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Jan Janas
Pavel Kurasov
Ari Laptev
Sergei Naboko
Editors

Operator Methods in Mathematical Physics

Conference on Operator Theory, Analysis and Mathematical Physics (OTAMP) 2010, Bedlewo, Poland

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This volume is dedicated
to the memory of

Israel Gohberg

Israel Gohberg (1928–2009)

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Introduction

This volume contains proceedings of the International Conference: Operator Theory, Analysis and Mathematical Physics – OTAMP 2010, held at the Mathematical Research and Conference Center in Bedlewo, Poland, in August. The Conference was the fifth one from the OTAMP series.

The current volume contains original results concerning among others the following domains: spectral properties of Jacobi and CMV matrices, inverse scattering for non-classical Schrödinger operators, Ginzburg-Landau theory for one-dimensional systems with contact interactions, commutator bounds and local approximation of observables, spectral minimal partitions for special domains with Neumann condition, eigenfunction expansions of the one-dimensional Schrödinger operator, ergodic theory and Krein theory of entire operators. The papers of the volume contain original material and were refereed by qualified experts in the field. The Editors thank all the referees who helped to improve several contributions.

We greatly appreciate financial support of the Institute of Mathematics of the Polish Academy of Sciences. We also thank the staff of the Banach Center in Bedlewo for essential help in transportation of the participants and smooth cooperation.

This volume is dedicated to the memory of Israel Gohberg an outstanding mathematician of the XX-th century Operator Theory. He supported OTAMP conferences from the beginning in particular by including all proceedings into the series Operator Theory: Advances and Applications.

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The Editors

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Inverse Scattering for Non-classical Impedance Schrödinger Operators

Sergio Albeverio, Rostyslav O. Hryniv, Yaroslav V. Mykytyuk and Peter A. Perry

Abstract. We review recent progress in the direct and inverse scattering theory for one-dimensional Schrödinger operators in impedance form. Two classes of non-smooth impedance functions are considered. Absolutely continuous impedances correspond to singular Miura potentials that are distributions from $W^{-1}_{2,\mathrm{loc}}(\mathbb{R})$; nevertheless, most of the classic scattering theory for Schrödinger operators with Faddeev–Marchenko potentials is carried over to this singular setting, with some weak decay assumptions. The second class consists of discontinuous impedances and generates Schrödinger operators with unusual scattering properties. In the model case of piece-wise constant impedance functions with discontinuities on a periodic lattice the corresponding reflection coefficients are periodic. In both cases, a complete description of the scattering data is given and the explicit reconstruction method is derived.

Mathematics Subject Classification (2010). Primary: 34L25, Secondary: 34L40, 47L10, 81U40.

Keywords. Schrödinger operator, impedance function, inverse scattering problem.

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1. Introduction

In this paper, we shall discuss inverse scattering problems for one-dimensional Schrödinger operators H in the impedance form,

$$H := -\frac{1}{p}\frac{\mathrm{d}}{\mathrm{d}x}p^2\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{p}, \tag{1.1}$$

for non-smooth impedance functions p. Our aim is two-fold: firstly, we shall show that the classic inverse scattering theory for Schrödinger operators as discussed in, e.g., [27, 31, 40, 54, 60, 61, 63] and which is well understood for Faddeev–Marchenko potentials $q \in L_1\big(\mathbb{R}, (1+|x|)\mathrm{d}x\big)$ (also called Jost–Bargmann potentials in the physical literature), can successfully be extended to a much wider class of operators, and shall give an account on a recent progress in this direction. Secondly, even though the general approach remains the same, we shall demonstrate that such extensions lead to scattering objects whose properties might differ drastically from those observed in the Faddeev–Marchenko case.

We note that the above impedance Schrödinger operators can often be written, at least for smooth enough p, in a more usual potential form; however, there are several reasons why our primary interest is in operators H in the impedance form (1.1). Firstly, Hamiltonians of many models of mathematical physics (e.g., in optics, electromagnetics etc.) take the form (1.1), or can easily be transformed to it; the corresponding example is given in Subsection 1.3. Secondly, (1.1) allows a reduction to a first-order Dirac-type (or Zakharov–Shabat) system that is much easier to work with. Finally, a non-negative Schrödinger operator in potential form can usually be recast as (1.1) for a suitable impedance function p, cf. [48], while for non-smooth p impedance Schrödinger operators may not possess a reasonable potential form; in this sense the class of operators (1.1) is larger.

Indeed, set $u := (\log p)' = p'/p$. For absolutely continuous p, the operator H can be written in the factorized form,

$$H = -\Big(\frac{\mathrm{d}}{\mathrm{d}x} + u\Big)\Big(\frac{\mathrm{d}}{\mathrm{d}x} - u\Big), \tag{1.2}$$

and becomes a Schrödinger operator in the potential form,

$$Hy = -y'' + qy, \tag{1.3}$$

for the *Miura potential* $q := u' + u^2$. For this to be a regular potential, u must be at least locally absolutely continuous and thus p a function from the Sobolev class $W^2_{1,\mathrm{loc}}(\mathbb{R})$. We, however, will not require any continuity of u. The first part of the paper will discuss the case where u is a function in $L_{2,\mathrm{loc}}(\mathbb{R})$ with additional decay properties and thus q will be a distribution that locally belongs to the Sobolev space $W_2^{-1}(\mathbb{R})$. In the second part, we will treat the case where the impedance p is discontinuous; then u contains the Dirac δ-functions and q – at least formally – involves their derivatives δ'. See the monographs [6] and [7] for detailed treatment of Schrödinger operators with singular potentials and extensive bibliography lists.

Yet another motivation for thinking of the Schrödinger operator H in terms of the function u rather than in terms of its potential q is given by Miura and is related to completely integrable dispersive equations, cf. [33]. Recall that the *Miura map* is defined as

$$\begin{aligned} B\ : L_{2,\mathrm{loc}}(\mathbb{R}) &\to W^{-1}_{2,\mathrm{loc}}(\mathbb{R}), \\ u &\mapsto u' + u^2. \end{aligned} \tag{1.4}$$

In 1968, Miura [62] observed that if $u(x,t)$ is a smooth solution of the mKdV equation, then

$$(Bu)(x,t) = \frac{\partial u}{\partial x}(x,t) + u^2(x,t)$$

is a smooth solution of the KdV equation. For this reason, the Miura map has played a fundamental role in the study of existence and well-posedness questions for these two equations. A suitable extension of the scattering theory for Schrödinger operators in the form (1.2) would allow to apply the inverse scattering transform method to study initial value problems for mKdV and other completely integrable dispersive equations with highly singular initial data; cf. [30] for a particular example of the defocussing non-linear Schrödinger (NLS) equation with the Dirac delta-functions in potentials.

We shall concentrate on two classes of operators H in (1.1) or (1.2), which are in a sense "extremal" and for which the direct and inverse scattering problems have recently been quite thoroughly discussed. The first is the class of (locally) absolutely continuous impedance functions p, for which the corresponding $u = p'/p$ have certain integrability at infinity and which still bears lots of properties found for problems with Faddeev–Marchenko potentials; see [35, 36, 46]. The second class is with piece-wise constant p [3, 4, 66, 67]; formally, the corresponding u is a discrete measure, i.e., the sum of the Dirac δ-functions. The Schrödinger operators (1.1) in this second class possess quite unusual scattering properties [9, 10]; in a certain sense, the corresponding scattering theory might be viewed as a "discrete" analogue of the classical one.

Despite the formal similarities in the way the inverse scattering problems are solved in both cases, there are essential differences that do not allow to combine the two methods and to treat generic piece-wise smooth impedances, i.e., generic measures $\mathrm{d}\log p$ without singular continuous components. Needless to say, such a unified theory would be of much interest for many applications, e.g., for electromagnetic scattering theory in stratified media.

1.1. Basic definitions

Now we recall the main objects of the scattering theory for Schrödinger operators in one dimension and describe in general terms the results we want to derive; see, e.g., [19, 27, 31, 58, 59, 64, 67] for a detailed exposition. We shall work in terms of the logarithmic derivative $u = p'/p$ of the impedance function p; the precise assumptions on u will be stated in the next sections. In particular, in the continuous case u will be in $L_2(\mathbb{R})$ with some decay at infinity, while for piece-wise constant p the function u is a measure.

Denote by $\mathfrak{l}$ the differential expression generated by either (1.1) or (1.2) on the maximal domain in $L_{2,\mathrm{loc}}(\mathbb{R})$. By definition, the Jost solutions $f_\pm(\cdot,\omega)$ for $\omega \in \mathbb{R}$ are solutions to the Schrödinger equation $\mathfrak{l}(y) = \omega^2 y$ that are asymptotic to $\mathrm{e}^{\pm\mathrm{i}\omega x}$ at $\pm\infty$, i.e., such that

$$\begin{aligned} f_+(x,\omega) &= \mathrm{e}^{\mathrm{i}\omega x}(1+o(1)), && x \to +\infty, \\ f_-(x,\omega) &= \mathrm{e}^{-\mathrm{i}\omega x}(1+o(1)), && x \to -\infty. \end{aligned}$$

The Jost solutions exist for quite a large class of impedance functions p (resp. u). For real nonzero ω, the solutions $f_-(\,\cdot\,,\omega)$ and $f_-(\,\cdot\,,-\omega)$ form a fundamental system of solutions of $\mathfrak{l}(y) = \omega^2 y$ and thus there exist coefficients $a(\omega)$ and $b(\omega)$ such that

$$f_+(x,\omega) = a(\omega)f_-(x,-\omega) + b(\omega)f_-(x,\omega). \tag{1.5}$$

As in the classic scattering theory for Schrödinger operators with potentials in the Faddeev–Marchenko class, the coefficients a and b will be shown to verify the identities $|a(\omega)|^2 - |b(\omega)|^2 = 1$, $a(-\omega) = \overline{a(\omega)}$, $b(-\omega) = \overline{b(\omega)}$, and the relation

$$f_-(x,\omega) = a(\omega)f_+(x,-\omega) - b(-\omega)f_+(x,\omega). \tag{1.6}$$

The corresponding right r_+ and left r_- *reflection coefficients* are introduced via

$$r_+(\omega) := -\frac{b(-\omega)}{a(\omega)}, \qquad r_-(\omega) := \frac{b(\omega)}{a(\omega)}, \tag{1.7}$$

and $t := 1/a$ is the *transmission* coefficient. The motivation for these terms comes from physics; indeed, the solution

$$t(\omega)f_+(x,\omega) = f_-(x,-\omega) + r_-(\omega)f_-(x,\omega)$$

describes the plane monochromatic wave $e^{i\omega x}$ sent in from $-\infty$ (the term $f_-(x;-\omega)$) that after interaction with the impedance p partly transmits to $+\infty$ (the term $t(\omega)f_+(x;\omega)$) and partly gets reflected back to $-\infty$ (the term $r_-(\omega)f_-(x;\omega)$).

These coefficients form the matrix

$$S(\omega) := \begin{pmatrix} t(\omega) & r_+(\omega) \\ r_-(\omega) & t(\omega) \end{pmatrix}$$

called the *scattering matrix* for H. This matrix is unitary on the real line and the above properties of the scattering coefficients a and b imply that S can uniquely be reconstructed from the right or left reflection coefficient alone. We observe that the impedance Schrödinger operator H is non-negative and thus has no bound states; therefore S comprises all the scattering information on H.

The direct scattering theory studies the properties of the scattering maps $\mathcal{S}_\pm$ defined via

$$\begin{aligned} \mathcal{S}_+ &: u \to r_+, \\ \mathcal{S}_- &: u \to r_-. \end{aligned}$$

The inverse scattering problem is to reconstruct the function u and thus the Schrödinger operator H from its scattering matrix (i.e., from its reflection coefficient r_+ or r_-). More exactly, for a given class of Schrödinger operators, i.e., for a given class of functions u, a complete solution of the inverse scattering problem consists in proving that the maps $\mathcal{S}_\pm$ are one-to-one, finding their images, and constructing the inverse maps $\mathcal{S}_\pm^{-1}$.

Next we discuss in some more detail two classes of problems we will mostly be interested in.

1.2. Miura potentials: the case of absolutely continuous p

To describe the first class of problems to be studied, we start with the observation that if a Schrödinger operator (1.3) has no bound states, then the corresponding potential q admits a Riccati representation given by the Miura map (1.4). Namely, for $q \in W_{2,\mathrm{loc}}^{-1}(\mathbb{R})$ real-valued and $\varphi \in C_0^\infty(\mathbb{R})$ define the Schrödinger form $\mathfrak{h}$ corresponding to (1.3) via

$$\mathfrak{h}(\varphi) := \int |\varphi'(x)|^2 \, \mathrm{d}x + \langle q, |\varphi|^2 \rangle,$$

where $\langle \cdot\,, \cdot \rangle$ is the pairing between $W_{2,\mathrm{loc}}^{-1}(\mathbb{R})$ and $W_{2,\mathrm{comp}}^{1}(\mathbb{R})$. Then, as shown in [48], if q is a real-valued distribution in $W_{2,\mathrm{loc}}^{-1}(\mathbb{R})$ for which the Schrödinger form $\mathfrak{h}$ is nonnegative, then q may be presented as $q = Bu$ for a function $u \in L_{2,\mathrm{loc}}(\mathbb{R})$. Such a function u need not be unique; we will call q a *Miura potential* and any function u satisfying $q = Bu$ a *Riccati representative* for q. It is easily seen that two Riccati representatives for a given q differ by a continuous function and that a Riccati representative u is the logarithmic derivative of a positive distributional solution to the zero-energy Schrödinger equation $-y'' + qy = 0$.

One may not hope for extension of the scattering theory that would reconstruct directly a singular Miura potential $q \in W^{-1}_{2,\mathrm{loc}}(\mathbb{R})$ of (1.3). However, the corresponding Riccati representative u is a regular function, and reconstruction of u from the scattering data of H might be possible. Since, however, a Miura potential q possesses many different Riccati representatives, one has to single out a distinguished u that should be recovered.

One such possibility was suggested in [36], where the class $\mathcal{Q}_0$ of Miura potentials admitting Riccati representatives $u \in L_1(\mathbb{R}) \cap L_2(\mathbb{R})$ was considered. In this case, such a Riccati representative is unique, thus giving a natural parametrization of Miura potentials q and Schrödinger operators (1.2) and (1.3). Below, we give several examples from [36] of Miura potentials generated this way.

Example 1.1. Let u be an even function that for $x > 0$ equals $x^{-\alpha} \sin x^{\beta}$. Assume that $\alpha > 1$ and $\beta > \alpha + 1$. Then u belongs to $L_1(\mathbb{R}) \cap L_2(\mathbb{R})$ and the corresponding Miura potential $q = u' + u^2$ is of the form

$$q(x) = \beta \,\mathrm{sign}\,(x)|x|^{\beta-\alpha-1} \cos |x|^{\beta} + \tilde{q}(x)$$

for some bounded function $\tilde{q}$. Thus q is unbounded and oscillatory; nevertheless, the corresponding Schrödinger operator possesses only absolutely continuous spectrum filling out the positive semi-axis and the scattering and inverse scattering on such potentials is well defined.

Example 1.2. Assume that $\phi \in C_0^{\infty}(\mathbb{R})$ is such that $\phi \equiv 1$ on $(-1, 1)$. Take $u(x) = \alpha\, \phi(x) \log |x|$ with $\alpha > 0$. Then $u \in L_1(\mathbb{R}) \cap L_2(\mathbb{R})$; moreover, since the distributional derivative of $\log |x|$ is the distribution P.v. $1/x$, the corresponding Miura potential q is smooth outside the origin and has there a Coulomb-type singularity. See, e.g., [16, 34, 57] and the references therein for discussion and rigorous treatment of Schrödinger operators with Coulomb potentials.

Example 1.3 (Frayer [35]). The Riccati representative $u = \alpha\chi_{[-1,1]}$, with α a nonzero real constant and χ_{Δ} the indicator function of a set Δ, corresponds to the Miura potential

$$q = \alpha\delta(\cdot + 1) - \alpha\delta(\cdot - 1) + \alpha^2 \chi_{[-1,1]},$$

δ being the Dirac delta-function centered at the origin.

The class $\mathcal{Q}_0$ of Miura potentials, however, is rather small in the sense that all the corresponding Schrödinger operators (1.2) possess *resonance* (or *half-bound* state) at the origin, see Section 2. In particular, $\mathcal{Q}_0$ includes neither the model singular potential $q = \alpha\delta$, with $\alpha > 0$ and δ being the Dirac delta function centered at the origin, nor generic (i.e., non-resonant) Faddeev–Marchenko potentials. For this reason a further extension of $\mathcal{Q}_0$ is desirable.

Such a wider class $\mathcal{Q}$ of Miura potentials q was suggested in [46]. Recall that any Riccati representative u gives rise to a strictly positive distributional solution y of the zero-energy Schrödinger equation $-y'' + qy = 0$ via

$$y(x) = \exp\left(\int_0^x u(s)\mathrm{d}s\right)$$

and, conversely, any positive solution $y \in H^1_{\mathrm{loc}}(\mathbb{R})$ gives rise to a Riccati representative $u(x) = y'(x)/y(x)$. Thus, the set of Riccati representatives for a given distribution potential q is parameterized by positive solutions y to the zero-energy Schrödinger equation normalized by $y(0) = 1$. Among all positive solutions to $y'' = qy$ there are extremal ones $y_\pm$ with the properties that

$$\int_0^\infty \frac{\mathrm{d}s}{y_+^2(s)} = \int_{-\infty}^0 \frac{\mathrm{d}s}{y_-^2(s)} = +\infty,$$

and then any positive solution y takes the form $y = \theta y_+ + (1-\theta)y_-$ for some $\theta \in [0,1]$. The corresponding extremal Riccati representatives $u_\pm = (\log y_\pm)'$ belong to $L_{2,\mathrm{loc}}(\mathbb{R})$; we will assume in addition that $u_\pm$ are in $L_2(\mathbb{R})$ and that u_+ is integrable at $+\infty$ and u_- is integrable at $-\infty$. The set of all potentials with the above properties is denoted by $\mathcal{Q}$, i.e.,

$$\mathcal{Q} := \{q = \overline{q} \in W_2^{-1}(\mathbb{R}) \,:\, \exists u_\pm \in L_2(\mathbb{R}) \cap L_1(\mathbb{R}^\pm) \text{ s.t. } q = u_+' + u_+^2 = u_-' + u_-^2\}.$$

We observe that the Riccati representatives u_+ and u_- with the above properties are unique [44, Ch. IX.2 (ix)] and that $\mathcal{Q}_0$ corresponds to the case where $u_- = u_+$, i.e., where the extremal solutions y_- and y_+ are linearly dependent. This condition is very unstable under perturbation of q, whence the case $q \in \mathcal{Q}_0$ might be considered "exceptional" and $q \in \mathcal{Q}_1 := \mathcal{Q} \setminus \mathcal{Q}_0$ "generic". A potential $q \in \mathcal{Q}$ is uniquely determined by the data $u_-|_{(-\infty,0)}$, $u_+|_{(0,\infty)}$, and the "jump" $(u_- - u_+)(0)$. The set $\mathcal{Q}$ contains all real-valued potentials of Faddeev–Marchenko class generating non-negative Schrödinger operators as well as many singular potentials (e.g., with Dirac delta-functions and Coulomb-like singularities). For instance, if $q = q_0 + q_1$ is such that $q_0 \in \mathcal{Q}$, $q_1 \in W_2^{-1}(\mathbb{R})$ is of compact support, and the corresponding operator H of (1.3) is non-negative, then $q \in \mathcal{Q}$; see [46].

In fact, a further extension is possible; namely, one can add a Miura potential from $\mathcal{Q}$ to any Faddeev–Marchenko potential; the resulting Schrödinger operator need not be non-negative any longer but will in general have a finite number of negative eigenvalues. A comprehensive direct and inverse scattering theory for such operators can be developed; this will be discussed in [47].

1.3. A physical example with discontinuous impedance

The second class of Schrödinger operators we shall treat are generated by (1.1) with discontinuous impedances. There are many physically relevant problems leading to such operators [3, 4, 66], and we present below one example.

Non-destructive testing of a layered isotropic medium is usually based on probing by electromagnetic waves and leads to the Maxwell system for the electric $E(\,\cdot\,,\omega)$ and magnetic $H(\,\cdot\,,\omega)$ components of the electromagnetic field [42]. For the planar probing wave of frequency ω and normal incidence (along the x-axis) this system takes the form

$$\begin{cases} \dfrac{dE(x,\omega)}{dx} + \mathrm{i}\omega\mu(x)H(x,\omega) = 0, \\ \dfrac{dH(x,\omega)}{dx} + \mathrm{i}\omega\varepsilon(x)E(x,\omega) = 0, \end{cases}$$

with μ and ε denoting respectively the permeability and permittivity of the medium. Under the Liouville transformation

$$s(x) := \int_0^x \sqrt{\varepsilon(x')\mu(x')}\,dx', \qquad p(s) := \sqrt[4]{\frac{\varepsilon(s)}{\mu(s)}},$$

the above Maxwell system assumes the form

$$\begin{cases} \dfrac{dE(s,\omega)}{ds} + \dfrac{\mathrm{i}\omega}{p^2(s)}H(s,\omega) = 0; \\ \dfrac{dH(s,\omega)}{ds} + \mathrm{i}\omega p^2(s)E(s,\omega) = 0, \end{cases}$$

and yields the impedance Schrödinger equation

$$-\bigl(p^2(s)E'(s,\omega)\bigr)' = \omega^2 p^2(s)E(s,\omega) \tag{1.8}$$

for the electric potential E. Clearly, the impedance p is discontinuous at the interface points between the layers.

The inverse scattering problem of interest is to reconstruct the impedance function p given the scattering data for the equation (1.8). Here, we consider the model case where p is piece-wise constant and has jumps at the points of a regular lattice $d\mathbb{Z}$, for some $d > 0$. Without loss of generality, we shall assume that $d = 1$, scaling appropriately the s-axis as necessary. Then in every interval $\Delta_j := (j, j+1)$ equation (1.8) takes the form $-E'' = \omega^2 E$, and the impedance p only determines the interface conditions at the lattice points $s \in \mathbb{Z}$.

We further set $y(s,\omega) = p(s)E(s,\omega)$ and find that y satisfies the equation

$$-\frac{1}{p(s)}\frac{d}{ds}p^2(s)\frac{d}{ds}\frac{y}{p(s)} = \omega^2 y, \tag{1.9}$$

for which the mathematical treatment of the corresponding direct and inverse scattering problems is easier. Since the asymptotic behavior of the solutions $E(\,\cdot\,,\omega)$ and $y(\,\cdot\,,\omega)$ of equations (1.8) and (1.9) are the same up to the factor $p(s)$, the scattering problems for the two equations are equivalent. Clearly, (1.9) is just the spectral problem $Hy = \omega^2 y$ for the impedance Scrödinger operator H of (1.1).

1.4. Some singular impedance Schrödinger operators not discussed

There are some other classes of Schrödinger operators that can be reduced to the impedance form. One of the examples is the Schrödinger operator H_κ on the half-line generated by differential expressions

$$\ell_\kappa(y) := -y'' + \frac{\kappa(\kappa+1)}{x^2}y + qy$$

with Bessel-type potentials $\kappa(\kappa+1)/x^2$, where $\kappa \in [-\frac{1}{2}, \frac{1}{2})$. For non-negative integer values of κ such operators arise in the decomposition in spherical harmonics of the three-dimensional Hamiltonian $-\Delta$, and then κ is the *angular momentum*, or *partial wave*, see [19, 26]. Operators of the form H_κ with non-integer values of κ arise in the study of scattering of waves and particles in conical domains (see, e.g., [20]), as well as in the study of the Aharonov–Bohm effect [2]. See also the related paper [56], where inverse scattering is discussed for long-range oscillating potentials leading to scattering functions with finite phase shifts.

We observe that for many q the differential expression ℓ_κ might be written in the factorized form (1.2)

$$-\Big(\frac{d}{dx} - \frac{\kappa}{x} + v\Big)\Big(\frac{d}{dx} + \frac{\kappa}{x} - v\Big)$$

with suitable v, thus taking the impedance form (1.1) with $p = x^{-\kappa}\exp\int v$. Recently, direct and inverse scattering problem for H_κ on the half-line was studied in [8]. It was demonstrated there that the scattering function F possesses some unusual properties, namely, that it is discontinuous at the origin and at infinity and $1-F$ does not tend to zero. In particular, in the model case $q \equiv 0$ the scattering function F was shown to take two different constant values for $\omega < 0$ and $\omega > 0$. As the scattering problems on half-line are formulated in somewhat different terms than on the whole line, we shall not discuss here the inverse scattering problems for the operator H_κ.

There are some works studying scattering problems for Hamiltonians on the half-line with Coulombic reference potential, see, e.g., [24, 25]. Although the Coulomb-type singularity can be modeled by Miura potentials treated here, see Example 1.2, taking $1/x$ as a reference potential again requires somewhat different techniques that could not be covered in this paper without significantly enlarging its size.

The paper is organized as follows. In Section 2, we discuss the general approach to solve the inverse scattering problem for the impedance operators H for continuous and discontinuous impedance functions. The continuous case leading to Schrödinger operators with Miura potentials is studied in Section 3, and the case of piece-wise constant impedances in Section 4. Finally, the Appendix contains some basic properties of Wiener-type Banach algebras.

2. The general approach and main results

The extension of the scattering theory we are going to present here builds upon the standard approach; however, we use extensively the Banach algebra and Banach space techniques and, whenever possible, avoid point evaluations of the functions involved.

We define the Fourier transforms $\mathcal{F}_+$ and $\mathcal{F}_-$ via

$$\begin{aligned}(\mathcal{F}_+ f)(x) &:= \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}sx} f(s)\,\mathrm{d}s,\\ (\mathcal{F}_- f)(x) &:= \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}sx} f(s)\,\mathrm{d}s\end{aligned} \tag{2.1}$$

for summable f and extend them in the usual manner to distributions. It will be convenient to work with the functions

$$F_+(x) := (\mathcal{F}_+ r_+)(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}sx} r_+(s)\,\mathrm{d}s, \tag{2.2}$$

$$F_-(x) := (\mathcal{F}_- r_-)(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}sx} r_-(s)\,\mathrm{d}s \tag{2.3}$$

and to analyze the mappings $u \mapsto F_+$ and $u \mapsto F_-$ given by $\mathcal{F}_+ \circ \mathcal{S}_+$ and $\mathcal{F}_- \circ \mathcal{S}_-$. The scattering mappings $\mathcal{S}_\pm$ are known to be close to the Fourier transforms in the sense that the mappings $\mathcal{F}_+ \circ \mathcal{S}_+$ and $\mathcal{F}_- \circ \mathcal{S}_-$ are close to the identity mapping and, in particular, act continuously in certain spaces of interest, see [45, 46].

We shall concentrate mostly on the case of absolutely continuous impedances generating Miura potentials; then u is in $L_2(\mathbb{R})$. The differences in the discrete case will be discussed at the end of this section; then u is a discrete measure.

2.1. The continuous case

In the continuous case, the Riccati representative u is supposed to generate the Miura potential $q \in \mathcal{Q}$. A generic $q \in \mathcal{Q}$ possesses two different representatives $u_\pm$ with the property that $u_\pm \in L_2(\mathbb{R}) \cap L_1(\mathbb{R}^\pm)$ and is uniquely determined by the triple $\{u_-|_{\mathbb{R}^-}, u_+|_{\mathbb{R}^+}, (u_- - u_+)(0)\}$, and in the exceptional case $u_- = u_+$. Set $X := L_1(\mathbb{R}) \cap L_2(\mathbb{R})$ with the norm $\|f\|_X = \|f\|_{L_1} + \|X\|_{L_2}$; then $\mathcal{Q}$ might be regarded as a subset of $X \oplus \mathbb{R}$, while $\mathcal{Q}_0$ is identified with X.

In what follows, we shall exploit the relation between the factorized Schrödinger operators (1.2) and the AKNS–Dirac systems [1], for which the inverse scattering theory is also well understood, at least for regular potentials [29, 38, 39, 43, 65, 68, 69]. Indeed, consider the reduced Dirac equation

$$LY := \Big(B\frac{d}{dx} + u_\pm J\Big)Y = \omega Y, \tag{2.4}$$

where

$$B = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad J = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{2.5}$$

It is straightforward to verify that if $Y = (y_1, y_2)^T$ solves (2.4) with say u_+, then y_1 and y_2 solve the respective Schrödinger equations $-y'' + q^{\pm} y = \omega^2 y$ with

$$q^{\pm} = \pm u'_+ + u_+^2.$$

The appearance of the operator L here should not be surprising since L is the first operator in the Lax pair for the modified Korteweg–de Vries equation.

The Jost solutions for the AKNS Dirac system (2.4) can be constructed in an explicit manner, and thus we can derive the representations for the Jost solutions f_- and f_+ for the Schrödinger operators H in the factorized form (1.2). Then we shall show that, for every fixed $x \in \mathbb{R}$, the Jost solutions f_- and f_+ are such that the functions

$$\mathrm{e}^{-\mathrm{i}\omega x} f_+(x, \omega) - 1 \quad \text{and} \quad \mathrm{e}^{\mathrm{i}\omega x} f_-(x, \omega) - 1 \tag{2.6}$$

are the Fourier transforms of some elements of X supported on the positive half-line $\mathbb{R}_+$. In particular, there is a kernel $K_+(x,t)$ such that, for every fixed $x \in \mathbb{R}$, the function $K_+(x, \cdot\,)$ is an element of X supported on the half-line $t > x$ and such that

$$f_+(x, \omega) = \mathrm{e}^{\mathrm{i}\omega x} + \int_x^\infty K_+(x,t) \mathrm{e}^{\mathrm{i}\omega t}\, \mathrm{d}t. \tag{2.7}$$

The kernel K_+ generates the corresponding *transformation operator*, see [59].

We regard the Fourier transforms $\widehat{h} = \mathcal{F}_+ h$ of functions $h \in X$ as elements of the corresponding Wiener-type algebra $\widehat{X}$ of continuous functions with the norm $\|\widehat{h}\|_{\widehat{X}} := \|h\|_X$. Adjoining the unity $\mathbf{1}$ to $\widehat{X}$, we then prove that the functions $\omega a(\omega)/(\omega + \mathrm{i})$ and $\omega b(\omega)/(\omega+\mathrm{i})$ are respectively elements of $\mathbf{1} \dotplus \widehat{X}$ and $\widehat{X}$, that a^{-1} belongs to $\mathbf{1} \dotplus \widehat{X}$ and a admits an extension into the upper-half complex plane $\mathbb{C}_+$ as an analytic function that is continuous and bounded on the closed upper-half plane $\overline{\mathbb{C}_+}$ outside the disks $|\omega| \le \varepsilon$, for every $\varepsilon > 0$. As a result, the scattering coefficient r_+ belongs to $\widehat{X}$; in particular, the function $F_+ = \mathcal{F}_+ r_+$ belongs to X. Next, symmetry properties of a and b result in the same symmetry for r_+, viz., $r_+(-\omega) = \overline{r_+(\omega)}$ for real ω; also, $|r_+(\omega)| < 1$ for real nonzero ω.

Concerning the value $\omega = 0$, two cases are possible. We say that the Schrödinger operator H has a *resonance* (also called *half-bound state*) at $\omega = 0$, if the zero-energy Jost solutions $f_-(\,\cdot\,, 0)$ and $f_+(\,\cdot\,, 0)$ are linearly dependent. In this case $q \in \mathcal{Q}_0$; moreover, a is then an element of $\mathbf{1} \dotplus \widehat{X}$ and, in particular, is bounded on the whole real line thus yielding the inequality $|r_+(0)| < 1$. Generically, $q \in \mathcal{Q}_1$ and H possesses no resonance at $\omega = 0$; then a is unbounded at the origin and $r_+(0) = -1$. Moreover, the explicit way r_+ depends on a and b leads to the conclusion that the regularized coefficient

$$\widetilde{r}_+(\omega) := \frac{1 - |r_+(\omega)|^2}{\omega^2}$$

belongs to $\widehat{X}$.

Introduce now the set

$$\mathcal{R} := \{r \in \widehat{X} \mid r(-\omega) = \overline{r(\omega)},\ |r(\omega)| < 1 \quad \text{for} \quad \omega \in \mathbb{R} \setminus \{0\}\}$$

and its subsets

$$\mathcal{R}_0 := \{r \in \mathcal{R} \mid \ |r(0)| < 1\} \tag{2.8}$$

and

$$\mathcal{R}_1 := \{r \in \mathcal{R} \mid r(0) = -1,\ \widetilde{r} \in \widehat{X},\ \widetilde{r}(0) \neq 0\}, \tag{2.9}$$

where $\widetilde{r}(\omega) := (1 - |r(\omega)|^2)/\omega^2$. The set $\mathcal{R}_0$ is endowed with the topology of $\widehat{X}$, while the topology of $\mathcal{R}_1$ is determined by the distance

$$d(r_1, r_2) = \|r_1 - r_2\|_{\widehat{X}} + \|\widetilde{r}_1 - \widetilde{r}_2\|_{\widehat{X}}.$$

One of our main results is that the sets $\mathcal{R}_0$ and $\mathcal{R}_1$ consist of the reflection coefficients for the class of Schrödinger operators under consideration in the resonant (i.e., exceptional $q \in \mathcal{Q}_0$) and non-resonant (i.e., generic $q \in \mathcal{Q}_1$) cases, respectively. More exactly, the typical result reads as follows. Denote by $X_{\mathbb{R}}$ the subset of real-valued functions in the space X; $X_{\mathbb{R}}$ is a real subspace of X under the inherited topology. Recall that $q \in \mathcal{Q}$ is parametrized by a pair $(w, \alpha) \in X \oplus \mathbb{R}^+$, in which $w\big|_{\mathbb{R}^\pm}$ are equal to $u_\pm\big|_{\mathbb{R}^\pm}$ and $\alpha = (u_- - u_+)(0)$; moreover, $\alpha = 0$ for $q \in \mathcal{Q}_0$ and $\alpha > 0$ for $q \in \mathcal{Q}_1$.

Theorem 2.1. *The maps*

$$\mathcal{S}_\pm : (w, \alpha) \mapsto r_\pm$$

are homeomorphic between $X_{\mathbb{R}}$ and $\mathcal{R}_0$ and between $X_{\mathbb{R}} \oplus \mathbb{R}^+$ and $\mathcal{R}_1$, respectively.

This gives a complete description of the scattering data for the class of operators under consideration, and thus solves the direct scattering problem and settles existence in the inverse problem. It remains to find the procedure to actually determine u given r_+ or r_-.

To this end we observe that equation (1.6) yields the relation

$$\frac{\mathrm{e}^{\mathrm{i}\omega x} f_-(x, \omega)}{a(\omega)} = \mathrm{e}^{\mathrm{i}\omega x} f_+(x, -\omega) + \mathrm{e}^{\mathrm{i}\omega x} r_+(\omega) f_+(x, \omega).$$

The properties of a and of the function $\mathrm{e}^{\mathrm{i}\omega x} f_-(x, \omega)$ of (2.6) imply that the left-hand side of the above equality is a function admitting a bounded analytic extension to the upper-half complex plane. Therefore the Fourier transform of the right-hand side is supported on the positive half-line; working it out on account of the representation (2.7) leads to the well-known *Marchenko equation* relating the Fourier transform F_+ of r_+ and the kernel K_+ of the transformation operator:

$$K_+(x, t) + F_+(x + t) + \int_x^\infty K_+(x, s) F_+(s + t)\, ds = 0, \qquad x < t. \tag{2.10}$$

For every fixed $x \in \mathbb{R}$, the above Marchenko equation is understood as an equality of X-valued functions of argument t for $t > x$. Given the reflection coefficient r_+ and thus the function F_+, one can solve this equation for $K_+(x, \cdot)$, for every fixed x. In the case of Faddeev–Marchenko potentials q the kernel K_+ is absolutely continuous in the domain $x \le t$, and the equality

$$q(x) = -2\frac{d}{dx}K_+(x,x)$$

holds almost everywhere.

For singular u, the kernel K_+ allows no restriction onto the diagonal $x = t$, and the above formula becomes useless. Moreover, our aim is to determine the Riccati representative u, and not the potential q.

To derive the main relation between u and the transformation operators, we assume for the time being that q is a Faddeev–Marchenko potential and consider along with (2.10) the equation

$$K_-(x,t) - F_+(x+t) - \int_x^\infty K_-(x,s)F_+(s+t)\,ds = 0, \qquad x < t,$$

in which F_+ is replaced with $-F_+$. In the resonant case this corresponds to taking $-r_+$ instead of r_+. Using the fact that the scattering maps $\mathcal{S}_\pm$ are odd in the resonant case, we conclude that $-r_+$ corresponds to the Riccati representative $-u$, so that

$$-2\frac{d}{dx}K_-(x,x) = -u'(x) + u^2(x).$$

Introducing the kernels

$$M_\pm(x,t) := \frac{1}{2}\Big[K_+(x,t) \pm K_-(x,t)\Big],$$

we see that

$$u(x) = -2M_-(x,x), \tag{2.11}$$

which is the desired relation. We note that the kernels $M_\pm$ satisfy the system of equations

$$F_+(x+t) + M_-(x,t) + \int_x^\infty M_+(x,s)F_+(s+t)\,ds = 0, \tag{2.12}$$

$$M_+(x,t) + \int_x^\infty M_-(x,s)F_+(s+t)\,ds = 0, \tag{2.13}$$

found in the inverse theory for Zakharov–Shabat systems [72].

It turns out [36, 46] that the same relations take place also for the case of Miura potentials in $\mathcal{Q}$. Therefore, given the reflection coefficient r_+, one can form the above Zakharov–Shabat system (2.12)–(2.13) with $F_+ = \mathcal{F}_+ r_+$, solve it for M_-, and determine u from (2.11).

In fact, the Riccati representative u determined via (2.11) will be integrable at $+\infty$ but need not be such at $-\infty$; in other words, u is the extremal Riccati representative u_+ of $q \in \mathcal{Q}$. To find the other extremal Riccati representative u_-

that is integrable at $-\infty$, we use the left reflection coefficient r_-, take its Fourier transform $F_- := \mathcal{F}_- r_-$ of (2.3), and form the "left" analogue

$$F_-(x+t) + M_-^-(x,t) + \int_{-\infty}^{x} M_+^-(x,s)F_-(s+t)\,ds = 0, \tag{2.14}$$

$$M_+^-(x,t) + \int_{-\infty}^{x} M_-^-(x,s)F_-(s+t)\,ds = 0 \tag{2.15}$$

of the Marchenko-type system (2.12)–(2.13); then $u_- = 2M_-^-(x,x)$.

The final and the most difficult step will be to prove that $Bu_+ = Bu_- =: q$ in the sense of distributions and that the Schrödinger operator H with Miura potential q has the reflection coefficient r_+ we have started with. The details are discussed in Section 3.

2.2. The discrete case

In the case where p is piece-wise constant, no direct analogue of (2.11) exists. However, there are meaningful analogues of the transformation operators but in a discretized form, see Section 4. Assume that p has jumps at the sites of a regular lattice $d\mathbb{Z}$; without loss of generality, we may take $d = 1$. The function $u = (\log p)'$ is now the discrete measure, $u = -\sum u_k \delta(\cdot - k)$, with

$$u_k := \log \frac{p(k+0)}{p(k-0)},$$

so that

$$p(x) = \exp\Big\{ \sum_{k:k>x} u_k \Big\}.$$

In other words, Riccati representatives u are now elements of the space X of measures $d\mu = \sum \mu_k \delta(\cdot - k)$ of finite total variation, i.e., with the sequences $\boldsymbol{\mu} := (\mu_k)$ belonging to $\ell_1(\mathbb{Z})$. Then the corresponding set $\widehat{X}$ of Fourier transforms of elements in X is the Wiener algebra of 2π-periodic functions with absolutely convergent Fourier series $\sum \mu_k \mathrm{e}^{\mathrm{i}ks}$. In particular, the scattering coefficients a and b and the reflection coefficients $r_\pm$ are elements of $\widehat{X}$, and $F_\pm = \mathcal{F}_\pm r_\pm$ are discrete measures supported by $\mathbb{Z}$.

The transformation operators exist and can be represented in the following way. Set $\Delta_j := [j, j+1)$ and denote by P_j the orthogonal projector in $L_2(\mathbb{R})$ onto $L_2(\Delta_j)$, $P_j g(x) = g(x)\chi_{\Delta_j}(x)$, with χ_{Δ_j} being the characteristic function of Δ_j. It is convenient to use the unitary equivalence of the spaces $L_2(\mathbb{R})$ and $L_2(0,1) \otimes \ell_2(\mathbf{Z})$ and to represent functions $g(x)$ in $L_2(\mathbb{R})$ as $g(y,k)$, with $y \in [0,1)$, $k \in \mathbb{Z}$, and $g(y,k) = g(y+k)$. Under this identification, every bounded operator T in $L_2(\mathbb{R})$ can be written in the matrix form $(T_{m,n})_{m,n\in\mathbb{Z}}$, with $T_{m,n} := P_m T P_n$.

In these notations, the transformation operator K for the Schrödinger operator H_u can be constructed in an explicit way and its components $K_{m,n}$ can be shown to be of the form $K(m,n)T^{m+n}$, there $K(m,n)$ is a number and T is the reflection operator in $L_2(\Delta_0)$, i.e., $(Tg)(y) = g(1-y)$. Further, set $R(k) := \widehat{r}_+(-k)$;

then the discrete analogue of the Marchenko equation reads

$$K_+(m,n) + R(m+n) + \sum_{\xi=m+1}^{\infty} K_+(m,\xi)R(\xi+n) = 0, \qquad m < n,$$

while the analogue of the Zakharov–Shabat system takes the form

$$\begin{aligned} M_+(m,n) + \sum_{\xi=m+1}^{\infty} M_-(m,\xi)R(\xi+n) &= 0, \\ M_-(m,n) + R(m+n) + \sum_{\xi=m+1}^{\infty} M_+(m,\xi)R(\xi+n) &= 0. \end{aligned}$$

As in the continuous case, the kernel M_- determines the function u, but the corresponding relation takes a somewhat different form, namely,

$$\tanh u_n = M_-(n-1, n+1), \qquad n \in \mathbb{Z}. \tag{2.16}$$

It is the difference between recovering u via (2.11) in the continuous case and (2.16) in the discrete case that does not allow to a unified approach to reconstructing measures u with both continuous and discrete components.

The details of solutions of the inverse scattering problems in the continuous and discrete cases respectively are given in Sections 3 and 4 below.

3. Inverse scattering for Miura potentials

The standard method of solution of the inverse scattering problem for Schrödinger operators is due to Marchenko and is based on the so-called transformation operators. As mentioned above, for impedance Schrödinger equations a more efficient approach is that of Zakharov and Shabat for the related Dirac system (2.4). Below, we explain the basic steps in the solution of the inverse scattering problem for the Schrödinger operator with Miura potentials using the reduced Dirac systems in AKNS form.

3.1. Jost solutions

We shall start with the simpler case where $q \in \mathcal{Q}_0$, i.e., where the Riccati representative u belongs to $X := L_1(\mathbb{R}) \cap L_2(\mathbb{R})$.

An effective construction of the Jost solution for $q = u' + u^2$ with given $u \in X$ uses the "conjugate" potentials $q^{(-)} = -u' + u^2$ corresponding to $-u$ and the associated reduced Dirac equation (2.4). Namely, we first construct a fundamental solution matrix for the Dirac system (2.4), i.e., a 2×2 matrix solution $U(\,\cdot\,, \omega)$ to

$$\Big(B\frac{d}{dx} + uJ\Big)U = \omega U$$

that approaches $\mathrm{e}^{-\omega x B}$ as x tends to $+\infty$ (recall that the matrices B and J were defined in (2.5)). Noting that B has eigenvalues $\lambda_1 = -\mathrm{i}$ and $\lambda_2 = +\mathrm{i}$ with the corresponding eigenvectors

$$v_1 = \begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix}, \qquad v_2 = \begin{pmatrix} 1 \\ \mathrm{i} \end{pmatrix},$$

we then see that the Jost solutions f_+ and $f_+^{(-)}$ for the potentials q and $q^{(-)}$ satisfy the relation

$$\begin{pmatrix} f_+(x,\omega) \\ -\mathrm{i} f_+^{(-)}(x,\omega) \end{pmatrix} = U(x,\omega) v_1. \tag{3.1}$$

Variation of constants formula leads to the integral equation

$$U(x,\omega) = \mathrm{e}^{-\omega x B} - \int_x^\infty \mathrm{e}^{-\omega(x-t)B} u(t) BJU(t,\omega)\,\mathrm{d}t.$$

Using the successive approximation method, we set

$$U_0(x,\omega) = \exp(-\omega x B)$$

and

$$U_n(x,\omega) = -\int_x^\infty \mathrm{e}^{-\omega(x-t)B} u(t) BJU_{n-1}(t,\omega)\,\mathrm{d}t$$

for $n \ge 1$; then U is formally given by the Volterra series $\sum_{n\ge 0} U_n$.

