ these are standard results of the theory of Fourier integral operators (see, for instance, [Shu, Section 19]). Complex-valued phase functions were considered in [LSV].

It is natural to call a_φ the *φ-symbol* of the operator A. Clearly, all the standard results of the classical theory of PDOs can be rewritten in terms of their φ-symbols. In particular, if $A, B \in \Psi^m_{1,0}$ then the φ-symbol of the composition AB is determined modulo $S^{-\infty}$ by an asymptotic series which involves φ-symbols of A and B and their derivatives. Similarly, the φ-symbol of the adjoint operator A^* is given by a series involving the derivatives of φ-symbol of A.

Obviously, the same formulae remain valid under milder assumptions about the symbols. Thus it should be possible to introduce symbol classes associated with the phase function φ and develop a symbolic calculus in these classes (as was done in [Sa2] for the special phase function φ_τ generated by a linear connection).

Such a general approach may allow one to extend results of Section 6 to other elliptic operators. It may also be useful for the study of solutions of hypoelliptic equations and operators on noncompact manifolds.

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