In a straightforward recursive manner one derives the formulas

$$U_{2n}(x,\omega) = \int_{x<t_1<\dots<t_{2n}} u(t_1)\cdots u(t_{2n}) \mathrm{e}^{-\omega(x-2\sigma_{2n}(\mathrm{t}))B}\,\mathrm{d}t_1\cdots\mathrm{d}t_{2n}$$

and

$$\begin{aligned} &U_{2n-1}(x,\omega) \\ &\qquad = -\int_{x<t_1<\dots<t_{2n-1}} u(t_1)\cdots u(t_{2n-1})\; BJ\,\mathrm{e}^{\omega(x-2\sigma_{2n-1}(\mathrm{t}))B}\,\mathrm{d}t_1\cdots\mathrm{d}t_{2n-1}, \end{aligned}$$

where

$$\sigma_n(\mathrm{t}) := \sum_{j=1}^n (-1)^{j+1} t_j$$

for $n \ge 1$ and $\mathrm{t} := (t_1, t_2, \dots, t_n)$. The proof uses the anti-commutation relation $BJ + BJ = 0$ (which implies that $J\exp(tB) = \exp(-tB)J$) together with the identity

$$\sigma_{n+1}(t_1,\dots,t_{n+1}) = t_1 - \sigma_n(t_2,\dots,t_{n+1}).$$

Note that $\left\|\mathrm{e}^{\omega x B}\right\| = 1$ for all real x and ω, with $\|\cdot\|$ being the operator norm on 2×2 matrices. Therefore, with

$$\eta(x) := \int_x^\infty |u(s)|\,\mathrm{d}s,$$

one easily shows that

$$\|U_n(x,\omega)\| \leq \frac{\big(\eta(x)\big)^n}{n!},$$

so the Volterra series for U converges uniformly in $\omega \in \mathbb{R}$ to a bounded continuous function $U(\,\cdot\,,\omega)$ on $\mathbb{R}$.

Since v_1 is an eigenvector of B and $Jv_1 = -iv_2$, we compute that

$$U_{2n}(x,\omega)v_1 = \left(\int_{x<t_1<\cdots<t_{2n}} u(t_1)\cdots u(t_{2n})\, e^{i\omega(x-2\sigma_{2n}(\mathrm{t}))}\,\mathrm{dt}\right) v_1$$

and

$$U_{2n-1}(x,\omega)v_1 = -\left(\int_{x<t_1<\cdots<t_{2n-1}} u(t_1)\cdots u(t_{2n-1})\, e^{-i\omega(x-2\sigma_{2n-1}(\mathrm{t}))}\,\mathrm{dt}\right) v_2.$$

Relation (3.1) now yields the representation

$$f_+(x,\omega) = a(x,\omega)\mathrm{e}^{\mathrm{i}\omega x} + b(x,\omega)\mathrm{e}^{-\mathrm{i}\omega x},$$

for the Jost solution f_+, with

$$a(x,\omega) = 1 + \sum_{n=1}^{\infty} a_{2n}(x,\omega),$$

$$b(x,\omega) = \sum_{n=1}^{\infty} b_{2n-1}(x,\omega),$$

where

$$a_{2n}(x,\omega) := \int_{x<t_1<\cdots<t_{2n}} u(t_1)\cdots u(t_{2n})\mathrm{e}^{-2\mathrm{i}\omega\sigma_{2n}(\mathrm{t})}\,\mathrm{dt} \tag{3.2}$$

and

$$b_{2n-1}(x,\omega) := -\int_{x<t_1<\cdots<t_{2n-1}} u(t_1)\cdots u(t_{2n-1})\mathrm{e}^{2\mathrm{i}\omega\sigma_{2n-1}(\mathrm{t})}\,\mathrm{dt}. \tag{3.3}$$

We can obtain a more useful representation for $a(x,\omega)$ and $b(x,\omega)$ by recasting (3.2) and (3.3) as follows. In (3.2), let $s = -\sigma_{2n}(\mathrm{t})$ and $y_j = t_{j+1}$. Note that $\sigma_{2n}(\mathrm{t}) \leq 0$ in the region of integration. We then have

$$a_{2n}(x,\omega) = \int_0^{\infty} \mathrm{e}^{2\mathrm{i}\omega s} A_{2n}(x,s)\,\mathrm{d}s$$

where

$$A_{2n}(x,s) = \int_{x<s-\sigma_{2n-1}(\mathrm{y})<y_1<\cdots<y_{2n-1}} u(s-\sigma_{2n-1}(\mathrm{y}))u(y_1)\cdots u(y_{2n-1})\,\mathrm{dy}$$

obeys the estimates

$$\|A_{2n}(x,\,\cdot\,)\|_{L_1(\mathbb{R}^+)} \leq \frac{\big(\eta(x)\big)^{2n}}{(2n)!}$$

for $u \in L_1(\mathbb{R})$ and

$$\|A_{2n}(x,\ \cdot\ )\|_{L_2(\mathbb{R}^+)} \le \|u\|_2 \frac{\bigl(\eta(x)\bigr)^{2n-1}}{(2n-1)!}$$

for $u \in X$. It follows that

$$a(x,\omega) = 1 + \int_0^\infty \mathrm{e}^{2\mathrm{i}\omega s} A(x,s)\,\mathrm{d}s$$

where

$$\|A(x,\ \cdot\ )\|_1 \le \cosh\eta(x) - 1$$

and

$$\|A(x,\ \cdot\ )\|_2 \le \|a\|_2 \sinh\eta(x).$$

Finally, it is easy to check that $\lim_{x\to\infty} A(x,\ \cdot\ ) = 0$ and that the limit $A(s) = \lim_{x\to-\infty} A(x,s)$ exists in $L_1(\mathbb{R}^+) \cap L_2(\mathbb{R}^+)$.

Next we consider $b(x,s)$. In (3.3), let $s = \sigma_{2n-1}(\mathrm{t})$ and note that $x < s$ in the region of integration. Thus with $y_j = t_{j+1}$ for $1 \le j \le 2n-2$ we get

$$b_{2n-1}(x,\omega) = -\int_x^\infty \mathrm{e}^{2\mathrm{i}\omega s} B_{2n-1}(x,s)\,\mathrm{d}s,$$

where

$$B_{2n-1}(x,s) = \int_{x<s+\sigma_{2n-2}(\mathrm{y})<y_1<\cdots<y_{2n-1}} u(s+\sigma_{2n-2}(\mathrm{y}))u(y_1)\cdots u(y_{2n-2})\,\mathrm{dy}$$

obeys multi-linear estimates similar to those for A_{2n}. In particular,

$$b(x,\omega) = -\int_x^\infty \mathrm{e}^{2\mathrm{i}\omega s} B(x,s)\ ds$$

where (taking X-norms on $\mathbb{R}$ and extending $B(x,s)$ to zero if $s < x$)

$$\|B(x,\ \cdot\ )\|_1 \le \sinh\eta(x)$$

and

$$\|B(x,\ \cdot\ )\|_2 \le \|u\|_2 \bigl(\cosh\eta(x) - 1\bigr).$$

We can show that the limit

$$B(s) = \lim_{x\to-\infty} B(x,s)$$

exists in X.

Finally, similar multi-linear estimates for the differences $A_{2n} - \widetilde{A}_{2n}$ and $B_{2n+1} - \widetilde{B}_{2n+1}$ of such functions constructed for u and $\widetilde{u}$ show that $u \mapsto A(x,\ \cdot\ )$ and $u \mapsto B(x,\ \cdot\ )$ are continuous mappings from X to $C(\mathbb{R};X)$.

Introduce the matrix

$$V := \begin{pmatrix} 1 & 1 \\ -\mathrm{i} & \mathrm{i} \end{pmatrix}$$

composed of the eigenvectors v_1 and v_2 of B and set $\Psi(x,\omega) := V^{-1}U(x,\omega)V$. Then Ψ is a solution of the AKNS-ZS system

$$\Psi' = \mathrm{i}\omega J_1\Psi + uJ\Psi$$

with $J_1 := \operatorname{diag}\{1, -1\}$, and one can verify in a straightforward manner that

$$\mathrm{e}^{-\mathrm{i}\omega J_1}\Psi(x,\omega) = \begin{pmatrix} a(x,\omega) & \overline{b(x,\omega)} \\ b(x,\omega) & \overline{a(x,\omega)} \end{pmatrix}$$

is an element of the group $SU(1,1)$; see [36]. In particular, we see that

$$|a(x,\omega)|^2 - |b(x,\omega)|^2 = 1.$$

From the computations above it is clear that the limits

$$\begin{aligned} a(\omega) &= \lim_{x\to-\infty} a(x,\omega) \\ b(\omega) &= \lim_{x\to-\infty} b(x,\omega) \end{aligned}$$

exist and define continuous functions of ω. Moreover,

$$|a(\omega)|^2 = |b(\omega)|^2 + 1 \tag{3.4}$$

so that $|a(\omega)| \geq 1$, while the symmetry relations

$$\overline{a(\omega)} = a(-\omega) \qquad \text{and} \qquad \overline{b(\omega)} = b(-\omega)$$

are inherited from those for $a(x,\omega)$ and $b(x,\omega)$. More importantly:

Proposition 3.1. *Suppose that $u \in L_1(\mathbb{R})$. Then the functions $a(\omega)$ and $b(\omega)$ admit integral representations*

$$\begin{aligned} a(\omega) &= 1 + \int_0^\infty \mathrm{e}^{2\mathrm{i}\omega s} A(s)\,\mathrm{d}s, \\ b(\omega) &= -\int_{-\infty}^\infty \mathrm{e}^{2\mathrm{i}\omega s} B(s)\,\mathrm{d}s, \end{aligned}$$

where

$$\begin{aligned} \|A\|_1 &\leq \cosh(\|u\|_1) - 1, \\ \|B\|_1 &\leq \sinh \|u\|_1\,, \end{aligned}$$

and the function $A \in L_1(\mathbb{R}^+)$ and $B \in L_1(\mathbb{R})$ depend continuously on u in $L_1(\mathbb{R})$. If, also, $u \in L_2(\mathbb{R})$, then

$$\begin{aligned} \|A\|_2 &\leq \|u\|_2 \sinh \|u\|_1\,, \\ \|B\|_2 &\leq \|u\|_2 \big(\cosh \|u\|_1 - 1\big), \end{aligned}$$

and the maps $u \mapsto A$ and $u \mapsto B$ are continuous as maps from X to $L_1(\mathbb{R}^+) \cap L_2(\mathbb{R}^+)$ and to X respectively.

Using this proposition, it is easy to derive the representation of the Jost solution f_+ in the form (2.7), with $K(x,\cdot)$ the function in X for every $x \in \mathbb{R}$.

3.2. The scattering data

It follows from Proposition 3.1 that for $u \in X$ the scattering coefficients a and b are elements of the Wiener algebras $\mathbf{1} \dotplus \widehat{X}$ and $\widehat{X}$, respectively. Since a is an invertible element of $\mathbf{1} \dotplus \widehat{X}$, we see that $r_+(\omega) := -b(-\omega)/a(\omega)$ belongs to $\widehat{X}$. The symmetry properties of a and b yield the relation $r(-\omega) = \overline{r(\omega)}$, while (3.4) implies that $|r(\omega)| < 1$ for all $\omega \in \mathbb{R}$. This establishes the direct part of the scattering problem, namely:

Proposition 3.2. *For every real-valued $u \in X$, the reflection coefficient r_+ of the corresponding Schrödinger operator H_u is an element of the set $\mathcal{R}_0$ of* (2.8).

In the case where $q = u_-' + u_-^2 = u_+' + u_+^2 \in \mathcal{Q}_1 := \mathcal{Q} \setminus \mathcal{Q}_0$ for some $u_\pm \in L_1(\mathbb{R}^\pm) \cap L_2(\mathbb{R})$, we cannot pass to the limit $x \to -\infty$ in the above formulas for $a(x,\omega)$, $b(x,\omega)$, $A(x,s)$, and $B(x,s)$. However, all the other arguments remain valid as they only require half-line integrability of u, which holds for u_+. Therefore, we get the following

Lemma 3.3. *The representation formulas*

$$f_+(x,\omega) = \mathrm{e}^{\mathrm{i}\omega x} + \int_x^\infty K_+(x,\zeta)\mathrm{e}^{\mathrm{i}\omega\zeta}d\zeta,$$

$$f_+^{[1]}(x,\omega) = \mathrm{i}\omega\left(\mathrm{e}^{\mathrm{i}\omega x} + \int_x^\infty K_{+,1}(x,\zeta)\mathrm{e}^{\mathrm{i}\omega\zeta}\,d\zeta\right)$$

hold, with $f_+^{[1]} := f' - u_+ f$ and the kernels $K_+(x,\,\cdot\,)$ and $K_{+,1}(x,\,\cdot\,)$ belonging to X for every fixed $x \in \mathbb{R}$.

The reason why *quasi-derivatives* $f^{[1]} := f' - u_+ f$ are used above comes from the fact that for f in the domain of the operator H_u, the derivative f' need not be continuous while $f^{[1]}$ is continuous. Denoting by $W_+\{f,g\} := f^{[1]}g - fg^{[1]}$ the modified Wronskian, we get from the above representations the equality

$$W_+\{f_+(x,\omega), f_+(x,-\omega)\} = -2\mathrm{i}\omega, \tag{3.5}$$

for every nonzero $\omega \in \mathbb{R}$.

Clearly, there are analogous construction for the left Jost solutions $f_-(x,\omega)$ and their quasi-derivatives $f_-^{[1]} := f_-' - u_- f_-$ that use the Riccati representative u_-. We then determine the coefficients a and b from the relations (1.5) and (3.5) as

$$a(\omega) = \frac{W_+\{f_-(x,\omega), f_+(x,\omega)\}}{2i\omega}, \tag{3.6}$$

$$b(\omega) = -\frac{W_+\{f_-(x,-\omega), f_+(x,\omega)\}}{2i\omega} \tag{3.7}$$

for real nonzero ω. Using now the integral representations for the Jost solutions $f_\pm$ and their quasi-derivatives, and recalling that $v := u_- - u_+$ is a non-negative continuous function, we arrive at the following conclusion.

Lemma 3.4. *Suppose that $q \in \mathcal{Q}$. Then the coefficients a and b admit the representation*

$$a(\omega) = 1 + \widehat{A}_1(\omega) - v(0)\left[\frac{1+\widehat{A}_2(\omega)}{2\mathrm{i}\omega}\right],$$

$$b(\omega) = \widehat{B}_1(\omega) + v(0)\left[\frac{1+\widehat{B}_2(\omega)}{2\mathrm{i}\omega}\right],$$

in which A_j and B_j, $j = 1, 2$, are real-valued functions in X, with A_i supported on $[0,\infty)$. Moreover, $A_2 = B_2 = 0$ if $q \in \mathcal{Q}_0$ and

$$1 + \widehat{A}_2(0) = 1 + \widehat{B}_2(0) = f_+(0,0)f_-(0,0)$$

is nonzero if $q \in \mathcal{Q}_1$. The maps $q \mapsto A_j$ and $q \mapsto B_j$ are continuous maps from $\mathcal{Q}$ into X.

It follows that in the generic case $q \in \mathcal{Q}_1$ the coefficients $\omega a(\omega)/(\omega+\mathrm{i})$ and $\omega b(\omega)/(\omega+\mathrm{i})$ are elements of the Wiener algebras $\mathbf{1} \dotplus \widehat{X}$ and $\widehat{X}$, respectively, but a and b themselves have singularity at the origin. The function a never vanishes on the real line so that $1/a$ is well defined and belongs to $\mathbf{1} \dotplus \widehat{X}$; as a result, $r_+(\omega) := -b(-\omega)/a(\omega)$ and $r_-(\omega) = b(\omega)/a(\omega)$ are well defined and belong to $\widehat{X}$. In particular, $r_\pm$ are continuous functions and $r_\pm(0) = -1$. More details are given in the following statement, where $w_\pm$ stand for the restrictions of the Riccati representatives $u_\pm$ onto the respective half-line $\mathbb{R}^\pm$ and the set $\mathcal{R}_1$ was introduced in (2.9).

Proposition 3.5. *Suppose that $q \in \mathcal{Q}_1$. Then $r_\pm \in \mathcal{R}_1$, and the maps*

$$\mathcal{S}_\pm : (w_+, w_-, v(0)) \mapsto r_\pm$$

and

$$(w_+, w_-, v(0)) \mapsto \widetilde{r}_\pm$$

are continuous.

3.3. Reconstruction of the transmission coefficient

Next, we show how to construct $t = 1/a$ given either one of the reflection coefficients. Again the case $q \in \mathcal{Q}_0$ is much simpler, and we shall concentrate on the non-resonant case $q \in \mathcal{Q}_1$.

We observe that formula (3.6) allows to extend a analytically in the open upper-half plane $\mathbb{C}^+$ and this extension has no zeros in $\overline{\mathbb{C}^+} \setminus \{0\}$. Thus the regularization

$$\widetilde{a}(\omega) := \frac{\omega}{\omega+\mathrm{i}}a(\omega)$$

of a extends to a bounded holomorphic function in the upper half-plane with no zeros in its closure. Using the Schwarz formula to reconstruct the function $\log\widetilde{a}$ from its real part $\operatorname{Re}\log\widetilde{a}(s) = \log|\widetilde{a}(s)|$, we get

$$\widetilde{a}(z) = \exp\left(\frac{1}{\pi\mathrm{i}}\int_{\mathbb{R}} \log|\widetilde{a}(s)|\,\frac{\mathrm{d}s}{s-z}\right). \tag{3.8}$$

It follows from (3.8) that

$$t(z) := 1/a(z) = \frac{z}{z+\mathrm{i}} \exp\left\{ \frac{1}{2\pi\mathrm{i}} \int_{\mathbb{R}} \log\left[\left(1 - |r_\pm(s)|^2\right) \frac{s^2+1}{s^2}\right] \frac{\mathrm{d}s}{s-z} \right\},$$

and t on the real line is given as a boundary value as $\operatorname{Im} z \to 0$. In terms of the Riesz projector $\mathcal{C}_+$, we get the formula

$$t(\omega) = \frac{\omega}{\omega+\mathrm{i}} \exp\left\{ \left(\mathcal{C}_+ \log\left[\left(1 - |r_\pm(s)|^2\right) \frac{s^2+1}{s^2}\right] \right)(\omega) \right\}. \tag{3.9}$$

In particular, the number $\theta := \lim_{\omega\to 0} [2\mathrm{i}\omega/t(\omega)]$ can be recovered from either reflection coefficient.

We next show that formula (3.9) makes sense for every element $r \in \mathcal{R}_1$. Indeed, the function

$$\left(1 - |r(\omega)|^2\right) \frac{\omega^2+1}{\omega^2} = 1 - r(\omega)r(-\omega) + \widetilde{r}(\omega) \tag{3.10}$$

belongs to the algebra $1 \dotplus \widehat{X}$, does not vanish on the real line, and tends to 1 at infinity. By the Wiener–Levi Lemma A.2, the function

$$\log\left[\left(1 - |r(\omega)|^2\right) \frac{\omega^2+1}{\omega^2}\right]$$

also belongs to $1 \dotplus \widehat{X}$; in fact, since it vanishes at infinity, it belongs to $\widehat{X}$. Finally, the Riesz projector $\mathcal{C}_+$ acts continuously in $\widehat{X}$, and exponentiation is a continuous operation in $1 \dotplus \widehat{X}$ by the Wiener–Levi lemma. We now define a function $\widetilde{t} \in 1 \dotplus \widehat{X}$ by (cf. (3.9))

$$\widetilde{t} = \exp\left\{ \mathcal{C}_+ \log\left[\left(1 - |r(\omega)|^2\right) \frac{\omega^2+1}{\omega^2}\right] \right\}. \tag{3.11}$$

Clearly, $\widetilde{t}$ is an invertible element of the Banach algebra $1 \dotplus \widehat{X}$. Moreover, the following holds:

Lemma 3.6. *The mappings*

$$\mathcal{R}_1 \ni r \mapsto \widetilde{t} \in 1 \dotplus \widehat{X} \qquad \textit{and} \qquad \mathcal{R}_1 \ni r \mapsto 1/\widetilde{t} \in 1 \dotplus \widehat{X}$$

are continuous.

We observe that since the function in (3.10) is even and the Riesz projector maps even functions into odd ones, the function $\widetilde{t}$ enjoys the symmetry property $\widetilde{t}(-\omega) = \overline{\widetilde{t}(\omega)}$. We set $t(\omega) = \omega\widetilde{t}(\omega)/(\omega+\mathrm{i})$; then the above considerations show that

$$\frac{t(\omega)}{t(-\omega)} = \frac{\omega-\mathrm{i}}{\omega+\mathrm{i}} \frac{\widetilde{t}(\omega)}{\widetilde{t}(-\omega)}$$

also belongs to $1 \dotplus \widehat{X}$. The function

$$r^{\#}(\omega) = -\frac{t(\omega)}{t(-\omega)} r(-\omega)$$

thus belongs to $\mathcal{R}_1$ and, as $|t(\omega)/t(-\omega)| = 1$, we have

$$\frac{1-\left|r^{\#}(\omega)\right|^2}{\omega^2} = \frac{1-|r(\omega)|^2}{\omega^2} \in \widehat{X}.$$

Hence:

Proposition 3.7. *For $r \in \mathcal{R}_1$, define $\widetilde{t}$ by (3.11) and set $t(\omega) = \omega\,\widetilde{t}(\omega)/(\omega+\mathrm{i})$. Then the nonlinear map*

$$\mathcal{I}\,:\,r \mapsto r^{\#}(\omega) := -\frac{t(\omega)}{t(-\omega)}r(-\omega)$$

is a continuous involution on $\mathcal{R}_1$.

We observe that if $r_\pm$ are the reflection coefficients for a Schrödinger operator H with Miura potential $q \in \mathcal{Q}$, then $\mathcal{I}r_\pm = r_\mp$.

3.4. The inverse problem

In this subsection we solve the inverse scattering problem by proving the following theorem.

Theorem 3.8. *Suppose that $r \in \mathcal{R}_j$, $j = 0, 1$. Then there exists a unique $q \in \mathcal{Q}_j$ having r as its right reflection coefficient; moreover, the map $r \mapsto q$ is continuous.*

The resonant case $r \in \mathcal{R}_0$ is much simpler and can be settled by the limiting procedure from the well-known results for smooth potentials q in the Schwartz class; we therefore concentrate on the case where $r \in \mathcal{R}_1$.

We thus suppose given a function $r \in \mathcal{R}_1$, presumed to be the right reflection coefficient corresponding to a potential q_0 to be found. From this data, we can construct $t(\omega)$ (and hence $a(\omega) := 1/t(\omega)$) using (3.9), and use the involution $\mathcal{I}$ to construct $r^{\#} = \mathcal{I}r$, a candidate for the left reflection coefficient. Clearly, b is defined as $r^{\#}a$.

We then form two Zakharov–Shabat systems like (2.12)–(2.13) but taking the putative reflection coefficients r and $r^{\#}$ instead of r_+ and r_- and prove that these equations are uniquely soluble for the kernels $M_\pm$ and $M_\pm^{\#}$. These kernels determine candidate right and left Riccati representatives w and $w^{\#}$, which give the Riccati data

$$\left(w|_{\mathbb{R}^+}, \left.w^{\#}\right|_{\mathbb{R}^-}, (w^{\#}-w)(0)\right) \tag{3.12}$$

of a distribution potential $q_0 \in \mathcal{Q}$. The construction exhibits continuity of the map from r to the data (3.12) as maps from $\mathcal{R}$ to $X^+ \times X^- \times \mathbb{R}^+$, with $X^\pm := L_1(\mathbb{R}^\pm) \cap L_2(\mathbb{R}^\pm)$.

The most difficult part of the problem is to justify the reconstruction by showing that $w' + w^2 = (w^{\#})' + (w^{\#})^2 = q_0$ and that q_0 has reflection coefficients r and $r^{\#}$. It then follows from the uniqueness result (whose proof is a simple variant of that for Levinson's theorem given in [27]) that q_0 is the correct reconstruction.

Now we explain some details of the above algorithm. Taking the Fourier transform F of the function r, we form the Marchenko-type system

$$F(x+t) + M_-(x,t) + \int_x^\infty M_+(x,s)F(s+t)\,\mathrm{d}s = 0, \tag{3.13}$$

$$M_+(x,t) + \int_x^\infty M_-(x,s)F(s+t)\,\mathrm{d}s = 0. \tag{3.14}$$

It is convenient to make change of variables $s = x+y$ in the above integrals and to introduce the linear operator $T_F(x)$ on X^+ by

$$T_F(x)\psi(y) := \int_0^\infty \psi(t)F(x+y+t)\ dt.$$

Since $F \in X$, this operator is compact in X^+. Substituting for M_+ from (3.14) in equation (3.13) and using the notation $F_x(\cdot) := F(x+\cdot)$, we then get the following equation for $\widetilde{M}_-(x,y) := M_-(x,x+y)$:

$$F_{2x}(y) + \widetilde{M}_-(x,y) - T_F^2(2x)\widetilde{M}_-(x,\cdot)(y) = 0,$$

or

$$\big(I - T_F^2(2x)\big)\widetilde{M}_-(x,\cdot) = -F_{2x}.$$

We now prove that the operator $I - T_F^2(2x)$ is boundedly invertible in X^+. Indeed, the inequality $|r(k)| < 1$ a.e. implies that $\ker_{L_2}(I \pm T_F(2x))$ is trivial (see, for example, the proof of Lemma 6.4.1 in [59]), and then compactness of $T_F(2x)$ in X^+ together with the Fredholm alternative gives the result. Therefore,

$$\widetilde{M}_-(x,\cdot) = -\big(I - T_F^2(2x)\big)^{-1}F_{2x}$$

is the solution we are looking for. Using the operator identity

$$(I-T)^{-1} = I + T(I-T)^{-1},$$

we can show that

$$\widetilde{M}_-(x,y) = -F(2x+y) + G(x,y)$$

for some function G that is jointly continuous in x and y. In particular,

$$w(x) := -2\widetilde{M}_-(x,0) = 2F(2x) - 2G(x,0)$$

is well defined and can be shown to belong to the space $L_1 \cap L_2$ on every half-line (c,∞).

"Left" analogues of the above objects constructed for $r^\#$ instead of r_- produce a function $w^\#$ that belongs to $L_1 \cap L_2$ on every half-line $(-\infty, c)$ and equals

$$w^\#(x) = 2\widetilde{M}_-^\#(x,0) = -2F^\#(2x) + 2G^\#(x,0)$$

for some continuous function $G^\#$. The difference $w^\# - w$ is continuous; indeed, it suffices to show that $F + F^\#$ is a continuous function. Recalling that $F = \mathcal{F}_+ r$

and $F^{\#} = \mathcal{F}_{-}r^{\#}$ (cf. (2.2)–(2.3)), we get that

$$F(x) + F^{\#}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\big(r(\omega) + r^{\#}(-\omega)\big)\,\mathrm{e}^{\mathrm{i}\omega x}\,\mathrm{d}\omega,$$
$$= \frac{1}{2\pi}\int_{-\infty}^{\infty}\Big(1 - \frac{t(-\omega)}{t(\omega)}\Big)\,r(\omega)\mathrm{e}^{\mathrm{i}\omega x}\,\mathrm{d}\omega.$$

We next observe that $t(-\omega)/t(\omega)$ belongs to the Wiener algebra $\mathbf{1} \dot{+} \widehat{X}$ and tends to 1 at infinity, so that $1 - t(-\omega)/t(\omega)$ is in $\widehat{X}$ and thus in $L_2(\mathbb{R})$; as a result, $F + F^{\#}$ is the Fourier transform of the integrable function $(1 - t(-\omega)/t(\omega))r(\omega)$ and thus is continuous.

The next step in the reconstruction algorithm is to show that w and $w^{\#}$ are the right and left extremal Riccati representatives of the potential $q_0 \in \mathcal{Q}$ corresponding to the data (3.12). We do this by first showing that $K := M_+ + M_-$ is the kernel of the transformation operator for the Schrödinger operator H_w with potential $q := w' + w^2$, i.e., that

$$f(x,\omega) := \mathrm{e}^{\mathrm{i}\omega x} + \int_x^{\infty} K(x,s)\mathrm{e}^{\mathrm{i}\omega s}\,\mathrm{d}s$$

is the right Jost solution for H_w. Similarly, the kernel $K^{\#} := M_+^{\#} + M_-^{\#}$ formed from the kernels $M_\pm^{\#}$ solving the "left" Marchenko-type system (2.14)–(2.15) but with F_- replaced by $F^{\#}$, is the kernel of the transformation operator for the Schrödinger operator $H_{w^{\#}}$ with potential $q^{\#} := (w^{\#})' + (w^{\#})^2$, i.e.,

$$f^{\#}(x,\omega) := \mathrm{e}^{-\mathrm{i}\omega x} + \int_{-\infty}^{x} K^{\#}(x,s)\mathrm{e}^{-\mathrm{i}\omega s}\,\mathrm{d}s$$

is the left Jost solution for $H_{w^{\#}}$.

It turns out that the functions f and $f^{\#}$ are related as follows.

Lemma 3.9. *The following holds:*

$$f^{\#}(x,\omega) = a(\omega)f(x,-\omega) - b(-\omega)f(x,\omega), \tag{3.15}$$
$$f(x,\omega) = a(\omega)f^{\#}(x,-\omega) + b(\omega)f^{\#}(x,\omega), \tag{3.16}$$

where a and b are constructed from r as explained at the beginning of this subsection.

As a result, we conclude that $f(\cdot,\omega)$ solves the equations $-y'' + qy = \omega^2 y$ and $-y'' + q^{\#}y = \omega^2 y$, which implies that $q = q^{\#} = q_0$ as distributions in $W^{-1}_{2,\mathrm{loc}}(\mathbb{R})$. It follows that f and $f^{\#}$ are respectively the right and left Jost solutions of the Schrödinger operator with Miura potential $q_0 \in \mathcal{Q}_1$, and now (3.15) and (3.16) show that r and $r^{\#}$ are respectively its right and left reflection coefficients. This completes the reconstruction procedure and the proof of Theorem 3.8.

3.5. Sobolev properties of the scattering mappings

One of the motivations for extending the inverse scattering theory is the possibility to study solvability of some completely integrable nonlinear partial differential equations with irregular initial data [14, 22, 33, 37]. For instance, the Cauchy problem for the modified Korteweg-de Vries (mKdV) equation on the line is

$$\begin{aligned} u_t + u_{xxx} + 6u^2 u_x &= 0;\\ u(x;0) &= u_0(x). \end{aligned} \tag{3.17}$$

The existence of global weak solutions for initial data in $L_2(\mathbb{R})$ was proven by Kato [51] and, independently, by Kruzhkov and Faminskiĭ [55]; see also [17] and [41]. Kato's result gives existence but no uniform continuity of the solution in the initial data. On the other hand, Kenig, Ponce, and Vega [52] showed local well-posedness for initial data in the Sobolev space $H^s(R)$ if $s \ge \frac{1}{4}$, while Colliander, Keel, Staffilani, Takaoka, and Tao [23] proved global well-posedness for initial data in $H^s(R)$ for $s > \frac{1}{4}$.

The classical inverse scattering method for mKdV on the line (see Wadati [71] and Tanaka [70], Beals and Coifman [11–13] and in a more general setting the monograph of Beals, Deift and Tomei [14]) constructs a classical solution using the inverse scattering transform for initial data u_0 in the Schwartz class $S(\mathbb{R})$. The crucial observation (made originally by C. Gardner, J. Green, M. Kruscal and R. Miura [37] in 1974 for the KdV equation) is that if the function $u(x,t)$ solves the mKdV equation (3.17), and $H(t)$ is the family of Schrödinger operators in the factorized form (1.2) with Riccati representatives $u(x,t)$,

$$H(t) := -\Big(\frac{\mathrm{d}}{\mathrm{d}x} + u(x,t)\Big)\Big(\frac{\mathrm{d}}{\mathrm{d}x} - u(x,t)\Big),$$

then the reflection coefficient $r(t)$ for $H(t)$ evolves in a straightforward manner in time, namely, $r(t,\omega) = \mathrm{e}^{8it\omega^3} r(0,\omega)$. Thus given the initial condition $u(x,0) = u_0(x)$, one finds the scattering data for the operator $H(0)$, calculates their time evolution, and then reconstructs the potential $u(x,t)$ of the operator $H(t)$ thus solving the mKdV equation.

The only obstacle to apply this method to initial data of low regularity is that the mKdV flow does not preserve the inclusion $r \in \mathcal{R}$. Therefore we need to find smaller classes of initial data u_0, for which the corresponding classes of reflection coefficients remain invariant. Similarly, the same questions arise in connection with using the inverse scattering for the ZS-AKNS systems [36] to solve the defocussing nonlinear Schrödinger equation. In other words, the problem is to study the properties of the scattering maps for various spaces of u.

Fourier-type properties of the map $q \mapsto r$ have been studied by many authors, including Cohen [21], Deift and Trubowitz [27], Faddeev [32], and Zhou [73]. These authors imposed weighted L_1 assumptions on q and obtained regularity results for r in terms of L_∞-norms of r and its derivatives. Kappeler and Trubowitz [49, 50] studied Sobolev space mapping properties of the scattering map and observed that, similarly to the Fourier transform, whenever q is integrable with the weight $\langle x\rangle^k :=$

$(1+|x|^2)^{k/2}$, $k \ge 3$, then the reflection coefficient r is $k-1$ times differentiable, while smoothness of q is reflected in the weight integrability of r. They extend their results to potentials with finitely many bound states in [50] and also prove analyticity and investigate the differential of the scattering map. Deift and Zhou in [28] discuss the long-time asymptotics of solutions to the non-linear Schrödinger equation with the initial data in weighted Sobolev spaces.

In our paper [45] we showed that, for any $s > \frac{1}{2}$, the mapping

$$\mathcal{S} \,:\, u \mapsto r$$

is locally invertible bi-Lipschitz map between real space $L_2(\mathbb{R}, \langle x\rangle^s dx)$ and special subspace of $W_2^s(\mathbb{R})$. However, the space $W_2^s(\mathbb{R})$ is not invariant under the mKdV-induced flow of r if $s > \frac{1}{2}$, whence this result is not directly applicable to solving the mKdV. It might be possible, however, to study the mKdV equation in the space $W_2^{2s}(\mathbb{R}, \langle x\rangle^s dx)$ since the corresponding space $W_2^s(\mathbb{R}, \langle x\rangle^{2s} dx)$ of the reflection coefficients is preserved under the mKdV flow. This and other related questions will be discussed elsewhere [18].

4. The case of discontinuous impedance function

In this section, we show that the case of discontinuous impedance functions leads to Schrödinger operators whose scattering matrices possess completely different properties than those observed in the previous section. The corresponding functions $u = (\log p)'$ now contain Dirac δ-functions and hence are not summable. Moreover, a common sense suggests that the scattering transforms $\mathcal{S}_\pm$ act approximately as the Fourier transforms and thus the reflection coefficients $r_\pm$ should have properties typical to those of the Fourier transform of u. We shall show that, indeed, $r_\pm$ contain (almost-) periodic components and, as a result, do not tend to zero at infinity, contrary to what was observed for singular Miura potentials in the previous section.

Inverse scattering for Schrödinger operators with discontinuous impedances were considered before (see, e.g., [3–5, 19, 66, 67], but only piece-wise smooth impedances with a finite number of discontinuities were allowed. Also, the so-called layer-stripping method was used, i.e., on every interval of continuity of p, the problem was transformed to the potential form and then solved by the standard methods, while the discontinuity in the impedance was determined form the asymptotics of the scattering data. One then had to recalculate the scattering data for the next interval of continuity, and then repeat the process until all discontinuities have been treated. Unfortunately, no method has been suggested that would automatically determine p along with all its jumps in a generic situation.

To better expose the main effects encountered in this problem, we shall concentrate on the model example of piece-wise constant impedance function p having jumps at points of a regular lattice, taken to be $\mathbb{Z}$ without loss of generality. We shall comment in Subsection 4.8 on possible extensions.

4.1. The operators

Throughout this section, the function p is assumed constant on the intervals $\Delta_j := (j, j+1)$ and hence takes the form

$$p(s) = \exp\Big\{ \sum_{j\,:\,j>s} u_j \Big\}$$

for some real numbers u_j. Since in applications only bounded and uniformly positive impedances are of interest, it is natural to assume that the sequence $\boldsymbol{u} := (u_j)$ belongs to $\ell_1(\mathbb{Z})$. Equation (1.9) is the spectral problem $Hy = \omega^2 y$ for the corresponding Schrödinger operator $H = H_{\boldsymbol{u}}$ generated by the differential expression

$$\mathfrak{l} := -\frac{1}{p(s)}\frac{d}{ds}p^2(s)\frac{d}{ds}\frac{1}{p(s)}.$$

The differential expression $\mathfrak{l}$ acts as $\mathfrak{l}y := -y''$ on its domain consisting of functions y such that both y/p and py' are locally absolutely continuous, i.e., of functions y satisfying the interface conditions

$$\begin{aligned} \mathrm{e}^{u_j} y(j+) &= y(j-), \\ \mathrm{e}^{-u_j} y'(j+) &= y'(j-) \end{aligned} \tag{IF$_j$}$$

at every lattice point $s = j$. The operator H is the realization of $\mathfrak{h}$ in $L_2(\mathbb{R})$, i.e., $Hy = -y''$ on the domain

$$\operatorname{dom} H = \{ y \in W_2^2(\mathbb{R} \setminus \mathbb{Z}) \mid \forall j \in \mathbb{Z}, \quad (\mathrm{IF}_j) \quad \text{holds}\}.$$

It is immediate to see that the operator H is symmetric; in fact [53], it is also self-adjoint on the above domain.

4.2. Jost solutions and the scattering data

The right Jost solution $f_+(\,\cdot\,, \omega)$, if exists, must be of the form

$$f_+(s,\omega) = a_j \mathrm{e}^{\mathrm{i}\omega s} + b_j \mathrm{e}^{-\mathrm{i}\omega s}$$

on each interval Δ_j. The interface conditions at the point $x = j$ force the relation

$$\begin{pmatrix} a_{j-1} \\ b_{j-1} \end{pmatrix} = M(j,\omega) \begin{pmatrix} a_j \\ b_j \end{pmatrix} \tag{4.1}$$

with

$$M(j,\omega) := \begin{pmatrix} \cosh u_j & \mathrm{e}^{-2\mathrm{i}\omega j}\sinh u_j \\ \mathrm{e}^{2\mathrm{i}\omega j}\sinh u_j & \cosh u_j \end{pmatrix}.$$

We observe that the matrix $M(j,\omega)$ for all $\omega \in \mathbb{R}$ belongs to the group $SU(1,1)$. Denoting by $|A|$ the norm of a matrix A and by $I_2 := \operatorname{diag}(1,1)$ the unity matrix in $\mathbb{C}^2$, we see that the inclusion $(\mu_j) \in \ell_1(\mathbb{Z})$ yields the inequality

$$\sum_{j\in\mathbb{Z}} |M(j,\omega) - I_2| < \infty,$$

whence for every $k \in \mathbb{Z}$ the product

$$M_k(\omega) := \overrightarrow{\prod_{j>k}} M(j,\omega) := \lim_{m\to\infty} M(k+1,\omega)\cdots M(m,\omega)$$

converges to an element of $SU(1,1)$. Also, by the same reason, the limit

$$M(\omega) := \lim_{n\to-\infty} M_n(\omega)$$

exists and belongs to $SU(1,1)$.

Set now

$$\begin{pmatrix} a_n(\omega) \\ b_n(\omega) \end{pmatrix} := M_n(\omega)\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \begin{pmatrix} a(\omega) \\ b(\omega) \end{pmatrix} := M(\omega)\begin{pmatrix} 1 \\ 0 \end{pmatrix};$$

then, for every fixed $\omega \in \mathbb{R}$, we have that $a_n(\omega) \to a(\omega)$ and $b_n(\omega) \to b(\omega)$ as $n \to -\infty$. Also, $M_n(\omega) \to I_2$ as $n \to \infty$ yields $a_n(\omega) \to 1$ and $b_n(\omega) \to 0$ as $n \to \infty$ and thus the $a_n(\omega)$ and $b_n(\omega)$ indeed determine the right Jost solution $f_+(\,\cdot\,,\omega)$ via (1.5).

The coefficients a_n and b_n possess some useful properties, which we now discuss. Assume first that a sequence $\boldsymbol{u} = (u_n)$ is such that, for some $m \in \mathbb{N}$, we have $u_n = 0$ if $|n| > m$. Then one can prove that, for every $n \in \mathbb{Z}$, the functions a_n and $\omega \mapsto \mathrm{e}^{-2\mathrm{i}\omega(n+1)} b_n(\omega)$ belong to the Hardy space H^+ of functions that are bounded and analytic in the upper-half complex plane $\mathbb{C}_+$. Moreover, for the Fourier series expansions of a_n and b_n,

$$a_n(\omega) = \sum_{m\ge 0} \widehat{a}_n(m)\mathrm{e}^{\mathrm{i}\omega m}, \qquad b_n(\omega) = \sum_{m\ge 2(n+1)} \widehat{b}_n(m)\mathrm{e}^{\mathrm{i}\omega m} \tag{4.2}$$

the interface condition (4.1) yields the relations

$$\widehat{a}_n(0) = \cosh\mu_{n+1}\widehat{a}_{n+1}(0), \qquad \widehat{b}_n(2n+2) = \sinh\mu_{n+1}\widehat{a}_{n+1}(0). \tag{4.3}$$

Passing to the limit as $m \to \infty$ shows that the above properties hold for all $\boldsymbol{u} \in \ell_1$. It follows that, for every fixed $\boldsymbol{u} \in \ell_1$ and $s = n + y$ with $n \in \mathbb{Z}$ and $y \in (0,1)$, the function of ω

$$\mathrm{e}^{-\mathrm{i}\omega s} f_+(s,\omega) = a_n(\omega) + \mathrm{e}^{-2\mathrm{i}\omega s} b_n(\omega)$$

belongs to the Hardy space H^+. In a similar manner, one concludes that

$$\mathrm{e}^{\mathrm{i}\omega s} f_-(s,\omega) \in H^+ \tag{4.4}$$

for every $x \in \mathbb{R}$. Observe also that none of a and a_n has zeros in the open upper-half plane $\mathbb{C}^+$ as otherwise the corresponding impedance Schrödinger operators would have non-positive eigenvalues, which is impossible.

We next recall the following

Definition 4.1. The *Wiener algebra* W is a complex Banach algebra of 2π-periodic continuous functions h with absolutely convergent Fourier series $\sum_{n\in\mathbb{Z}} h_n \mathrm{e}^{\mathrm{i}nx}$ under the point-wise multiplication and the norm $\|h\|_W := \sum_{n\in\mathbb{Z}} |h_n|$.

The above considerations might be summarized as follows:

Proposition 4.2. *The functions a_n, b_n, a, and b are π-periodic elements of the Wiener algebra W, depend therein continuously on $\boldsymbol{u} \in \ell_{1,\mathbb{R}}$ and satisfy the estimates*

$$\|a_n\|_W + \|b_n\|_W, \|a\|_W + \|b\|_W \le \exp\{\|\boldsymbol{u}\|\}.$$

The Wiener algebra W has a nice property that the spectrum of an element $h \in W$ is the range $\operatorname{Ran} h := \{h(x) \mid x \in \mathbb{R}\}$; as a result, h is invertible in W whenever h does not vanish on $\mathbb{R}$. Now, the inclusion $M(\omega) \in SU(1,1)$ yields the relation

$$|a(\omega)|^2 - |b(\omega)|^2 = 1$$

for real ω; therefore a does not vanish on $\mathbb{R}$ and thus is invertible in W. It follows that the reflection coefficients $r_-(\omega) = b(\omega)/a(\omega)$ and $r_+(\omega) = -b(-\omega)/a(\omega)$ belong to W as well. Set

$$\mathscr{R} := \{r \in W \mid r(x+\pi) = r(x), \quad r(-\omega) = \overline{r(\omega)}, \quad \|r\|_\infty < 1\}; \tag{4.5}$$

then the above reasoning establish the direct part of the inverse problem, namely:

Corollary 4.3. *For every real-valued sequence $\boldsymbol{u} \in \ell_1$ the reflection coefficients r_- and r_+ of the corresponding Schrödinger operator $H_{\boldsymbol{u}}$ belong to $\mathscr{R}$.*

The next step is to show that, firstly, the reflection coefficients determine uniquely the corresponding scattering coefficients a and b, and, in fact, that every $r \in \mathscr{R}$ generates some a and b that have properties the genuine scattering coefficients do. Secondly, a continuous involution $\mathcal{I}$ on $\mathscr{R}$ exists such that the right and left reflection coefficients for every Schrödinger operator $H_{\boldsymbol{u}}$ with $\boldsymbol{u} \in \ell_{1,\mathbb{R}}$ are related via $r_- = \mathcal{I} r_+$.

Lemma 4.4.

(i) *Every $r \in \mathscr{R}$ admits a unique representation in the form $r = b/a$ with $a, b \in W$ such that a is invertible in W, zero-free in $\mathbb{C}^+$, and satisfies $\widehat{a}(0) > 0$ and $|a|^2 = (1 - |r|^2)^{-1}$.*

(ii) *For $r \in \mathscr{R}$, take a and b as in part* (i) *and set $r^\#(\omega) := -b(-\omega)/a(\omega)$. Then the function $r^\#$ also belongs to $\mathscr{R}$ and the mapping*

$$\mathcal{I} : r \mapsto r^\#$$

is a continuous involution on $\mathscr{R}$.

(iii) *Assume that $\boldsymbol{u} \in \ell_{1,\mathbb{R}}$ and that $r_\pm$ are the reflection coefficients for the Schrödinger operator $H_{\boldsymbol{u}}$; then $\mathcal{I} r_\pm = r_\mp$.*

(iv) *For every $r \in \mathscr{R}$, the mapping $[0,1] \ni z \to (zr)^\# \in \mathscr{R}$ is real analytic.*

4.3. Transformation operators

The Jost solution $f_+(\,\cdot\,,\omega)$ can also be represented via the transformation operator. We shall need such a representation only for the values of f_+ at the lattice points $s \in \mathbb{Z}$. Using the Fourier series expansions (4.2) of a_s and b_s in (1.5), we see that

$$\begin{aligned} f_+(s+0,\omega) &= a_s(\omega)\mathrm{e}^{\mathrm{i}\omega s} + b_s(\omega)\mathrm{e}^{-\mathrm{i}\omega s} \\ &= \sum_{t\ge s} \mathrm{e}^{\mathrm{i}\omega t}\Big[\widehat{a}_s(t-s) + \widehat{b}_s(t+s)\Big]. \end{aligned}$$

For $s, t \in \mathbb{Z}$, we set

$$M_+(s,t) := \frac{\widehat{a}_s(t-s)}{\widehat{a}_s(0)} - \delta(s,t), \qquad M_-(s,t) := \frac{\widehat{b}_s(t+s)}{\widehat{a}_s(0)}, \tag{4.6}$$

$$K_\pm(s,t) := M_+(s,t) \pm M_-(s,t), \tag{4.7}$$

where $\delta(s,t)$ is the Kronecker delta. It then follows that, for all $\omega \in \mathbb{R}$ and $s \in \mathbb{Z}$,

$$f_+(s+0,\omega) = \widehat{a}_s(0)\Big(\mathrm{e}^{\mathrm{i}\omega s} + \sum_{t=s+1}^{\infty} K_+(s,t)\mathrm{e}^{\mathrm{i}\omega t}\Big). \tag{4.8}$$

Equalities (4.3) yield the crucial relation

$$M_-(s-1,s+1) = \tanh u_s, \qquad s \in \mathbb{Z}\,,$$

that allows one to uniquely reconstruct the numbers u_s from the kernel M_-. Observe that analogous procedure in the continuous case gives the value of u as the restriction of M_- on the diagonal, cf. (2.11).

Remark 4.5. The "genuine" transformation operator for $H_{\boldsymbol{u}}$ can be constructed in a similar manner. Using the unitary equivalence of $L_2(\mathbb{R})$ and $\ell_2(\mathbb{Z}) \otimes L_2(0,1)$, we can represent every function $g \in L_2(\mathbb{R})$ via the sequence $(g(n,y))_{n\in\mathbb{Z}}$ of its restrictions onto Δ_n, with $g(n,y) := g(n+y)$ for $n \in \mathbb{Z}$ and $y \in (0,1)$. For ease of notation, we shall write $g(n,\cdot)$ as g_n.

Substituting the Fourier series expansions for a_n and b_n in the expression for f at the point $s = n + y \in \Delta_n$, we get

$$\begin{aligned} f_n(y) &= \sum_{m\ge n} \widehat{a}_n(m-n)\mathrm{e}^{\mathrm{i}\omega(m+y)} + \sum_{m\ge n+2} \widehat{b}_n(m+n)\mathrm{e}^{\mathrm{i}\omega(m-y)} \\ &=: \widehat{a}_n(0)\Big[\mathrm{e}^{\mathrm{i}\omega(n+\cdot)} + \sum_{m>n} [A(n,m) + B(n,m)]\mathrm{e}^{\mathrm{i}\omega(m+\cdot)}\Big](y), \end{aligned}$$

where $A(n,m)$ and $B(n,m)$ are operators in $L_2(0,1)$ given by

$$A(n,m) = \frac{\widehat{a}_n(m-n)}{\widehat{a}_n(0)}I, \qquad B(n,m) = \frac{\widehat{b}_n(m+n+1)}{\widehat{a}_n(0)}T$$

and T is the reflection operator in $L_2(0,1)$ defined via $Tf(y) = f(1-y)$.

It turns out that the operator $\mathcal{K}$ in $L_2(\mathbb{R})$ given by

$$(\mathcal{K}g)_n = \widehat{a}_n(0)\Big[g_n + \sum_{m>n}(A(n,m)+B(n,m))g_m\Big]$$

is the transformation operator for $H_{\boldsymbol{u}}$. In other words, for every $g \in W_2^2(\mathbb{R})$, the function $\mathcal{K}g$ belongs to the domain of $H_{\boldsymbol{u}}$ and $H_{\boldsymbol{u}}\mathcal{K}g = -\mathcal{K}g''$. Indeed, the fact that the function $\mathcal{K}g$ belongs to W_2^2 outside the integer points and satisfies the interface conditions can be verified in a straightforward manner first for g of support contained in $(j-\frac{1}{2}, j+\frac{1}{2})$, for some $j \in \mathbb{Z}$ and then using the linearity. Finally, one can show that the operator $\mathcal{K}$ is boundedly invertible and performs similarity of the operators $H_{\boldsymbol{u}}$ and $H_{\mathbf{0}}$. We shall not need this fact in what follows.

4.4. Derivation of the Marchenko equation

The Marchenko equation relating the kernel of the transformation operator and the Fourier transform of the reflection coefficient can now be derived in a standard manner. The only difference is that, because r_+ is a periodic function and the kernel K is in a sense piece-wise constant, the discrete Fourier transform should be used.

Assume that $f_\pm$ are the Jost solution for the operator $H_{\boldsymbol{u}}$, with some $\boldsymbol{u} \in \ell_{1,\mathbb{R}}$, and that a, b, and $r = r_+$ are the corresponding scattering and reflection coefficients. Since a never vanishes on the real line, the relations (1.6) and (1.7) imply that

$$\frac{\mathrm{e}^{\mathrm{i}\omega x}f_-(x,\omega)}{a(\omega)} = \mathrm{e}^{\mathrm{i}\omega x}f_+(x,-\omega) + r(\omega)\mathrm{e}^{\mathrm{i}\omega x}f_+(x,\omega).$$

By (4.4), for every $x \in \mathbb{R}$ the function $\omega \mapsto \mathrm{e}^{\mathrm{i}\omega x}f_-(x,\omega)$ belongs to the algebra $W^+ := W \cap H^+$, and thus the same is true of the function

$$g(x,\omega) := \mathrm{e}^{\mathrm{i}\omega x}f_+(x,-\omega) + r(\omega)\mathrm{e}^{\mathrm{i}\omega x}f_+(x,\omega).$$

Set

$$R(s) := \widehat{r}(-s), \qquad s \in \mathbb{Z}; \tag{4.9}$$

then equality (4.8) for each $s \in \mathbb{Z}$ yields

$$\begin{aligned}\frac{g(s+0,\omega)}{\widehat{a}_s(0)} &= 1 + \sum_{t=s+1}^{\infty} K_+(s,t)\mathrm{e}^{-\mathrm{i}\omega(t-s)} + \sum_{n\in\mathbb{Z}} \widehat{r}(n)\mathrm{e}^{\mathrm{i}\omega(n+2s)} \\ &\quad + \sum_{\xi=s+1}^{\infty}\sum_{n\in\mathbb{Z}} \widehat{r}(n)K_+(s,\xi)\mathrm{e}^{\mathrm{i}\omega(\xi+s+n)} \\ &= 1 + \sum_{t\in\mathbb{Z}} L_+(s,t)\mathrm{e}^{-\mathrm{i}\omega(t-s)},\end{aligned}$$

where

$$L_+(s,t) := K_+(s,t) + R(s+t) + \sum_{\xi=s+1}^{\infty} K_+(s,\xi)R(\xi+t).$$

Recalling that $g(s+0,\,\cdot\,) \in W^+$, we derive the following discrete analogue of the Marchenko equation for all $s, t \in \mathbb{Z}$ with $s < t$:

$$K_+(s,t) + R(s+t) + \sum_{\xi=s+1}^{\infty} K_+(s,\xi)R(\xi+t) = 0. \tag{4.10}$$

4.5. Derivation of the Zakharov–Shabat system

It follows from the analysis of Subsection 4.2 that the sign change $\boldsymbol{u} \mapsto -\boldsymbol{u}$ does not affect the functions a_n, while b_n change to $-b_n$; as a result, we have $r_{\pm,-\boldsymbol{u}} = -r_{\pm,\boldsymbol{u}}$. Therefore the counterpart of (4.10) for K_- reads

$$K_-(s,t) - R(s+t) - \sum_{\xi=s+1}^{\infty} K_-(s,\xi)R(\xi+t) = 0. \tag{4.11}$$

Recalling the definition of the kernels M_+ and M_- in (4.6), one can recast the system (4.10)–(4.11) as

$$M_+(s,t) + \sum_{\xi=s+1}^{\infty} M_-(s,\xi)R(\xi+t) = 0, \tag{4.12}$$

$$M_-(s,t) + R(s+t) + \sum_{\xi=s+1}^{\infty} M_+(s,\xi)R(\xi+t) = 0 \tag{4.13}$$

for $s, t \in \mathbb{Z}$ and $s < t$, which is a discrete analogue of the Zakharov–Shabat system.

4.6. Solution of the Zakharov–Shabat system

Take now an arbitrary element r of $\mathscr{R}$; our aim is to show that it is the right reflection coefficient for a Schrödinger operator $H_{\boldsymbol{u}}$ with some real-valued sequence $\boldsymbol{u} \in \ell_1$. We shall do this by first solving the Zakharov–Shabat system with the sequence R defined via (4.9) and then determining $\boldsymbol{u}$ via (2.16).

The sequence $R(n)$ generates a continuous operator $\mathcal{R}$ in $\ell_2 := \ell_2(\mathbb{Z})$ via

$$(\mathcal{R}x)(s) := \sum_{t\in\mathbb{Z}} R(s+t)x(t). \tag{4.14}$$

Taking the (inverse) Fourier transform of (4.14), we see that

$$\|\mathcal{R}\| = \sup_{\omega\in\mathbb{R}} |r(\omega)| \le \|R\|_1,$$

where $\|R\|_1$ denotes the ℓ_1-norm of the sequence R. In particular, $\|\mathcal{R}\| < 1$; this inequality is used crucially to establish the unique solvability of the Zakharov–Shabat system. For $s \in \mathbb{Z}$, we denote by $\mathcal{P}_s$ an orthoprojector in ℓ_2 given by

$$(\mathcal{P}_s x)(t) := \begin{cases} x(t) & \text{if} \quad t > s, \\ 0 & \text{otherwise,} \end{cases}$$

and set $\mathcal{R}_s := \mathcal{P}_s\mathcal{R}\mathcal{P}_s$. Also, $\mathscr{X}$ shall stand for the set of all complex-valued functions on

$$\Omega := \{(s,t) \in \mathbb{Z}^2 \mid s < t\}$$

with

$$\|X\|_{\mathscr{X}}^2 := \sup_{s\in\mathbb{Z}} \sum_{t=s+1} |X(s,t)|^2$$

finite; the set $\mathscr{X}$ is a Banach space with respect to the norm $\|\cdot\|_{\mathscr{X}}$. Also, $\mathscr{X}_0$ stands for the subspace of $\mathscr{X}$ defined by

$$\mathscr{X}_0 := \{X \in \mathscr{X} \mid \lim_{s\to+\infty} \sum_{t>s} |X(s,t)|^2 = 0\}.$$

Then the following holds.

Theorem 4.6. *For every $r \in \mathscr{R}$, define $R \in \ell_1(\mathbb{Z})$ via $R(n) := \widehat{r}(-n)$. Then the Zakharov–Shabat system* (4.12)–(4.13) *has a unique solution (M_+, M_-) belonging to the space $\mathscr{X}_0 \times \mathscr{X}$. This solution is given by*

$$\begin{aligned} M_+(s,t) &= \langle (I-\mathcal{R}_s^2)^{-1}\mathcal{R}_s\mathcal{R}e_s, e_t\rangle,\\ M_-(s,t) &= -\langle (I-\mathcal{R}_s^2)^{-1}\mathcal{P}_s\mathcal{R}e_s, e_t\rangle, \end{aligned} \tag{4.15}$$

with $\langle\,\cdot\,,\,\cdot\,\rangle$ denoting the scalar product in ℓ_2 and (e_s) the standard orthonormal basis therein, and depends continuously in $\mathscr{X}_0 \times \mathscr{X}$ on $r \in \mathscr{R}$.

We shall also need a related uniqueness result stating that no two different $r \in \mathscr{R}$ can share the same solutions of the corresponding Zakharov–Shabat systems. This will be crucial in the inverse scattering problem of the next subsection.

Theorem 4.7. *Assume that $r_1, r_2 \in \mathscr{R}$ are such that the solutions $M_\pm$ of the related Zakharov–Shabat systems* (4.12)–(4.13) *coincide. Then $r_1 = r_2$.*

Proof. Denote by R_1 and R_2 the corresponding ℓ_1-sequences formed from the Fourier coefficients of r_1 and r_2 (namely, $R_j(n) := \widehat{r}_j(-n)$) and recall that K_+ is given by $K_+ = M_+ + M_-$. Set $R := R_1 - R_2$; then R satisfies the relations

$$R(s+t) + \sum_{\xi=s+1}^{\infty} K_+(s,\xi)R(\xi+t) = 0 \tag{4.16}$$

for all $s \in \mathbb{Z}$ and all $t > s$. Using properties of the kernel K_+ and (4.16), we shall show that

(i) there is $N \in \mathbb{Z}$ such that $R(n) = 0$ for all $n \geq N$;
(ii) the N above can be taken arbitrary;

which results in $R \equiv 0$.

For (i), it suffices to show existence of $s \in \mathbb{Z}$ such that

$$\sum_{\xi>s} |K_+(s,\xi)| < 1; \tag{4.17}$$

indeed, (4.16) yields the inequality

$$\max_{n>2s} |R(n)| \leq \max_{n>2s} |R(n)| \cdot \sum_{\xi>s} |K_+(s,\xi)|,$$

which by (4.17) forces that $R(n) = 0$ for all $n > 2s$. This is proved by using the explicit formulae (4.15) for solutions $M_\pm$ and the fact that $\sum_{t>s} |R_j(t)|$ tends to zero as $s \to +\infty$. Part (ii) is then established by induction. $\square$

4.7. The inverse scattering problem

Finally we show that every $r \in \mathscr{R}$ is a right reflection coefficient for a Schrödinger operator $H_{\boldsymbol{u}}$ corresponding to a unique sequence $\boldsymbol{u} = (u_j)_{j\in\mathbb{Z}} \in \ell_{1,\mathbb{R}}$. The considerations of the previous sections imply that such a $\boldsymbol{u}$ must verify the relation

$$\tanh u_j = M_-(j-1, j+1), \qquad j \in \mathbb{Z},$$

where the kernel M_- satisfies the Zakharov–Shabat system (4.12)–(4.13), in which $R(j) := \widehat{r}(-j)$.

This suggests the following reconstruction algorithm:

(1) given $r \in \mathscr{R}$, form the sequence $R = \big(R(n)\big) \in \ell_{1,\mathbb{R}}$ with $R(n) := \widehat{r}(-n)$;
(2) solve the Zakharov–Shabat system (4.12)–(4.13) with the given R to get $(M_+, M_-) \in \mathscr{X}_0 \times \mathscr{X}$ and form the sequence $\mathbf{v} := (v(j))$ with $v(j) := M_-(j-1, j+1)$ for $j \in \mathbb{Z}$;
(3) define $u_j \in \mathbb{R}$ via $\tanh u_j := v(j)$ and form $\boldsymbol{u} := (u_j)_{j\in\mathbb{Z}}$.

By Theorem 4.6 step (2) can always be performed, but $\boldsymbol{u}$ can only be defined if $\|\mathbf{v}\|_\infty < 1$. We shall prove this is the case and, moreover, that so-defined $\boldsymbol{u}$ belongs to ℓ_1. The final step is to show that the Schrödinger operator corresponding to this $\boldsymbol{u}$ has r we have started with as its right reflection coefficient.

We first start with r of small norm.

Lemma 4.8. *Assume that $r \in \mathscr{R}$ is such that $\|r\|_W \le \frac{1}{2}$; then the corresponding sequence $\mathbf{v}$ belongs to ℓ_1 and $\|\mathbf{v}\|_1 \le \frac{2}{3}$.*

This can be derived from the explicit formula (4.15) for the solution M_- of the Zakharov–Shabat system. Therefore $\boldsymbol{u}$ is well defined; we then consider the corresponding Schrödinger operator $H_{\boldsymbol{u}}$ and determine its right reflection coefficient $r_{\boldsymbol{u},+}$ and the corresponding kernels $M_{\boldsymbol{u},\pm}$. In fact, both $M_\pm$ and $M_{\boldsymbol{u},\pm}$ satisfy the discrete hyperbolic system with the same initial conditions determined by $\mathbf{v}$ and therefore coincide [10]. It follows that the sequence $R_{\boldsymbol{u}}(n) := \widehat{r}_{\boldsymbol{u},+}(-n)$ along with $R(n)$ verifies the Zakharov–Shabat system with the same $M_\pm$; by Theorem 4.7, $r_{\boldsymbol{u},+} = r$. This completes the solution of the inverse scattering problem in the case when $\|r\|_W < \frac{1}{2}$.

In a generic case, we first show that the sequence $\mathbf{v}$ belongs to ℓ_1 at $+\infty$. To this end we observe that, by (4.15), the values of $v(n)$ for $n > N$ only depend on $R(n)$ with $n > N$; choosing N so that $\sum_{n>N} |R(n)| < \frac{1}{2}$ and using the above reasonings yields the result.

At the second step we exploit the way $\boldsymbol{u}$ and $r_\pm$ behave under the reflection $x \mapsto -x$ to show that $\mathbf{v} \in \ell_1$. Namely, set $r^\# := \mathcal{I}r$, with the involution $\mathcal{I}$ defined in Lemma 4.4. Regarding r as a putative right reflection coefficient for the Schrödinger operator to be found, we conclude that $r^\#$ will then be its left reflection coefficient. If r were a genuine right reflection coefficient for some Schrödinger operator $H_{\boldsymbol{u}}$

and $\boldsymbol{u}^\# = u(n, r^\#)$ is the sequence constructed for $r^\#$ instead of r, then we would have the relation

$$u(n, r^\#) = -u(-n, r)$$

for all $n \in \mathbb{Z}$. In particular, this relation holds whenever the W-norm of r is sufficiently small. Using now the analytic dependence on a small parameter ε of the sequences $\boldsymbol{u}$ and $\mathbf{v}$ constructed from εr, we can establish the above equality for an arbitrary $r \in \mathscr{R}$. This shows that the sequence $\mathbf{v}$ constructed for every $r \in \mathscr{R}$ belongs to ℓ_1. The final step is to use the same analyticity to prove that $\|\mathbf{v}\|_\infty < 1$; see [10] for details.

Thus given any $r \in \mathscr{R}$, we can successfully perform the steps (i) to (iii) in the above reconstruction algorithm and to determine a real-valued sequence $\boldsymbol{u}$ in ℓ_1. The fact that the corresponding Schrödinger operator $H_{\boldsymbol{u}}$ has the right reflection coefficient equal to the r we have started from is again justified using the uniqueness result of Theorem 4.7. This completes the solution of the inverse scattering problem for the class of impedance Schrödinger operators under consideration.

4.8. Some generalizations

Most of the above considerations can be generalized for the situation where the discontinuity points x_k of the impedance function p do not form a periodic lattice. Assume that the set $\{x_k\}$ does not have finite accumulation points, that x_k are labelled in increasing order, and determine the sequence u_k from the relation

$$p(x) = \exp\Bigl\{ \sum_{k: x_k > x} u_k \Bigr\}.$$

Then under the assumption that the sequence (u_k) belongs to ℓ_1 we can define the scattering coefficients $a(\omega)$ and $b(\omega)$ as in Subsection 4.2. They are no longer elements of the Wiener algebra W; however, they are almost-periodic functions with absolutely summable Fourier series [15] and thus elements of a generalized Wiener-type algebra W_{ap}. The spectrum of an element in this algebra is the closure of its range over $\mathbb{R}$; thus we again get that a is invertible in W_{ap} and $r \in W_{ap}$.

Next, the function a belongs to the Hardy space H^+, and this opens the door to deriving an analogue of the Marchenko equation. It takes the form (4.10), where the variables s and t belong to the additive group Γ spanned by $\{x_j\}$ and the summation in ξ is over Γ as well.

Due to the condition $\|r\|_\infty < 1$, the corresponding Zakharov–Shabat system might be shown to possess a unique solution in $\ell_2(\Gamma)$. The difficult part of the inverse scattering problem is to find a replacement for the relation (2.16) and thus actually determine the sequence (u_k) and then justify that the corresponding Schrödinger operator $H_{\boldsymbol{u}}$ has the reflection coefficient r have started with. This will be discussed in a future work that is currently in progress.

Appendix

Let us denote by $\widehat{L^1}(\mathbb{R})$ the Wiener algebra of Fourier transforms (2.1) of functions in $L^1(\mathbb{R})$ with norm $\|\hat{f}\|_{\widehat{L^1}} := \|f\|_{L^1}$, and by $\widehat{X}$ the Banach algebra that is the image of $X = L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ under the Fourier transform, equipped with the norm $\|\hat{f}\|_{\widehat{X}} := \|f\|_X$. We also denote by $\mathbf{1} \dotplus \widehat{X}$ the unital extension of $\widehat{X}$ obtained by adding the constant functions and norming $1 \dotplus \widehat{X}$ with the norm

$$\|c + \hat{f}\|_{1 \dotplus \widehat{X}} = |c| + \|\hat{f}\|_{\widehat{X}};$$

we similarly define $1 \dotplus \widehat{L^1}(\mathbb{R})$. The Fourier transform extends to $1 \dotplus \widehat{X}$ by mapping the constant 1 into the convolution identity δ.

We will need the following results.

Lemma A.1. *Suppose that $f = \alpha + \widehat{h} \in 1 \dotplus \widehat{X}$. Then f is invertible in the Banach algebra $1 \dotplus \widehat{X}$ if and only if f is non-vanishing on $\mathbb{R}$ and $\alpha \neq 0$.*

Proof. If f is invertible in $1 \dotplus \widehat{X}$ it is also invertible in $1 \dotplus \widehat{L^1}(\mathbb{R})$, so the condition is necessary by the Wiener theorem. If, on the other hand, f does not vanish on $\mathbb{R}$ and $\alpha \neq 0$, then f is invertible in $1 \dotplus \widehat{L^1}(\mathbb{R})$ with $f^{-1} = \alpha^{-1} + \widehat{g}$ for $g \in L^1(\mathbb{R})$. We need to check that $g \in L^2(\mathbb{R})$. Without loss we take $\alpha = 1$ and compute that $\widehat{g} = -(1 + \widehat{h})^{-1}\widehat{h}$, which shows that $g \in L^2(\mathbb{R})$ as required. □

We now have an analogue of the Wiener–Levi theorem for $1 \dotplus \widehat{X}$.

Lemma A.2. *Assume that $f \in 1 \dotplus \widehat{X}$ and that ϕ is a function that is analytic in an open neighborhood Ω of the closure of the range of f. Then $\phi \circ f \in 1 \dotplus \widehat{X}$ and, moreover, the map*

$$f \mapsto \phi \circ f$$

is an analytic map from $1 \dotplus \widehat{X}$ into itself when restricted to functions with range contained in a fixed compact subset of Ω.

Proof. It suffices to note that, according to the above, the spectrum of f in $1 \dotplus \widehat{X}$ coincides with the closure of its range. Then the standard functional calculus for Banach algebras applies, thus yielding the result. □

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Finite and Infinite Gap Jacobi Matrices

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Abstract. The present paper reviews the theory of bounded Jacobi matrices whose essential spectrum is a finite gap set, and it explains how the theory can be extended to also cover a large number of infinite gap sets. Two of the central results are generalizations of Denisov–Rakhmanov's theorem and Szegő's theorem, including asymptotics of the associated orthogonal polynomials. When the essential spectrum is an interval, the natural limiting object J_0 has constant Jacobi parameters. As soon as gaps occur, ℓ say, the complexity increases and the role of J_0 is taken over by an ℓ-dimensional isospectral torus of periodic or almost periodic Jacobi matrices.

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1. Introduction

Let $d\mu$ be a probability measure on $\mathbb{R}$ with moments of all orders, that is,

$$\int_{\mathbb{R}} |x|^n d\mu(x) < \infty \text{ for all } n \geq 0. \tag{1.1}$$

When $d\mu$ is nontrivial (i.e., supp$(d\mu)$ is infinite), we can apply the Gram–Schmidt process to $1, x, x^2, \ldots$ and obtain a sequence $\{P_n\}_{n\geq 0}$ of orthonormal polynomials

$$\langle P_n, P_m \rangle := \int_{\mathbb{R}} P_n(x) P_m(x) d\mu(x) = \delta_{nm}, \tag{1.2}$$

where each P_n has positive leading coefficient and is of degree n. It is a basic fact that such polynomials satisfy a three-term recurrence relation of the form

$$xP_n(x) = a_{n+1}P_{n+1}(x) + b_{n+1}P_n(x) + a_nP_{n-1}(x), \quad n \geq 0 \tag{1.3}$$

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with $a_n = \langle P_{n-1}, xP_n\rangle > 0$ and $b_n = \langle P_{n-1}, xP_{n-1}\rangle \in \mathbb{R}$ for $n \geq 1$ (by convention, $P_{-1}(x) \equiv 0$). To see this, simply expand xP_n in terms of $P_0, P_1, \dots, P_{n+1}$ and use the orthogonality relation (1.2). Note also that

$$P_n(x) = \frac{1}{a_1 \cdots a_n}\Big(x^n - (b_1 + \cdots + b_n)x^{n-1} + \cdots\Big) \text{ for } n \geq 1. \tag{1.4}$$

The spectral theorem for orthonormal polynomials (also known as Favard's theorem) states that *for any pair of sequences* $\{a_n, b_n\}_{n=1}^{\infty} \in (0,\infty)^{\mathbb{N}} \times \mathbb{R}^{\mathbb{N}}$*, there exists a probability measure* $d\mu$ *on* $\mathbb{R}$ *such that the polynomials generated by* (1.3)*, with* $P_0(x) = 1$*, satisfy the orthogonality relation* (1.2). In general, this measure of orthogonality need not be unique. But when the recurrence coefficients are bounded, say $a_n, |b_n| \leq C$, then $d\mu$ is indeed unique and $\mathrm{supp}(d\mu)$ is contained in $[-3C, 3C]$. Conversely, if $d\mu$ has compact support, then the associated recurrence coefficients are bounded by

$$\max_{x \in \mathrm{supp}(d\mu)} |x| < \infty$$

and the polynomials are dense in $L^2(d\mu)$. We shall henceforth assume that $\mathrm{supp}(d\mu)$ is compact.

The three-term recurrence relation (1.3) links orthogonal polynomials to Jacobi matrices, that is, tridiagonal matrices of the form

$$J = \begin{pmatrix} b_1 & a_1 & & & \\ a_1 & b_2 & a_2 & & \\ & a_2 & b_3 & a_3 & \\ & & \ddots & \ddots & \ddots \end{pmatrix} \tag{1.5}$$

with $a_n > 0$ and $b_n \in \mathbb{R}$. In fact, the matrix J in (1.5) represents the operator of multiplication by the identity function x in the Hilbert space $L^2(d\mu)$ with respect to the orthonormal basis $\{P_n\}_{n\geq 0}$. When J is viewed as an operator on $\ell^2(\mathbb{N})$, its spectrum $\sigma(J)$ coincides with $\mathrm{supp}(d\mu)$ and we shall refer to $d\mu$ as the spectral measure of J.

In spectral theory for orthogonal polynomials, one studies the relation between nontrivial probability measures $d\mu$ satisfying (1.1) on one hand and pairs of sequences $\{a_n, b_n\}_{n=1}^{\infty} \in (0,\infty)^{\mathbb{N}} \times \mathbb{R}^{\mathbb{N}}$ on the other hand. The aim of the present paper is to give a general view of the situation where $d\mu$ is compactly supported and the recurrence coefficients (also known as Jacobi parameters) are bounded sequences. As already mentioned, there is a one-one correspondence between these two classes of objects and we shall focus on results that explain how qualitative features of the Jacobi parameters, say, are reflected in the measure of orthogonality, and vice versa.

Throughout, we shall write the probability measure $d\mu$ as

$$d\mu = f(x)dx + d\mu_{\mathrm{s}}, \tag{1.6}$$

with $d\mu_{\mathrm{s}}$ singular to dx. Rather than $\sigma(J)$, many of the results are more suitably formulated in terms of $\sigma_{\mathrm{ess}}(J)$, the essential spectrum of J. By definition,

$$\sigma_{\mathrm{ess}}(J) := \{x \in \sigma(J) \mid x \text{ is } \textit{not} \text{ an isolated eigenvalue of } J\}. \tag{1.7}$$

As regards proofs, in particular, a key role is played by the m-function (or Stieltjes transform of $d\mu$) defined by

$$m(z) := m_\mu(z) = \int \frac{d\mu(x)}{x-z}, \quad z \in \mathbb{C} \setminus \operatorname{supp}(d\mu). \tag{1.8}$$

This analytic function is known to be a Nevanlinna–Pick function (i.e., $\operatorname{Im} m(z) \gtrless 0$ for $\operatorname{Im} z \gtrless 0$) and we have

$$m(z) = -1/z + \mathcal{O}(z^{-2}) \tag{1.9}$$

near ∞. In fact, one can write down the Laurent expansion of m_μ around ∞ in terms of the moments of $d\mu$. More importantly, the boundary values $m(x+i0) := \lim_{\varepsilon\downarrow 0} m(x+i\varepsilon)$ exist for a.e. $x \in \mathbb{R}$ and

$$\frac{1}{\pi} \operatorname{Im} m_\mu(x+i\varepsilon)\, dt \xrightarrow{w} d\mu \text{ as } \varepsilon \downarrow 0. \tag{1.10}$$

To be even more specific,

$$f(x) = \frac{1}{\pi} \operatorname{Im} m_\mu(x+i0) \text{ a.e. on } \mathbb{R} \tag{1.11}$$

and

$$\mu_{\mathrm{s}}\big(\{x\}\big) = \lim_{\varepsilon\to 0} \varepsilon \operatorname{Im} m_\mu(x+i\varepsilon) \text{ for all } x \in \mathbb{R}. \tag{1.12}$$

So isolated mass points of $d\mu$ (or isolated eigenvalues of J) are poles of m.

The simplest compact subsets of $\mathbb{R}$ that have positive measure are intervals of the form $[\alpha, \beta]$ with $-\infty < \alpha < \beta < \infty$. In Section 2, we shall consider the situation when $\sigma_{\mathrm{ess}}(J)$ has this form and without loss of generality we may assume that $-\alpha = \beta = 2$. The associated Jacobi parameters are often – but not always – close to 1 and 0 as $n \to \infty$. Orthogonal polynomials on a compact interval are intimately related to Jacobi parameters that are asymptotically constant. As we shall see, the theory is well developed and many precise results are available.

In Section 3, we generalize our studies to finite gap sets $\mathfrak{e}$, that is, finite unions of closed intervals. When $\mathfrak{e}$ is the union of two or more disjoint intervals, the complement $\overline{\mathbb{C}} \setminus \mathfrak{e}$ is no longer simply connected. This is to be overcome by using the universal covering map. Perhaps more seriously, the structure of the Jacobi parameters changes. They are no longer asymptotically constant but rather asymptotically periodic or almost periodic. The natural limit point (viz., the free Jacobi matrix) also has to be replaced by an ℓ-dimensional torus, where ℓ counts the number of gaps in $\mathfrak{e}$.

Finally, in Section 4 we consider infinite gap sets of Parreau–Widom type. This notion of regular compact sets includes Cantor sets of positive measure, among others. The theory is less developed, but many results that hold for finite gap sets can be extended to the infinite gap setting.

2. Perturbations of the free Jacobi matrix

The most natural choice of Jacobi parameters is

$$a_n \equiv 1 \text{ and } b_n \equiv 0. \tag{2.1}$$

As is well known, the associated orthogonal polynomials are Chebyshev of the 2nd kind

$$U_n(x) = \frac{\sin(n+1)\theta}{\sin\theta}, \quad x = 2\cos\theta.$$

They are orthogonal on the interval $[-2,2]$ with respect to the semicircle law $f_0(x) = \sqrt{4-x^2}/2\pi$. We shall follow the standard terminology and refer to

$$J_0 = \begin{pmatrix} 0 & 1 & & & \\ 1 & 0 & 1 & & \\ & 1 & 0 & 1 & \\ & & \ddots & \ddots & \ddots \end{pmatrix} \tag{2.2}$$

as the free Jacobi matrix.

If $a_n \to 1$ and $b_n \to 0$, then $J = \{a_n, b_n\}_{n=1}^\infty$ is a compact perturbation of J_0 and hence $\sigma_{\mathrm{ess}}(J) = [-2,2]$ by Weyl's theorem. There may be points in $\mathrm{supp}(d\mu) \setminus [-2,2]$, but these are all isolated mass points that can only accumulate at ± 2. Moreover, a result of Nevai [14] states that the ratio $P_{n+1}(x)/P_n(x)$ has a limit for $x \notin \sigma(J)$.

The condition $\sigma_{\mathrm{ess}}(J) = [-2,2]$, on the other hand, is by itself not strong enough to imply $a_n \to 1$ and $b_n \to 0$ (see, e.g., [21, Section 1.4] for a counterexample). An extra condition is needed and for $d\mu$ as in (1.6), the Denisov–Rakhmanov theorem [9] states that *if* $\sigma_{\mathrm{ess}}(J) = [-2,2]$ *and* $f(x) > 0$ *a.e. on* $[-2,2]$*, then* $a_n \to 1$ *and* $b_n \to 0$. Denoting by J_n the n times stripped Jacobi matrix (i.e., the matrix obtained from J by removing the first n rows and columns), the above conclusion can also be formulates as $J_n \to J_0$ strongly.

The more detailed spectral analysis involves the rate of convergence of the Jacobi parameters. Of particular interest are the cases of Hilbert–Schmidt and trace-class perturbations of J_0. A deep result of Killip and Simon [12] classifies the spectral measures of all Jacobi matrices $J = \{a_n, b_n\}_{n=1}^\infty$ for which

$$\sum_{n=1}^{\infty} (a_n - 1)^2 + b_n^2 < \infty. \tag{2.3}$$

They all have

$$\mathrm{supp}(d\mu) = [-2,2] \cup \{x_k\},$$

where $\{x_k\}$ is a countable set of isolated mass points, possibly empty, and are precisely those probability measures of the form (1.6) that satisfy

$$\int_{-2}^{2} \log f(x) \sqrt{4-x^2}\, dx > -\infty \tag{2.4}$$

and

$$\sum_k \bigl(|x_k| - 2\bigr)^{3/2} < \infty. \tag{2.5}$$

The proof of Killip–Simon's theorem relies on sum rules, obtained from a factorization of the m-function. More precisely, one shows that

$$M(z) := -m(z + 1/z), \quad |z| < 1 \tag{2.6}$$

is a meromorphic Herglotz function and hence of the form $M = B \cdot O$, where B is an alternating Blaschke product and O an outer function (see [18] for details). The sum rules now result from computing the Taylor coefficients of $\log(M(z)/z)$ in two different ways.

Note that

$$\phi(z) := z + 1/z \tag{2.7}$$

is the unique conformal mapping of the unit disk $\mathbb{D}$ onto $\overline{\mathbb{C}}\backslash[-2,2]$ for which $\phi(0) = \infty$ and $\lim_{z\to 0} z\phi(z) = 1$. The use of ϕ in the theory of orthogonal polynomials goes back at least to Szegő.

Compared to (2.3), the a priori stronger condition

$$\sum_{n=1}^{\infty} |a_n - 1| + |b_n| < \infty \tag{2.8}$$

was conjectured by Nevai [13] and later proven by Killip and Simon [12] to imply the Szegő condition, that is,

$$\int_{-2}^{2} \frac{\log f(x)}{\sqrt{4 - x^2}} dx > -\infty. \tag{2.9}$$

In turn, (2.9) is closely related to

$$a_1 \cdots a_n \not\to 0 \tag{2.10}$$

and

$$\sum_k \bigl(|x_k| - 2\bigr)^{1/2} < \infty. \tag{2.11}$$

What is known as Szegő's theorem states that *if* (2.11) *holds, then* (2.9) *is equivalent to* (2.10). Moreover, (2.9)–(2.10) implies (2.11) so as formulated by Simon and Zlatoš [22], *any two imply the third*. In the setting of Szegő's theorem (i.e., when (2.9)–(2.11) hold), the product in (2.10) has a positive limit, (2.3) is satisfied, and both of the series

$$\sum_{n=1}^{\infty} (a_n - 1), \quad \sum_{n=1}^{\infty} b_n \tag{2.12}$$

are conditionally convergent. Furthermore, a result of Peherstorfer and Yuditskii [15] states that

$$z^n P_n(z + 1/z) \to \frac{B(z)D(z)}{1 - z^2} \tag{2.13}$$

uniformly on compact subsets of $\mathbb{D}$, where B is the Blaschke product

$$B(z) = \prod_k \frac{|z_k|}{z_k} \frac{z_k - z}{1 - z_k z}, \quad z_k = \frac{1}{2}\Big(x_k - \sqrt{x_k^2 - 4}\Big)$$

and D the outer function

$$D(z) = \exp\biggl\{ \int_0^{2\pi} \frac{e^{i\theta} + z}{e^{i\theta} - z} \log\biggl(\frac{|\sin\theta|}{\pi f(2\cos\theta)}\biggr) \frac{d\theta}{4\pi} \biggr\}.$$

This type of power asymptotic behavior is known as Szegő asymptotics. Note that since

$$U_n(z + 1/z) = \frac{z^{n+1} - z^{-n-1}}{z - z^{-1}} \sim \frac{z^{-n}}{1 - z^2},$$

we can replace z^n by $1/U_n(z + 1/z)$ on the left-hand side in (2.13) if the factor $1 - z^2$ on the right-hand side is removed too.

While the Szegő condition implies Szegő asymptotics, as has long been known, it is not a necessary condition. Examples for which (2.11) fails and yet the left-hand side of (2.13) has a limit are given by Damanik and Simon in [8]. More importantly, [8] proves that $z^n P_n(z + 1/z)$ has a limit for all $z \in \mathbb{D}$ if and only if (2.3) holds and the series in (2.12) are conditionally convergent. The right-hand side of (2.13), however, is only correct when (2.9) holds.

3. Finite gap Jacobi matrices

In this section, we shall consider Jacobi matrices $J = \{a_n, b_n\}_{n=1}^{\infty}$ for which $\sigma_{\mathrm{ess}}(J)$ is a finite gap set, that is, a set of the form

$$\mathfrak{e} = \bigcup_{j=1}^{\ell+1} [\alpha_j, \beta_j], \quad \alpha_1 < \beta_1 < \alpha_2 < \cdots < \beta_{\ell+1}. \tag{3.1}$$

Apart from a single interval, such a finite union of closed intervals is the simplest type of compact sets in $\mathbb{R}$ with positive measure (and no isolated points). Note that ℓ counts the number of gaps in $\mathfrak{e}$ and when $\ell \geq 1$, two questions arise:

- Is there a natural choice of J that can serve as a limit point, like J_0 did for the interval $[-2, 2]$?
- What replaces the conformal mapping ϕ in (2.7) when $\overline{\mathbb{C}} \setminus \mathfrak{e}$ is no longer simply connected?

The answer to the first question is negative. There is no single J that will take over the role of J_0. Even when $\mathfrak{e}$ only has one gap, say $\mathfrak{e} = [-2, -1] \cup [1, 2]$, there are several sequences of periodic Jacobi parameters with period 2 (i.e., $a_{n+2} = a_n$ and $b_{n+2} = b_n$ for all n) leading to the right spectrum, namely $\mathfrak{e}$. And it seems impossible to pick out one that should be more natural than all the others. In fact, the Denisov–Rakhmanov theorem is known to fail when $[-2, 2]$ is replaced by a finite gap set with at least one gap. The Jacobi parameters need not approach a single point. Rather, they approach a set which is topologically a circle (or a 1-dimensional torus) when $\ell = 1$.

For a general finite gap set $\mathfrak{e}$ as in (3.1), Simon [19,20] suggested to introduce the so-called isospectral torus $\mathcal{T}_{\mathfrak{e}}$ of dimension ℓ. The structure of this limiting object is carefully described in [4]. It consists of all Jacobi matrices whose m-function is a minimal Herglotz function on the two-sheeted Riemann surface $\mathcal{S}$ associated with $\mathfrak{e}$. Loosely speaking, one can think of $\mathcal{S}$ as two copies of $\mathbb{C} \setminus \mathfrak{e}$ glued together suitably. Alternatively, $\mathcal{T}_{\mathfrak{e}}$ is the collection of all two-sided Jacobi matrices $J = \{a_n, b_n\}_{n=-\infty}^{\infty}$ that have spectrum $\mathfrak{e}$ and are reflectionless on $\mathfrak{e}$ (see, e.g., [17, 23] for more details).

The isospectral torus is invariant under coefficient stripping, a very useful fact. If J' is a point on $\mathcal{T}_{\mathfrak{e}}$, then the Jacobi parameters $\{a'_n, b'_n\}_{n=1}^{\infty}$ are periodic or almost periodic sequences, depending on whether the intervals in $\mathfrak{e}$ all have rational harmonic measure (i.e., whether $\mu_{\mathfrak{e}}\big([\alpha_j, \beta_j]\big) \in \mathbb{Q}$ for all j, where $d\mu_{\mathfrak{e}}$ is the equilibrium measure of $\mathfrak{e}$). We say that $\mathfrak{e}$ is periodic if all $[\alpha_j, \beta_j]$ have rational harmonic measure. The spectral measure of J' is also very regular. It is purely absolutely continuous on $\mathfrak{e}$ with a density that satisfies the Szegő condition (see (3.3) below). Besides, it has at most one mass point in each of the ℓ gaps in $\mathfrak{e}$ and no other singular part. For later use, we pick $J^\sharp$ to be a suitable reference point on $\mathcal{T}_{\mathfrak{e}}$, namely a Jacobi matrix whose spectral measure has no singular part at all.

A remarkable result of Remling [17] generalizes the Denisov–Rakhmanov theorem to finite gap sets. It states that *if* $\sigma_{\mathrm{ess}}(J) = \mathfrak{e}$ *and* $f(x) > 0$ *a.e. on* $\mathfrak{e}$*, then the orbit of* J *under coefficient stripping approaches the isospectral torus* $\mathcal{T}_{\mathfrak{e}}$. The sequence of J_n's need not have a limit, but any of its accumulation points (essentially right limits) lie on $\mathcal{T}_{\mathfrak{e}}$. In order to ensure convergence to some point on the isospectral torus and not only the torus as a set, stronger assumptions on J are needed.

We say that a Jacobi matrix $J = \{a_n, b_n\}_{n=1}^{\infty}$ with spectral measure $d\mu$ of the form (1.6) belongs to the Szegő class for $\mathfrak{e}$ if

$$\mathrm{supp}(d\mu) = \mathfrak{e} \cup \{x_k\},$$

where $\{x_k\}$ is a countable set of isolated mass points satisfying the Blaschke condition

$$\sum_k \mathrm{dist}(x_k, \mathfrak{e})^{1/2} < \infty \tag{3.2}$$

and f obeys the Szegő condition

$$\int_{\mathfrak{e}} \frac{\log f(x)}{\mathrm{dist}(x, \mathbb{R} \setminus \mathfrak{e})^{1/2}} dx > -\infty. \tag{3.3}$$

It is proven in [5] that *when* (3.2) *holds,* (3.3) *is equivalent to*

$$\frac{a_1 \cdots a_n}{\mathrm{Cap}(\mathfrak{e})^n} \not\to 0. \tag{3.4}$$

In fact, just as for Szegő's theorem on $[-2,2]$, *any two of* (3.2)–(3.4) *imply the third.* While the sequence in (3.4) no longer has a limit, it turns out to be asymptotically periodic/almost periodic.

Another result of Christiansen, Simon, and Zinchenko [5] states that *if J belongs to the Szegő class for $\mathfrak{e}$, there is a unique point $J' \in \mathcal{T}_{\mathfrak{e}}$ so that*

$$|a_n - a_n'| + |b_n - b_n'| \to 0. \tag{3.5}$$

Equivalently, this means that $J_n - J_n' \to 0$ strongly (i.e., the orbit of J under coefficient stripping approaches the orbit of J' on $\mathcal{T}_{\mathfrak{e}}$). To explain which point on the torus to pick and to make a statement about the asymptotics of P_n, we first need to answer the second question.

In short, the role of ϕ is taken over by the universal covering map of $\mathbb{D}$ onto $\Omega := \overline{\mathbb{C}} \setminus \mathfrak{e}$. This is the standard tool for 'lifting' functions on multiply connected domains to the unit disk. The universal covering map $\psi : \mathbb{D} \to \Omega$ is only locally one-to-one and each point in Ω has infinitely many preimages in $\mathbb{D}$. These are related to one another through a Fuchsian group Γ of Möbius transformations,

$$\psi(z) = \psi(w) \iff \exists \gamma \in \Gamma : \ z = \gamma(w).$$

We fix ψ uniquely by also requiring that $\psi(0) = \infty$ and $\lim_{z\to 0} z\psi(z) > 0$. Γ is isomorphic to the fundamental group $\pi_1(\Omega)$ and hence a free group on ℓ generators, say $\gamma_1, \ldots, \gamma_\ell$.

To get a better picture of Γ, we introduce the open set

$$\mathbb{F} := \big\{ z \in \mathbb{D} : |\gamma'(z)| < 1 \text{ for all } \gamma \neq \mathrm{id} \big\}. \tag{3.6}$$

This is a fundamental domain for Γ, that is, no two points of $\mathbb{F}$ are equivalent under Γ and $\overline{\mathbb{F}}$ contains at least one point from each Γ-orbit. Geometrically, $\mathbb{F}$ is symmetric in the real line and consists of the unit disk with 2ℓ orthocircles (and their interior) removed. The circular arcs in the upper (or lower) half-disk, say $C_1, \ldots, C_\ell$, are in one-one correspondence with the gaps in $\mathfrak{e}$ under the covering map ψ. In fact, one can take the generator γ_j to be reflection in C_j following complex conjugation.

The multiplicative group of characters on Γ, denoted Γ^*, turns out to play an important role. Since an element in Γ^* is determined from its values on the generators of Γ, we can think of Γ^* as an ℓ-dimensional torus. The point is that $\mathcal{T}_{\mathfrak{e}}$ and Γ^* are homeomorphic. To get hold of a homeomorphism between these two ℓ-dimensional tori, we first introduce the Jost function of an element in the Szegő class. Let $d\mu^\sharp = f^\sharp(x)dx$ be the spectral measure of $J^\sharp$, our reference point on $\mathcal{T}_{\mathfrak{e}}$. For J in the Szegő class of $\mathfrak{e}$, we define its Jost function by

$$u(z; J) = \prod_k B(z, z_k) \exp\left\{ \int_0^{2\pi} \frac{e^{i\theta} + z}{e^{i\theta} - z} \log\left(\frac{f^\sharp(\psi(e^{i\theta}))}{f(\psi(e^{i\theta}))} \right) \frac{d\theta}{4\pi} \right\}, \quad z \in \mathbb{D} \tag{3.7}$$

where $\{z_k\}$ are the unique points in $\overline{\mathbb{F}}$ with $\mathrm{Im}\, z_k \geq 0$ and $\psi(z_k) = x_k$. This analytic function turns out to be character automorphic, that is, there exists $\chi_{{}_J} \in \Gamma^*$ such that

$$u(\gamma(\cdot); J) = \chi_{_J}(\gamma) u(\,\cdot\,; J) \text{ for all } \gamma \in \Gamma. \tag{3.8}$$

Most importantly, the map

$$\mathcal{T}_{\mathfrak{e}} \ni J \longrightarrow \chi_{_J} \in \Gamma^*, \tag{3.9}$$

essentially the Abel map, is a homeomorphism (see, e.g., [4] for details).

We are now able to explain which point J' on $\mathcal{T}_{\mathfrak{e}}$ is the right one for (3.5) to hold: *Take the unique point for which* $\chi_{_{J'}} = \chi_{_J}$. This fact is proven in [5] by use of Remling's theorem, the homeomorphism (3.9), and a technical lemma stating that strong convergence to a point on the torus implies convergence of the associated characters. We repeat the proof here as it merely takes a few lines.

For contradiction, suppose that

$$|a_n - a_n'| + |b_n - b_n'| \not\to 0.$$

Then there is a subsequence $\{n_k\}$ so that J and J' have different right limits, say $K \neq K'$. Due to Remling's theorem, both K and K' lie on $\mathcal{T}_{\mathfrak{e}}$, and we have

$$\chi_{_{J_{n_k}}} \longrightarrow \chi_{_K} \text{ and } \chi_{_{J'_{n_k}}} \longrightarrow \chi_{_{K'}}$$

since $J_{n_k} \to K$ and $J'_{n_k} \to K'$ strongly. As $\chi_{_J} = \chi_{_{J'}}$, we also have $\chi_{_{J_n}} = \chi_{_{J'_n}}$ so that $\chi_{_K} = \chi_{_{K'}}$. This contradicts the fact that $K \neq K'$.

The Jost function also enters the picture in connection with the asymptotic behavior of P_n. With P_n' the orthonormal polynomials associated with J' (not to be confused with the derivative), we have

$$\frac{P_n(\psi(z))}{P_n'(\psi(z))} \longrightarrow \frac{u(z; J)}{u(z; J')} \tag{3.10}$$

uniformly on compact subsets of $\mathbb{F}$, the fundamental domain for Γ. This result should be compared with (2.13) and the fact that $u(z; J_0) = 1$.

Along the lines of [8], Christiansen, Simon, and Zinchenko [6] set out to find weaker assumptions than the Szegő condition that still imply Szegő asymptotics (in the sense that the left-hand side of (3.10) has a limit). At first sight, it may look like

$$\sum_{n=1}^{\infty} (a_n - a_n')^2 + (b_n - b_n')^2 < \infty \tag{3.11}$$

and conditional convergence of

$$\sum_{n=1}^{\infty} (a_n - a_n'), \quad \sum_{n=1}^{\infty} (b_n - b_n') \tag{3.12}$$

will be sufficient. But a more careful analysis shows that the periodicity/almost periodicity has to be taken into account and one needs to replace the conditional convergence with a more involved set of assumptions involving the harmonic measures $\mu_{\mathfrak{e}}([\alpha_j, \beta_j])$ for all j. The reader is referred to [6] for more details.

The generalized Nevai conjecture has recently been proved in the finite gap setting by Frank and Simon [10]. They answer in the affirmative that *if* $J = \{a_n, b_n\}_{n=1}^{\infty}$ *is a Jacobi matrix with spectral measure* $d\mu$ *of the form* (1.6) *and*

$$\sum_{n=1}^{\infty} |a_n - a_n'| + |b_n - b_n'| < \infty \tag{3.13}$$

for some point J' *on* $\mathcal{T}_{\mathfrak{e}}$, *then the Szegő condition* (3.3) *holds.* Hence there is some understanding of ℓ^1-convergence to $\mathcal{T}_{\mathfrak{e}}$. Among other things, [10] relies on an improved Birman–Schwinger bound in the gaps of $\mathfrak{e}$.

The situation of ℓ^2-convergence to $\mathcal{T}_{\mathfrak{e}}$, on the other hand, is much less understood. Whether or not the Killip–Simon theorem can be proved for all finite gap sets is still an open question. That it is true when $\mathfrak{e}$ is periodic has proven by Damanik, Killip, and Simon [7]. The ingenious idea of [7] is to handle the periodic case by use of matrix orthogonal polynomials. But this method only applies to periodic $\mathfrak{e}$. The proof of Killip–Simon's theorem for $[-2, 2]$ relies among other things on the explicit form of ϕ. The universal covering map, in turn, is much more complicated. Even if one succeeds in finding ψ explicitly, the expression at hand will still be too difficult to work with. New insight is needed to really understand the concept of ℓ^2-convergence to the isospectral torus.

4. Infinite gap Jacobi matrices

Every compact set $\ \subset \mathbb{R}$ can be written in the form

$$\ = [\alpha, \beta] \setminus \bigcup\nolimits_j (\alpha_j, \beta_j), \tag{4.1}$$

where $\cup_j$ is a countable union of disjoint open subintervals of $[\alpha, \beta]$. We shall refer to (α_j, β_j) as a 'gap' in   and now mainly focus on the situation of infinitely many gaps. In order to develop the theory, a few restrictions have to be put on . But among others, there will still be room for Cantor sets of positive measure.

First of all, we shall always assume that $|\ \ | > 0$ to allow for an absolutely continuous part of $d\mu$. This in particular implies that the logarithmic capacity of , denoted Cap( ), is positive so that the domain $\Omega = \overline{\mathbb{C}} \setminus\ $ has a Green's function. We denote by g the Green's function for Ω with pole at ∞. This function is known to be positive and harmonic on Ω, and

$$g(z) = \log|z| + \gamma(\ \ ) + o(1)$$

near ∞, where $e^{-\gamma(\ )} = \mathrm{Cap}(\ )$.

To avoid dealing with isolated points in the essential spectrum, we assume that   is regular, that is,

$$\lim_{\Omega \ni z \to x} g(z) = 0 \ \text{ for all } x \in\ \ . \tag{4.2}$$

Hence g has precisely one critical point in each gap of . Denoting by c_j the critical point in (α_j, β_j), we impose the so-called Parreau–Widom condition,

$$\sum\nolimits_j g(c_j) < \infty. \tag{4.3}$$

While Widom was interested in Riemann surfaces with sufficiently many analytic functions, the notion becomes useful to us as the equilibrium measure $d\mu$ of   turns out to be absolutely continuous (see, e.g., [2] for a detailed proof). Moreover, the m-function for measures supported on   is of bounded characteristic when lifted to $\mathbb{D}$.

The Parreau–Widom condition (4.3) is known to be satisfied for compact sets that are homogeneous in the sense of Carleson [1]. By definition, this means there is an $\varepsilon > 0$ such that

$$\frac{|(x-\delta, x+\delta) \cap \quad|}{\delta} \geq \varepsilon \text{ for all } x \in \quad \text{ and all } \delta < \operatorname{diam}(\quad). \tag{4.4}$$

Carleson introduced this geometric condition to avoid the possibility of certain parts of   to be very thin, compared to Lebesgue measure. To get an explicit example of an infinite gap set which is homogeneous, remove the middle $1/4$ from the interval $[0,1]$ and continue removing subintervals of length $1/4^n$ from the middle of each of the 2^{n-1} remaining intervals. The set   of what is left in $[0,1]$ is a Cantor set of length $1/2$, and the reader may check that $|(x-\delta, x+\delta) \cap \quad| \geq \delta/4$ for all $x \in$ and all $\delta < 1$.

Just as in the finite gap setting, we can make use of the covering space formalism. In fact, the seminal paper [23] of Sodin and Yuditskii deals with infinite gap sets of Parreau–Widom type. Let $J = \{a_n, b_n\}_{n=1}^{\infty}$ be a Jacobi matrix with $\sigma_{\text{ess}}(J) =$ and spectral measure $d\mu$ of the form (1.6). Denote by $\{x_k\}$ the possible mass points of $d\mu$ outside . We say that $d\mu$ (or J) satisfies the Szegő condition if

$$\int \log f(x)\, d\mu \;\, (x) > -\infty. \tag{4.5}$$

As follows at once when recalling the explicit form of $d\mu_{\mathfrak{e}}$ (see, e.g., [21, Chap. 5]), this is the natural way of generalizing (3.3). On condition that

$$\sum\nolimits_k g(x_k) < \infty, \tag{4.6}$$

Sodin and Yuditskii [23] showed that $M := m \circ \psi$ is of bounded characteristic on $\mathbb{D}$ and without a singular inner part. Hence it admits a factorization of the form

$$M(z) = B_\infty(z) \exp\left\{ \int_0^{2\pi} \frac{e^{i\theta}+z}{e^{i\theta}-z} \log\bigl|M(e^{i\theta})\bigr| \frac{d\theta}{2\pi} \right\} \tag{4.7}$$

with B_∞ the Blaschke product of zeros and poles, and this paves the way for step-by-step sum rules. Comparing the constant terms in (4.7) and iterating n times lead to

$$\log\left(\frac{a_1 \cdots a_n}{\operatorname{Cap}(\quad)^n}\right) = \sum_k \bigl(g(x_k) - g(x_{n,k})\bigr) + \frac{1}{2} \int \log\left(\frac{f(t)}{f_n(t)}\right) d\mu \;\, (t), \tag{4.8}$$

where $\{x_{n,k}\}$ are the eigenvalues of J_n outside and f_n is the absolutely continuous part of its spectral measure. Interpreting the integral on the right-hand side in terms of relative entropies, one can show that *the Szegő condition is equivalent to*

$$\frac{a_1 \cdots a_n}{\mathrm{Cap}(\ )^n} \not\to 0 \tag{4.9}$$

provided that (4.6) *holds.* The details are given in [2] and the proof also shows that the sequence in (4.9) is bounded above and below. While one direction is straightforward using (4.8), the other involves some cutting and pasting in the Jacobi matrix before applying (4.8).

For general Parreau–Widom sets, the isospectral torus $\mathcal{T}$ will be infinite dimensional and we equip it with the product topology. It is known that Remling's theorem generalizes and one can ask if elements in the Szegő class still approach a point on $\mathcal{T}$ and not only the isospectral torus as a set. Provided the Abel map remains a homeomorphism, the same proof as in Section 3 should work. For this to hold, an extra condition on turns out to be needed. The so-called direct Cauchy theorem has to be valid (see [24], [11]). These and related issues are treated in the upcoming paper [3]. A recent article of Yuditskii [25] points out that Parreau–Widom sets for which the direct Cauchy theorem holds are still more general than homogeneous sets. Asymptotics of orthogonal polynomials on homogeneous sets were treated by Peherstorfer and Yudiskii in [16].

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Derivation of Ginzburg-Landau Theory for a One-dimensional System with Contact Interaction

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Abstract. In a recent paper [7] we give the first rigorous derivation of the celebrated Ginzburg-Landau (GL) theory, starting from the microscopic Bardeen-Cooper-Schrieffer (BCS) model. Here we present our results in the simplified case of a one-dimensional system of particles interacting via a δ-potential.

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1. Introduction and main results

1.1. Introduction

In 1950 Ginzburg and Landau [1] presented the first satisfactory mathematical description of the phenomenon of superconductivity. Their model examined the *macroscopic* properties of a superconductor in a phenomenological way, without explaining its microscopic mechanism. In the GL theory the superconducting state is represented by a complex order parameter $\psi(x)$, which is zero in the normal state and non-zero in the superconducting state. The order parameter $\psi(x)$ can be considered as a macroscopic wave-function whose square $|\psi(x)|^2$ is proportional to the density of superconducting particles.

In 1957 Bardeen, Cooper and Schrieffer [2] formulated the first *microscopic* explanation of superconductivity starting from a first principle Hamiltonian. In a major breakthrough they realized that this phenomenon can be described by the *pairing-mechanism*. The superconducting state forms due to an instability of the normal state in the presence of an attraction between the particles. In the case of a metal the attraction is made possible by an interaction through the lattice. For other systems, like superfluid cold gases, the interaction is of local type. In the BCS theory the superconducting state, which is made up by pairs of particles of opposite spin, the *Cooper-pairs*, is described by a two-particle wave-function $\alpha(x, y)$.

A connection between the two approaches, the phenomenological GL theory and the microscopic BCS theory, was made by Gorkov [3] who showed that, close to the critical temperature, the order parameter $\psi(x)$ and the pair-wavefunction $\alpha(x, y)$ are proportional. A simpler argument was later given by de Gennes [4].

Recently we presented in [7] a mathematical proof of the equivalence of the two models, GL and BCS, in the limit when the temperature T is close to the critical temperature T_c, i.e., when $h = [(T_c - T)/T_c]^{1/2} \ll 1$, where T_c is the critical temperature for the translation-invariant BCS equation. The mathematical aspects of this equation where studied in detail in [8, 6, 9, 10, 11]. In the present paper we present this result in the simplified case a of one-dimensional system where the particles interact via an attractive contact interaction potential of the form

$$V(x-y) = -a\delta(x-y) \quad \text{with } a > 0\,. \tag{1.1}$$

We assume that the system is subject to a weak external potential W, which varies on a large scale $1/h$ compared to the microscopic scale of order 1. Since variations of the system on the macroscopic scale cause a change in energy of the order h^2, we assume that the external potential W is also of the order h^2. Hence we write it as $h^2 W(hx)$, with x being the microscopic variable. The parameter h will play the role of a semiclassical parameter.

We will prove that, to leading order in h, the Cooper pair wave function $\alpha(x, y)$ and the GL function $\psi(x)$ are related by

$$\alpha(x,y) = \psi\left(h\frac{x+y}{2}\right)\alpha^0(x-y) \tag{1.2}$$

where α^0 is the translation invariant minimizer of the BCS functional. In particular, the argument $\bar{x}$ of the order parameter $\psi(\bar{x})$ describes the *center-of-mass* motion of the BCS state, which varies on the macroscopic scale. To be precise, we shall prove that $\alpha(x, y) = \frac{1}{2}(\psi(hx) + \psi(hy))\alpha^0(x - y)$ to leading order in h, which agrees with (1.2) to this order.

For simplicity we restrict our attention to contact potentials of the form (1.1), but our method can be generalized to other kinds of interactions; see [7] for details. The proof presented here is simpler than the general proof in [7] which applies to any dimension $d \leq 3$. There are several reasons for this. First, there is no magnetic field in one dimension. Second, for a contact interaction the translation invariant problem is particularly simple and the corresponding gap equation has an explicit solution. Finally, several estimates are simpler in one dimension due the boundedness of the Green's function for the Laplacian.

1.2. The BCS functional

We consider a macroscopic sample of a fermionic system, in one spatial dimension. Let $\mu \in \mathbb{R}$ denote the chemical potential and $T > 0$ the temperature of the sample.

The fermions interact through the attractive two-body potential given in (1.1). In addition, they are subject to an external force, represented by a potential $W(x)$.

In BCS theory the state of the system can be conveniently described in terms of a 2×2 operator-valued matrix

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \bar{\alpha} & 1-\bar{\gamma} \end{pmatrix}$$

satisfying $0 \leq \Gamma \leq 1$ as an operator on $L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$. The bar denotes complex conjugation, i.e., $\bar{\alpha}$ has the integral kernel $\overline{\alpha(x,y)}$. In particular, Γ is assumed to be hermitian, which implies that γ is hermitian and α is symmetric (i.e., $\gamma(x,y) = \overline{\gamma(y,x)}$ and $\alpha(x,y) = \alpha(y,x)$.) There are no spin variables in Γ. The full, spin dependent Cooper pair wave function is the product of α with an antisymmetric spin singlet.

We are interested in the effect of weak and slowly varying external fields, described by a potential $h^2W(hx)$. In order to avoid having to introduce boundary conditions, we assume that the system is infinite and periodic with period h^{-1}. In particular, W should be periodic. We also assume that the state Γ is periodic. The aim then is to calculate the free energy per unit volume.

We find it convenient to do a rescaling and use macroscopic variables instead of the microscopic ones. In macroscopic variables, the BCS functional has the form

$$\mathcal{F}^{\mathrm{BCS}}(\Gamma) := \mathrm{Tr}\left(-h^2\nabla^2 - \mu + h^2W(x)\right)\gamma - T\,S(\Gamma) - ah\int_{\mathcal{C}} |\alpha(x,x)|^2\,dx \tag{1.3}$$

where $\mathcal{C}$ denotes the unit interval $[0,1]$. The entropy equals $S(\Gamma) = -\mathrm{Tr}\,\Gamma\ln\Gamma$. The BCS state of the system is a minimizer of this functional over all admissible Γ.

The symbol Tr in (1.3) stands for the trace per unit volume. More precisely, if B is a periodic operator (meaning that it commutes with translation by 1), then $\mathrm{Tr}\,B$ equals, by definition, the (usual) trace of χB, with χ the characteristic function of $\mathcal{C}$. The location of the interval is obviously of no importance. It is not difficult to see that the trace per unit volume has the usual properties like cyclicity, and standard inequalities like Hölder's inequality hold. This is discussed in more detail in [7].

Assumption 1.1. *We assume that W is a bounded, periodic function with period* 1 *and* $\int_{\mathcal{C}} W(x)\,dx = 0$.

1.2.1. The translation-invariant case. In the translation-invariant case $W = 0$ one can restrict $\mathcal{F}^{\mathrm{BCS}}$ to translation-invariant states. We write a general translation-invariant state in form of the 2×2 matrix

$$\Gamma = \begin{pmatrix} \tilde{\gamma}(-ih\nabla) & \tilde{\alpha}(-ih\nabla) \\ \overline{\tilde{\alpha}(-ih\nabla)} & 1-\overline{\tilde{\gamma}(-ih\nabla)} \end{pmatrix}, \tag{1.4}$$

that is, $\gamma = [\Gamma]_{11}$ and $\alpha = [\Gamma]_{12}$ have integral kernels

$$\gamma(x,y) = \frac{1}{2\pi}\int_{\mathbb{R}} \tilde{\gamma}(hp)e^{ip(x-y)}\,dp \quad \text{and} \quad \alpha(x,y) = \frac{1}{2\pi}\int_{\mathbb{R}} \tilde{\alpha}(hp)e^{ip(x-y)}\,dp\,.$$

The fact that Γ is admissible means that $\tilde\alpha(p) = \overline{\tilde\alpha(-p)}$, that $0 \le \tilde\gamma(p) \le 1$ and $|\tilde\alpha(p)|^2 \le \tilde\gamma(p)(1-\tilde\gamma(-p))$ for any $p \in \mathbb{R}$. For states of this form the BCS functional becomes

$$\mathcal{F}^{\rm BCS}(\Gamma) = \int_{\mathbb{R}} (h^2p^2-\mu)\tilde\gamma(hp)\,\frac{dp}{2\pi} - T\int_{\mathbb{R}} S(\tilde\Gamma(hp))\frac{dp}{2\pi} - ah\left|\int_{\mathbb{R}} \tilde\alpha(hp)\frac{dp}{2\pi}\right|^2 , \quad (1.5)$$

with $S(\tilde\Gamma(p)) = -\operatorname{Tr}_{\mathbb{C}^2}\tilde\Gamma(p)\ln\tilde\Gamma(p)$ and $\tilde\Gamma(p)$ the 2×2 matrix obtained by replacing $-i\nabla$ by p in (1.4).

In the following, we are going to summarize some well-known facts about the translation-invariant functional (1.5). For given $a > 0$, we define the critical temperature $T_c > 0$ by the equation

$$\frac{1}{a} = \int_{\mathbb{R}} \frac{\tanh\left(\frac{p^2-\mu}{2T_c}\right)}{p^2-\mu}\frac{dp}{2\pi}\,. \quad (1.6)$$

This is the form in which the gap-equation is usually presented in the physics literature, see, e.g., [13, 4]. The fact that there is a unique solution to this equation follows from the strict monotonicity of $t/\tanh t$ for $t>0$. If $T \ge T_c$, then the minimizer of (1.5) satisfies $\tilde\alpha \equiv 0$ and $\tilde\gamma(hp) = (1+\exp((h^2p^2-\mu)/T))^{-1}$. If $0<T<T_c$, on the other hand, then there is a unique solution $\Delta_0 > 0$ of the *BCS gap equation*

$$\frac{1}{a} = \int_{\mathbb{R}} \frac{1}{K_T^0(p)}\frac{dp}{2\pi}\,, \quad (1.7)$$

where

$$K_T^0(p) = \frac{\sqrt{(p^2-\mu)^2+\Delta_0^2}}{\tanh\left(\frac{1}{2T}\sqrt{(p^2-\mu)^2+\Delta_0^2}\right)}\,. \quad (1.8)$$

Moreover, the minimizer of (1.5) is given by

$$\tilde\Gamma^0(hp) = \left(1+\exp\left(\tfrac{1}{T}H^0_{\Delta_0}(hp)\right)\right)^{-1} \quad (1.9)$$

with

$$H^0_{\Delta_0}(p) = \begin{pmatrix} p^2-\mu & -\Delta_0 \\ -\Delta_0 & -p^2+\mu \end{pmatrix}.$$

Writing $\tilde\alpha^0(hp) = [\tilde\Gamma^0(hp)]_{12}$ one easily deduces from (1.9) that

$$\tilde\alpha^0(p) = \frac{\Delta_0}{2K_T^0(p)}\,. \quad (1.10)$$

To summarize, in the case $W\equiv 0$ the functional $\mathcal{F}^{\rm BCS}$ has a minimizer Γ^0 for $0<T<T_c$ whose off-diagonal element does not vanish and has the integral kernel

$$\alpha^0((x-y)/h) = \frac{\Delta_0}{2}\int_{\mathbb{R}} \frac{1}{K_T^0(hp)}e^{ip(x-y)}\,\frac{dp}{2\pi}\,. \quad (1.11)$$

We emphasize that the function α^0 depends on T. For T close to T_c, which is the case of interest, we have $\Delta_0 \sim \mathrm{const}(1-T/T_c)^{1/2}$.

1.3. The GL functional

Let ψ be a periodic function in $H^1_{\mathrm{loc}}(\mathbb{R})$. For numbers $b_1, b_3 > 0$ and $b_2 \in \mathbb{R}$ the Ginzburg-Landau (GL) functional is given by

$$\mathcal{E}(\psi) = \int_{\mathcal{C}} \left(b_1 |\psi'(x)|^2 + b_2 W(x) |\psi(x)|^2 + b_3 \left(1 - |\psi(x)|^2\right)^2 \right) dx \,. \tag{1.12}$$

We denote its ground state energy by

$$E^{\mathrm{GL}} = \inf\{\mathcal{E}(\psi) \,|\, \psi \in H^1_{\mathrm{per}}\} \,.$$

Under our assumptions on W it is not difficult to show that there is a corresponding minimizer, which satisfies a second-order differential equation known as the GL equation.

1.4. Main results

Recall the definition of the BCS functional $\mathcal{F}^{\mathrm{BCS}}$ in (1.3). We define the energy $F^{\mathrm{BCS}}(T, \mu)$ as the difference between the infimum of $\mathcal{F}^{\mathrm{BCS}}$ over all admissible Γ and the free energy of the normal state

$$\Gamma_0 := \begin{pmatrix} \gamma_0 & 0 \\ 0 & 1 - \bar{\gamma}_0 \end{pmatrix} \tag{1.13}$$

with $\gamma_0 = (1 + e^{(-h^2\nabla^2 + h^2 W(x) - \mu)/T})^{-1}$. That is,

$$F^{\mathrm{BCS}}(T, \mu) = \inf_{\Gamma} \mathcal{F}^{\mathrm{BCS}}(\Gamma) - \mathcal{F}^{\mathrm{BCS}}(\Gamma_0) \,. \tag{1.14}$$

Note that

$$\mathcal{F}^{\mathrm{BCS}}(\Gamma_0) = -T \,\operatorname{Tr} \ln \left(1 + \exp\left(-\left(-h^2\nabla^2 - \mu + h^2 W(x)\right)\right)/T\right) \,. \tag{1.15}$$

For small h this behaves like an (explicit) constant times h^{-1}. Under further regularity assumptions on W, (1.15) can be expanded in powers of h. We do not need this, however, since we are only interested in the difference $F^{\mathrm{BCS}}(T, \mu)$.

Since Γ_0 is an admissible state, one always has $F^{\mathrm{BCS}}(T, \mu) \leq 0$. If the strict inequality $F^{\mathrm{BCS}}(T, \mu) < 0$ holds, then the system is said to be in a superconducting (or superfluid, depending on the physical interpretation) state.

Theorem 1.2. *Let Assumption* 1.1 *be satisfied, and let $T_c > 0$ be the critical temperature in the translation invariant case, defined in* (1.6). *Let $D > 0$. Then there are coefficients b_1, b_2 and b_3, given explicitly in* (1.20)–(1.22) *below, such that*

$$F^{\mathrm{BCS}}(T_c(1 - Dh^2), \mu) = h^3 \left(E^{\mathrm{GL}} - b_3\right) + o(h^3) \tag{1.16}$$

as $h \to 0$. More precisely, the error term $o(h^3)$ satisfies

$$-\operatorname{const} h^{3+\frac{1}{3}} \leq o(h^3) \leq \operatorname{const} h^5 \,.$$

Moreover, if Γ is an approximate minimizer of $\mathcal{F}^{\mathrm{BCS}}$ at $T = T_c(1 - h^2 D)$, in the sense that

$$\mathcal{F}^{\mathrm{BCS}}(\Gamma) \leq \mathcal{F}^{\mathrm{BCS}}(\Gamma_0) + h^3 \left(E^{\mathrm{GL}} - b_3 + \epsilon\right) \tag{1.17}$$

for some small $\epsilon > 0$, then the corresponding α can be decomposed as

$$\alpha(x,y) = \frac{1}{2}\big(\psi(x)+\psi(y)\big)\alpha^0(h^{-1}(x-y)) + \sigma(x,y) \tag{1.18}$$

with $\mathcal{E}^{\rm GL}(\psi) \le E^{\rm GL} + \epsilon + \mathrm{const}\, h^{\frac{1}{3}}$, α^0 defined in (1.11), *and*

$$\int_{\mathcal{C}\times\mathbb{R}} |\sigma(x,y)|^2\, dx\, dy \le \mathrm{const}\, h^{3+\frac{1}{3}}\,. \tag{1.19}$$

1.5. The coefficients in the GL functional

In order to give explicit expressions for the coefficients in the GL functional we introduce the functions

$$g_0(z) = \frac{\tanh(z/2)}{z}\,, \qquad g_1(z) = \frac{e^{2z}-2ze^z-1}{z^2(1+e^z)^2}\,, \qquad g_2(z) = \frac{2e^z\,(e^z-1)}{z\,(e^z+1)^3}\,.$$

Setting, as usual, $\beta_c = T_c^{-1}$ we define

$$c = \frac{2\int_{\mathbb{R}}\big[g_0(\beta_c(q^2-\mu)) - \beta_c(q^2-\mu)g_1(\beta_c(q^2-\mu))\big]\, dq}{\beta_c\int_{\mathbb{R}} \frac{g_1(\beta_c(q^2-\mu))}{q^2-\mu}\, dq}\,.$$

The three coefficients of the GL functional turn out to be as follows,

$$b_1 = cD\,\frac{\beta_c^2}{16}\int_{\mathbb{R}}\big(g_1(\beta_c(q^2-\mu)) + 2\beta_c q^2\, g_2(\beta_c(q^2-\mu))\big)\,\frac{dq}{2\pi}\,, \tag{1.20}$$

$$b_2 = cD\,\frac{\beta_c^2}{4}\int_{\mathbb{R}} g_1(\beta_c(q^2-\mu))\,\frac{dq}{2\pi} \tag{1.21}$$

and

$$b_3 = (cD)^2\,\frac{\beta_c^2}{16}\int_{\mathbb{R}} \frac{g_1(\beta_c(q^2-\mu))}{q^2-\mu}\,\frac{dq}{2\pi}\,. \tag{1.22}$$

We shall now discuss the signs of these coefficients. First note that $g_0(z) - zg_1(z) = (zg_0(z))' > 0$ and $g_1(z)/z > 0$, which implies that $c > 0$. Using $g_1(z)/z > 0$ again, we see that $b_3 > 0$. In contrast, the coefficient b_2 may have either sign, depending on the value of $\beta_c\mu$ (which depends on a and μ). The coefficient b_1 is again positive, as the following computation shows: using the fact that $g_2(z) = g_1'(z) + (2/z)g_1(z)$ we find

$$\begin{aligned}
b_1 &= cD\,\frac{\beta_c^2}{16}\int_{\mathbb{R}}\left(g_1(\beta_c(q^2-\mu)) + 2\beta_c q^2\left(g_1'(\beta_c(q^2-\mu)) + \frac{2g_1(\beta_c(q^2-\mu))}{\beta_c(q^2-\mu)}\right)\right)\frac{dq}{2\pi}\\
&= cD\,\frac{\beta_c^2}{16}\int_{\mathbb{R}}\left(g_1(\beta_c(q^2-\mu)) + q\frac{d}{dq}\big(g_1(\beta_c(q^2-\mu))\big) + 4q^2\,\frac{g_1(\beta_c(q^2-\mu))}{q^2-\mu}\right)\frac{dq}{2\pi}\\
&= cD\,\frac{\beta_c^2}{4}\int_{\mathbb{R}} q^2\,\frac{g_1(\beta_c(q^2-\mu))}{q^2-\mu}\,\frac{dq}{2\pi}\,.
\end{aligned}$$

The claimed positivity is now again a consequence of $g_1(z)/z > 0$.

2. Sketch of the proof

In the following we will consider temperatures $T = T_c(1 - Dh^2)$. It is not difficult to see that the solution Δ_0 of the BCS gap equation (1.7) is of order $\Delta_0 = O(h)$.

It is useful to rewrite the BCS functional in a more convenient way. Define Δ to be the multiplication operator

$$\Delta = \Delta(x) = -\psi(x)\Delta_0,$$

where Δ_0 is the solution of the BCS equation (1.7) for temperature T, and ψ a periodic function in $H^2_{\mathrm{loc}}(\mathbb{R})$. Define further

$$H_\Delta = \begin{pmatrix} -h^2\nabla^2 - \mu + h^2 W(x) & \Delta \\ \overline{\Delta} & h^2\nabla^2 + \mu - h^2 W(x) \end{pmatrix}. \tag{2.1}$$

Formally, we can write the BCS functional as

$$\begin{aligned} \mathcal{F}^{\mathrm{BCS}}(\Gamma) = &- \operatorname{Tr}(-h^2\nabla^2 - \mu + h^2 W) + \frac{1}{2}\operatorname{Tr} H_\Delta \Gamma - TS(\Gamma) \\ &+ \frac{1}{4ha}\Delta_0^2 \int_{\mathcal{C}} |\psi(x)|^2 dx - ha \int_{\mathcal{C}} \left| \frac{\Delta_0 \psi(x)}{2ha} - \alpha(x,x) \right|^2 dx\,. \end{aligned} \tag{2.2}$$

The first two terms on the right are infinite, of course, only their sum is well defined. For an upper bound, we can drop the very last term. The terms on the first line are minimized for $\Gamma_\Delta = 1/(1 + e^{\frac{1}{T}H_\Delta})$, which we choose as a trial state. Then

$$\begin{aligned} F^{\mathrm{BCS}}(T,\mu) &\le \mathcal{F}^{\mathrm{BCS}}(\Gamma_\Delta) - \mathcal{F}^{\mathrm{BCS}}(\Gamma_0) \\ &\le -\frac{T}{2}\operatorname{Tr}\left[\ln(1 + e^{-\frac{1}{T}H_\Delta}) - \ln(1 + e^{-\frac{1}{T}H_0})\right] + \frac{1}{4ha}\Delta_0^2 \int_{\mathcal{C}} |\psi(x)|^2 dx\,. \end{aligned} \tag{2.3}$$

To complete the upper bound, we have to evaluate $\operatorname{Tr}[\ln(1 + e^{-H_\Delta/T}) - \ln(1 + e^{-H_0/T})]$. This is done via a contour integral representation and semiclassical types of estimates.

The lower bound is divided into several steps. We first aim at an a priori bound on α for a general state Γ, which has lower energy than the translation-invariant state. With

$$H^0_{\Delta_0} = \begin{pmatrix} -h^2\nabla^2 - \mu & \Delta_0 \\ \Delta_0 & -h^2\nabla^2 + \mu \end{pmatrix},$$

we can rewrite the BCS functional in the form

$$\begin{aligned} \mathcal{F}^{\mathrm{BCS}}(\Gamma) = &- \operatorname{Tr}(-h^2\nabla^2 - \mu + h^2 W) + \frac{1}{2}\operatorname{tr} H^0_{\Delta_0}\Gamma - TS(\Gamma) \\ &+ h^2 \operatorname{Tr} W\gamma + \frac{1}{4ha}\Delta_0^2 - ha \int_{\mathcal{C}} \left| \frac{\Delta_0}{2ha} - \alpha(x,x) \right|^2 dx. \end{aligned} \tag{2.4}$$

From the BCS equation and the definition of α^0 in (1.11) we conclude that

$$\alpha^0(0) = \frac{1}{2\pi h} \int_{\mathbb{R}} \frac{\Delta_0}{2K^0_T(p)} dp = \frac{\Delta_0}{2ah}, \tag{2.5}$$

and hence

$$\mathcal{F}^{\rm BCS}(\Gamma)-\mathcal{F}^{\rm BCS}(\Gamma^0)\geq\frac{T}{2}\mathcal{H}(\Gamma,\Gamma^0)+h^2\,\mathrm{Tr}\,W(\gamma-\gamma^0)-ah\int_{\mathcal{C}}|\alpha(x,x)-\alpha^0(0)|^2dx, \tag{2.6}$$

where $\mathcal{H}$ denotes the relative entropy

$$\begin{aligned}\mathcal{H}(\Gamma,\Gamma^0)&=\frac{2}{T}\left(\frac{1}{2}\,\mathrm{tr}\,H^0_{\Delta_0}\Gamma-TS(\Gamma)+\frac{1}{2}\,\mathrm{tr}\,H^0_{\Delta_0}\Gamma^0-TS(\Gamma^0)\right)\\&=\mathrm{Tr}\left[\Gamma\left(\ln\Gamma-\ln\Gamma^0\right)+(1-\Gamma)\left(\ln(1-\Gamma)-\ln(1-\Gamma^0)\right)\right].\end{aligned} \tag{2.7}$$

Note that the left side of (2.6) is necessarily non-positive for a minimizing state Γ.

One of the essential steps in our proof, which is used on several occasions, is Lemma 5.1. This lemma presents a lower bound on the relative entropy of the form

$$\begin{aligned}\mathcal{H}(\Gamma,\Gamma^0)&\geq\mathrm{Tr}\left[H^0\left(\Gamma-\Gamma^0\right)^2\right]\\&\quad+\frac{1}{3}\frac{\left(\mathrm{Tr}\,\Gamma(1-\Gamma)-\mathrm{Tr}\,\Gamma_0(1-\Gamma^0)\right)^2}{|\mathrm{Tr}\,\Gamma(1-\Gamma)-\mathrm{Tr}\,\Gamma^0(1-\Gamma^0)|+\mathrm{Tr}\,\Gamma^0(1-\Gamma^0)},\end{aligned} \tag{2.8}$$

where $H^0=(1-2\Gamma_0)^{-1}\ln((1-\Gamma^0)/\Gamma^0)$. In our case here, it equals $K^0_T(-ih\nabla)/T$, with K^0_T defined in (1.8). From (2.6) we deduce that for a minimizer Γ

$$\begin{aligned}0\geq\mathcal{F}^{\rm BCS}(\Gamma)-\mathcal{F}^{\rm BCS}(\Gamma^0)&\geq\mathrm{Tr}\,K^0_T(\gamma-\gamma^0)^2+h^2\,\mathrm{Tr}\,W(\gamma-\gamma^0)\\&\quad+\int_{\mathcal{C}}\langle\alpha(\,\cdot\,,y)-\alpha^0(\tfrac{\cdot\,-y}{h})|K^0_T(-ih\nabla)-a\delta(\tfrac{\cdot\,-y}{h})|\alpha(\,\cdot\,,y)-\alpha^0(\tfrac{\cdot\,-y}{h})\rangle\,dy\\&\quad+\frac{1}{3}\frac{T\left(\mathrm{Tr}\left[\gamma(1-\gamma)-\gamma^0(1-\gamma^0)-|\alpha|^2+|\alpha^0|^2\right]\right)^2}{|\mathrm{Tr}\left[\gamma(1-\gamma)-\gamma^0(1-\gamma^0)-|\alpha|^2+|\alpha^0|^2\right]|+\mathrm{Tr}\left[\gamma^0(1-\gamma^0)-|\alpha^0|^2\right]},\end{aligned} \tag{2.9}$$

where $\langle\cdot|\cdot\rangle$ denotes the inner product in $L^2(\mathbb{R})$. Observe that the term in the second line is a convenient way to write $\mathrm{Tr}\,K^0_T(\alpha-\alpha^0)^*(\alpha-\alpha^0)-ah\int_{\mathcal{C}}|\alpha(x,x)-\alpha^0(0)|^2dx$. From the first line on the right side and the Schwarz inequality together with the fact that $K^0_T-a\delta\geq 0$, we obtain first that $\mathrm{Tr}\,K^0_T(\gamma-\gamma^0)^2\leq O(h^3)$. Together with the last line this further gives the a priori bound $\|\alpha\|_2^2\leq O(h)$.

Next, we use that $K^0_T-a\delta$ has α^0 as unique zero energy ground state, with a gap of order one above zero, and we can further conclude from (2.9) that α is necessarily of the form

$$\alpha(x,y)=\tfrac{1}{2}(\psi(x)+\psi(y))\alpha^0((x-y)/h)+\beta(x,y),$$

with $\|\beta\|_2^2\leq O(h^3)$. This information about the decomposition of α then allows us to deduce, again by means of a lower bound of the type (2.8), that the difference $\mathcal{F}^{\rm BCS}(\Gamma)-\mathcal{F}^{\rm BCS}(\Gamma_\Delta)$ is very small compared to h^3. This reduces the problem to the computation we already did in the upper bound.

3. Semiclassics

One of the key ingredients in both the proof of the upper and the lower bound are detailed semiclassical asymptotics for operators of the form

$$H_\Delta = \begin{pmatrix} -h^2\nabla^2 - \mu + h^2 W(x) & \Delta(x) \\ \overline{\Delta(x)} & h^2\nabla^2 + \mu - h^2 W(x) \end{pmatrix} . \tag{3.1}$$

Here $\Delta(x) = -h\psi(x)$ with a periodic function ψ, which is of order one as $h \to 0$ (but might nevertheless depend on h). We are interested in the regime $h \to 0$. In contrast to traditional semiclassical results [12, 16] we work under minimal smoothness assumptions on ψ and W. To be precise, we assume Assumption 1.1 for W and that ψ is a periodic function in $H^2_{\mathrm{loc}}(\mathbb{R})$.

Our first result concerns the free energy.

Theorem 3.1. *Let*

$$f(z) = -\ln\left(1 + e^{-z}\right) , \tag{3.2}$$

and define

$$g_0(z) = \frac{f'(-z) - f'(z)}{z} = \frac{\tanh\left(\frac{1}{2}z\right)}{z} , \tag{3.3}$$

$$g_1(z) = -g_0'(z) = \frac{f'(-z) - f'(z)}{z^2} + \frac{f''(-z) + f''(z)}{z} = \frac{e^{2z} - 2ze^z - 1}{z^2(1+e^z)^2} \tag{3.4}$$

and

$$g_2(z) = g_1'(z) + \frac{2}{z}\, g_1(z) = \frac{f'''(z) - f'''(-z)}{z} = \frac{2e^z\left(e^z - 1\right)}{z\left(e^z+1\right)^3} . \tag{3.5}$$

Then, for any $\beta > 0$,

$$\frac{h}{\beta}\,\mathrm{Tr}\left[f(\beta H_\Delta) - f(\beta H_0)\right] = h^2 E_1 + h^4 E_2 + O(h^6)\left(\|\psi\|^6_{H^1(\mathcal{C})} + \|\psi\|^2_{H^2(\mathcal{C})}\right) , \tag{3.6}$$

where

$$E_1 = -\frac{\beta}{2}\|\psi\|_2^2 \int_{\mathbb{R}} g_0(\beta(q^2 - \mu))\,\frac{dq}{2\pi}$$

and

$$\begin{aligned} E_2 = &\frac{\beta^2}{8}\|\psi'\|_2^2 \int_{\mathbb{R}} \left(g_1(\beta(q^2-\mu)) + 2\beta q^2 g_2(\beta(q^2-\mu))\right)\frac{dq}{2\pi} \\ &+ \frac{\beta^2}{2}\langle\psi|W|\psi\rangle \int_{\mathbb{R}} g_1(\beta(q^2-\mu))\,\frac{dq}{2\pi} \\ &+ \frac{\beta^2}{8}\|\psi\|_4^4 \int_{\mathbb{R}} \frac{g_1(\beta(q^2-\mu))}{q^2-\mu}\,\frac{dq}{2\pi} . \end{aligned}$$

More precisely, we claim that the diagonal entries of the 2×2 matrix-valued operator $f(\beta H_\Delta) - f(\beta H_0)$ are locally trace class and that the sum of their traces per unit volume is given by (3.6). We sketch the proof of Theorem 3.1 in Subsection 6.2 below and refer to [7] for some technicalities.

Our second semiclassical result concerns the behavior of $(1+\exp(\beta H_\Delta))^{-1}$ in the limit $h \to 0$. More precisely, we are interested in $[(1+\exp(\beta H_\Delta))^{-1}]_{12}$, where $[\,\cdot\,]_{12}$ denotes the upper off-diagonal entry of an operator-valued 2×2 matrix. For this purpose, we define the H^1 norm of a periodic operator η by

$$\|\eta\|_{H^1}^2 = \operatorname{Tr}\left[\eta^*(1-h^2\nabla^2)\eta\right]\,. \tag{3.7}$$

In Subsection 6.3 we shall prove

Theorem 3.2. *Let*

$$\rho(z) = (1+e^z)^{-1} \tag{3.8}$$

and let g_0 *be as in* (3.3). *Then*

$$[\rho(\beta H_\Delta)]_{12} = \frac{\beta h}{4}\left(\psi(x)\, g_0(\beta(-h^2\nabla^2-\mu)) + g_0(\beta(-h^2\nabla^2-\mu))\,\psi(x)\right) + \eta_1 + \eta_2$$

where

$$\|\eta_1\|_{H^1}^2 \le Ch^5\|\psi\|_{H^2(\mathcal{C})}^2 \tag{3.9}$$

and

$$\|\eta_2\|_{H^1}^2 \le Ch^5\left(\|\psi\|_{H^1(\mathcal{C})}^2 + \|\psi\|_{H^1(\mathcal{C})}^6\right)\,. \tag{3.10}$$

4. Upper bound

We assume that $T = T_c(1-Dh^2)$ with a fixed $D>0$ and denote by Δ_0 the solution of the BCS gap equation (1.7). In the following we write, as usual, $\beta = T^{-1} = \beta_c(1-Dh^2)^{-1}$ with $\beta_c = T_c^{-1}$. It is well known that the Ginzburg-Landau functional has a minimizer ψ, which is a periodic $H^2_{\mathrm{loc}}(\mathbb{R})$ function. We put

$$\Delta(x) = -\Delta_0\psi(x),$$

and define H_Δ by (2.1).

To obtain an upper bound for the energy we use the trial state

$$\Gamma_\Delta = \left(1+e^{\beta H_\Delta}\right)^{-1}\,.$$

Denoting its off-diagonal element by $\alpha_\Delta = [\Gamma_\Delta]_{12}$, we have the upper bound

$$\begin{aligned}\mathcal{F}^{\mathrm{BCS}}(\Gamma_\Delta) - \mathcal{F}^{\mathrm{BCS}}(\Gamma_0) &= -\frac{1}{2\beta}\operatorname{Tr}\left[\ln(1+e^{-\beta H_\Delta}) - \ln(1+e^{-\beta H_0})\right]\\ &\quad + \frac{\Delta_0^2}{4ha}\|\psi\|_2^2 - ha\int_C\left|\frac{\Delta_0\psi(x)}{2ha} - \alpha_\Delta(x,x)\right|^2 dx \qquad (4.1)\\ &\le -\frac{1}{2\beta}\operatorname{Tr}\left[\ln(1+e^{-\beta H_\Delta}) - \ln(1+e^{-\beta H_0})\right] + \frac{\Delta_0^2}{4ha}\|\psi\|_2^2\,.\end{aligned}$$

The first term on the right side was evaluated in Theorem 3.1.

Applying this theorem with ψ replaced by $(\Delta_0/h)\psi$ we obtain that

$$\begin{aligned}
&\mathcal{F}^{\mathrm{BCS}}(\Gamma_\Delta) - \mathcal{F}^{\mathrm{BCS}}(\Gamma_0) \\
&\leq -\frac{h\beta}{4}\frac{\Delta_0^2}{h^2}\|\psi\|_2^2 \int_{\mathbb{R}} g_0(\beta(q^2-\mu))\,\frac{dq}{2\pi} \\
&\quad + \frac{h^3}{2}\left[\frac{\beta^2}{8}\frac{\Delta_0^2}{h^2}\|\psi'\|_2^2 \int_{\mathbb{R}} (g_1(\beta(q^2-\mu)) + 2\beta q^2 g_2(\beta(q^2-\mu)))\,\frac{dq}{2\pi}\right. \\
&\qquad \left. + \frac{\beta^2}{2}\frac{\Delta_0^2}{h^2}\langle\psi|W|\psi\rangle \int_{\mathbb{R}} g_1(\beta(q^2-\mu))\,\frac{dq}{2\pi} + \frac{\beta^2}{8}\frac{\Delta_0^4}{h^4}\|\psi\|_4^4 \int_{\mathbb{R}} \frac{g_1(\beta(q^2-\mu))}{q^2-\mu}\,\frac{dq}{2\pi}\right] \\
&\quad + \frac{\Delta_0^2}{4ha}\|\psi\|_2^2 + O(h^5)\,. \qquad (4.2)
\end{aligned}$$

In the estimate of the remainder we used that ψ is H^2 and that $\Delta_0 \leq Ch$.

Next, we use that by definition (1.7) of Δ_0 the first and the last term on the right side of (4.2) cancel to leading order and that one has

$$\begin{aligned}
&-\frac{h\beta}{4}\frac{\Delta_0^2}{h^2}\|\psi\|_2^2 \int_{\mathbb{R}} g_0(\beta(q^2-\mu))\,\frac{dq}{2\pi} + \frac{\Delta_0^2}{4ha}\|\psi\|_2^2 \\
&\quad = \frac{h\beta}{4}\frac{\Delta_0^2}{h^2}\|\psi\|_2^2 \int_{\mathbb{R}} \left(g_0(\beta\sqrt{(q^2-\mu)^2+\Delta_0^2}) - g_0(\beta(q^2-\mu))\right)\,\frac{dq}{2\pi} \\
&\quad = -\frac{h^3\beta^2}{8}\frac{\Delta_0^4}{h^4}\|\psi\|_2^2 \int_{\mathbb{R}} \frac{g_1(\beta(q^2-\mu))}{q^2-\mu}\,\frac{dq}{2\pi} + O(h^5)\,.
\end{aligned}$$

We conclude that

$$\begin{aligned}
&\mathcal{F}^{\mathrm{BCS}}(\Gamma_\Delta) - \mathcal{F}^{\mathrm{BCS}}(\Gamma_0) \\
&\leq \frac{h^3}{2}\left[\frac{\beta^2}{8}\frac{\Delta_0^2}{h^2}\|\psi'\|_2^2 \int_{\mathbb{R}} (g_1(\beta(q^2-\mu)) + 2\beta q^2 g_2(\beta(q^2-\mu)))\,\frac{dq}{2\pi}\right. \\
&\qquad + \frac{\beta^2}{2}\frac{\Delta_0^2}{h^2}\langle\psi|W|\psi\rangle \int_{\mathbb{R}} g_1(\beta(q^2-\mu))\,\frac{dq}{2\pi} + \frac{\beta^2}{8}\frac{\Delta_0^4}{h^4}\|\psi\|_4^4 \int_{\mathbb{R}} \frac{g_1(\beta(q^2-\mu))}{q^2-\mu}\,\frac{dq}{2\pi} \\
&\qquad \left. - \frac{\beta^2}{4}\frac{\Delta_0^4}{h^4}\|\psi\|_2^2 \int_{\mathbb{R}} \frac{g_1(\beta(q^2-\mu))}{q^2-\mu}\,\frac{dq}{2\pi}\right] + O(h^5)\,. \qquad (4.3)
\end{aligned}$$

Up to an error of the order $O(h^5)$ we can replace $\beta = \beta_c(1-Dh^2)^{-1}$ by β_c on the right side. Our last task is then to compute the asymptotics of Δ_0/h. To do so, we rewrite the BCS gap equation (1.7) as

$$\beta_c \int_{\mathbb{R}} g_0(\beta_c(q^2-\mu))\,\frac{dq}{2\pi} = \frac{1}{a} = \beta \int_{\mathbb{R}} g_0\left(\beta\sqrt{(q^2-\mu)^2+\Delta_0^2}\right)\,\frac{dq}{2\pi}\,.$$

A simple computation shows that

$$\Delta_0^2 = Dh^2\,\frac{\int_{\mathbb{R}}\left[g_0(\beta_c(q^2-\mu)) - \beta_c(q^2-\mu)g_1(\beta_c(q^2-\mu))\right]\,dq}{\beta_c\int_{\mathbb{R}}\frac{g_1(\beta_c(q^2-\mu))}{2(q^2-\mu)}\,dq}\left(1+O(h^2)\right)\,.$$

Inserting this into (4.3) and using the fact that $\mathcal{E}(\psi) = E^{\rm GL}$ we arrive at the upper bound claimed in Theorem 1.2.

5. Lower bound

5.1. The relative entropy

As a preliminary to our proof of the lower bound, we present a general estimate for the relative entropy. In this subsection H^0 and $0 \leq \Gamma \leq 1$ are arbitrary self-adjoint operators in a Hilbert space, not necessarily coming from BCS theory. Let $\Gamma^0 := \left(1+\exp(\beta H^0)\right)^{-1}$. It is well known that

$$\mathcal{H}(\Gamma,\Gamma^0) = \operatorname{Tr}\left(\beta H^0\Gamma + \Gamma\ln\Gamma + (1-\Gamma)\ln(1-\Gamma) + \ln\left(1+\exp(-\beta H_0)\right)\right)$$

is non-negative and equals to zero if and only if $\Gamma = \Gamma^0$. Solving this equation for H^0, i.e., $H^0 = \beta^{-1}(\ln(1-\Gamma^0) - \ln\Gamma^0)$, we can rewrite $\mathcal{H}(\Gamma,\Gamma^0)$ as a relative entropy,

$$\mathcal{H}(\Gamma,\Gamma^0) = \operatorname{Tr}\left[\Gamma\left(\ln\Gamma - \ln\Gamma^0\right) + (1-\Gamma)\left(\ln(1-\Gamma) - \ln(1-\Gamma^0)\right)\right]. \tag{5.1}$$

The following lemma quantifies the positivity of $\mathcal{H}$ and improves an earlier result from [5].

Lemma 5.1. *For any $0 \leq \Gamma \leq 1$ and any Γ_0 of the form $\Gamma^0 = (1+e^{\beta H^0})^{-1}$,*

$$\begin{aligned}\mathcal{H}(\Gamma,\Gamma^0) \geq \operatorname{Tr}&\left[\frac{\beta H^0}{\tanh(\beta H^0/2)}\left(\Gamma-\Gamma^0\right)^2\right] \\ &+ \frac{1}{3}\frac{\left(\operatorname{Tr}\Gamma(1-\Gamma) - \operatorname{Tr}\Gamma^0(1-\Gamma^0)\right)^2}{\left|\operatorname{Tr}\Gamma(1-\Gamma) - \operatorname{Tr}\Gamma^0(1-\Gamma^0)\right| + \operatorname{Tr}\Gamma^0(1-\Gamma^0)}.\end{aligned}$$

Proof. It is tedious, but elementary, to show that for real numbers $0 < x, y < 1$,

$$x\ln\frac{x}{y} + (1-x)\ln\frac{1-x}{1-y} \geq \frac{\ln\frac{1-y}{y}}{1-2y}(x-y)^2 + \frac{1}{3}\frac{\left(x(1-x)-y(1-y)\right)^2}{|x(1-x)-y(1-y)| + y(1-y)}.$$

Using joint convexity we see that

$$\begin{aligned}&\frac{\left(x(1-x)-y(1-y)\right)^2}{|x(1-x)-y(1-y)| + y(1-y)} \\ &\qquad = 4\sup_{0<b<1}\left[b(1-b)\,|x(1-x)-y(1-y)| - b^2y(1-y)\right].\end{aligned}$$

Let us replace on the right side the modulus $|a|$ by $\max\{a,-a\}$, and then use Klein's inequality [15, Section 2.1.4] for either of the expressions. This implies the result. $\square$

5.2. A priori estimates on α

We begin by briefly reviewing some facts about the translation-invariant case $W \equiv 0$; see also Subsection 1.2.1. Recall that Γ^0 denotes the minimizer of $\mathcal{F}$ in the translation-invariant case. It can be written as $\Gamma^0 = (1 + e^{\beta H^0_{\Delta_0}})^{-1}$ with

$$H^0_{\Delta_0} = \begin{pmatrix} -h^2\nabla^2 - \mu & -\Delta_0 \\ -\Delta_0 & h^2\nabla^2 + \mu \end{pmatrix}.$$

Here Δ_0 is the solution of the BCS gap-equation (1.7) and $\beta^{-1} = T = T_c(1 - Dh^2)$. Notice the distinction between Γ^0 and Γ_0 which was defined in (1.13). The latter one, Γ_0, contains the external potential W and has no off-diagonal term.

Recall also that we denote the kernel of the off-diagonal entry $\alpha^0 = [\Gamma^0]_{12}$ by $\alpha^0((x-y)/h)$, which is explicitly given in (1.11). From this explicit representation and the fact that $\Delta_0 \le Ch$ we conclude, in particular, that

$$\|\alpha^0\|_2^2 = \int_0^1 dy \int_{\mathbb{R}} dx\, |\alpha^0((x-y)/h)|^2 = h \int_{\mathbb{R}} |\alpha^0(x)|^2\, dx \le Ch\,. \tag{5.2}$$

Moreover, the BCS gap-equation (1.7) is equivalent to

$$(K_T^0(-ih\nabla) - ah\delta(x))\alpha^0(x/h) = 0\,. \tag{5.3}$$

This implies, in particular, that

$$\mathrm{Tr}\, K_T^0(-ih\nabla)\alpha^0\overline{\alpha^0} - ah|\alpha^0(0)|^2 = 0\,. \tag{5.4}$$

Now we turn to the case of general W. Our goal in this subsection is to prove that the α of *any* low-energy state satisfies bounds similar to (5.2) and (5.4).

Proposition 5.2. *Any admissible* Γ *with* $\mathcal{F}^{\mathrm{BCS}}(\Gamma) \le \mathcal{F}^{\mathrm{BCS}}(\Gamma^0)$ *satisfies*

$$\|\alpha\|_2^2 = \int_0^1 dx \int_{\mathbb{R}} dy\, |\alpha(x,y)|^2 \le Ch \tag{5.5}$$

and

$$0 \le \mathrm{Tr}\, K_T^0(-ih\nabla)\alpha\overline{\alpha} - ah\int_{\mathcal{C}} |\alpha(x,x)|^2\, dx \le Ch^3\,, \tag{5.6}$$

where $\alpha = [\Gamma]_{12}$.

Proof. We divide the proof into two steps.

Step 1. Our starting point is the representation

$$\mathcal{F}^{\mathrm{BCS}}(\Gamma) - \mathcal{F}^{\mathrm{BCS}}(\Gamma^0) = \tfrac{1}{2\beta}\,\mathcal{H}(\Gamma,\Gamma^0) + h^2\,\mathrm{Tr}\,\gamma W - ah\int_{\mathcal{C}} |\alpha(x,x) - \alpha^0(0)|^2\, dx \tag{5.7}$$

for any admissible Γ, with the relative entropy $\mathcal{H}(\Gamma,\Gamma^0)$ defined in (5.1). We note that Γ^0 is of the form $(1 + e^{\beta H^0})^{-1}$ with $H^0 = H^0_{\Delta_0}$. We use Lemma 5.1 to bound

$\mathcal{H}(\Gamma,\Gamma^0)$ from below. Since $x \mapsto x/\tanh x$ is even, we can replace $H^0_{\Delta_0}$ by its absolute value $E(-ih\nabla) = \sqrt{(-h^2\nabla^2-\mu)^2+\Delta_0^2}$, and thus

$$\begin{aligned}\operatorname{Tr}\left[\frac{H^0_{\Delta_0}}{\tanh\frac{\beta}{2}H^0_{\Delta_0}}(\Gamma-\Gamma_0)^2\right] &= \operatorname{Tr}\left[K_T^0(-ih\nabla)(\Gamma-\Gamma_0)^2\right]\\ &= 2\operatorname{Tr}K_T^0(-ih\nabla)(\gamma-\gamma^0)^2 + 2\operatorname{Tr}K_T^0(-ih\nabla)(\alpha-\alpha^0)(\overline{\alpha-\alpha^0})\end{aligned}$$

with

$$K_T^0(hp) = \frac{E(hp)}{\tanh\frac{\beta E(hp)}{2}}$$

from (1.8). With the aid of Lemma 5.1 and the assumption $\mathcal{F}^{\mathrm{BCS}}(\Gamma) \leq \mathcal{F}^{\mathrm{BCS}}(\Gamma^0)$ we obtain from (5.7) the basic inequality

$$\begin{aligned}0 \geq\ & \operatorname{Tr}K_T^0(-ih\nabla)(\gamma-\gamma^0)^2 + h^2\operatorname{Tr}\gamma W \\ &+ \operatorname{Tr}K_T^0(-ih\nabla)(\alpha-\alpha^0)(\overline{\alpha-\alpha^0}) - ah\int_{\mathcal{C}}|\alpha(x,x)-\alpha^0(0)|^2\,dx \\ &+ \frac{T}{3}\frac{\left(\operatorname{Tr}\left[\gamma(1-\gamma)-\gamma^0(1-\gamma^0)-\alpha\overline{\alpha}+\alpha^0\overline{\alpha^0}\right]\right)^2}{\left|\operatorname{Tr}\left[\gamma(1-\gamma)-\gamma^0(1-\gamma^0)-\alpha\overline{\alpha}+\alpha^0\overline{\alpha^0}\right]\right| + \operatorname{Tr}\left[\gamma^0(1-\gamma^0)-\alpha^0\overline{\alpha^0}\right]}\,.\end{aligned} \tag{5.8}$$

In the following step we shall derive the claimed a priori estimates on α from this inequality.

Step 2. We begin by discussing the first line on the right side of (5.8). Using the fact that $\operatorname{Tr}W\gamma^0 = 0$ (since W has mean value zero) and the Schwarz inequality we obtain the lower bound

$$\begin{aligned}&\operatorname{Tr}K_T^0(-ih\nabla)(\gamma-\gamma^0)^2 + h^2\operatorname{Tr}W\gamma\\ &\quad= \tfrac12\operatorname{Tr}K_T^0(-ih\nabla)(\gamma-\gamma^0)^2 + \tfrac12\operatorname{Tr}K_T^0(\gamma-\gamma^0)^2 + h^2\operatorname{Tr}W(\gamma-\gamma^0)\\ &\quad\geq \tfrac12\operatorname{Tr}K_T^0(-ih\nabla)(\gamma-\gamma^0)^2 - h^4\tfrac12\operatorname{Tr}W\left(K_T^0(-ih\nabla)\right)^{-1}W\\ &\quad\geq \tfrac12\operatorname{Tr}K_T^0(-ih\nabla)(\gamma-\gamma^0)^2 - Ch^3\,.\end{aligned} \tag{5.9}$$

The last step used that $\operatorname{Tr}W\left(K_T^0(-ih\nabla)\right)^{-1}W \leq \|W\|_\infty^2\operatorname{Tr}K_T^0(-ih\nabla)^{-1} \leq Ch^{-1}$.

Next, we treat the second line on the right side of (5.8). Recall that the BCS gap equation in the form (5.3) says that the operator $K_T^0(-ih\nabla) - ah\delta(x)$ has an eigenvalue zero with eigenfunction $\alpha^0(x/h)$. Hence

$$\begin{aligned}&\operatorname{Tr}K_T^0(-ih\nabla)(\alpha-\alpha^0)(\overline{\alpha-\alpha^0}) - ah\int_{\mathcal{C}}|\alpha(x,x)-\alpha^0(0)|^2\,dx\\ &\quad= \operatorname{Tr}K_T^0(-ih\nabla)\alpha\overline{\alpha} - ah\int_{\mathcal{C}}|\alpha(x,x)|^2\,dx\,.\end{aligned}$$

Since a delta potential creates at most one bound state, zero must be the ground state energy of $K_T^0(-ih\nabla) - ah\delta(x)$, and we deduce that

$$\operatorname{Tr} K_T^0(-ih\nabla)\alpha\overline{\alpha} - ah\int_{\mathcal{C}} |\alpha(x,x)|^2\, dx \geq 0\,.$$

This information, together with (5.9) and (5.8), yields

$$\operatorname{Tr}(1-h^2\nabla^2)(\gamma-\gamma^0)^2 \leq C \operatorname{Tr} K_T^0(-ih\nabla)(\gamma-\gamma^0)^2 \leq Ch^3\,, \tag{5.10}$$

$$\operatorname{Tr} K_T^0(-ih\nabla)\alpha\overline{\alpha} - ah\int_{\mathcal{C}} |\alpha(x,x)|^2\, dx \leq Ch^3 \tag{5.11}$$

and

$$\frac{\left(\operatorname{Tr}\left[\gamma(1-\gamma)-\gamma^0(1-\gamma^0)-\alpha\overline{\alpha}+\alpha^0\overline{\alpha^0}\right]\right)^2}{\left|\operatorname{Tr}\left[\gamma(1-\gamma)-\gamma^0(1-\gamma^0)-\alpha\overline{\alpha}+\alpha^0\overline{\alpha^0}\right]\right| + \operatorname{Tr}\left[\gamma^0(1-\gamma^0)-\alpha^0\overline{\alpha^0}\right]} \leq Ch^3\,. \tag{5.12}$$

We know that $\operatorname{Tr}\left[\gamma^0(1-\gamma^0)-\alpha^0\overline{\alpha^0}\right] \leq Ch^{-1}$ from the explicit solution in the translation invariant case, and therefore (5.12) yields

$$\left|\operatorname{Tr}\left[\gamma(1-\gamma)-\gamma^0(1-\gamma^0)-\alpha\overline{\alpha}+\alpha^0\overline{\alpha^0}\right]\right| \leq Ch\,. \tag{5.13}$$

In order to derive from this an a priori estimate on α we use (5.10) and the Schwarz inequality to bound

$$\left|\operatorname{Tr}(\gamma-\gamma^0)\right| \leq h^{-2}\operatorname{Tr} K_T^0(-ih\nabla)(\gamma-\gamma^0)^2 + h^2 \operatorname{Tr}\left(K_T^0(-ih\nabla)\right)^{-1} \leq Ch$$

and

$$\left|\operatorname{Tr}(\gamma^2-(\gamma^0)^2)\right| = \left|\operatorname{Tr}(\gamma-\gamma^0)(\gamma+\gamma^0)\right| \leq h^{-2}\operatorname{Tr}(\gamma-\gamma^0)^2 + h^2\operatorname{Tr}(\gamma+\gamma^0)^2 \leq Ch\,.$$

Finally, since $\operatorname{Tr}\alpha^0\overline{\alpha^0} \leq Ch$ (see (5.2)), we conclude from (5.13) that $\operatorname{Tr}\alpha\overline{\alpha} \leq Ch$, as claimed. □

5.3. Decomposition of $\boldsymbol{\alpha}$

Here we quantify in which sense $\alpha(x,y)$ is close to $\frac{1}{2}\left(\psi(x)+\psi(y)\right)\alpha^0(h^{-1}(x-y))$. There is one technical point that we would like to discuss before stating the result. The asymptotic form $\frac{1}{2}\left(\psi(x)+\psi(y)\right)\alpha^0(h^{-1}(x-y))$ will allow us in the next subsection to use the semiclassical results in a similar way as in the proof of the upper bound. Our semiclassics, however, require ψ to be in H^2. While we naturally get an H^1 condition, the H^2 condition is achieved by introducing an additional parameter $\epsilon > 0$, which will later chosen to go to zero as $h \to 0$.

Proposition 5.3. *Let Γ be admissible with $\mathcal{F}^{\mathrm{BCS}}(\Gamma) \leq \mathcal{F}^{\mathrm{BCS}}(\Gamma^0)$. Then for every sufficiently small $\epsilon \geq h > 0$, the operator $\alpha = [\Gamma]_{12}$ can be decomposed as*

$$\alpha(x,y) = \tfrac{1}{2}\left(\psi(x)+\psi(y)\right)\alpha^0(h^{-1}(x-y)) + \sigma(x,y) \tag{5.14}$$

with a periodic function $\psi \in H^2(\mathcal{C})$ satisfying

$$\|\psi\|_{H^1} \leq C\,, \qquad \|\psi\|_{H^2} \leq C\epsilon h^{-1} \tag{5.15}$$

and with

$$\|\sigma\|_{H^1}^2 \leq C\epsilon^{-2}h^3 \,. \tag{5.16}$$

More precisely, one has $\sigma = \sigma_1 + \sigma_2$ *with*

$$\|\sigma_1\|_{H^1}^2 \leq Ch^3 \tag{5.17}$$

and with σ_2 *of the form*

$$\sigma_2(x,y) = \tfrac{1}{2}\left(\tilde{\psi}(x) + \tilde{\psi}(y)\right)\alpha^0(h^{-1}(x-y))\,,$$

where the Fourier transform of $\tilde{\psi}$ *supported in* $\{|p| \geq \epsilon h^{-1}\}$*. The Fourier transform of* ψ *is supported in* $\{|p| < \epsilon h^{-1}\}$*.*

We recall that the H^1 norm of an operator was introduced in (3.7).

Proof. Step 1. We can write (5.6) as

$$0 \leq \int_{\mathcal{C}} \langle \alpha(\,\cdot\,,y)|K_T^0(-ih\nabla) - ah\delta(\cdot\,-y)|\alpha(\,\cdot\,,y)\rangle\, dy \leq Ch^3\,. \tag{5.18}$$

Here, the operator $K_T^0(-ih\nabla)$ acts on the x variable of $\alpha(x,y)$, and $\langle\,\cdot\,|\,\cdot\,\rangle$ denotes the standard inner product on $L^2(\mathbb{R})$.

Now we recall that the operator $K_T^0 - ah\delta(\cdot - y)$ on $L^2(\mathbb{R})$ has a unique ground state, proportional to $\alpha^0(h^{-1}(\cdot - y))$, with ground state energy zero. There are no further eigenvalues and the bottom of its essential spectrum is $\Delta_0/\tanh\left[\frac{\Delta_0}{2T}\right] \geq 2T$. In particular, there is a lower bound, independent of h, on the gap. We write

$$\psi_0(y) = \left(h\int_{\mathbb{R}^d} |\alpha^0(x)|^2\, dx\right)^{-1} \int_{\mathbb{R}^d} \alpha^0(h^{-1}(x-y))\alpha(x,y)\, dx \tag{5.19}$$

and decompose

$$\alpha(x,y) = \psi_0(y)\alpha^0(h^{-1}(x-y)) + \sigma_0(x,y)\,.$$

Then (5.18) together with the uniform lower bound on the gap of $K_T^0 - ah\delta(\,\cdot\, - y)$ yields the bound $\|\sigma_0\|_2^2 \leq Ch^3$. We can also symmetrize and write

$$\sigma_1(x,y) = \sigma_0(x,y) + \tfrac{1}{2}\left(\psi(x) - \psi(y)\right)\alpha^0(h^{-1}(x-y))\,. \tag{5.20}$$

Then

$$\alpha(x,y) = \tfrac{1}{2}\left(\psi_0(x) + \psi_0(y)\right)\alpha^0(h^{-1}(x-y)) + \sigma_1(x,y) \tag{5.21}$$

again with

$$\|\sigma_1\|_2^2 \leq Ch^3\,. \tag{5.22}$$

This proves the first half of (5.17). Before proving the second half in Step 4 below we need to study ψ.

Step 2. We claim that

$$\int_{\mathcal{C}} |\psi_0(x)|^2\, dx \leq C \tag{5.23}$$

and

$$\int_{\mathcal{C}} |\psi_0'(x)|^2\, dx \leq C\,. \tag{5.24}$$

The first inequality follows by Schwarz's inequality

$$\int_{\mathcal{C}} |\psi_0(x)|^2\, dx \leq \frac{\|\alpha\|_2^2}{h\int_{\mathbb{R}} |\alpha^0(x)|^2 dx}$$

and our bounds (5.5) and (5.2). In order to prove (5.24) we use again Schwarz's inequality,

$$\int_{\mathcal{C}} |\psi_0'(x)|^2\, dx \leq \frac{\int_{\mathbb{R}\times\mathcal{C}} \left|(\nabla_x + \nabla_y)\, \alpha(x,y)\right|^2\, dx\, dy}{h\int |\alpha^0(x)|^2 dx}\,. \tag{5.25}$$

Lemma 5.4 below bounds the numerator by a constant times

$$h^{-2}\int_{\mathcal{C}} \langle \alpha(\,\cdot\,,y)|K_T^0(-ih\nabla) - ah\delta(\cdot\, - y)|\alpha(\,\cdot\,,y)\rangle\, dy\,,$$

and therefore (5.24) is a consequence of (5.18) and (5.2).

Step 3. Next, we establish the remaining bound $\|\nabla\sigma_1\|_2^2 \leq Ch$ in (5.17). We use formula (5.20) for σ_1. First of all, using the fact that

$$K(-ih\nabla) \geq c(1 - h^2\nabla^2)$$

one easily deduces from (5.18) that $\|\nabla\sigma_0\|_2^2 \leq Ch$. Moreover, because of (5.2) and (5.24)

$$\int_{\mathcal{C}} |\psi_0'(x)|^2 \int_{\mathbb{R}} |\alpha^0(h^{-1}(x-y))|^2 dx\, dy \leq Ch\,.$$

Finally,

$$\begin{aligned}
&h^{-2}\int_{\mathcal{C}\times\mathbb{R}} |\psi_0(x) - \psi_0(y)|^2 |(\alpha^0)'(h^{-1}(x-y))|^2\, dx\, dy \\
&\quad = h^{-1} 4 \sum_{p\in 2\pi\mathbb{Z}} |\hat{\psi}_0(p)|^2 \int_{\mathbb{R}} \left|(\alpha^0)'(x)\right|^2 \sin^2\left(\tfrac{1}{2}hpx\right)\, dx \\
&\quad \leq h \sum_{p\in 2\pi\mathbb{Z}} |p|^2 |\hat{\psi}_0(p)|^2 \int_{\mathbb{R}} \left|(\alpha^0)'(x)\right|^2 x^2\, dx \leq Ch\,,
\end{aligned}$$

where we used (5.24) and the fact that $\int_{\mathbb{R}} \left|(\alpha^0)'(x)\right|^2 x^2 dx$ is finite. This is a simple consequence of the fact that the Fourier transform of α^0 is given by the smooth function $\frac{\Delta_0}{2(2\pi)^{1/2}}\left(K_T^0\right)^{-1}$. This completes the proof of (5.17).

Step 4. Finally, for each $\epsilon \geq h$ we decompose $\psi_0 = \psi + \tilde{\psi}$, where the Fourier transforms of ψ and $\tilde{\psi}$ are supported in $\{|p| < \epsilon h^{-1}\}$ and $\{|p| \geq \epsilon h^{-1}\}$, respectively. Clearly, the bounds (5.23) and (5.24) imply (5.15).

Moreover, $\|\tilde{\psi}\|_2 \leq C\epsilon^{-1}h$ and $\|\tilde{\psi}'\|_2 \leq C$, and hence

$$\sigma_2(x,y) = \tfrac{1}{2}\left(\tilde{\psi}(x) + \tilde{\psi}(y)\right)\alpha^0(h^{-1}(x-y))$$

satisfies $\|\sigma_2\|_{H^1}^2 \leq h^3\epsilon^{-2}$. This completes the proof of the proposition. $\square$

In the previous proof we made use of the following

Lemma 5.4. *For some constant $C > 0$,*

$$\begin{aligned} & h^2 \int_{\mathbb{R}\times\mathcal{C}} \left|(\nabla_x + \nabla_y)\, \alpha(x,y)\right|^2 \, dx\, dy \\ & \leq C \int_{\mathcal{C}} \langle \alpha(\,\cdot\,,y) | K_T^0(-ih\nabla) - ah\delta(\cdot\, - y) | \alpha(\,\cdot\,,y)\rangle \, dy \end{aligned} \tag{5.26}$$

for all periodic and symmetric α (i.e., $\alpha(x,y) = \alpha(y,x)$).

Proof. By expanding $\alpha(x,y)$ in a Fourier series

$$\alpha(x,y) = \sum_{p\in 2\pi\mathbb{Z}} e^{ip(x+y)/2} \alpha_p(x-y) \tag{5.27}$$

and using that $\alpha_p(x) = \alpha_p(-x)$ for all $p \in 2\pi\mathbb{Z}$ we see that (5.26) is equivalent to

$$K_T^0(-ih\nabla + hp/2) + K_T^0(-ih\nabla - hp/2) - 2a\,\delta(x/h) \geq \frac{2}{C} h^2 p^2 \tag{5.28}$$

for all $p \in 2\pi\mathbb{Z}$. This inequality holds for all $p \in \mathbb{R}$, in fact, for an appropriate choice of $C > 0$, as we shall now show.

Since $K_T^0 \geq \mathrm{const}(1 + h^2(-i\nabla + p/2)^2)$, it suffices to consider the case of hp small. If $\kappa = \Delta_0 / \tanh\left[\frac{\Delta_0}{2T}\right] \geq 2T$ denotes the gap in the spectrum of $K_T^0(-ih\nabla) - ah\delta$ above zero, and $h^{-1/2}\phi_0(x/h)$ its normalized ground state, proportional to $\alpha^0(x/h)$,

$$\begin{aligned} & K_T^0(-ih\nabla + hp/2) + K_T^0(-ih\nabla - hp/2) - 2ah\delta \\ & \geq \kappa \left[e^{ihxp/2} \left(1 - |\phi_0\rangle\langle\phi_0|\right) e^{-ihxp/2} + e^{-ihxp/2} \left(1 - |\phi_0\rangle\langle\phi_0|\right) e^{ihxp/2} \right] \\ & \geq \kappa \left[1 - \left| \int |\phi_0(x)|^2 e^{-ihxp} dx \right| \right] . \end{aligned} \tag{5.29}$$

In order to see the last inequality, simply rewrite the term as $\kappa(2 - |f\rangle\langle f| - |g\rangle\langle g|)$, where $|\langle f|g\rangle|^2 = \left|\int |\phi_0(x)|^2 e^{-ihxp} dx\right|$, and compute the smallest eigenvalue of the corresponding 2×2 matrix. Since ϕ_0 is reflection symmetric, normalized and satisfies $\int x^2 |\phi_0|^2 \, dx < \infty$ (see Step 4 in the proof of Proposition 5.3), we have

$$1 - \left| \int |\phi_0(x)|^2 e^{-ihxp} dx \right| = \int |\phi_0(x)|^2 \left(1 - \cos(hpx)\right) dx \geq c h^2 p^2 \,.$$

This completes the proof of (5.28). $\square$

5.4. The lower bound

Pick a Γ with $\mathcal{F}^{\mathrm{BCS}}(\Gamma) \leq \mathcal{F}^{\mathrm{BCS}}(\Gamma^0)$ and let ψ be as in Proposition 5.3 (depending on some parameter $\epsilon \geq h$ to be chosen later). As before we let $\Delta(x) = -\psi(x)\Delta_0$ and define H_Δ by (2.1). We also put $\Gamma_\Delta = (1 + \exp(\beta H_\Delta))^{-1}$.

Our starting point is the representation

$$\mathcal{F}^{\mathrm{BCS}}(\Gamma) - \mathcal{F}^{\mathrm{BCS}}(\Gamma_0) = -\frac{T}{2}\,\mathrm{Tr}\left[\ln(1+e^{-\beta H_\Delta}) - \ln(1+e^{-\beta H_0})\right] + \frac{T}{2}\,\mathcal{H}(\Gamma,\Gamma_\Delta) + \Delta_0\,\mathrm{Re}\int_{\mathcal{C}} \overline{\psi(x)}\alpha(x,x)dx - ha\int_{\mathcal{C}} |\alpha(x,x)|^2 dx\,. \quad (5.30)$$

(Compare with (5.7).) According to the decomposition (5.14) which, in view of the BCS gap equation (1.7), reads on the diagonal

$$\alpha(x,x) = \psi(x)\alpha^0(0) + \sigma(x,x) = \frac{\Delta_0\psi(x)}{2ah} + \sigma(x,x)\,,$$

we can obtain the lower bound

$$\mathcal{F}^{\mathrm{BCS}}(\Gamma) - \mathcal{F}^{\mathrm{BCS}}(\Gamma_0) \geq -\frac{T}{2}\,\mathrm{Tr}\left[\ln(1+e^{-\beta H_\Delta}) - \ln(1+e^{-\beta H_0})\right] + \frac{T}{2}\,\mathcal{H}(\Gamma,\Gamma_\Delta) - ah\int_{\mathcal{C}} |\sigma(x,x)|^2\, dx\,.$$

For the first two terms on the right side we apply the semiclassics from Theorem 3.1. Arguing as in the proof of the upper bound and taking into account the bounds on ψ from Proposition 5.3 we obtain

$$\mathcal{F}^{\mathrm{BCS}}(\Gamma) - \mathcal{F}^{\mathrm{BCS}}(\Gamma_0) \geq h^3\left(\mathcal{E}^{\mathrm{GL}}(\psi) - b_3\right) - C\epsilon^2 h^3 + \tfrac{T}{2}\,\mathcal{H}(\Gamma,\Gamma_\Delta) - ah\int_{\mathcal{C}} |\sigma(x,x)|^2\, dx\,. \quad (5.31)$$

Our final task is to bound the last two terms from below. In the remainder of this subsection we shall show that

$$\tfrac{T}{2}\,\mathcal{H}(\Gamma,\Gamma_\Delta) - ah\int_{\mathcal{C}} |\sigma(x,x)|^2\, dx \geq -C\left(\epsilon h^3 + \epsilon^{-2}h^4\right)\,. \quad (5.32)$$

The choice $\epsilon = h^{1/3}$ will then lead to

$$\mathcal{F}^{\mathrm{BCS}}(\Gamma) - \mathcal{F}^{\mathrm{BCS}}(\Gamma_0) \geq h^3\left(E^{\mathrm{GL}} - b_3\right) - Ch^{3+1/3}\,,$$

which is the claimed lower bound.

In order to prove (5.32) we again use the lower bound on the relative entropy from Lemma 5.1 to estimate

$$T\,\mathcal{H}(\Gamma,\Gamma_\Delta) \geq \mathrm{Tr}\left[\frac{H_\Delta}{\tanh\frac{1}{2T}H_\Delta}\,(\Gamma-\Gamma_\Delta)^2\right]\,. \quad (5.33)$$

The next lemma will allow us to replace the operator H_Δ in this bound by H_0.

Lemma 5.5. *There is a constant $c>0$ such that for all sufficiently small $h>0$*

$$\frac{H_\Delta}{\tanh\frac{1}{2T}H_\Delta} \geq (1-ch)\,K_T^0(-ih\nabla)\otimes \mathbb{I}_{\mathbb{C}^2}\,. \quad (5.34)$$

Proof. An application of Schwarz's inequality yields that for every $0 < \eta < 1$

$$H_\Delta^2 \geq (1-\eta)\left(H_{\Delta_0}^0\right)^2 - \eta^{-1}(\Delta_0^2\|\psi-1\|_\infty^2 + h^2\|W\|_\infty^2)\,.$$

The expansion formula [14, (4.3.91)]

$$\frac{x}{\tanh(x/2)} = 2 + \sum_{k=1}^\infty \left(2 - \frac{2k^2\pi^2}{x^2/4+k^2\pi^2}\right)$$

shows that $x \mapsto \sqrt{x}/\tanh\sqrt{x}$ is an operator monotone function. This operator monotonicity implies that

$$\begin{aligned}
K_T^0(-ih\nabla)\otimes\mathbb{I}_{\mathbb{C}^2} &\leq \frac{(1-\eta)^{-1/2}\sqrt{H_\Delta^2+\eta^{-1}(\Delta_0^2\|\psi-1\|_\infty^2+h^2\|W\|_\infty^2)}}{\tanh\frac{1}{2T}(1-\eta)^{-1/2}\sqrt{H_\Delta^2+\eta^{-1}(\Delta_0^2\|\psi-1\|_\infty^2+h^2\|W\|_\infty^2)}}\\
&\leq (1-\eta)^{-1/2}\frac{\sqrt{H_\Delta^2+\eta^{-1}(\Delta_0^2\|\psi-1\|_\infty^2+h^2\|W\|_\infty^2)}}{\tanh\frac{1}{2T}\sqrt{H_\Delta^2+\eta^{-1}(\Delta_0^2\|\psi-1\|_\infty^2+h^2\|W\|_\infty^2)}}\\
&\leq (1-\eta)^{-1/2}\left(1+\tfrac{1}{4T^2\eta}(\Delta_0^2\|\psi-1\|_\infty^2+h^2\|W\|_\infty^2)\right)\frac{H_\Delta}{\tanh\frac{1}{2T}H_\Delta}
\end{aligned}$$

for $0<\eta<1$. The Sobolev inequality and (5.15) show that $\|\psi\|_\infty \leq C\|\psi\|_{H^1}\leq C$, and hence the lemma follows by choosing $\eta = h$. □

To proceed, we denote $\alpha_\Delta = [\Gamma_\Delta]_{12}$ and recall from Theorem 3.2 that

$$\begin{aligned}
\alpha_\Delta &= \frac{\Delta_0}{4}\left(\psi K_T^0(-ih\nabla)^{-1} + K_T^0(-ih\nabla)^{-1}\psi\right) + \eta_1 + \eta_2\\
&= \frac{1}{2}\left(\psi\alpha^0 + \alpha^0\psi\right) + \eta_1+\eta_2
\end{aligned}$$

with η_1 and η_2 satisfying the bounds (3.9) and (3.10). The second equality follows from the explicit form (1.10) of α^0. Comparing this with (5.14) we infer that

$$\alpha = \alpha_\Delta + \sigma - \eta_1 - \eta_2\,. \tag{5.35}$$

Then (5.33) and (5.34) imply that

$$\begin{aligned}
&\tfrac{T}{2}\,\mathcal{H}(\Gamma,\Gamma_\Delta) - ah\int_{\mathcal{C}}|\sigma(x,x)|^2\,dx\\
&\quad\geq (1-ch)\,\mathrm{Tr}\,K_T^0(-ih\nabla)(\alpha-\alpha_\Delta)(\overline{\alpha-\alpha_\Delta}) - ah\int_{\mathcal{C}}|\sigma(x,x)|^2\,dx\\
&\quad\geq (1-ch)\,\mathrm{Tr}\,K_T^0(-ih\nabla)\sigma\overline{\sigma} - ah\int_{\mathcal{C}}|\sigma(x,x)|^2\,dx\\
&\qquad - (1-ch)2\,\mathrm{Re}\,\mathrm{Tr}\,K_T^0(-ih\nabla)\sigma(\overline{\eta_1+\eta_2})\,.
\end{aligned}\tag{5.36}$$

In order to bound the first term on the right side from below we are going to choose a parameter $\rho\geq 0$ such that $ch+\rho\leq 1/2$. Here c is the constant from

(5.34). (Eventually, we will pick either $\rho = 0$ or $\rho = 1/4$, say.) Note that

$$(1 - ch)\,\mathrm{Tr}\, K_T^0(-ih\nabla) - ah\delta = \rho K_T^0(-ih\nabla) + (1 - 2ch - 2\rho)(K_T^0(-ih\nabla) - ah\delta) + (ch + \rho)(K_T^0(-ih\nabla) - 2ah\delta)\,.$$

We recall that the operator $K_T^0(-ih\nabla) - ah\delta$ is non-negative and that the operator $K_T^0(-ih\nabla) - 2ah\delta$ has a negative eigenvalue of order one (by the form boundedness of δ with respect to $K_T^0(-i\nabla)$). Hence $K_T^0(-ih\nabla) - 2ah\delta \geq -C_1$ with a constant C_1 independent of h. (In the following it will be somewhat important to keep track of various constants, therefore we introduce here a numbering.) Moreover, using the fact that $K_T^0(-ih\nabla) \geq c_1(1 - h^2\nabla^2)$ we arrive at the lower bound

$$(1 - ch)\,\mathrm{Tr}\, K_T^0(-ih\nabla) - ah\delta \geq c_1\rho(1 - h^2\nabla^2) - C_1(ch + \rho)\,,$$

which means for the first term on the right side of (5.36) that

$$(1-ch)\,\mathrm{Tr}\, K_T^0(-ih\nabla)\sigma\overline{\sigma} - ah\int_{\mathcal{C}} |\sigma(x,x)|^2\, dx \geq c_1\rho\|\sigma\|_{H^1}^2 - C_1(ch+\rho)\|\sigma\|_2^2\,. \quad (5.37)$$

We now turn to the second term on the right side of (5.36). Theorem 3.2, together with the bounds (5.15) on ψ, implies that $\|\eta_1+\eta_2\|_{H^1}^2 \leq C\epsilon^2 h^3$. This bound, combined with $\|\sigma\|_{H^1}^2 \leq C\epsilon^{-2}h^3$ from Lemma 5.3, however, is not good enough. (It leads to an error of order h^3.) Instead, we shall make use of the observation that in the decompositions $\sigma = \sigma_1 + \sigma_2$ and $\eta_1 + \eta_2$ one has

$$\mathrm{Tr}\, K_T^0(-ih\nabla)\sigma_2\overline{\eta_1} = 0\,.$$

This can be seen by writing out the trace in momentum space and recalling that the Fourier transform of the ψ involved in σ_2 has support in $\{|p| \geq \epsilon h^{-1}\}$, whereas the one of the ψ involved in η_1 has support in $\{|p| < \epsilon h^{-1}\}$ (see also (6.22)).

Using the estimates (5.17) and (3.10) on σ_1 and η_2 we conclude that

$$\begin{aligned}\left|\mathrm{Tr}\, K_T^0(-ih\nabla)\sigma(\overline{\eta_1 + \eta_2})\right| &\leq \left|\mathrm{Tr}\, K_T^0(-ih\nabla)\sigma_1\overline{\eta_1}\right| + \left|\mathrm{Tr}\, K_T^0(-ih\nabla)\sigma\overline{\eta_2}\right| \\ &\leq C_2\left(\epsilon h^3 + h^{5/2}\|\sigma\|_{H^1}\right)\,. \end{aligned} \quad (5.38)$$

Combining (5.36), (5.37) and (5.38) we find that

$$\begin{aligned}&\tfrac{T}{2}\,\mathcal{H}(\Gamma,\Gamma_\Delta) - ah\int_{\mathcal{C}} |\sigma(x,x)|^2\, dx \\ &\quad \geq c_1\rho\|\sigma\|_{H^1}^2 - C_1(ch+\rho)\|\sigma\|_2^2 - 2C_2\left(\epsilon h^3 + h^{5/2}\|\sigma\|_{H^1}\right)\,. \end{aligned} \quad (5.39)$$

Next, we are going to distinguish two cases, according to whether $4C_1\|\sigma\|_2^2 \leq c_1\|\sigma\|_{H^1}^2$ or not. In the first case, we choose $\rho = 1/4$ and h so small that $ch + \rho \leq 1/2$. In this way we can bound the previous expression from below by

$$\tfrac{1}{8}c_1\|\sigma\|_{H^1}^2 - 2C_2\left(\epsilon h^3 + h^{5/2}\|\sigma\|_{H^1}\right) \geq -8c_1^{-1}C_2^2 h^5 - 2C_2\epsilon h^3\,.$$

This proves the claimed (indeed, a better) bound (5.32) in this case.

Now assume, conversely, that $4C_1\|\sigma\|_2^2 > c_1\|\sigma\|_{H^1}^2$. Then we choose $\rho = 0$ and bound (5.39) from below by

$$\begin{aligned} & - C_1 ch\|\sigma\|_2^2 - 2C_2\left(\epsilon h^3 + h^{5/2}\|\sigma\|_{H^1}\right) \\ & \geq -C_1 ch\|\sigma\|_2^2 - 2C_2\left(\epsilon h^3 + h^{5/2}\left(4C_1/c_1\right)^{1/2}\|\sigma\|_2\right) . \end{aligned}$$

The bound (5.16) on $\|\sigma\|_2$ now leads again to the claimed lower bound (5.32).

This concludes the proof of the lower bound to the free energy in Theorem 1.2. Concerning the statement about approximate minimizers we note that $\mathcal{F}^{\mathrm{BCS}}(\Gamma^0) - \mathcal{F}^{\mathrm{BCS}}(\Gamma_0) = O(h^3)$ and that our a-priori bounds on α in Proposition 5.3 remain true under the weaker condition that $\mathcal{F}^{\mathrm{BCS}}(\Gamma) \leq \mathcal{F}^{\mathrm{BCS}}(\Gamma^0) + Ch^3$. We leave the details to the reader.

6. Proof of semiclassical asymptotics

In this section we shall sketch the proofs of Theorems 3.1 and 3.2 containing the semiclassical asymptotics. We shall skip some technical details and refer to [7] for a thorough discussion.

6.1. Preliminaries

It will be convenient to use the following abbreviations

$$k = -h^2\nabla^2 - \mu + h^2 W(x), \qquad k_0 = -h^2\nabla^2 - \mu . \tag{6.1}$$

We will frequently have to bound various norms of the resolvents $(z-k)^{-1}$ for z in the contour Γ defined by $\operatorname{Im} z = \pm\pi/(2\beta)$ for $\beta > 0$. We state these auxiliary bounds separately.

For $p \geq 1$, we define the p-norm of a periodic operator A by

$$\|A\|_p = \left(\operatorname{Tr}|A|^p\right)^{1/p} \tag{6.2}$$

where Tr stands again for the trace per unit volume. We note that for a Fourier multiplier $A(-ih\nabla)$, these norms are given as

$$\|A(-ih\nabla)\|_p = h^{-1/p}\left(\int_{\mathbb{R}} |A(q)|^p \frac{dq}{2\pi}\right)^{1/p} . \tag{6.3}$$

The usual operator norm will be denoted by $\|A\|_\infty$.

Lemma 6.1. *For $z = t \pm i\pi/(2\beta)$ and all sufficiently small h one has*

$$\left\|(z-k)^{-1}\right\|_p \leq C\, h^{-1/p} \times \begin{cases} t^{-1/(2p)} & \text{for } t \gg 1 \\ |t|^{-1+1/(2p)} & \text{for } t \ll -1 \end{cases} \qquad \text{if } 1 \leq p \leq \infty , \tag{6.4}$$

as well as

$$\left\|(z-k)^{-1}\right\|_\infty \leq C \times \begin{cases} 1 & \text{for } t \gg 1 \\ |t|^{-1} & \text{for } t \ll -1 \end{cases} . \tag{6.5}$$

Proof. The estimates are easily derived with k_0 instead of k by evaluating the corresponding integral. Since the spectra of k and k_0 agree up to $O(h^2)$ the same bounds hold for k. $\square$

6.2. Proof of Theorem 3.1

The function f in (3.2) is analytic in the strip $|\operatorname{Im} z| < \pi$, and we can write

$$f(\beta H_\Delta) - f(\beta H_0) = \frac{1}{2\pi i} \int_\Gamma f(\beta z) \left[\frac{1}{z - H_\Delta} - \frac{1}{z - H_0} \right] dz\,,$$

where Γ is the contour $z = r \pm i\frac{\pi}{2\beta}$, $r \in \mathbb{R}$. We emphasize that this contour representation is not true for the operators $f(\beta H_\Delta)$ and $f(\beta H_0)$ separately (because of a contribution from infinity), but only for their difference.

We claim that

$$[f(\beta H_\Delta)]_{11} = \overline{[f(\beta H_\Delta)]_{22}} - \beta\overline{[H_\Delta]_{22}}\,. \tag{6.6}$$

Recall that $[\,\cdot\,]_{ij}$ denotes the ij element of an operator-valued 2×2 matrix. To see (6.6), we introduce the unitary matrix

$$U = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

and note that

$$[f(\beta H_\Delta)]_{11} = -\,[U f(\beta H_\Delta) U]_{22}\,.$$

On the other hand, $U H_\Delta U = -\overline{H_\Delta}$, which implies that

$$U f(\beta H_\Delta) U = f(-\beta \overline{H_\Delta}) = \overline{f(-\beta H_\Delta)}\,.$$

The claim (6.6) now follows from the fact that $f(-z) = f(z) - z$.

Subtracting (6.6) and the corresponding formula for H_0 and noting that H_Δ and H_0 coincide on the diagonal we find that the two diagonal entries of $f(\beta H_\Delta) - f(\beta H_0)$ are complex conjugates of each other. Since their trace is real we conclude that

$$\operatorname{Tr}\left[f(\beta H_\Delta) - f(\beta H_0)\right] = \frac{1}{\pi i} \int_\Gamma f(\beta z)\, \operatorname{Tr} \left[\frac{1}{z - H_\Delta} - \frac{1}{z - H_0} \right]_{11} dz\,.$$

(For technical details concerning the interchange of the trace and the integral we refer to [7].)

The resolvent identity and the fact that

$$\delta := H_\Delta - H_0 = -h \begin{pmatrix} 0 & \psi(x) \\ \overline{\psi(x)} & 0 \end{pmatrix} \tag{6.7}$$

is off-diagonal (as an operator-valued 2×2 matrix) implies that

$$\begin{aligned}\operatorname{Tr}\left[\frac{1}{z-H_\Delta}-\frac{1}{z-H_0}\right]_{11} &= \operatorname{Tr}\left[\frac{1}{z-H_0}\left(\delta\frac{1}{z-H_0}\right)^2\right]_{11} \\ &\quad + \operatorname{Tr}\left[\frac{1}{z-H_0}\left(\delta\frac{1}{z-H_0}\right)^4\right]_{11} + \operatorname{Tr}\left[\frac{1}{z-H_\Delta}\left(\delta\frac{1}{z-H_0}\right)^6\right]_{11} \\ &=: I_1 + I_2 + I_3\,.\end{aligned}$$

In the following we shall prove that

$$\begin{aligned}\frac{1}{\pi i}\int_\Gamma f(\beta z) I_1\,dz = &-\frac{h\beta^2}{2}\|\psi\|_2^2\int_{\mathbb{R}} g_0(\beta(q^2-\mu))\,\frac{dq}{2\pi} \\ &+\frac{h^3\beta^3}{8}\|\psi'\|_2^2\int_{\mathbb{R}}\left(g_1(\beta(q^2-\mu))+2\beta q^2 g_2(\beta(q^2-\mu))\right)\frac{dq}{2\pi} \\ &+\frac{h^3\beta^3}{2}\langle\psi|W|\psi\rangle\int_{\mathbb{R}} g_1(\beta(q^2-\mu))\,\frac{dq}{2\pi} \\ &+O(h^5)\|\psi\|_{H^2}^2\,, \end{aligned} \tag{6.8}$$

$$\frac{1}{\pi i}\int_\Gamma f(\beta z) I_2\,dz = \frac{h^3\beta^3}{8}\|\psi\|_4^4\int_{\mathbb{R}}\frac{g_1(\beta(q^2-\mu))}{q^2-\mu}\,\frac{dq}{2\pi} + O(h^5)\|\psi\|_{H^1}^3\|\psi\|_{H^2} \tag{6.9}$$

and

$$\frac{1}{\pi i}\int_\Gamma f(\beta z) I_3\,dz = O(h^5)\|\psi\|_{H^1}^6\,. \tag{6.10}$$

This will clearly prove (3.6). We will treat the three terms I_3, I_2 and I_1 (in this order) separately.

I_3: With the notation k introduced in (6.1) at the beginning of this section, we have

$$I_3 = \operatorname{Tr}\left[\frac{1}{z-H_\Delta}\right]_{11}\Delta\frac{1}{z+k}\Delta^\dagger\frac{1}{z-k}\Delta\frac{1}{z+k}\Delta^\dagger\frac{1}{z-k}\Delta\frac{1}{z+k}\Delta^\dagger\frac{1}{z-k}\,.$$

Using Hölder's inequality for the trace per unit volume (see [7]) and the fact that $|z-H_\Delta| \geq \pi/(2\beta)$, we get

$$|I_3| \leq \frac{2\beta}{\pi}h^6\|\psi\|_\infty^6\left\|(z-k)^{-1}\right\|_6^3\left\|(z+k)^{-1}\right\|_6^3\,.$$

Together with (6.4), this yields

$$|I_3| \leq \frac{Ch^5}{1+|z|^3}\|\psi\|_\infty^6\,.$$

Here it was important to get a decay faster than $|z|^{-2}$, since we need to integrate I_3 against the function f which behaves linearly at $-\infty$. Since $\|\psi\|_\infty \leq C\|\psi\|_{H^1}$ by Sobolev inequalities we have completed the proof of (6.10).

***I*₂**: We continue with

$$I_2 = \operatorname{Tr} \frac{1}{z-k}\Delta\frac{1}{z+k}\Delta^\dagger\frac{1}{z-k}\Delta\frac{1}{z+k}\Delta^\dagger\frac{1}{z-k}\,.$$

By the resolvent identity we have

$$\frac{1}{z-k} = \frac{1}{z-k_0} + \frac{1}{z-k_0}h^2W\frac{1}{z-k}\,. \tag{6.11}$$

Using Hölder as above, we can bound

$$\begin{aligned}&\left|\operatorname{Tr}\left(\frac{1}{z-k}-\frac{1}{z-k_0}\right)\Delta\frac{1}{z+k}\Delta^\dagger\frac{1}{z-k}\Delta\frac{1}{z+k}\Delta^\dagger\frac{1}{z-k}\right|\\ &\quad\le h^6\|W\|_\infty\left\|(z-k_0)^{-1}\right\|_\infty\|\psi\|_\infty^4\|(z-k)^{-1}\|_3^3\|(z+k)^{-1}\|_\infty^2\,.\end{aligned} \tag{6.12}$$

By (6.4) and (6.5) this is bounded by $Ch^5\|\psi\|^4_{H^1(\mathcal{C})}(1+|z|^{5/2})^{-1}$. What we effectively have achieved for this error is, therefore, to replace one factor of $(z-k)^{-1}$ in I_2 by a factor of $(z-k_0)^{-1}$

In exactly the same way we proceed with the remaining factors $(z-k)^{-1}$ and $(z+k)^{-1}$ in I_2. The only difference is that k might now be replaced by k_0 in the terms we have already treated, but this does not effect the bounds.

The final result is that $(\pi i)^{-1}\int_\Gamma f(\beta z)\, I_2\, dz$ equals

$$\frac{1}{\pi i}\int_\Gamma f(\beta z)\operatorname{Tr}\left[\frac{1}{z-k_0}\Delta\frac{1}{z+k_0}\Delta^\dagger\frac{1}{z-k_0}\Delta\frac{1}{z+k_0}\Delta^\dagger\frac{1}{z-k_0}\right]dz + O(h^5)\|\psi\|^4_{H^1}\,,$$

and it remains to compute the asymptotics of the integral.

Let us indicate how to perform the trace per unit volume $\operatorname{Tr}[\ldots]$. In terms of integrals the trace can be written as

$$\begin{aligned}&\frac{h^4}{(2\pi)^4}\int_0^1 dx_1\int_{\mathbb{R}}dx_2\int_{\mathbb{R}}dx_3\int_{\mathbb{R}}dx_4\int_{\mathbb{R}^4}dp_1dp_2dp_3dp_4\;\overline{\psi(x_1)}\psi(x_2)\overline{\psi(x_3)}\psi(x_4)\\ &\quad\times\frac{e^{ip_1(x_1-x_2)}}{(z-(h^2p_1^2-\mu))^2}\frac{e^{ip_2(x_2-x_3)}}{z+(h^2p_2^2-\mu)}\frac{e^{ip_3(x_3-x_4)}}{z-(h^2p_3^2-\mu)}\frac{e^{ip_4(x_4-x_1)}}{z+(h^2p_4^2-\mu)}\,.\end{aligned} \tag{6.13}$$

Since ψ is periodic with period one we have

$$\psi(x_j) = \sum_{l_j\in 2\pi\mathbb{Z}}\hat\psi(l_j)e^{ix_jl_j}\,.$$

We insert this into the above integral and perform the integrals over x_2, x_3, x_4. This leads to δ-distributions such that we can subsequently perform the integrals over p_2, p_3, p_4, as well as the integral over x_1. In this way we obtain

$$\begin{aligned}&\frac{1}{\pi i}\int_\Gamma f(\beta z)\operatorname{Tr}\left[\frac{1}{z-k_0}\Delta\frac{1}{z+k_0}\Delta^\dagger\frac{1}{z-k_0}\Delta\frac{1}{z+k_0}\Delta^\dagger\frac{1}{z-k_0}\right]dz\\ &\quad= h^3\sum_{p_1,p_2,p_3\in 2\pi\mathbb{Z}}\widehat{\psi}(p_1)\widehat{\psi^*}(p_2)\widehat{\psi}(p_3)\widehat{\psi^*}(-p_1-p_2-p_3)F(hp_1,hp_2,hp_3)\end{aligned}$$

with

$$F(p_1,p_2,p_3) = \frac{\beta^4}{\pi i}\int_\Gamma dz\, f(\beta z)\int_{\mathbb{R}}\frac{dq}{2\pi}\frac{1}{\left(z-\beta((q+p_1+p_2+p_3)^2+\mu)\right)^2}$$
$$\times \frac{1}{z+\beta((q+p_1+p_2)^2-\mu)}\,\frac{1}{z-\beta((q+p_1)^2-\mu)}\,\frac{1}{z+\beta(q^2-\mu)}\,.$$

The leading behavior is given by

$$F(0,0,0)\sum_{p_1,p_2,p_3\in 2\pi\mathbb{Z}}\widehat{\psi}(p_1)\widehat{\psi^*}(p_2)\widehat{\psi}(p_3)\widehat{\psi^*}(-p_1-p_2-p_3) = F(0,0,0)\|\psi\|_4^4\,.$$

The integral $F(0,0,0)$ can be calculated explicitly and we obtain

$$F(0,0,0) = \frac{\beta^3}{8}\int_{\mathbb{R}}\frac{g_1(\beta(q^2-\mu))}{q^2-\mu}\,\frac{dq}{2\pi}$$

with g_1 from (3.4). In order to estimate the remainder we use the fact that [7]

$$|F(p_1,p_2,p_3)-F(0,0,0)| \leq \text{const}\left(p_1^2+p_2^2+p_3^2\right)\,.$$

Using Schwarz and Hölder we can bound

$$\sum_{p_1,p_2,p_3\in 2\pi\mathbb{Z}} p_1^2\left|\widehat{\psi}^*(p_1)\widehat{\psi}^*(p_2)\widehat{\psi}(p_3)\widehat{\psi}(-p_1-p_2-p_3)\right| \leq \text{const}\,\|\psi\|_{H^2}\|\psi\|_{H^1}^3$$

and equally with p_1^2 replaced by p_2^2 and p_3^2. Hence we conclude that

$$\begin{aligned}
&\frac{1}{\pi i}\int_\Gamma f(\beta z)\, I_2\, dz\\
&= h^3\sum_{p_1,p_2,p_3\in 2\pi\mathbb{Z}}\widehat{\psi}(p_1)\widehat{\psi^*}(p_2)\widehat{\psi}(p_3)\widehat{\psi^*}(-p_1-p_2-p_3)F(hp_1,hp_2,hp_3) + O(h^5)\|\psi\|_{H^1}^4\\
&= h^3F(0,0,0)\|\psi\|_4^4 + O(h^5)\|\psi\|_{H^1}^3\|\psi\|_{H^2}\,.
\end{aligned}$$

This is what we claimed in (6.9).

$\boldsymbol{I_1}$: Finally, we examine the contribution of

$$I_1 = \operatorname{Tr}\left[\frac{1}{z-k}\Delta\frac{1}{z+k}\Delta^\dagger\frac{1}{z-k}\right]\,.$$

Using the resolvent identity (6.11) we can write $I_1 = I_1^a + I_1^b + I_1^c$, where

$$I_1^a = \operatorname{Tr}\left[\frac{1}{z-k_0}\Delta\frac{1}{z+k_0}\Delta^\dagger\frac{1}{z-k_0}\right]$$

and

$$I_1^b = \mathrm{Tr}\Bigg[\frac{1}{z-k_0}(k-k_0)\frac{1}{z-k_0}\Delta\frac{1}{z+k_0}\Delta^\dagger\frac{1}{z-k_0} + \frac{1}{z-k_0}\Delta\frac{1}{z+k_0}(k_0-k)\frac{1}{z+k_0}\Delta^\dagger\frac{1}{z-k_0} + \frac{1}{z-k_0}\Delta\frac{1}{z+k_0}\Delta^\dagger\frac{1}{z-k_0}(k-k_0)\frac{1}{z-k_0}\Bigg].$$

The part I_1^c consists of the rest. We claim that

$$\frac{1}{\pi i}\int_\Gamma f(\beta z)\, I_1^a\, dz = -\frac{h\beta^2}{2}\|\psi\|_2^2\int_{\mathbb{R}} g_0(\beta(q^2-\mu))\,\frac{dq}{2\pi} + \frac{h^3\beta^3}{8}\|\psi'\|_2^2\int_{\mathbb{R}}\big(g_1(\beta(q^2-\mu)) + 2\beta q^2 g_2(\beta(q^2-\mu))\big)\,\frac{dq}{2\pi} + O(h^5)\|\psi\|_{H^2}^2\,, \tag{6.14}$$

$$\frac{1}{\pi i}\int_\Gamma f(\beta z)\, I_1^b\, dz = \frac{h^3\beta^3}{2}\langle\psi|W|\psi\rangle\int_{\mathbb{R}} g_1(\beta(q^2-\mu))\,\frac{dq}{2\pi} + O(h^5)\|\psi\|_{H^2}\|\psi\|_{H^1} \tag{6.15}$$

and

$$\frac{1}{\pi i}\int_\Gamma f(\beta z)\, I_1^c\, dz = O(h^5)\|\psi\|_{H^1}^2\,. \tag{6.16}$$

Clearly, this will imply (6.8).

We begin with I_1^c. These terms contain at least five resolvents, where at least two terms are of the form $(z-k_\#)^{-1}$ and at least one term of the form $(z+k_\#)^{-1}$. (Here $k_\#$ stands for any of the operators k or k_0.) Moreover, they contain at least two factors of $k-k_0$. The terms are either of the type

$$A = \mathrm{Tr}\,\frac{1}{z-k_0}(k-k_0)\frac{1}{z-k}\Delta\frac{1}{z+k_0}(k_0-k)\frac{1}{z+k}\Delta^\dagger\frac{1}{z-k_0} \tag{6.17}$$

(at least three minus signs) or of the type

$$B = \mathrm{Tr}\,\frac{1}{z-k_0}\Delta\frac{1}{z+k_0}(k_0-k)\frac{1}{z+k_0}(k_0-k)\frac{1}{z+k}\Delta^\dagger\frac{1}{z-k} \tag{6.18}$$

(only two minus signs). Terms of the first type we bound by

$$|A| \leq Ch^6\|W\|_\infty^2\|\psi\|_\infty^2\|(z-k_0)^{-1}\|_\infty^2\|(z+k_0)^{-1}\|_3\|(z+k)^{-1}\|_3\|(z-k)^{-1}\|_3\,.$$

By (6.4) and (6.5) this can be estimated by $Ch^5|z|^{-2+1/6}$ if $\mathrm{Re}\, z \geq 1$ and by $Ch^5|z|^{-2-1/6}$ if $\mathrm{Re}\, z \leq -1$. This bound is finite when integrated against $f(\beta z)$.

Terms of type B can be bounded similarly by replacing z by $-z$. Indeed, we note that since $\int_\Gamma z\, B\, dz = 0$, we can replace $f(\beta z)$ by $f(-\beta z) = f(\beta z) - \beta z$ in the integrand without changing the value of the integral. I.e., we can integrate B against a function that decays exponentially for negative t and increases linearly for positive t, instead of the other way around. These considerations lead to the estimate (6.16).

Next, we discuss the term I_1^a. After doing the contour integral the term I_1^a gives

$$(\pi i)^{-1} \int_\Gamma f(\beta z)\, I_1^a \, dz = h \sum_{p \in 2\pi\mathbb{Z}} |\hat\psi(p)|^2 G(hp)$$

with

$$G(p) = -\frac{\beta}{2} \int_{\mathbb{R}} \frac{\tanh\left(\frac12 \beta((q+p)^2-\mu)\right) + \tanh\left(\frac12\beta(q^2-\mu)\right)}{(p+q)^2+q^2-2\mu} \, \frac{dq}{2\pi} \, .$$

By definition (3.3) we have

$$G(0) = -\frac{\beta^2}{2} \int_{\mathbb{R}} g_0(\beta(q^2-\mu)) \, \frac{dq}{2\pi} \, .$$

Integrating by parts we can write

$$G''(0) = \frac{\beta^3}{4} \int_{\mathbb{R}} \left(g_1(\beta(q^2-\mu)) + 2\beta q^2 g_2(\beta(q^2-\mu)) \right) \, \frac{dq}{2\pi}$$

with g_1 and g_2 from (3.4) and (3.5). Moreover, one can show that [7]

$$\left| G(p) - G(0) - \tfrac12 p^2 G''(0) \right| \leq C p^4 \, .$$

From this we conclude that

$$\begin{aligned} \frac{1}{\pi i} \int_\Gamma f(\beta z)\, I_1^a \, dz &= h \sum_{p \in 2\pi\mathbb{Z}} |\hat\psi(p)|^2 \left(G(0) + \tfrac12 G''(0) h^2 p^2 \right) + O(h^5) \|\psi\|_{H^2}^2 \\ &= hG(0) \|\psi\|_2^2 + \tfrac12 G''(0) h^3 \|\psi'\|_2^2 + O(h^5)\|\psi\|_{H^2}^2 \, , \end{aligned}$$

which is what we claimed in (6.14).

Finally, we proceed to I_1^b. After the contour integration we find

$$\frac{1}{\pi i} \int_\Gamma f(\beta z)\, I_1^b \, dz = h^3 \sum_{p,q \in 2\pi\mathbb{Z}} \widehat{\psi}^*(p) \widehat{\psi}(q) \widehat{W}(-p-q) L(hp,hq) \, ,$$

where

$$L(p,q) = \beta^3 \int_{\mathbb{R}} L(p,q,k) \, \frac{dk}{2\pi}$$

with

$$\begin{aligned} L(p,q,k) = \frac{1}{\pi i} \int_\Gamma & \ln\left(2 + e^{-\beta z} + e^{\beta z}\right) \frac{1}{z+k^2-\mu} \frac{1}{z-p^2+\mu} \frac{1}{z-q^2+\mu} \\ & \times \left(\frac{1}{z-p^2+\mu} + \frac{1}{z-q^2+\mu} + \frac{1}{z+k^2-\mu} \right) dz \, . \end{aligned}$$

We have

$$L(0,0) = \frac{\beta^3}{2} \int_{\mathbb{R}} g_1(\beta(k^2-\mu)) \, \frac{dk}{2\pi}$$

and (see [7] for details)

$$|L(p,q) - L(0,0)| \leq C \left(p^2 + q^2 \right) \, .$$

By the Schwarz inequality we can bound

$$\sum_{p,q\in 2\pi\mathbb{Z}} \left|\widehat{\psi}^*(p)\widehat{\psi}(q)\widehat{W}(-p-q)(p^2+q^2)\right| \leq C\|W\|_2\|\psi\|_{H^2}\|\psi\|_{H^1}\,,$$

and obtain

$$\begin{aligned}\frac{1}{\pi i}\int_\Gamma f(\beta z)\, I_1^b\, dz &= h^3 L(0,0)\sum_{p,q\in 2\pi\mathbb{Z}} \widehat{\psi}^*(-p)\widehat{\psi}(q)\widehat{W}(p-q) + O(h^5)\|\psi\|_{H^2}\|\psi\|_{H^1} \\ &= \frac{h^3\beta^3}{2}\langle\psi|W|\psi\rangle \int_{\mathbb{R}} g_1(\beta(k^2-\mu))\,\frac{dk}{2\pi} + O(h^5)\|\psi\|_{H^2}\|\psi\|_{H^1}\,.\end{aligned}$$

This concludes the proof of Theorem 3.1.

6.3. Proof of Theorem 3.2

Since the function ρ in (3.8) is analytic in the strip $|\operatorname{Im} z| < \pi$, we can write $[\rho(\beta H_\Delta)]_{12}$ with the aid of a contour integral representation as

$$[\rho(\beta H_\Delta)]_{12} = \frac{1}{2\pi i}\int_\Gamma \rho(\beta z)\left[\frac{1}{z-H_\Delta}\right]_{12} dz\,, \tag{6.19}$$

where Γ is again the contour $\operatorname{Im} z = \pm\pi/(2\beta)$. We expand $(z-H_\Delta)^{-1}$ using the resolvent identity and note that, since $H_\Delta = H_0 + \delta$ with a H_0 *diagonal* and δ *off-diagonal*, only the terms containing an odd number of δ's contribute to the 12-entry of $(z-H_\Delta)^{-1}$. In this way arrive at the decomposition

$$[\rho(\beta H_\Delta)]_{12} = \eta_0 + \eta_1 + \eta_2^a + \eta_2^b\,, \tag{6.20}$$

where

$$\eta_0 = -\frac{h}{4\pi i}\int_\Gamma \rho(\beta z)\left(\psi\;\frac{1}{z^2-k_0^2} + \frac{1}{z^2-k_0^2}\;\psi\right) dz\,, \tag{6.21}$$

$$\eta_1 = \frac{h}{4\pi i}\int_\Gamma \rho(\beta z)\left(\frac{1}{z-k_0}\,[\psi,k_0]\,\frac{1}{z^2-k_0^2} + \frac{1}{z^2-k_0^2}[\psi,k_0]\frac{1}{z+k_0}\right) dz\,, \tag{6.22}$$

$$\eta_2^a = -\frac{h^3}{2\pi i}\int_\Gamma \rho(\beta z)\frac{1}{z-k_0}\left(W\frac{1}{z-k}\psi + \psi\frac{1}{z+k_0}W\right)\frac{1}{z+k}\,dz \tag{6.23}$$

and

$$\eta_2^b = -\frac{h^3}{2\pi i}\int_\Gamma \rho(\beta z)\frac{1}{z-k}\psi\frac{1}{z+k}\bar{\psi}\frac{1}{z-k}\psi\left[\frac{1}{z-H_\Delta}\right]_{22} dz\,. \tag{6.24}$$

A simple residue computation yields

$$\begin{aligned}\eta_0 &= -\frac{h}{4}\left(\psi\;\frac{\rho(\beta k_0)-\rho(-\beta k_0)}{k_0} + \frac{\rho(\beta k_0)-\rho(-\beta k_0)}{k_0}\;\psi\right) \\ &= \frac{h\beta}{4}\left(\psi\; g_0(\beta k_0) + g_0(\beta k_0)\;\psi\right)\,,\end{aligned}$$

which is the main term claimed in the theorem. In the following we shall prove that

$$\|\eta_1\|_{H^1}^2 \le Ch^5\|\psi\|_{H^2}^2\,, \tag{6.25}$$

$$\|\eta_2^a\|_{H^1}^2 \le Ch^5\|\psi\|_{H^1}^2\,, \tag{6.26}$$

and

$$\|\eta_2^b\|_{H^1}^2 \le Ch^5\|\psi\|_{H^1}^6\,. \tag{6.27}$$

This clearly implies Theorem 3.2.

$\boldsymbol{\eta_1}$: The square of the H^1 norm of η_1 is given by

$$\|\eta_1\|_{H^1}^2 = h\sum_{p\in 2\pi\mathbb{Z}} |\hat\psi(p)|^2 J(hp)$$

with

$$J(p) = \frac{\beta^4}{4}\int_{\mathbb{R}} \left((q+p)^2-q^2\right)^2\left(1+q^2\right)|F(q+p,q)-F(q,q+p)|^2\,\frac{dq}{2\pi}$$

and $F(p,q)$ equals

$$\frac{1}{p^2-\mu}\frac{1}{1+e^{\beta(p^2-\mu)}}\frac{1}{1+e^{\beta(q^2-\mu)}}\left(\frac{e^{\beta(p^2-\mu)}-e^{\beta(q^2-\mu)}}{p^2-q^2}+\frac{e^{\beta(p^2+q^2-2\mu)}-1}{p^2+q^2-2\mu}\right).$$

One can show that $0\le J(p)\le Cp^4$ [7], which yields the desired bound (6.25).

$\boldsymbol{\eta_2^a}$: This term is a sum of two terms and we begin by bounding the first one, that is, $-h^3(2\pi i)^{-1}\int\rho(\beta z)(z-k_0)^{-1}W(z-k)^{-1}\psi(z+k)^{-1}\,dz$. Using Hölder's inequality for the trace per unit volume we find that the square of the H^1 norm of the integrand can be bounded by

$$\begin{aligned}&\operatorname{Tr}\left[\frac{1-h^2\nabla^2}{|z-k_0|^2}W\frac{1}{z-k}\psi\frac{1}{|z+k|^2}\overline{\psi}\frac{1}{\bar z-k}W\right]\\ &\quad\le\left\|\frac{1-h^2\nabla^2}{|z-k_0|^2}\right\|_\infty\|W\|_\infty^2\|\psi\|_\infty^2\|(z-k)^{-1}\|_\infty^2\|(z+k)^{-1}\|_2^2\,.\end{aligned}$$

In order to bound this we use (6.4) and (6.5), as well as the fact that $\|(1-h^2\nabla^2)|z-k_0|^{-2}\|_\infty$ is bounded by $C|z|^{-1}$ if $\operatorname{Re}z\le -1$ and by $C|z|$ if $\operatorname{Re}z\ge 1$. (This follows similarly as (6.5).) In particular, we conclude that for $\operatorname{Re}z\le -1$ the previous quantity is bounded by $Ch^{-1}\|\psi\|_\infty^2|z|^{-7/2}$. The square root of this is integrable against $\rho(\beta z)$ and we arrive at the bound $Ch^{5/2}\|\psi\|_\infty$ for the H^1 norm. For the positive z direction, we notice that $\rho(\beta z)$ decays exponentially leading to a finite result after z integration.

For the second term in η_2^a we proceed similarly. It is important to first notice that $\rho(z)=1-\rho(-z)$, however, and that the 1 does not contribute anything but integrates to zero. Proceeding as above we arrive at (6.26).

$\boldsymbol{\eta_2^b}$: Finally, we consider η_2^b. Using Hölder's inequality for the trace per unit volume and bounding $[(z-H_\Delta)^{-1}]_{22}$ by $2\beta/\pi$ for $z\in\Gamma$ we find that the square of the H^1 norm of the integrand is bounded by

$$\frac{4\beta^2}{\pi^2}\|\psi\|_\infty^6 \left\| \frac{1-h^2\nabla^2}{|z-k_0|^2} \right\|_\infty \|(z-k)^{-1}\|_\infty^2 \|(z+k)^{-1}\|_2^2 \,.$$

Similarly as in the bound for η_2^a one can show that for $\operatorname{Re} z \leq -1$ this is bounded by $Ch^{-1}\|\psi\|_\infty^6 |z|^{-7/2}$. This leads to (6.27).

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Eigenfunction Expansions Associated with the One-dimensional Schrödinger Operator

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Abstract. We consider the form of eigenfunction expansions associated with the time-independent Schrödinger operator on the line, under the assumption that the limit point case holds at both of the infinite endpoints. It is well known that in this situation the multiplicity of the operator may be one or two, depending on properties of the potential function. Moreover, for values of the spectral parameter in the upper half complex plane, there exist Weyl solutions associated with the restrictions of the operator to the negative and positive half-lines respectively, together with corresponding Titchmarsh-Weyl functions.

In this paper, we establish some alternative forms of the eigenfunction expansion which exhibit the underlying structure of the spectrum and the asymptotic behaviour of the corresponding eigenfunctions. We focus in particular on cases where some or all of the spectrum is simple and absolutely continuous. It will be shown that in this situation, the form of the relevant part of the expansion is similar to that of the singular half-line case, in which the origin is a regular endpoint and the limit point case holds at infinity. Our results demonstrate the key role of real solutions of the differential equation which are pointwise limits of the Weyl solutions on one of the half-lines, while all solutions are of comparable asymptotic size at infinity on the other half-line.

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1. Introduction

The study of eigenfunction expansions associated with singular differential operators of the Sturm-Liouville type was initiated by Weyl [6], [19], and subsequently generalised by Stone, Kodaira, Titchmarsh, and others [16], [14], [17], [18]. Particularly well known are the Fourier, Hermite and Legendre expansions, the Laguerre polynomials and the Fourier-Bessel series, all of which have widespread applications in engineering and the physical sciences. It therefore seems worthwhile to explore the general behaviour of the eigenfunctions which contribute to such expansions, to investigate the relationship between the eigenfunctions and spectral properties, and to consider under what circumstances the formal structure of the standard expansions can be improved.

In the case of singular Sturm-Liouville operators, the eigenfunctions are themselves solutions of the differential equations. If the multiplicity of the spectrum is two then every solution of $Lu = \lambda u$ may be regarded as an eigenfunction, but since the dimension of the solution space is also two, we expect not more than two linearly independent solutions to feature as integral kernels in the expansions. In a similar way, it seems reasonable to expect that when the spectrum, or a part of the spectrum, is simple then for each relevant value of λ, precisely one linearly independent solution should feature in the expansion. This expectation has recently been confirmed for some specific classes of singular Sturm-Liouville operators, which include cases where both singular endpoints are limit point (see, e.g., [7], [8]).

It is the purpose of this paper to demonstrate that, in the case where part or all of the absolutely continuous spectrum is simple, the corresponding part of the expansion can always be reformulated in such a way that the integral kernels are, up to scalar multiples, the unique eigenfunctions themselves. To achieve this result we start from the Weyl-Kodaira expansion formula [3], [14], and following the method of Kac [12], [13], diagonalise the spectral density matrix in order to identify the eigenfunctions and simplify the expansion. It turns out that in the process of reformulating the part of the expansion where the spectral multiplicity is one, the contribution of the half-line operators $H_{-\infty}$ and H_{∞} is reflected through their respective Titchmarsh-Weyl m-functions and corresponding spectral densities. This information enables the asymptotic behaviour of the eigenfunctions at $\pm\infty$ to be determined in terms of the theory of subordinacy [10], [11], and details of the process will be demonstrated through worked examples.

Note. Throughout the paper the use of the term "eigenfunctions" is not restricted to specific real solutions of the differential equation which are in $L_2(\mathbf{R})$, but also includes "eigendifferentials" in the terminology of Weyl [4], [19], as well as other relevant solutions associated with the essential spectrum. Where appropriate we will distinguish between singular eigenfunctions and absolutely continuous eigenfunctions depending on whether the corresponding λ-values are in the minimal supports of the singular, respectively absolutely continuous parts of the spectral measure, and the term generalised eigenfunction will be used to refer to an eigenfunction of either type.

2. Mathematical background

In this section we briefly summarize the relevant underlying theory from which the main results of this paper are obtained.

Consider the differential operator H on $L_2(-\infty,\infty)$ associated with

$$Lu := -u'' + q(r)u = \lambda u, \qquad -\infty < r < \infty,$$

where $q(r) : \mathbf{R} \to \mathbf{R}$ is locally integrable, $\lambda \in \mathbf{R}$ is the spectral parameter, and the differential expression L is in Weyl's limit point case at $\pm\infty$. In this case the unique self-adjoint operator H is defined by

$$Hf = Lf, \qquad f \in \mathcal{D}(H),$$

where $f \in \mathcal{D}(H)$ if

(i) $f, Lf \in L_2(\mathbf{R})$,
(ii) f, f' are locally absolutely continuous on $\mathbf{R}$.

We refer to H as the Schrödinger operator on the line.

It is convenient in this context to use the so-called splitting method to analyse the spectrum of H and derive appropriate formulations of the associated eigenfunction expansion. We first define the half-line operator H_∞ to be the restriction of H to $L_2([0,\infty))$ with a Dirichlet boundary condition at $r=0$, and choose a fundamental set of solutions $\{u_1(r,z), u_2(r,z)\}$ of $Lu = zu$, $z \in \mathbf{C}$, to satisfy

$$u_1(0,z) = u_2'(0,z) = 0, \qquad u_2(0,z) = u_1'(0,z) = 1, \tag{2.1}$$

where for $i = 1,2$, $u_i'(0,z)$ denotes the value at $r=0$ of the derivative of $u_i(r,z)$ with respect to r. Associated with H_∞, there exists a Herglotz function $m_\infty(z) : \mathbf{C}^+ \to \mathbf{C}^+$ known as the Titchmarsh-Weyl function, such that the solution $u_2(r,z) + m_\infty(z)\,u_1(r,z)$ of $Lu = zu$ is in $L_2([0,\infty))$ for all $z \in \mathbf{C}^+$. The related spectral function $\rho_\infty(\lambda) : \mathbf{R} \to \mathbf{R}$ is non-decreasing, continuous on the right and generates a non-negative Borel-Stieltjes measure μ_∞ on $\mathbf{R}$. Its derivative, the spectral density function $\rho_\infty'(\lambda)$, exists and satisfies

$$\rho_\infty'(\lambda) = \lim_{z\downarrow\lambda} \frac{1}{\pi}\,\mathrm{Im}\, m_\infty(z), \quad z = \lambda + \mathrm{i}\epsilon, \tag{2.2}$$

for Lebesgue and μ_∞-almost all $\lambda \in \mathbf{R}$, and the spectrum $\sigma(H_\infty)$ may be defined by

$$\sigma(H_\infty) := \mathbf{R} \setminus \{\lambda \in \mathbf{R} : \rho_\infty \text{ is constant in a neighbourhood } N(\lambda) \text{ of } \lambda\},$$

which is the smallest closed set containing the points of increase of $\rho_\infty(\lambda)$.

The half-line operator $H_{-\infty}$ on $L_2((-\infty,0])$ is defined in a similar way, the principal difference being that the Titchmarsh-Weyl function $m_{-\infty}(z)$ has negative imaginary part on $\mathbf{C}^+$, so that the spectral density $\rho_{-\infty}'(\lambda)$ satisfies

$$\rho_{-\infty}'(\lambda) = -\lim_{z\uparrow\lambda} \frac{1}{\pi}\,\mathrm{Im}\, m_{-\infty}(z), \quad z = \lambda + \mathrm{i}\epsilon, \tag{2.3}$$

for Lebesgue and $\mu_{-\infty}$-almost all $\lambda \in \mathbf{R}$. We note that the spectrum of both half-line operators is simple, that is to say, both H_∞ and $H_{-\infty}$ have spectral multiplicity one.

The standard form of the eigenfunction expansion associated with the self-adjoint operator H_∞ is as follows for $f(r) \in L_2([0,\infty))$:

$$f(r) = \underset{\omega\to\infty}{\text{l.i.m.}} \int_{-\omega}^{\omega} u_1(r,\lambda)\, G(\lambda)\, d\rho_\infty(\lambda), \tag{2.4}$$

where $u_1(r,\lambda)$, $0 \le r < \infty$, satisfies the boundary condition in (2.1) with $z = \lambda \in \mathbf{R}$, and

$$G(\lambda) = \underset{\eta\to\infty}{\text{l.i.m.}} \int_0^{\eta} u_1(r,\lambda)\, f(r)\, dr,$$

where convergence in the mean is in $L_2([0,\infty))$ and $L_2(\mathbf{R}; d\rho_\infty(\lambda))$ respectively [2]. Note that $G(\lambda)$ only contributes to the expansion (2.4) for those λ which are points of increase of ρ_∞, or more precisely, belong to a minimal support of μ_∞ (see Definition 2 below). We see that the integral kernel of both transform and inverse transform is a solution of $Lu = \lambda u$ satisfying the Dirichlet boundary condition at $r = 0$, namely $u_1(r,\lambda)$, and it follows that $u_1(r,\lambda)$ is an eigenfunction of H_∞ for those λ contributing to the spectrum of the operator. Note that the spectral function $\rho_\infty(\lambda)$ is constant on each open interval of the resolvent set, so that there is no contribution to the integral in (2.4) when λ is in the resolvent set. The expansion associated with the operator $H_{-\infty}$ has a similar form, with obvious adjustments.

In the case of the full line operator H, the analogue of the Titchmarsh-Weyl m-function is a 2×2 M-matrix, which is defined in terms of the scalar m-functions associated with $H_{-\infty}$ and H_∞ by

$$M(z) := \frac{1}{m_{-\infty} - m_\infty} \begin{pmatrix} m_{-\infty} m_\infty & \frac{1}{2}(m_{-\infty} + m_\infty) \\ \frac{1}{2}(m_{-\infty} + m_\infty) & 1 \end{pmatrix} \tag{2.5}$$

for $z \in \mathbf{C}^+$. The associated matrix spectral function for $\lambda \in \mathbf{R}$,

$$(\rho_{ij}(\lambda)) := \begin{pmatrix} \rho_{11}(\lambda) & \rho_{12}(\lambda) \\ \rho_{21}(\lambda) & \rho_{22}(\lambda) \end{pmatrix},$$

is continuous on the right, has bounded variation on compact subintervals of the real line, and generates a Borel-Stieltjes measure (μ_{ij}) which is positive semi-definite [14]. The components of the corresponding density matrix $\left(\rho'_{ij}(\lambda)\right)$ satisfy

$$\rho'_{ij}(\lambda) = \lim_{z\downarrow\lambda} \frac{1}{\pi} \operatorname{Im} M_{ij}(z), \quad z = \lambda + \mathrm{i}\epsilon, \tag{2.6}$$

Lebesgue and μ_{ij}-almost everywhere on $\mathbf{R}$ for each $i,j = 1,2$, and the spectrum of H is given by

$$\sigma(H) := \mathbf{R} \setminus \{\lambda \in \mathbf{R} : (\rho_{ij}) \text{ is constant in a neighbourhood } N(\lambda) \text{ of } \lambda\}.$$

As noted above, both the half-line operators, $H_{-\infty}$ and H_∞, have spectral multiplicity one; however, in the case of the full line operator H where both endpoints are limit point, some or all of the spectrum may have multiplicity two. Here the standard formulation of the expansion in its most general form is given by the Weyl-Kodaira formula [3], [14], from which we have for $f \in L_2(\mathbf{R})$,

$$f(r) = \underset{\omega\to\infty}{\text{l.i.m.}} \int_{-\omega}^{\omega} \sum_{i=1}^{2}\sum_{j=1}^{2} u_i(r,\lambda)\ F_j(\lambda)\ d\rho_{ij}(\lambda), \tag{2.7}$$

where

$$F(\lambda) = \{F_1(\lambda), F_2(\lambda)\} = \underset{\eta\to\infty}{\text{l.i.m.}} \left\{ \int_{-\eta}^{\eta} u_1(r,\lambda) f(r) dr, \int_{-\eta}^{\eta} u_2(r,\lambda) f(r) dr \right\},$$

and $u_1(r,\lambda)$, $u_2(r,\lambda)$, satisfy (2.1) at $r = 0$, with $z = \lambda \in \mathbf{R}$, convergence of the integrals being in $L_2(\mathbf{R})$ and $L_2(\mathbf{R}; d\rho_{ij}(\lambda))$, respectively. An advantage of this form of the eigenfunction expansion is that it has very general application, so that with suitable adjustments it may also be applied to cases where

- the endpoints $-\infty$, ∞, are replaced by a, b, respectively, and the decomposition point 0 by c, where $-\infty \le a < c < b \le \infty$,
- the boundary condition at the decomposition point $c \in \mathbf{R}$ is $\cos(\alpha)u(c,\lambda) + \sin(\alpha)u'(c,\lambda) = 0$ for some $\alpha \in [0,\pi)$,
- one or both of the endpoints is in the limit circle case.

For further details, see [10].

However, a significant drawback of the Weyl-Kodaira formula is that in the case of simple spectrum those solutions of the differential equation which are eigenfunctions of the operator H cannot be identified directly from the expansion as it stands. We note that the formulation (2.7) contains four terms, whereas the multiplicity of the spectrum, and hence the dimension of the eigenspaces, is at most two. It will be shown that whenever the spectrum of H has multiplicity one, the expansion can be reduced to a much simpler form which replicates many of the features of (2.4) in the half-line case. In this situation the eigenfunctions are the integral kernels in the simplified expansion and can be completely characterised in terms of their subordinacy properties.

To clarify the relevance of the theory of subordinancy in this context, we first briefly introduce some key features. A subordinate solution of $Lu = \lambda u$, $r \ge 0$, when L is regular at 0 and in the limit point case at infinity, is defined as follows:

Definition 1. A solution $u_s(r,\lambda)$ of $Lu = \lambda u$, $-\infty < \lambda < \infty$, $0 \le r < \infty$, is said to be *subordinate* at infinity if

$$\lim_{N\to\infty} \frac{\| u_s(r,\lambda) \|_N}{\| u(r,\lambda) \|_N} = 0,$$

where $\| \, . \, \|_N$ denotes $(\int_0^N |\, . \,|^2 dr)^{1/2}$, and $u(r,\lambda)$ denotes any solution of $Lu = \lambda u$ which is linearly independent from $u_s(r,\lambda)$.

Thus a subordinate solution is unique up to multiplication by scalars or functions of λ, and is asymptotically smaller than any linearly independent solution of the same equation, in the sense of limiting ratios of Hilbert space norms. To contribute to the eigenfunction expansion associated with H_∞, a solution $u(r,\lambda)$ of $Lu = \lambda u$ must either

(a) satisfy the boundary condition at $r = 0$ in the case where no solution is subordinate at infinity, or
(b) satisfy the boundary condition at $r = 0$ and be subordinate at infinity,

since the set of all $\lambda \in \mathbf{R}$ for which no solution satisfies (a) or (b) has μ_∞-measure zero [11]. In fact the solutions of $Lu = \lambda u$, $r \geq 0$ which satisfy (a) are absolutely continuous eigenfunctions of H_∞, and solutions which satisfy (b) are singular eigenfunctions of H_∞. The definition of subordinate solutions and the distinguishing properties of the eigenfunctions are entirely analogous in the case of $H_{-\infty}$.

The relationship between the eigenfunctions and the corresponding parts of the spectrum of H can be made more precise using the concept of a minimal support of a Borel-Stieltjes measure.

Definition 2. A subset S of $\mathbf{R}$ is said to be a *minimal support* of a measure ν on $\mathbf{R}$ if the following conditions hold:

(i) $\nu(\mathbf{R} \setminus S) = 0$,
(ii) if S_0 is a subset of S such that $\nu(S_0) = 0$, then $\mid S_0 \mid= 0$,

where $\mid . \mid$ denotes Lebesgue measure.

Note that a minimal support of a measure ν is unique up to sets of ν- and Lebesgue measure zero and, in the case of a spectral measure, provides an indication of where the spectrum is concentrated (for further details, see [11]). Corresponding to the decomposition of a Borel-Stieltjes measure ν into absolutely continuous and singular parts, $\nu_{a.c.}$ and $\nu_{s.}$, there exist minimal supports, $S(\nu_{a.c.})$ and $S(\nu_{s.})$ respectively such that $S(\nu_{a.c.}) \cup S(\nu_{s.}) = S(\nu)$ and $S(\nu_{a.c.}) \cap S(\nu_{s.}) = \emptyset$, where $S(\nu)$ is a minimal support of ν. For H_∞, as shown in [11], minimal supports $\mathcal{M}_{a.c.}(H_\infty)$, $\mathcal{M}_{s.}(H_\infty)$ of the absolutely continuous and singular parts respectively of μ_∞ are as follows:

$$\mathcal{M}_{a.c}(H_\infty) = \{\lambda \in \mathbf{R} : \text{no solution of } Lu = \lambda u \text{ is subordinate at } \infty\},$$

$$\begin{aligned}\mathcal{M}_{s.}(H_\infty) = \{\lambda \in \mathbf{R} : &\text{ there exists a solution of } Lu = \lambda u \text{ which satisfies the} \\ &\text{Dirichlet boundary condition at 0 and is subordinate at } \infty\}\end{aligned}$$

Minimal supports, $\mathcal{M}_{a.c}(H_{-\infty})$ and $\mathcal{M}_{s.}(H_{-\infty})$, of the absolutely continuous and singular parts of $\mu_{-\infty}$ are obtained by replacing ∞ with $-\infty$ in the above equations. Note that the Lebesgue measure of a minimal support of a spectral measure and the Lebesgue measure of the corresponding spectrum are not in general equal. For example, in the case where there is dense singular spectrum on a real interval $[c,d]$, the singular spectrum, being a closed set, will contain $[c,d]$, so that the Lebesgue measure of the interval is $d - c$; however, the minimal support of the singular part of a spectral measure will always have Lebesgue measure zero. A similar situation can also arise in relation to the absolutely continuous spectrum (see, e.g., Example 6.5 in [10]).

In the case of a full-line operator H on $L_2(\mathbf{R})$ with two limit point end-points and spectral measure μ, a minimal support of μ is given by $\mathcal{M} = \mathcal{M}_{a.c.}(H) \cup \mathcal{M}_{s.}(H)$, where

$$\begin{aligned}\mathcal{M}_{a.c.}(H) = \{\lambda \in \mathbf{R} : &\text{ either no solution of } Lu = \lambda u \text{ exists which is}\\ &\text{subordinate at } -\infty, \text{ or no solution of } Lu = \lambda u \text{ exists}\\ &\text{which is subordinate at } +\infty, \text{ or both}\}\\ \mathcal{M}_{s.}(H) = \{\lambda \in \mathbf{R} : &\text{ a solution of } Lu = \lambda u \text{ exists which is}\\ &\text{subordinate at both} \pm \infty\}\end{aligned}$$

(see [9]). The nature of the eigenfunctions when H has simple spectrum will be considered in Section 4.

3. Diagonalising the spectral density matrix

In order to simplify the eigenfunction expansion in the case where both endpoints are limit point, we follow the method of I.S. Kac [12], [13], and begin by introducing a spectral density matrix. Let $M_\tau(z)$ denote the trace of the M-matrix in (2.5), so that for $z \in \mathbf{C}^+$

$$\begin{aligned}M_\tau(z) &:= M_{11}(z) + M_{22}(z)\\ &= \frac{m_{-\infty}(z)\, m_\infty(z) + 1}{m_{-\infty}(z) - m_\infty(z)}.\end{aligned} \tag{3.1}$$

Since $m_{-\infty}$ and m_∞ are anti-Herglotz and Herglotz functions respectively, it is straightforward to check that $M_\tau(z)$ is Herglotz, so that $\operatorname{Im} M_\tau(z) > 0$ for $z \in \mathbf{C}^+$. It follows that a non-decreasing function $\rho_\tau(\lambda) : \mathbf{R} \to \mathbf{R}$ exists such that

$$\rho_\tau'(\lambda) = \lim_{z \downarrow \lambda} \frac{1}{\pi} \operatorname{Im} M_\tau(z), \quad z = \lambda + i\epsilon, \tag{3.2}$$

exists and is satisfied for Lebesgue and μ_τ-almost all $\lambda \in \mathbf{R}$, where μ_τ is the non-negative Borel-Stieltjes measure generated by $\rho_\tau(\lambda)$. Moreover, since $(\rho_{ij}(\lambda))$ is positive semi-definite, μ_{ij} is absolutely continuous with respect to μ_τ for each $i, j = 1, 2$, from which it may be inferred that for $\lim_{z\downarrow\lambda} \operatorname{Im} M_\tau(z) \neq 0$,

$$d\rho_{ij}(\lambda) = \frac{d\rho_{ij}}{d\rho_\tau}(\lambda) d\rho_\tau(\lambda) = \lim_{z\downarrow\lambda} \frac{\mathrm{Im} M_{ij}(z)}{\mathrm{Im} M_\tau(z)} d\rho_\tau(\lambda), \quad z = \lambda + \mathrm{i}\epsilon, \tag{3.3}$$

Lebesgue and μ_τ-almost everywhere on $\mathbf{R}$ (see [10], Lemma 5.3). We refer to

$$\left(\frac{d\rho_{ij}}{d\rho_\tau}(\lambda)\right) = \begin{pmatrix} \frac{d\rho_{11}}{d\rho_\tau}(\lambda) & \frac{d\rho_{12}}{d\rho_\tau}(\lambda) \\ \frac{d\rho_{21}}{d\rho_\tau}(\lambda) & \frac{d\rho_{22}}{d\rho_\tau}(\lambda) \end{pmatrix} \tag{3.4}$$

as the spectral density matrix for H. Since the set

$$S_0 := \{\lambda \in \mathbf{R} : \lim_{z \downarrow \lambda} \operatorname{Im} M_\tau(z) = 0\}$$

has μ_τ-measure zero, we may take

$$\left(\frac{d\rho_{ij}}{d\rho_\tau}(\lambda)\right) = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \qquad \text{for all } \lambda \in S_0. \tag{3.5}$$

Also, noting that the limits as $z \downarrow \lambda$ in (3.3) exist for Lebesgue and μ_τ-almost all $\lambda \in \mathbf{R} \setminus S_0$, we have that

$$\frac{d\rho_{11}}{d\rho_\tau}(\lambda) = \frac{\operatorname{Im} m_{-\infty}(\lambda) \mid m_\infty(\lambda) \mid^2 - \operatorname{Im} m_\infty(\lambda) \mid m_{-\infty}(\lambda) \mid^2}{D(\lambda)}, \tag{3.6}$$

$$\begin{aligned} \frac{d\rho_{12}}{d\rho_\tau}(\lambda) &= \frac{d\rho_{21}}{d\rho_\tau}(\lambda) \\ &= \frac{\operatorname{Im} m_{-\infty}(\lambda) \operatorname{Re} m_\infty(\lambda) - \operatorname{Im} m_\infty(\lambda) \operatorname{Re} m_{-\infty}(\lambda)}{D(\lambda)}, \end{aligned} \tag{3.7}$$

$$\frac{d\rho_{22}}{d\rho_\tau}(\lambda) = \frac{\operatorname{Im} m_{-\infty}(\lambda) - \operatorname{Im} m_\infty(\lambda)}{D(\lambda)}, \tag{3.8}$$

almost everywhere on $\mathbf{R} \setminus S_0$, where

$$D(\lambda) = \operatorname{Im} m_{-\infty}(\lambda) \left(1 + \mid m_\infty(\lambda) \mid^2\right) - \operatorname{Im} m_\infty(\lambda) \left(1 + \mid m_{-\infty}(\lambda) \mid^2\right),$$

and $m_{-\infty}(\lambda)$, $m_\infty(\lambda)$, denote the normal limits of $m_{-\infty}(z)$, $m_\infty(z)$, respectively as $z \downarrow \lambda \in \mathbf{R}$.

The following theorem establishes a rigorous correlation between the rank of the spectral density matrix and the multiplicity of the spectrum of H.

Theorem 1 (Kac). *The spectral multiplicity of H is two if and only if the μ_τ-measure of the set*

$$\mathcal{M}_2 := \left\{\lambda \in E : \operatorname{rank}\left(\frac{d\rho_{ij}}{d\rho_\tau}(\lambda)\right) = 2\right\}$$

is strictly positive, where

$$E := \left\{\lambda \in \mathcal{M} : \left(\frac{d\rho_{ij}}{d\rho_\tau}(\lambda)\right) \textit{ exists}\right\}$$

for some minimal support $\mathcal{M}$ of μ_τ. The set $\mathcal{M}_2$ is a maximal set of multiplicity 2, and for μ_τ-almost all $\lambda \in (\mathbf{R} \setminus \mathcal{M}_2)$, H has multiplicity one with

$$\operatorname{rank}\left(\frac{d\rho_{ij}}{d\rho_\tau}(\lambda)\right) = 1.$$

An important consequence of the theorem, as recognized by Kac, is the following.

Corollary 1. *Let*

$$S_d := \{\lambda \in \mathbf{R} : \operatorname{Im} m_{-\infty}(\lambda) < 0,\ \operatorname{Im} m_\infty(\lambda) > 0\}.$$

Then $\mu_\tau(\mathcal{M}_2 \triangle S_d) = 0$, where $\triangle$ denotes the symmetric difference.

The corollary implies that only the absolutely continuous part of the spectrum can have multiplicity two, or contain a non-trivial subset with multiplicity two. It also implies that the degenerate spectrum is supported on

$$S' := \{\lambda \in \mathbf{R} : \text{no solution of } Lu = \lambda u \text{ is subordinate at either } -\infty \text{ or at } \infty\},$$

where $\mu_\tau(S_d \triangle S') = 0$ (see [10] for further details).

We now use the spectral density matrix to rearrange the Weyl-Kodaira formulation (2.7) in such a way that the generalised eigenfunctions of H are exhibited explicitly in the expansion. Using (3.3)–(3.5), it is straightforward to see that the integral on the right-hand side of (2.7) may be expressed as follows:

$$\int_{-\omega}^{\omega} \sum_{i=1}^{2} \sum_{j=1}^{2} u_i(r,\lambda) F_j(\lambda) d\rho_{ij}(\lambda) = \int_{-\omega}^{\omega} (U(r,\lambda))^T \left(\frac{d\rho_{ij}}{d\rho_\tau}(\lambda) \right) F(\lambda) d\rho_\tau(\lambda) \quad (3.9)$$

where the superfix T denotes the transpose, and

$$U(r,\lambda) = \begin{pmatrix} u_1(r,\lambda) \\ u_2(r,\lambda) \end{pmatrix}, \qquad F(\lambda) = \begin{pmatrix} F_1(\lambda) \\ F_2(\lambda) \end{pmatrix},$$

with $F_1(\lambda)$ and $F_2(\lambda)$ as in (2.7). Since the spectral density matrix (3.4) is real and symmetric, we may decompose it in such a way that

$$\left(\frac{d\rho_{ij}}{d\rho_\tau}(\lambda) \right) = P^T \, D \, P, \quad (3.10)$$

where

$$D = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

according as the rank of the spectral density matrix is 1 or 2 respectively, and P is a 2×2 matrix given by

$$P = \begin{pmatrix} \sigma_{11}^{1/2} & \sigma_{11}^{-1/2} \sigma_{12} \\ 0 & \sigma_{11}^{-1/2} (\sigma_{11}\sigma_{22} - \sigma_{12}{}^2)^{1/2} \end{pmatrix} \quad (3.11)$$

for $\sigma_{11} \neq 0$, where for each $i,j = 1,2$, σ_{ij} denotes $(d\rho_{ij}/d\rho_\tau)(\lambda)$. Note that $P^T \, P = (\sigma_{ij}(\lambda))$ and that P has full rank if and only if the determinant, $\sigma_{11}\sigma_{22} - \sigma_{12}^2$, of the spectral density matrix is strictly positive. For non-trivial cases where $\sigma_{11} = 0$, we have

$$D = P = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad (3.12)$$

taking into account the positive semi-definite property of the spectral density matrix and the fact that $0 \leq \mid \sigma_{ij} \mid \leq 1$ for $i,j = 1,2$ (see [10]).

Let $\mathcal{M}_1$ denote the set of all $\lambda \in E$ such that $((d\rho_{ij}/d\rho_\tau)(\lambda))$ has multiplicity one. From (2.7), (3.9) and (3.10), we have for $f(r) \in L_2(\mathbf{R})$,

$$\begin{aligned} f(r) &= \underset{\omega\to\infty}{\text{l.i.m.}} \int_{-\omega}^{\omega} (U(r,\lambda))^T \; P^T \, D \, P \; F(\lambda) \; d\rho_\tau(\lambda) \\ &= \underset{\omega\to\infty}{\text{l.i.m.}} \int_{-\omega}^{\omega} (V(r,\lambda))^T \; D \; G(\lambda) \; d\rho_\tau(\lambda), \end{aligned} \tag{3.13}$$

where

$$P\,U(r,\lambda) = V(r,\lambda) = \begin{pmatrix} v_1(r,\lambda) \\ v_2(r,\lambda) \end{pmatrix}, \quad P\,F(\lambda) = G(\lambda) = \begin{pmatrix} G_1(\lambda) \\ G_2(\lambda) \end{pmatrix}, \tag{3.14}$$

and convergence is in $L_2(\mathbf{R})$. Using (3.11)–(3.14), this leads to

$$\begin{aligned} f(r) = \; \underset{\omega\to\infty}{\text{l.i.m.}} & \left\{ \int_{(-\omega,\omega)\cap\mathcal{M}_1} v(r,\lambda) \;\; G(\lambda) \;\; d\rho_\tau(\lambda) \right. \\ & \left. + \sum_{i=1}^{2} \int_{(-\omega,\omega)\cap\mathcal{M}_2} v_i(r,\lambda) \;\; G_i(\lambda) \;\; d\rho_\tau(\lambda) \right\}, \end{aligned} \tag{3.15}$$

where

$$G(\lambda) = \underset{\eta\to\infty}{\text{l.i.m.}} \int_{-\eta}^{\eta} v(r,\lambda) \; f(r) \; dr,$$

with

$$v(r,\lambda) = \begin{cases} \sigma_{11}^{1/2} \; u_1(r,\lambda) + \sigma_{11}^{-1/2} \sigma_{12} \; u_2(r,\lambda) & \sigma_{11} \neq 0 \\ u_2(r,\lambda) & \sigma_{11} = 0, \end{cases} \tag{3.16}$$

and for $i = 1, 2$,

$$G_i(\lambda) = \underset{\eta\to\infty}{\text{l.i.m.}} \int_{-\eta}^{\eta} v_i(r,\lambda) \; f(r) \; dr,$$

with

$$\begin{aligned} v_1(r,\lambda) &= \sigma_{11}^{1/2} \; u_1(r,\lambda) + \sigma_{11}^{-1/2} \; \sigma_{12} \; u_2(r,\lambda), \\ v_2(r,\lambda) &= \sigma_{11}^{-1/2} \; (\sigma_{11} \, \sigma_{22} - {\sigma_{12}}^2)^{1/2} \; u_2(r,\lambda). \end{aligned}$$

Also for $k = 1,\ 2$,

$$\mathcal{M}_k := \left\{ \lambda \in \mathbf{R} : \operatorname{rank} \left(\frac{d\rho_{ij}}{d\rho_\tau}(\lambda) \right) = k \right\},$$

and convergence of the integrals is in $L_2(\mathbf{R})$ and $L_2(\mathbf{R}; d\rho_\tau(\lambda))$, respectively.

From (3.15), $v(r,\lambda)$ is an eigenfunction of H for each $\lambda \in \mathcal{M}_1$, and for each $\lambda \in \mathcal{M}_2$, a basis for the eigenspace is $\{v_1(r,\lambda), v_2(r,\lambda)\}$. Note from Kac's theorem, that if $\mu_\tau(\mathcal{M}_2) = 0$ the spectrum of H is simple so that the second term in (3.15) is null and the expansion has a similar form to that of the half-line case in (2.4).

4. The case of simple spectrum

In this section, we focus on the particular case where the spectrum of H is simple and purely absolutely continuous. In this situation $\mu_\tau(\mathcal{M}_2) = 0$, and hence as shown in Section 3, the expansion in (3.15) reduces to a simpler form, so that for $f(r) \in L_2(\mathbf{R})$

$$f(r) = \underset{\omega\to\infty}{\text{l.i.m.}} \int_{-\omega}^{\omega} v(r,\lambda)\, G(\lambda)\, d\rho_\tau(\lambda) \tag{4.1}$$

where $v(r,\lambda)$ is as in (3.16), and

$$G(\lambda) = \underset{\eta\to\infty}{\text{l.i.m.}} \int_{-\eta}^{\eta} v(r,\lambda)\, f(r)\, dr,$$

with convergence in the mean in $L_2(\mathbf{R})$ and $L_2(\mathbf{R}; d\rho_\tau(\lambda))$ respectively.

We now investigate the structure of the eigenfunction $v(r,\lambda)$ in terms of its relationship to the Titchmarsh-Weyl functions, $m_{-\infty}$, m_∞, and the corresponding Weyl solutions associated with $H_{-\infty}$ and H_∞, respectively. This will enable the asymptotic behaviour of $v(r,\lambda)$ as $r \to \pm\infty$ to be ascertained in terms of the theory of subordinacy.

From (3.11) and (3.14), we have for $\sigma_{11} \neq 0$, $\sigma_{22} \neq 0$,

$$v(r,\lambda) = \begin{pmatrix} \sigma_{11}^{1/2} & \sigma_{11}^{-1/2}\,\sigma_{12} \end{pmatrix} \begin{pmatrix} u_1(r,\lambda) \\ u_2(r,\lambda) \end{pmatrix}, \tag{4.2}$$

since by Kac's theorem the assumption that H has simple spectrum implies that $\det(\sigma_{ij}) = 0$, and hence that the second row of P in (3.11) is zero. In cases where $\sigma_{11} = 0$ or $\sigma_{22} = 0$, it follows from (3.12) and (3.11) that $v(r,\lambda) = u_2(r,\lambda)$ or $v(r,\lambda) = u_1(r,\lambda)$, respectively.

From (4.2), $v(r,\lambda)$ is a linear combination of $u_1(r,\lambda)$ and $u_2(r,\lambda)$, whose coefficients are functions of λ which reflect the nature of the spectrum at λ. In order to determine the coefficients, we first introduce the following disjoint sets:

$$\begin{aligned}
S_1 &:= \{\lambda \in \mathbf{R} : m_{-\infty}(\lambda) \in \mathbf{C}^-,\;\; m_\infty(\lambda) \in \mathbf{R}\cup\{\infty\}\} \\
S_2 &:= \{\lambda \in \mathbf{R} : m_{-\infty}(\lambda) \in \mathbf{R}\cup\{\infty\},\;\; m_\infty(\lambda) \in \mathbf{C}^+\} \\
S_3 &:= \{\lambda \in \mathbf{R} : m_{-\infty}(\lambda) = m_\infty(\lambda) \in \mathbf{R}\cup\{\infty\}\} \\
S_4 &:= \{\lambda \in \mathbf{R} : m_{-\infty}(\lambda) \in \mathbf{C}^-,\; m_\infty(\lambda) \in \mathbf{C}^+\}
\end{aligned}$$

Note that $S_1 \cup S_2$ is a minimal support of the absolutely continuous part of the spectral measure μ_τ in $\mathcal{M}_1$. The set S_3 is a minimal support of the singular part of μ_τ and always has Lebesgue measure zero. Altogether the set $\{S_i : i = 1,\ldots,3\}$ constitutes a minimal support of the part of the spectral measure μ_τ corresponding to the simple part of the spectrum, so is equal to $\mathcal{M}_1$ up to sets of μ_τ- and Lebesgue measure zero. Also from Corollary 1, S_4 and $\mathcal{M}_2$ differ at most by μ_τ- and Lebesgue null sets, so that the degenerate part of the spectrum is supported on those values of λ on which both $m_{-\infty}(\lambda)$ and $m_\infty(\lambda)$ are strictly complex (see also [10]). Note that the resolvent set is the largest open set in $\mathbf{R}\backslash\{S_i : i = 1,\ldots,4\}$.

In this section we concentrate particularly on S_1 and S_2 which are associated with the simple part of the absolutely continuous spectrum. In fact it is sufficient to consider S_1 in detail, since the derivations and results are almost entirely analogous for S_2.

For simplicity of exposition, suppose in the first instance that $S_1 = \mathbf{R}$. If $\lambda \in S_1$, so that $m_\infty(\lambda) \in \mathbf{R} \cup \{\infty\}$, then since $m_{-\infty}(\lambda) \in \mathbf{C}^-$, we have from (3.6) and (3.7),

$$\sigma_{11} = \frac{(m_\infty(\lambda))^2}{1+(m_\infty(\lambda))^2}, \qquad \sigma_{12} = \frac{m_\infty(\lambda)}{1+(m_\infty(\lambda))^2} \tag{4.3}$$

and hence from (4.2),

$$v(r,\lambda) = \frac{u_2(r,\lambda) + m_\infty(\lambda)\, u_1(r,\lambda)}{(1+(m_\infty(\lambda))^2)^{1/2}}, \tag{4.4}$$

which is a real solution of the differential equation and a scalar multiple of the pointwise limit of the Weyl solution for H_∞, viz. $u_2(r,z)+m_\infty(z)\, u_1(r,z)$, as $z \downarrow \lambda$. Note also that if $m_\infty(z) \to \infty$ as $z \downarrow \lambda \in \mathbf{R}$, it follows from (4.3) that $\sigma_{11} = 1$ and $\sigma_{12} = 0$, so that $v(r,\lambda) = u_1(r,\lambda)$, which is an eigenfunction of H_∞; this is also directly evident from (4.4) above. Thus we see that for all λ in S_1, $v(r,\lambda)$ is a real solution of $Lu = \lambda u$ which is subordinate at ∞. Also, since $m_{-\infty}(\lambda)$ is strictly complex for $\lambda \in S_1$, we infer from the theory of subordinacy that all solutions are of comparable asymptotic size as $r \to -\infty$ [11]. Substituting for $v(r,\lambda)$ from (4.4) into (4.1) now yields for $f(r) \in L_2(\mathbf{R})$,

$$f(r) = \operatorname*{l.i.m.}_{\omega\to\infty} \int_{-\omega}^{\omega} \frac{u_2(r,\lambda) + m_\infty(\lambda)\, u_1(r,\lambda)}{(1+(m_\infty(\lambda))^2)^{1/2}}\, G(\lambda)\, d\rho_\tau(\lambda), \tag{4.5}$$

where

$$G(\lambda) = \operatorname*{l.i.m.}_{\eta\to\infty} \int_{-\eta}^{\eta} \frac{u_2(r,\lambda) + m_\infty(\lambda)\, u_1(r,\lambda)}{(1+(m_\infty(\lambda))^2)^{1/2}}\, f(r)\, dr,$$

with convergence as before.

We illustrate the process outlined above by considering two operators, both of which are in the limit point case at $\pm\infty$ and have purely absolutely continuous spectrum.

Example 1. Let

$$q(r) = \begin{cases} 0 & -\infty < r < 0, \\ 1 & 0 \le r < \infty, \end{cases} \tag{4.6}$$

and define a fundamental set of solutions $\{u_1(r,z), u_2(r,z)\}$ of $Lu = zu$ on $\mathbf{R}$ to satisfy the conditions in (2.1). By choosing the $\sqrt{z}$-plane to have positive imaginary part in $\mathbf{C}^+$, we have for $\mathrm{Im} z > 0$,

$$\exp(-\mathrm{i}\sqrt{z}r) \in L_2(\mathbf{R}^-), \qquad \exp(\mathrm{i}\sqrt{z-1}r) \in L_2(\mathbf{R}^+),$$

from which it is straightforward to show that for $z \in \mathbf{C}^+$,

$$m_{-\infty}(z) = -\mathrm{i}\sqrt{z}, \qquad m_\infty(z) = \mathrm{i}\sqrt{z-1},$$

so that the boundary values for $z = \lambda \in \mathbf{R}$ are given by

$$m_{-\infty}(\lambda) = -\mathrm{i}\sqrt{\lambda}, \qquad m_{\infty}(\lambda) = \mathrm{i}\sqrt{\lambda - 1}, \tag{4.7}$$

respectively. We remark that $m_{-\infty}(\lambda)$ is real for $\lambda \leq 0$ and complex for $\lambda > 0$, while $m_{\infty}(\lambda)$ is real for $\lambda \leq 1$ and complex for $\lambda > 1$. Thus we have $S_1 = (0, 1]$, $S_2 = S_3 = \emptyset$ and $S_4 = S_d = (1, \infty)$, where S_d is as in Corollary 1. Since both $m_{-\infty}(\lambda)$ and $m_{\infty}(\lambda)$ are real for $\lambda \leq 0$, we may take $(\sigma_{ij}(\lambda))$ to be the zero matrix as in (3.5) for $-\infty < \lambda \leq 0$, and note that the resolvent set is $(-\infty, 0)$.

It is straightforward to determine the spectral density matrix explicitly for $\lambda > 0$, using (3.4)–(3.8). For $0 < \lambda \leq 1$, we note that $m_{\infty}(\lambda) = -\sqrt{1-\lambda}$ to obtain

$$\left(\frac{d\rho_{ij}}{d\rho_\tau}(\lambda)\right) = \frac{1}{2-\lambda}\begin{pmatrix} 1-\lambda & -\sqrt{1-\lambda} \\ -\sqrt{1-\lambda} & 1 \end{pmatrix}, \tag{4.8}$$

which has rank 1, from which it follows by Theorem 1 that the spectrum of H is simple on $0 < \lambda \leq 1$. The spectral density matrix for $\lambda > 1$ is obtained in a similar way and has full rank (see [10], Example 5.10), so that $S_2 = (1, \infty) = \mathcal{M}_2$.

The spectral density matrix for $\lambda \in S_1$ in (4.8) may be decomposed as in (3.10), to give

$$D = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad P = \frac{1}{\sqrt{2-\lambda}}\begin{pmatrix} -\sqrt{1-\lambda} & 1 \\ 0 & 0 \end{pmatrix}, \tag{4.9}$$

and hence from (4.7) and (4.9),

$$\begin{aligned} PU &= \left(-\frac{\sqrt{1-\lambda}}{\sqrt{2-\lambda}}u_1(r,\lambda) + \frac{1}{\sqrt{2-\lambda}}u_2(r,\lambda)\right) \\ &= \frac{u_2(r,\lambda) + m_\infty(\lambda)u_1(r,\lambda)}{(1 + (m_\infty(\lambda))^2)^{\frac{1}{2}}} \\ &= v(r,\lambda), \end{aligned} \tag{4.10}$$

for $\lambda \in (0, 1]$, where $u_1(r, \lambda)$, $u_2(r, \lambda)$ satisfy

$$u_1(r,\lambda) = \begin{cases} \frac{1}{2\sqrt{1-\lambda}}\left(e^{\sqrt{1-\lambda}r} - e^{-\sqrt{1-\lambda}r}\right), & r \geq 0 \\ \frac{\sin(\sqrt{\lambda}r)}{\sqrt{\lambda}}, & r < 0 \end{cases} \tag{4.11}$$

$$u_2(r,\lambda) = \begin{cases} \frac{1}{2}\left(e^{\sqrt{1-\lambda}r} + e^{-\sqrt{1-\lambda}r}\right), & r \geq 0 \\ \cos\left(\sqrt{\lambda}r\right), & r < 0 \end{cases} \tag{4.12}$$

It follows from (4.11) and (4.12) that for $\lambda \in (0, 1]$, no solution of $Lu = \lambda u$ is subordinate at $-\infty$, and that the real-valued eigenfunction $v(r, \lambda)$ in (4.10) satisfies (4.5) and is subordinate at ∞. Moreover, since $m_{\infty}(\lambda)$ is real on $(0, 1]$, we have from (3.1) and (3.2),

$$\begin{aligned} \rho_\tau'(\lambda) &= -\frac{1}{\pi}\,\frac{\operatorname{Im} m_{-\infty}(\lambda)\left(1 + (m_\infty(\lambda))^2\right)}{\mid m_{-\infty}(\lambda) - m_\infty(\lambda)\mid^2}, \qquad 0 < \lambda \leq 1, \\ &= (2-\lambda)\,\rho_{-\infty}'(\lambda), \end{aligned} \tag{4.13}$$

noting that on this λ-interval,

$$\rho'_{-\infty}(\lambda) = -\frac{1}{\pi}\,\mathrm{Im}\, m_{-\infty}(\lambda), \qquad 1 + (m_\infty(\lambda))^2 = 2 - \lambda,$$

and

$$| \, m_{-\infty}(\lambda) - m_\infty(\lambda) \, |^2 = 1.$$

Since $m_\infty(\lambda)$ is finite for all values of λ, we may multiply (4.10) by $(1+(m_\infty(\lambda))^2)^{\frac{1}{2}}$ and divide (4.13) by $(1 + (m_\infty(\lambda))^2)$ to obtain a simpler form of the expansion (4.5) which holds on $S_1 = (0, 1]$. The part of the expansion corresponding to the simple spectrum of H on $S_1(\lambda)$ then reduces to the following spectral projection:

$$\mathcal{P}_{(0,1]} f(r) = \int_0^1 e^{-\sqrt{1-\lambda}\, r}\, G(\lambda)\, \sqrt{\lambda}\, d\lambda,$$

where

$$G(\lambda) = \int_{-\infty}^{\infty} e^{-\sqrt{1-\lambda}\, r}\, f(r)\, dr,$$

and the integrals converge absolutely. Note that the full expansion for H would also include the set $S_4 = (1, \infty)$, on which the spectrum is purely absolutely continuous with multiplicity 2.

Example 2. Consider the Airy operator associated with the singular Sturm-Liouville equation,

$$-u''(r, \lambda) + r\, u(r, \lambda) = \lambda u(r, \lambda), \qquad -\infty < r < \infty. \tag{4.14}$$

It is well known that a fundamental set of solutions for (4.14) is given by $\{A\mathrm{i}(r - \lambda), B\mathrm{i}(r - \lambda)\}$, and that the differential equation is in the limit point case at both endpoints [5]. Moreover, Ai and Bi can be expressed in terms of Bessel functions [1], [15], and the solution $A\mathrm{i}(r - \lambda)$, $\lambda \in \mathbf{R}$, is real valued and square integrable at infinity with respect to r for all $\lambda \in \mathbf{R}$. It follows that $A\mathrm{i}(r - \lambda)$ is subordinate at infinity [11], from which it may be inferred that

$$m_\infty(\lambda) = \lim_{z \downarrow \lambda} \left. \frac{A\mathrm{i}'(r - z)}{A\mathrm{i}(r - z)} \right|_{r=0}, \tag{4.15}$$

for all $\lambda \in \mathbf{R}$, where $'$ denotes differentiation with respect to r.

To investigate the asymptotic behaviour of solutions of (4.14) at $-\infty$, we first note that the conditions for validity of the Liouville-Green approximation are satisfied in this case (see [15], Chapter 6). Hence the asymptotic behaviour of a fundamental set, $\{u_+(r, \lambda), u_-(r, \lambda)\}$, of solutions of (4.14) as $r \to -\infty$ is given by:

$$u_\pm(r, \lambda) = \frac{1}{(r - \lambda)^{\frac{1}{4}}} \exp\left(\int^r \pm (r - \lambda)^{\frac{1}{2}}\, dr \right) (1 + o(1)). \tag{4.16}$$

Since for each fixed $\lambda \in \mathbf{R}$, $(r - \lambda)$ is eventually negative as $r \to -\infty$, we may write

$$u_\pm(r, \lambda) = K\, \frac{1}{(\lambda - r)^{\frac{1}{4}}} \exp\left(\int^r \pm \mathrm{i} (\lambda - r)^{\frac{1}{2}}\, dr \right) (1 + o(1)), \tag{4.17}$$

as $r \to -\infty$ for each $\lambda \in \mathbf{R}$, where K is a constant which is independent of r and λ. It may be deduced from (4.17) that for every real value of λ, no solution of (4.14) is subordinate at $-\infty$, so that $m_{-\infty}(\lambda) \in \mathbf{C}^-$ for all $\lambda \in \mathbf{R}$ [11]. This, together with (4.15), which implies that $m_\infty(\lambda) \in \mathbf{R} \cup \{\infty\}$ for all $\lambda \in \mathbf{R}$, shows that $S_1 = \mathbf{R}$.

Thus we have shown that in the case of the Airy operator, the spectrum of H is purely absolutely continuous with multiplicity one on the whole real line, and that the absolutely continuous eigenfunctions which feature in the expansion (4.1) are given by

$$v(r,\lambda) = \frac{u_2(r,\lambda) + m_\infty(\lambda) u_1(r,\lambda)}{(1 + (m_\infty(\lambda))^2)^{1/2}}, \tag{4.18}$$

where $m_\infty(\lambda)$ is as in (4.15). Note that $v(r,\lambda)$ is a scalar multiple of $A\mathrm{i}(r-\lambda)$, and that when λ is an eigenvalue of H_∞, so that $m_\infty(z) \to \infty$ as $z \downarrow \lambda$, it follows from (4.18) that $v(r,\lambda) = u_1(r,\lambda)$.

To determine the scalar Herglotz function, $M(z)$, explicitly it is first necessary to identify (up to a scalar multiple) the Weyl solution of $Lu = z\,u$, which is in $L_2(\mathbf{R}^-)$ for $z \in \mathbf{C}^+$. Then $m_{-\infty}$ can be obtained by evaluating the logarithmic derivative of the Weyl solution at $r = 0$, as in (4.15). We omit the technical details.

These examples confirm that when part or all of the spectrum is absolutely continuous with multiplicity one, the corresponding eigenfunctions in the expansion (4.1) are solutions of $L\,u = \lambda u$ which are subordinate at one of the limit point endpoints, and are of comparable asymptotic size to all linearly independent solutions of the same equation at the other endpoint. In cases where both S_1 and S_2 have positive μ_τ-measure, but S_3 and S_4 are empty, the simplified expansions will still be valid on the relevant λ-sets, but non-overlapping spectral projections are needed to separate the corresponding parts of the expansion. Thus we expect the absolutely continuous eigenfunctions associated with S_1 and S_2 respectively to be real scalar multiples of $u_2(r,\lambda) + m_\infty\, u_1(r,\lambda)$ and $u_2(r,\lambda) + m_{-\infty}\, u_1(r,\lambda)$, and the corresponding spectral densities to be positive scalar multiples of $\rho_{-\infty}(\lambda)$ and $\rho_\infty(\lambda)$, noting that there may be some λ dependence in the scalar multiples. We have for $f(r) \in L_2(-\infty,\infty)$,

$$\begin{aligned} f(r) = \underset{\omega\to\infty}{\text{l.i.m.}} \Bigg\{ &\int_{(-\omega,\omega)\cap S_1} \frac{u_2(r,\lambda) + m_\infty(\lambda) u_1(r,\lambda)}{\mid m_{-\infty}(\lambda) - m_\infty(\lambda) \mid}\, G_+(\lambda)\, d\rho_{-\infty}(\lambda) \\ &+ \int_{(-\omega,\omega)\cap S_2} \frac{u_2(r,\lambda) + m_{-\infty}(\lambda)\, u_1(r,\lambda)}{\mid m_{-\infty}(\lambda) - m_\infty(\lambda) \mid}\, G_-(\lambda)\, d\rho_\infty(\lambda) \Bigg\} \end{aligned} \tag{4.19}$$

where

$$G_+(r,\lambda) = \underset{\eta\to\infty}{\text{l.i.m.}} \int_{-\eta}^{\eta} \frac{u_2(r,\lambda) + m_\infty(\lambda) u_1(r,\lambda)}{\mid m_{-\infty}(\lambda) - m_\infty(\lambda) \mid} f(r)\, dr,$$

$$G_-(r,\lambda) = \underset{\eta\to\infty}{\text{l.i.m.}} \int_{-\eta}^{\eta} \frac{u_2(r,\lambda) + m_{-\infty}(\lambda) u_1(r,\lambda)}{\mid m_{-\infty}(\lambda) - m_\infty(\lambda) \mid} f(r)\, dr.$$

with convergence in $L_2(\mathbf{R})$, $L_2(\mathbf{R}; d\rho_{-\infty})$ and $L_2(\mathbf{R}; d\rho_{\infty})$ respectively. Noting that for $\lambda \in S_1(\lambda)$,

$$\rho'_\tau(\lambda) = -\frac{1}{\pi}\,\frac{\operatorname{Im} m_{-\infty}(\lambda)\left(1 + (m_\infty(\lambda))^2\right)}{|\, m_{-\infty}(\lambda) - m_\infty(\lambda)\,|^2}, \qquad 0 < \lambda \le 1, \tag{4.20}$$

we may write

$$d\rho_\tau(\lambda) = \frac{\left(1 + (m_\infty(\lambda))^2\right)}{|\, m_{-\infty}(\lambda) - m_\infty(\lambda)\,|^2}\, d\rho_{-\infty}(\lambda), \qquad 0 < \lambda \le 1.$$

We see that the form of the first integrand in (4.19) is derived from (4.5), by cancellation of the term $(1 + (m_\infty(\lambda))^2)$ in the numerator of the expression for $\rho'_\tau(\lambda)$ in (4.20) with the denominator of the eigenfunctions in (4.5), and by removal of the term $|\, m_{-\infty}(\lambda) - m_\infty(\lambda)\,|^2$, which is strictly positive for $\lambda \in S_1 \cup S_2$, from the denominator of $\rho'_\tau(\lambda)$ in (4.20) to the denominators of the eigenfunction in (4.19). The argument is entirely analogous for $\lambda \in S_2(\lambda)$, with ∞ and $-\infty$ interchanged. Note that the expansion in (4.19) is still valid if $m_\infty(z)$ or $m_{-\infty}(z) \downarrow \infty$ as $z \downarrow \lambda$ for λ in S_1 or S_2 respectively, in which case the eigenfunctions are given by $u_1(r, \lambda)$.

The form of the expansion in (4.19) clearly demonstrates the relationships between properties of the simple part of the absolutely continuous spectrum and the asymptotic behaviour of the corresponding absolutely continuous eigenfunctions; it also exposes the contribution of the Titchmarsh-Weyl m-functions and associated spectral densities of the half-line operators, $H_{-\infty}$ and H_∞, to the structure of the expansion in this case. We expect to extend this work to cases where the spectrum includes non-trivial singular and/or degenerate parts in a separate publication.

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Spectral Minimal Partitions for a Thin Strip on a Cylinder or a Thin Annulus like Domain with Neumann Condition

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Abstract. We analyze "Neumann" spectral minimal partitions for a thin strip on a cylinder or for the thin annulus.

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1. Introduction

In previous papers, sometimes in collaborations with other colleagues, we have analyzed spectral minimal partitions for some specific open subsets of $\mathbb{R}^2$ and for the sphere $\mathbb{S}^2$. See [4] for some of the basic results and for more detailed definitions. In contrast with two-dimensional eigenvalue problems for which a few examples exist where the eigenvalues and the eigenfunctions are explicitly known – rectangles, the disk, sectors, the equilateral triangle, $\mathbb{S}^2$ and the torus – explicit non-nodal examples for minimal partitions are lacking. Up to now we only have been able to work out explicitly $\mathfrak{L}_3$ for the 2-sphere, [5].

Here we find other examples of non-nodal minimal partitions for problems for which the circle $\mathbb{S}^1$ is a deformation retract. Note that the Laplacian on the circle $\mathbb{S}^1_*$ (with perimeter 1) can be interpreted as the Laplacian on an interval $(0, 1)$ with periodic boundary conditions. For this one-dimensional problem we can work out the partition eigenvalues (see below for a definition) $\mathfrak{L}_k(\mathbb{S}^1_*)$ explicitly. We have $\mathfrak{L}_k = \pi^2 k^2$. Observe that for odd $k \geq 3$ the $\mathfrak{L}_k$ are not eigenvalues, whereas for k even they are. The corresponding k-partitions are given by partitioning the circle into k equal parts, hence $D_1 = (0, 1/k), D_2 = (1/k, 2/k), \dots, D_k = ((k-1)/k, 1)$ identifying 0 with 1.

We will consider a strip on a cylinder or the annulus with suitable boundary conditions. All these domains are homotopic to $\mathbb{S}^1_*$. For those domains we are going to investigate the corresponding minimal 3-partitions.

We recall some notation and definitions. Consider a k-partition $\mathcal{D}_k = (D_1, \dots, D_k)$, i.e., k disjoint open subsets D_i of some Ω. Here Ω can be a bounded domain in $\mathbb{R}^2$ or in a 2-dimensional C^∞ Riemannian manifold.

Consider first $-\Delta$ on Ω where Δ can be the usual Laplacian or in the case of a manifold (with boundary or without boundary) the corresponding Laplace-Beltrami operator. For the case with boundary we can impose Dirichlet or Neumann but we could also have mixed boundary conditions.

We associate with $\mathcal{D}_k$

$$\Lambda(\mathcal{D}_k) = \sup_{1\leq i\leq k} \lambda_1(D_i)$$

where $\lambda_1(D_i)$ denotes

- either the lowest eigenvalue of the Dirichlet Laplacian in D_i
- or the lowest eigenvalue of the Laplacian in D_i where we put the Dirichlet boundary condition on $\partial D_i \subset \Omega$ and the Neumann boundary condition on $\partial D_i \cap \partial\Omega$.

It is probably worth to explain rigorously what we mean above by $\lambda_1(D_i)$ in the case of measurable D_i's.

Definition 1.1. For any measurable $\omega \subset \Omega$, let $\lambda_1^D(\omega)$ (resp. $\lambda_1^N(\omega)$) denotes the first eigenvalue of the Dirichlet realization (resp. $\partial\Omega$-Neumann) of the operator in the following generalized sense. We define

$$\lambda_1^{D\,or\,N}(\omega) = +\infty\ ,$$

if $\big\{u \in W^1(\Omega)\,, u \equiv 0 \text{ a.e. on } \Omega\setminus\omega\big\} = \{0\}$,

$$\lambda_1^D(\omega) = \inf\left\{\frac{\int_\Omega |\nabla u(x)|^2\,dx}{\int_\Omega |u(x)|^2\,dx}\ :\ u \in W_0^1(\Omega)\setminus\{0\}\,, u\equiv 0 \text{ a.e. on } \Omega\setminus\omega\right\}\ ,$$

$$\lambda_1^N(\omega) = \inf\left\{\frac{\int_\Omega |\nabla u(x)|^2\,dx}{\int_\Omega |u(x)|^2\,dx}\ :\ u \in W^1(\Omega)\setminus\{0\}\,, u\equiv 0 \text{ a.e. on } \Omega\setminus\omega\right\}\ ,$$

otherwise.

We call groundstate any function ϕ achieving the above infimum.

Of course, if $\omega \subset\subset \Omega$, we have $\lambda_1^D(\omega) = \lambda_1^N(\omega)$.

The kth partition-eigenvalue $\mathfrak{L}_k(\Omega)$ is then defined by

$$\mathfrak{L}_k(\Omega) = \inf_{\mathcal{D}} \Lambda(\mathcal{D})\,, \tag{1.1}$$

where the infimum is considered[1] over the k-partitions.

Any k-partition $\mathcal{D}$ for which

$$\mathfrak{L}_k(\Omega) = \Lambda(\mathcal{D}) \tag{1.2}$$

is called spectral minimal k-partition, for short minimal k-partition.

[1] We refer to [4] for a more precise definition of the considered class of k-partitions and the notion of regular representatives.

If needed we will write $\mathfrak{L}_k^D(\Omega)$ or $\mathfrak{L}_k^N(\Omega)$ to indicate if we choose the Dirichlet condition or the $\partial\Omega$-Neumann condition in the above definitions.

Although not explicitly written in [4], all the results obtained in the case of Dirichlet are also true in the case of Neumann. In particular, minimal partitions exist and have regular representatives.

One of the main results in [4] concerns the characterization of the case of equality in Courant's nodal theorem. Consider an eigenvalue problem $-\Delta u_k = \lambda_k$ with suitable homogeneous boundary conditions (as previously defined) and order the eigenvalues in increasing order $\lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_k \ldots$. If we assume that u_k is real, then Courant's nodal theorem says that the number of its nodal domains $\mu(u_k)$ satisfies $\mu(u_k) \leq k$. Note that Courant's nodal theorem holds in greater generality, in higher dimensions and with a potential. Here a nodal domain is a component of $\Omega \setminus N(u_k)$ where Ω is the domain in Ω or the manifold and $N(u_k) = \overline{\{x \in \Omega \mid u_k(x) = 0\}}$. We call u_k and λ_k **Courant sharp** if $\mu(u_k) = k$. In [4] we have also described some properties of minimal partitions. In many respects they are related to nodal domains. Nodal domains have many interesting properties. In particular in neighboring nodal domains the corresponding eigenfunction has different signs. Thereby two nodal domains D_i, D_j are said to be neighbors if $\overline{\mathrm{Int}\, D_i \cup D_j}$ is connected. We can associate with any (not necessarily nodal) partition, say $\mathcal{D}_k = (D_1, \ldots, D_k)$, a simple graph in the following way: we associate to each D_i a vertex and draw an edge between two vertices i, j if the corresponding D_i, D_j are neighbors. This amounts to say that nodal graphs $\mathcal{G}(\mathcal{D}_k)$ are **bipartite** graphs.

The relation with Courant's nodal theorem is now the following, which is valid in the Dirichlet or Neumann case:

Theorem 1.2 (Dirichlet). *If for a bounded domain Ω with smooth boundary a minimal k-partition $\mathcal{D}$ with associated partition eigenvalue $\mathfrak{L}_k^D$ has a bipartite graph $\mathcal{G}(\mathcal{D})$, then this minimal k-partition is produced by the nodal domains of an eigenfunction u which is* **Courant sharp** *so that $-\Delta^D u = \lambda_k^D u$ in Ω and $\lambda_k^D = \mathfrak{L}_k^D$.*

Theorem 1.3 ($\partial\Omega$-Neumann). *If for a bounded domain Ω with smooth boundary a minimal k-partition $\mathcal{D}$ with associated partition eigenvalue $\mathfrak{L}_k^N$ has a bipartite graph $\mathcal{G}(\mathcal{D})$, then this minimal k-partition is produced by the nodal domains of an eigenfunction u which is* **Courant sharp** *so that $-\Delta^N u = \lambda_k^N u$ in Ω and $\lambda_k^N = \mathfrak{L}_k^N$.*

Note that by the minimax principle $\lambda_k^D \leq \mathfrak{L}_k^D$, resp. $\lambda_k^N \leq \mathfrak{L}_k^N$ and that, by Pleijel's Theorem [10], for each Ω there is a $k(\Omega)$ such that for each $k > k(\Omega)$ any associated eigenfunction u has strictly less than k nodal domains. That implies that, for sufficiently high k, the spectral minimal k-partitions are non-nodal.

Note also that we will also meet mixed cases, when either Dirichlet or Neumann boundary conditions are assumed on different components of $\partial\Omega$.

2. Neumann problem for a strip on the cylinder

We start with the a strip $C(1,b)=C(b)$ on a cylinder where

$$C(b)=\mathbb{S}^1_* \times (0,b)\,. \tag{2.1}$$

If needed, we can represent the strip by a rectangle $R(1,b)=(0,1)\times(0,b)$ with identification of $x=0$ and $x=1$. But the open sets of the partition are always considered as open sets on the strip.

We consider Neumann boundary conditions at $y=0$ and $y=b$. The spectrum for the Laplacian Δ^N with these boundary conditions is discrete and is given by

$$\sigma(-\Delta^N)=\left\{\pi^2\Big(4m^2+\frac{n^2}{b^2}\Big)_{(m,n)\in\mathbb{N}^2}\right\}. \tag{2.2}$$

Note that eigenvalues for $m\geq 1$ have at least multiplicity two. Identifying $L^2(C(1,b))$ and $L^2(R(1,b))$, a corresponding orthonormal basis of eigenfunctions is given by the functions on $R(1,b)$ $(x,y)\mapsto\cos(2\pi m x)\cos(\pi n\frac{y}{b})$ $((m,n)\in\mathbb{N}^2)$ and $(x,y)\mapsto\sin(2\pi m x)\cos(\pi n\frac{y}{b})$ $((m,n)\in\mathbb{N}^*\times\mathbb{N})$, where $\mathbb{N}^*=\mathbb{N}\setminus\{0\}$. We can now distinguish the following cases:

(i) If $b<\frac{1}{2}$,

$$\lambda_1^N=0\,,\ \lambda_2^N=\lambda_3^N=4\pi^2<\lambda_4^N\,.$$

(ii) If $\frac{1}{2}<b<1$,

$$\lambda_1^N=0\,,\ \lambda_2^N=\frac{\pi^2}{b^2}\,,\ \lambda_3^N=\lambda_4^N=4\pi^2<\lambda_5^N\,.$$

(iii) If $b=1$,

$$\lambda_1^N=0\,,\ \lambda_2^N=\pi^2\,,\ \lambda_3^N=\lambda_4^N=\lambda_5^N=4\pi^2<\lambda_6^N\,.$$

(iv) If $b>1$,

$$\lambda_1^N=0\,,\ \lambda_2^N=\pi^2\,,\ \lambda_3^N=4\pi^2<\lambda_4^N\,.$$

In particular, we see that $\lambda_3^N(C(1,b))$ is Courant sharp if and only if $b\geq 1$. Note also that, for $b\in(\frac{1}{2},1]$, $\lambda_4^N(C(1,b))$ cannot be Courant sharp, and that $\lambda_5^N(C(1,1))$ cannot be Courant sharp.

Before we state the main result for the strip on the cylinder, we look also at its double covering $C(2,b)$, whose associated rectangle is given by $(0,2)\times(0,b)$.

Lemma 2.1. *The Neumann eigenvalues for $C(2,b)$ are given, assuming that*

$$b\leq 1/3, \tag{2.3}$$

by

$$\lambda_1^N=0,\ \lambda_2^N=\lambda_3^N=\pi^2,\ \lambda_4^N=\lambda_5^N=4\pi^2,\ \lambda_6^N=\lambda_7^N=9\pi^2. \tag{2.4}$$

Note that $\lambda_6^N(C(2,b))$ is **Courant sharp** *if $b\leq 1/3$.*

Remark 2.2. Note that $\lambda_2^N=\lambda_3^N$ implies that $\mathfrak{L}_3^N>\lambda_3^N$ and that by Theorem 1.3 the associated $\mathcal{D}_3$ is **non-nodal**.

Note that for $b\geq 1$, we get by the same theorem that $\lambda_3^N(b)=\mathfrak{L}_3^N(b)=\frac{4\pi^2}{b^2}$.

Remark 2.3. The Neumann boundary conditions imply that the zero's hit the boundary not as in the Dirichlet case. More precisely consider the cylinder $C(1,b)$ with associated rectangle $R(1,b)$ and assume that the zero hits at $(x_0,0)$. In polar coordinates (r,ω) centered at this point the zeroset looks locally like the zeroset of $r^m \cos m\omega$, $m = 1,2,\ldots$. This is in contrast with the Dirichlet case where we would have $r^m \sin m\omega$. The r^m factor is just included to point out that eigenfunctions near zero's behave to leading order as harmonic homogeneous polynomials.

Here comes the main result for the minimal 3-partition for the strip on the cylinder.

Theorem 2.4. *For*

$$b \leq b_0 = \frac{1}{2\sqrt{5}}\,, \tag{2.5}$$

we have

$$\mathfrak{L}_3^N(C(b)) = 9\pi^2. \tag{2.6}$$

The associated minimal 3*-partition* $\mathcal{D}_3(b) = (D_1, D_2, D_3)$ *is up to rotation represented by*

$$D_\ell = ((\ell-1)/3, \ell/3) \times (0,b), \tag{2.7}$$

in $R(1,b)$.

Before giving the proof it might be appropriate to consider the case $b_0 < b \leq 1$. In this direction, we have:

Proposition 2.5. *For* $b \in [2/3, 1)$ *the spectral minimal* 3*-partition* $\mathcal{D}_3(b)$ *is not the one given by* (2.7) *and* $\mathfrak{L}_3^N(C(b)) < 9\pi^2$ *for* $2/3 < b < 1$.

Proof. It is immediate that the eigenfunction associated with $m = 0$ and $n = 2$ $(x,y) \mapsto \cos(2\pi\frac{y}{b})$ has three nodal domains with energy $\frac{4\pi^2}{b^2}$ which is less than $9\pi^2$. $\square$

Proof of the theorem. Note that by definition of $\mathfrak{L}_3^N$, we have in any case

$$\mathfrak{L}_3^N(C(b)) \leq 9\pi^2. \tag{2.8}$$

We first sketch the main ideas for the proof. There are two arguments which will be crucial for the proof:

(1) Take any candidate for a minimal 3-partition, $\mathcal{D}_3 = (D_1, D_2, D_3)$. If we can show that $\Lambda(\mathcal{D}_3) > 9\pi^2$ then this $\mathcal{D}_3$ cannot be a minimal partition due to the definition of $\mathfrak{L}_3^N(C(b))$.

(2) Assume $b \leq 1/3$. A 3-partition $\mathcal{D}_3$ is said to have **property B** if it becomes on the double covering $C(2,b)$ a 6-partition.

Assume that there is **minimal** 3-partition $\mathcal{D}_3$ with **property B**. Then $\Lambda(\mathcal{D}_3)$, the energy of this partition is larger than or equal to $\lambda_6^N(C(2,b))$. To see this just note that by Lemma 2.1, $\lambda_6^N(C(2,b))$ is Courant sharp. The corresponding minimal 6-partition $\mathcal{D}_6 = (D_1,\ldots,D_6)$ is given by

$$D_\ell = (\,(\ell-1)/3\,,\, \ell/3) \times (0,b), \quad \ell = 1,2,\ldots,6. \tag{2.9}$$

Furthermore $\mathcal{D}_6$ for $C(2,b)$ is just the lifted 3-partition of $C(1,b)$ given in Theorem 2.4.

Hence it suffices to show that the candidates for minimal partitions have the property B.

We also observe that the only candidates for minimal 3-partitions, assuming $b<1$, are non-nodal and further that, if we have a candidate for $\mathcal{D}_3=(D_1,D_2,D_3)$ for a minimal partition, each D_i is nice, that means

$$\operatorname{Int}(\overline{D}_i)=D_i. \tag{2.10}$$

If not we could lower the energy by removing an arc inside $\overline{D}_i$ without reducing the number of the D_i. Here we neglect sets of capacity 0.

The assumption on D_i implies by monotonicity that

$$\lambda_1^D(D_i)>\lambda_1^D(C(1,b))=\pi^2/b^2.$$

Hence if $\pi^2/b^2>9\pi^2$ the associated partition must already lead to a $\Lambda_3(\mathcal{D}_3)>9\pi^2$, so **(1)** applies. □

We proceed by showing that any minimal 3-partition has property **B**. To show this it suffices that in any minimal 3-partition $\mathcal{D}_3=(D_1,D_2,D_3)$ all the D_i are 0-homotopic. This implies that lifting this partition to the double covering yields a 6-partition and the argument **(2)** applies. We assume for contradiction that D_3 is not contractible, hence contains a path of index 1. We first observe that D_1 and D_2 must be neighbours (if not the partition would be nodal). Then let us introduce $D_{12}=\operatorname{Int}(\bar{D}_1\cup\bar{D}_2)$. Because D_3 contains a path of index 1, $\overline{D_{12}}$ cannot touch one component of the boundary of the cylinder and we have $\lambda_2^N(D_{12})=\mathfrak{L}_3^N$. By domain monotonicity (this is not the Dirichlet monotonicity result but the proof can be done either by reflection or by a density argument), the second eigenvalue $\lambda_2^N(D_{12})=\lambda_1^N(D_1)$ must be be larger than the second eigenvalue of the Dirichlet-Neumann problem of the cylinder. But we have, with λ_i^{ND} denoting the eigenvalues with Neumann and Dirichlet boundary conditions on the two components of the boundary of the strip,

$$\lambda_1^{ND}=\frac{\pi^2}{4b^2},\ \lambda_2^{ND}=\pi^2\min\Big(\frac{1}{b^2},\ \frac{1}{4b^2}+4\Big). \tag{2.11}$$

Hence

$$\lambda_2^N(D_{1,2})>\lambda_2^{ND}\,, \tag{2.12}$$

and we get a contradiction if $\lambda_2^{ND}\geq 9\pi^2$. We just have to work out the condition on b such that

$$\min\big(\frac{1}{b^2},\ \frac{1}{4b^2}+4\big)\geq 9. \tag{2.13}$$

This is achieved for $b\leq(2\sqrt{5})^{-1}$ as claimed in (2.5) in Theorem 2.4.

Remark 2.6. We recall that, although there is a natural candidate (which is nodal on the double covering), the minimal 3-partition problem with Dirichlet conditions for the annulus (also in the case of a thin annulus) or the disk is still open.

Remark 2.7. In view of the considerations above and of Proposition 2.5 the question arises whether for some $b < 1$ the corresponding minimal partition has the property that it has one or two points in its zero set where 3 arcs meet, hence having locally a **Y**-structure as discussed for instance in [5]. As in the case of the rectangle considered in [1], we can observe that in the case $b = 1$, the eigenfunction $\cos 2\pi x - \cos 2\pi y$ has a nodal set described in $R(1,1)$ by the two diagonals of the square and that it determines indeed a nodal 3-partition. The guess is then that when $1 - \epsilon < b < 1$ (with $\epsilon > 0$ small enough) this nodal 3-partition will be deformed into a non nodal minimal 3-partition keeping the symmetry $(x, y) \mapsto (x, 1 - y)$. We expect two critical points from which three arcs start.

3. Extension to minimal k-partitions of $C(b)$

One can also consider for $\Omega = C(b)$ minimal k-partitions with k odd ($k \geq 3$) and Neumann condition and assume

$$b < \frac{1}{k}\,. \tag{3.1}$$

The theorem of the previous section can be extended to the case $k > 3$.
First one observes that, if the closure of one open set of the minimal k-partition contains a line joining the two components of the boundary, then one can go to the double covering and obtain a $(2k)$-partition. If (3.1) is satisfied, $\lambda_k^N(C(0, 2b))$ is Courant sharp, and get as in the previous section that the energy of this partition is necessarily higher than $k^2\pi^2$.

So there is no D_i whose boundary has nonempty intersection with both parts of the boundary of the strip. Hence there exists one component of $\partial\Omega$ and at least $\frac{k+1}{2}$ D_i of the k-partition such that their boundaries ∂D_i's do not intersect with this component. We immediately deduce that if $b \leq \frac{1}{k}$:

$$\min\left(\mathfrak{L}^{DN}_{\frac{k+1}{2}}(\Omega), \mathfrak{L}^{ND}_{\frac{k+1}{2}}(\Omega)\right) \geq k^2\pi^2\,, \tag{3.2}$$

we have $\mathfrak{L}_k^N(\Omega) = k^2\pi^2$.

Here $\mathfrak{L}_\ell^{DN}$ corresponds to the ℓth spectral partition eigenvalue for the strip with Dirichlet boundary condition on $y = 0$ and Neumann boundary condition for $y = b$ and $\mathfrak{L}_\ell^{ND}$ is defined by exchange of the boundary conditions on the two boundaries. In our special case, due to the symmetry with respect to $y = \frac{b}{2}$, we have actually $\mathfrak{L}_\ell^{DN}(C(b)) = \mathfrak{L}_\ell^{ND}(C(b))$.

Having in mind that[2] $\lambda_\ell^{DN} \leq \mathfrak{L}_\ell^{DN}$, (3.2) is a consequence of

$$\lambda^{DN}_{\frac{k+1}{2}} \geq k^2\pi^2.$$

If $b < \frac{1}{k}$, we get in the case when $k = 4p + 3$ ($p \in \mathbb{N}$) the additional condition

$$\frac{1}{4b^2} + 4(p+1)^2 \geq (4p+3)^2\,.$$

[2]Note that we have equality for ℓ even and $b < \frac{1}{\ell}$.

Similarly, we get in the case when $k = 4p + 1$ ($p \in \mathbb{N}^*$)

$$\frac{1}{4b^2} + 4p^2 \geq (4p+1)^2\,.$$

We have consequently proven:

Theorem 3.1. *If*

- $k = 4p + 3$ ($p \in \mathbb{N}$) *and* $b \leq 1/\sqrt{(3k+1)(k-1)}$,
  or
- $k = 4p + 1$ ($p \in \mathbb{N}^*$) *and* $b \leq 1/\sqrt{(3k-1)(k+1)}$,

then

$$\mathfrak{L}_k(C(b)) = k^2\pi^2\,,$$

and a minimal k-partition is given by $D_\ell = ((\ell-1)/k, \ell/k)) \times (0, b)$, *for* $\ell = 1, \ldots, k$.

4. Generalization to other thin domains

The previous proof is more general than it seems at the first look. At the price of less explicit results we have a similar result for an annulus like domain Ω. We mention first the case $k = 3$ where the conditions read

- The eigenfunction associated with $\lambda_6^N(\Omega^R)$ is Courant sharp and antisymmetric with respect to the deck transformation from Ω^R onto Ω,
- $$\lambda_6^N(\Omega^R) \leq \inf(\lambda_2^{DN}(\Omega), \lambda_2^{ND}(\Omega))\,. \tag{4.1}$$

Here Ω^R is the double covering of Ω and (DN) (respectively (ND)) corresponds to the Dirichlet-Neumann problem (Dirichlet inside, Neumann outside), respectively (Dirichlet outside, Neumann inside). In the case of the annulus, these conditions can be made more explicit.

Here is a typical result which can be expected. For $b > 0$ and two regular functions $h_1(\theta)$ and $h_2(\theta)$ on the circle such that $h_1 < h_2$, we consider an annulus like domain around the unit circle defined in polar coordinates by

$$A(b) = \{(x, y)\,:\,1 + bh_1(\theta) < r < 1 + bh_2(\theta)\}\,.$$

It is clear from [8] together with Poincaré's inequality that there exists $b_0 > 0$ such that, if $0 < b \leq b_0$, condition (4.1) is satisfied.

One must verify the condition for Courant sharpness, which is true for the sixth eigenvalue of the lifted Laplacian on the double covering of the annulus and should be also true for our more general situation but for which we have no references, (see however [2] for thin curved tubes and [9]).

Remark 4.1. Although not explicit, condition (4.1) can be analyzed by perturbative method. This is indeed a purely spectral question. There is a huge literature concerning thin domains, see for example [3, 8] (and references therein).

Remark 4.2. Similar considerations lead also to extensions to higher k odd for the thin annulus with Neumann boundary conditions.

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Jacobi and CMV Matrices with Coefficients of Generalized Bounded Variation

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Abstract. We consider Jacobi and CMV matrices with coefficients satisfying an ℓ^p condition and a generalized bounded variation condition. This includes discrete Schrödinger operators on a half-line or line with finite linear combinations of Wigner–von Neumann type potentials $\cos(n\phi + \alpha)/n^\gamma$ with $\gamma > 0$.

Our results show preservation of the absolutely continuous spectrum, absence of singular continuous spectrum, and that embedded pure points in the continuous spectrum can only occur in an explicit finite set.

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For a bounded sequence $\{a_n, b_n\}_{n=1}^\infty$ with $a_n > 0$, $b_n \in \mathbb{R}$, the corresponding Jacobi matrix is the tridiagonal matrix acting on $\ell^2(\mathbb{N})$,

$$J(a,b) = \begin{pmatrix} b_1 & a_1 & & \\ a_1 & b_2 & a_2 & \\ & a_2 & b_3 & \ddots \\ & & \ddots & \ddots \end{pmatrix}. \tag{1}$$

For a sequence $\{\alpha_n\}_{n=0}^\infty$ with $|\alpha_n| < 1$, the corresponding CMV matrix [1] is a five-diagonal unitary matrix which acts on $\ell^2(\mathbb{N})$, defined by

$$\mathcal{C}(\alpha) = \begin{pmatrix} \Theta_0 & & & \\ & \Theta_2 & & \\ & & \Theta_4 & \\ & & & \ddots \end{pmatrix} \begin{pmatrix} 1 & & & \\ & \Theta_1 & & \\ & & \Theta_3 & \\ & & & \ddots \end{pmatrix} \tag{2}$$

where 1 stands for a single entry of 1 and Θ_j are unitary 2×2 blocks

$$\Theta_j = \begin{pmatrix} \bar{\alpha}_j & \sqrt{1-|\alpha_j|^2} \\ \sqrt{1-|\alpha_j|^2} & -\alpha_j \end{pmatrix} \tag{3}$$

CMV matrices arise naturally in the study of orthogonal polynomials on the unit circle (see [1, 11]).

It is well known that bounded variation combined with decay to the free case implies preservation of a.c. spectrum. These results are often cited as Weidmann's theorem, who proved the result for Schrödinger operators [13]. The analogous Jacobi and CMV results are due to Máté–Nevai [7] and Peherstorfer–Steinbauer [9].

Interest in operators with decaying harmonic oscillations dates at least to the work of Wigner and von Neumann [8] (see also [10, XIII.13]), who constructed on $\mathbb{R}^3$ a radial potential $V(r)$ with the asymptotic behavior

$$V(r) = -8\frac{\sin(2r)}{r} + O(r^{-2}), \quad r \to \infty \tag{4}$$

with the peculiar property that the Schrödinger operator $-\Delta + V$ has an eigenvalue at $+1$ embedded in the a.c. spectrum $[0, +\infty)$. We are interested in a class of Jacobi and CMV matrices with similar behavior. This motivates our use of the notion of *generalized bounded variation*:

Definition 1. A sequence $\beta = \{\beta_n\}_{n=N}^{\infty}$ (N can be finite or $-\infty$) has *rotated bounded variation* with phase ϕ if

$$\sum_{n=N}^{\infty} |e^{i\phi}\beta_{n+1} - \beta_n| < \infty. \tag{5}$$

A sequence $\alpha = \{\alpha_n\}_{n=N}^{\infty}$ has *generalized bounded variation* with the set of phases $A = \{\phi_1, \dots, \phi_L\}$ if it can be expressed as a finite sum

$$\alpha_n = \sum_{l=1}^{L} \beta_n^{(l)} \tag{6}$$

of L sequences $\beta^{(1)}, \dots, \beta^{(L)}$, such that the lth sequence $\beta^{(l)}$ has rotated bounded variation with phase ϕ_l. We will denote by $GBV(A)$ the set of sequences with generalized bounded variation with set of phases A.

For an example of rotated bounded variation with phase ϕ, take $\beta_n = e^{-i(n\phi+\alpha)}\gamma_n$, with $\{\gamma_n\}_{n=N}^{\infty}$ any sequence of bounded variation. Generalized bounded variation may seem like an unnatural condition for real-valued sequences, but by combining rotated bounded variation with phases ϕ and $-\phi$, one gets $e^{-i(n\phi+\alpha)}\gamma_n + e^{+i(n\phi+\alpha)}\gamma_n = \cos(n\phi+\alpha)\gamma_n$. It is then clear that a linear combination of Wigner–von Neumann type potentials plus an ℓ^1 part,

$$V_n = \sum_{k=1}^{K} \lambda_k \cos(n\phi_k + \delta_k)/n^{\gamma_k} + q_n \tag{7}$$

with $\gamma_k > 0$ and $\{q_n\} \in \ell^1$, has generalized bounded variation.

Wong [14] has the first result for CMV matrices with generalized bounded variation, proving Theorem 2 in the case $\{\alpha_n\}_{n=0}^{\infty} \in \ell^2$. For discrete Schrödinger operators, Janas–Simonov [3] analyzed the potential $V_n = \cos(\phi n + \delta)/n^{\gamma} + q_n$, with $\gamma > 1/3$ and $\{q_n\}_{n=1}^\infty \in \ell^1$, and obtained for this potential the same spectral results as our Corollary 3.

We can now state the main results:

Theorem 1 (Lukic [6]). *Let J be a Jacobi matrix with coefficients $\{a_n, b_n\}_{n=1}^\infty$. Let p be a positive integer, $A \subset \mathbb{R}$ a finite set of phases, and make one of these sets of assumptions:*

1° $\{a_n^2 - 1\}_{n=1}^\infty, \{b_n\}_{n=1}^\infty \in \ell^p \cap GBV(A)$
2° $\{a_n - 1\}_{n=1}^\infty, \{b_n\}_{n=1}^\infty \in \ell^p \cap GBV(A)$

Then

(i) $\sigma_{\mathrm{ac}}(J) = [-2, 2]$
(ii) $\sigma_{\mathrm{sc}}(J) = \emptyset$
(iii) $\sigma_{\mathrm{pp}}(J) \cap (-2, 2)$ *is the subset of an explicit finite set,*

$$\sigma_{\mathrm{pp}}(J) \cap (-2,2) \subset \left\{\pm 2\cos(\eta/2) \middle| \eta \in \underbrace{\tilde{A} + \cdots + \tilde{A}}_{p-1 \ \textit{times}}\right\} \tag{8}$$

where $\tilde{A} = A \cup \{0\}$ in case 1° and $\tilde{A} = (A + A) \cup A \cup \{0\}$ in case 2°.

Theorem 2 (Lukic [6]). *Let $\mathcal{C} = \mathcal{C}(\alpha)$ be a CMV matrix with coefficients $\{\alpha_n\}_{n=0}^\infty$ such that*

$$\{\alpha_n\}_{n=0}^\infty \in \ell^p \cap GBV(A)$$

for a positive odd integer $p = 2q + 1$ and a finite set $A \subset \mathbb{R}$. Then

(i) $\sigma_{\mathrm{ac}}(\mathcal{C}) = \partial\mathbb{D}$, *where $\partial\mathbb{D}$ is the unit circle*
(ii) $\sigma_{\mathrm{sc}}(\mathcal{C}) = \emptyset$
(iii) $\sigma_{\mathrm{pp}}(\mathcal{C})$ *is the subset of an explicit finite set,*

$$\sigma_{\mathrm{pp}}(\mathcal{C}) \subset \left\{\exp(i\eta) \middle| \eta \in (\underbrace{A + \cdots + A}_{q \ \textit{times}}) - (\underbrace{A + \cdots + A}_{q-1 \ \textit{times}})\right\} \tag{9}$$

Remark 1. If a sequence $\{\beta_n\}$ has rotated q-bounded variation, i.e., $\sum |e^{i\phi}\beta_{n+q} - \beta_n| < \infty$, then it also has generalized bounded variation so our results trivially extend to such sequences (with the appropriate adjustment of the set A).

In the special case $a_n = 1$, Theorem 1 becomes a result on discrete Schrödinger operators on a half-line. By a standard pasting argument, this also implies a result for discrete Schrödinger operators on a line.

Corollary 3. *Let*

$$(Hx)_n = x_{n+1} + x_{n-1} + V_n x_n \tag{10}$$

be a discrete Schrödinger operator on a half-line or line, with $\{V_n\}$ in ℓ^p with generalized bounded variation with set of phases A.

Then

(i) $\sigma_{\mathrm{ac}}(H) = [-2,2]$
(ii) $\sigma_{\mathrm{sc}}(H) = \emptyset$
(iii) $\sigma_{\mathrm{pp}}(H) \cap (-2,2)$ *is a finite set,*

$$\sigma_{\mathrm{pp}}(H) \cap (-2,2) \subset \left\{ \pm 2\cos(\eta/2) \,\middle|\, \eta \in \bigcup_{k=1}^{p-1} (\underbrace{A + \cdots + A}_{k \text{ times}}) \right\}$$

This corollary applies in particular to linear combinations of Wigner–von Neumann potentials (7).

All the results discussed so far concern perturbation of the free operator by generalized bounded variation. For perturbations of other operators the situation is more complicated. For instance, in contrast to Weidmann's theorem, Last [5] has shown that for some classes of potentials V_0, perturbing the discrete Schrödinger operator $-\Delta + V_0$ by a perturbation V of bounded variation can destroy a.c. spectrum.

In another direction, one can relax the bounded variation condition to an ℓ^2 condition on q-variation, namely $\sum_n |x_{n+q} - x_n|^2 < \infty$. Kaluzhny–Shamis [4], using in part ideas from Denisov [2] who studied the case $a_n \equiv 1$, have shown that this kind of perturbation with $x_n \to 0$ preserves the a.c. spectrum of periodic Jacobi operators.

In yet another direction, Stolz [12] takes Δ to be the forward difference operator $(\Delta x)_n = x_{n+1} - x_n$ and analyzes discrete Schrödinger potentials with $\Delta^j V \in \ell^{k/j}$ for $1 \le j \le k$, showing that a.c. spectrum persists precisely on the interval $[-2 + \limsup_{n\to\infty} V_n, 2 + \liminf_{n\to\infty} V_n]$.

As communicated to us by Yoram Last, this problem can also be motivated in a different way: let $V_n = \lambda_n W_n$, with $\lambda_n > 0$ monotone decaying to 0, and let H be given by (10). For different classes of potentials W, what kind of decay do we need to ensure preservation of a.c. spectrum? For W from a large class of almost periodic potentials, our results state that any $\{\lambda_n\} \in \ell^p$, $p < \infty$, suffices:

Corollary 4. *Let* (10) *be a discrete Schrödinger operator on a half-line or line with* $V_n = \lambda_n W_n$, $\{\lambda_n\} \in \ell^p$ *of bounded variation* (*with* $p < \infty$) *and* W *a trigonometric polynomial,*

$$W_n = \sum_{l=1}^{L} a_l \cos(2\pi\alpha_l n + \phi_l)$$

Then with $A = \{\pm 2\pi\alpha_1, \ldots, \pm 2\pi\alpha_l\}$, *all conclusions of Corollary* 3 *hold.*

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Order Convergence Ergodic Theorems in Rearrangement Invariant Spaces

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Abstract. We find necessary and sufficient conditions for order convergence of Cesáro averages of positive absolute contractions in rearrangement invariant spaces. We study the case, when the considered measure is infinite. The investigation of order convergence includes both Dominated and Individual Ergodic Theorems.

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1. Introduction

Let $(\mathbf{\Omega}, \mu)$ be an infinite σ-finite non-atomic measure space, $\mathbf{L}_p = \mathbf{L}_p(\mathbf{\Omega}, \mu)$, $1 \leq p \leq +\infty$ and $\mathbf{L}_0 = \mathbf{L}_0(\mathbf{\Omega}, \mu)$ be the set of all μ-measurable functions $f \colon \mathbf{\Omega} \to \mathbf{R}$.

We write: $\mathbf{L}_0 = \mathbf{L}_0(\mathbf{R}_+, \mathbf{m})$ in the particular case, when $\mathbf{\Omega} = \mathbf{R}_+ = [0, \infty)$ and $\mu = \mathbf{m}$ is the usual Lebesgue measure on $[0, +\infty)$.

A linear operator $T : \mathbf{L}_1 + \mathbf{L}_\infty \to \mathbf{L}_1 + \mathbf{L}_\infty$ is said to be an *absolute contraction or* $(\mathbf{L}_1, \mathbf{L}_\infty)$*-contraction* if T is a contraction in $\mathbf{L}_1$ and in $\mathbf{L}_\infty$ as well. The operator T is said to be *positive* if $Tf \geq 0$ for all $f \geq 0$. Let us denote by $\mathcal{PAC}$ the set of all positive absolute contractions.

For any $T \in \mathcal{PAC}$ and $f \in \mathbf{L}_1 + \mathbf{L}_\infty$ we consider the Cesáro averages

$$A_{n,T} f = \frac{1}{n} \sum_{k=1}^{n} T^{k-1} f$$

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and the corresponding dominant function

$$B_T f = \sup_{n\geq 1} A_{n,T}|f| = \sup_{n\geq 1} \frac{1}{n}\sum_{k=1}^{n} T^{k-1} f.$$

Notice that $B_T f \in \mathbf{L}_0$ for all $f \in \mathbf{L}_1 + \mathbf{L}_\infty$ (see [9], Ch. 8, §4 and [22], Ch. 1, §6).

A Banach space $\mathbf{E}$ of measurable functions on $(\mathbf{\Omega}, \mu)$ is called *rearrangement invariant* (r.i.) if

$$f \in \mathbf{L}_0\ ,\ g \in \mathbf{E},\ f^* \leq g^* \implies f \in \mathbf{E}\ ,\ \|f\|_{\mathbf{E}} \leq \|g\|_{\mathbf{E}}\ .$$

Here f^* denotes the decreasing right-continuous rearrangement of $|f|$. It can be defined as the right-continuous generalized inverse

$$f^*(x) := \inf\{y \in [0, +\infty) \colon \mathbf{n}_f(y) \leq x\}, \qquad x \in [0, \infty)$$

of the distribution function $\mathbf{n}_f$ of $|f|$, which is

$$\mathbf{n}_f(x) = \mu\{u \in \mathbf{\Omega} \colon |f(u)| > x\}\ ,$$

The function f^* is well defined if $\mathbf{n}_f(x) < +\infty$ for some $x \geq 0$.

In the case $(\mathbf{\Omega}, \mu) = (\mathbf{R}_+, \mathbf{m})$ r.i. spaces $\mathbf{E} = \mathbf{E}(\mathbf{R}_+, \mathbf{m})$ will be called *standard*. For any r.i. space $\mathbf{E}(\mathbf{\Omega}, \mu)$ on an arbitrary measure space $(\mathbf{\Omega}, \mu)$ there is a unique standard r.i. space $\mathbf{E}(\mathbf{R}_+, \mathbf{m})$ on $(\mathbf{R}_+, \mathbf{m})$ (called standard realization of $\mathbf{E}$) such that

$$f \in \mathbf{E}(\mathbf{\Omega}, \mu) \iff f^* \in \mathbf{E}(\mathbf{R}_+, \mathbf{m})$$

(see [21], Ch. II, §8). In general we do not assume that the measure space $(\mathbf{\Omega}, \mu)$ is separable and isomorphic to the standard measure space $(\mathbf{R}_+, \mathbf{m})$.

It is known (see [21], Ch. II, §4.1 or [24], Ch. 2.a), that for every r.i. space $\mathbf{E}$ there exist continuous inclusions

$$\mathbf{L}_1 \cap \mathbf{L}_\infty \subseteq \mathbf{E} \subseteq \mathbf{L}_1 + \mathbf{L}_\infty \subseteq \mathbf{L}_0\ ,$$

where $\mathbf{L}_0$ is considered as a complete topological linear space with respect to the stochastic convergence, i.e., the measure convergence on all finite measure sets.

On the other hand, every r.i. Banach space $\mathbf{E}$ is a Banach lattice and a sublattice of the lattice $\mathbf{L}_0$, equipped with the usual partial order on functions (see [17], Ch. 10 and [24], Ch. 1.c.). The lattice $\mathbf{L}_0$ is order σ-complete and also order complete, since the measure μ is σ-finite.

Remind that a subset F_0 of a partially ordered set F is said to be *order bounded* in F if $f \leq g$ for all $f \in F_0$ and some $g \in F$. The set F is called order complete if every order bounded subset $F_0 \subseteq F$ has the least upper bound $\sup F_0 \in F$ and the greatest lower bound $\inf F_0 \in F$ in F.

Further, a sequence $\{f_n\}_{n=1}^{\infty}$ of elements of a partially ordered set F is said to be *order convergent* to $f \in F$in F ($f_n \xrightarrow{(o)} f$), if there exist $g_n \in F$ and $h_n \in F$ such that

$$g_n \uparrow f\ \ ,\ \ h_n \downarrow f\ \ ,\ \ f = \sup_{n\geq 1} g_n = \inf_{n\geq 1} h_n \in F\ .$$

If, in addition, F is an order σ-complete lattice then $f_n \xrightarrow{(o)} f \in F$ iff $\{f_n\,,\, n \geq 1\}$ is order bounded in F and

$$f = \sup_{n\geq 1} \inf_{m\geq n} f_m = \inf_{n\geq 1} \sup_{m\geq n} f_m \in F\,.$$

Let $\mathbf{E} \subseteq \mathbf{L}_0(\mathbf{\Omega}, \mu)$ be an r.i. Banach space on $(\mathbf{\Omega}, \mu)$. Then

- $\mathbf{E}$ is a order complete sublattice of the order complete lattice $\mathbf{L}_0$.
- A sequence $\{f_n\}_{n=1}^{\infty}$ is order convergent in $\mathbf{E}$ ($f_n \xrightarrow{(o)} f \in \mathbf{E}$) iff the set $\{f_n\,,\, n \geq 1\}$ is order bounded in $\mathbf{E}$ and the sequence $\{f_n\}_{n=1}^{\infty}$ is order convergent in $\mathbf{L}_0$.
- $f_n \xrightarrow{(o)} f \in \mathbf{L}_0$) iff $f_n \to f$ almost everywhere on $(\mathbf{\Omega}, \mu)$).

Keeping in mind these facts we can formulate the following two problems that will be under our consideration:

Problem 1. Let $\mathbf{E}$ be an r.i. Banach space and $T \in \mathcal{PAC}$. What is the subset

$$\mathbf{E}^T := \{f \in \mathbf{E}\colon \{A_{n,T}f\}_{n=1}^{\infty} \text{ is order convergent in } \mathbf{E}\ \}\ ?$$

Problem 2. What is the subclass of all r.i. Banach spaces such that $\mathbf{E}^T = \mathbf{E}$ for all $T \in \mathcal{PAC}$, i.e., the sequence of Cesáro averages $\{A_{n,T}f\}_{n=1}^{\infty}$ is order convergent in $\mathbf{E}$ for all $f \in \mathbf{E}$ and $T \in \mathcal{PAC}$?

Notice again that the sequence $\{A_{n,T}f\}_{n=1}^{\infty}$ of Cesáro averages is (o)-convergent in $\mathbf{E}$ iff the corresponding dominant function $B_T f$ belongs to $\mathbf{E}$, while the sequence $\{A_{n,T}f\}_{n=1}^{\infty}$ itself converges almost everywhere on $(\mathbf{\Omega}, \mu)$.

This means that the setup includes both Dominated Ergodic Theorem ($\mathcal{DET}$) and Individual (Pointwise) Ergodic Theorem ($\mathcal{IET}$) in the classical case of spaces $\mathbf{L}_p$ and Zygmund's classes $\mathcal{Z}_r = \mathbf{L}\log^r \mathbf{L}$ (see, e.g., [9], Ch. VIII, §6 or [22], Ch. I, §1.6).

First individual and dominated ergodic theorems where proved in [12], [40],[2] and [18] for measure preserving transformations. One can find detailed explanation, various generalizations and relevant references in [22], and also in [1], where the case of infinite measure is treated in more details. Dunford and Schwartz ([8], [9] considered ergodic theorems for positive absolute contractions in spaces $\mathbf{L}_p$, $1 \leq p < \infty$. The Converse Dominated Ergodic Theorem in $\mathbf{L}_1$ was proved by Ornstein [34] for finite measure preserving transformations (see [22], pp. 54–56, where the infinite measure case is also described).

A. Veksler and A. Fedorov began to study Ergodic Theorems for general rearrangement invariant spaces. They investigated in [38] and [39] conditions of strong operator convergence of the Cesáro averages $A_{n,T}$, $T \in \mathcal{PAC}$ in r.i. Banach spaces $\mathbf{E}$. In particular they described the class of r.i. spaces $\mathbf{E}$, for which the Statistical (Mean) Ergodic Theorem holds on $\mathbf{E}$, i.e., the sequence of Cesáro averages $\{A_{n,T}f\}_{n=1}^{\infty}$ is convergent in norm $\|\cdot\|_{\mathbf{E}}$ for all $f \in \mathbf{E}$ and $T \in \mathcal{PAC}$.

Dominated Ergodic Theorems in r.i. spaces on finite measure spaces were studied in [4]. Some recent results on Ergodic Theorems in Orlicz and Lorentz spaces one can find in [30] [31], [32] and [33].

In this paper we solve Problems 1 and 2. Our main results Theorems 2.1–2.4 and some their consequences are formulated in Section 2.

These theorems follow in turn immediately from corresponding Dominated Ergodic Theorem, Converse Dominated Ergodic Theorem and Individual Ergodic Theorem, which are proved in Section 3, 4, and 5, respectively.

In the important particular cases, when the r.i. space $\mathbf{E}$ is an Orlicz space $\mathbf{E} = \mathbf{L}_\Phi$ or a Lorentz space $\mathbf{\Lambda}_W$, Problems 1 and 2 are solved in Section 6 in terms of corresponding Orlicz functions Φ and weight functions W.

The corresponding classical results for space $\mathbf{L}_p$ and for Zygmund classes $\mathbf{L}\log^r \mathbf{L}$ also follow.

2. Main results

To estimate the dominant functions $B_T f$, $f \in \mathbf{E}$, we use the *maximal Hardy-Littlewood function* f^{**}, which is defined for any function $f \in \mathbf{L}_1 + \mathbf{L}_\infty$ by

$$f^{**}(x) := \frac{1}{x}\int_0^x f^*(u)\,du, \qquad x \in (0,\infty)\ .$$

Let $\mathbf{E} = \mathbf{E}(\mathbf{\Omega},\mu)$ be an r.i. space on a measure space $(\mathbf{\Omega},\mu)$, and $\mathbf{E}(\mathbf{R}_+,\mathbf{m})$ be the corresponding standard r.i. space. *The Hardy core* of $\mathbf{E}$ is

$$\mathbf{E_H} = \mathbf{E_H}(\mathbf{\Omega},\mu) := \{f \in (\mathbf{L}_1 + \mathbf{L}_\infty)(\mathbf{\Omega},\mu)\colon f^{**} \in \mathbf{E}(\mathbf{R}_+,\mathbf{m})\}\ .$$

Evidently, $f^* \le f^{**}$ for every $f \in \mathbf{E}$, whence $\mathbf{E_H} \subseteq \mathbf{E}$. Moreover, it can be verified that $\mathbf{E_H}$ is an r.i. space with the norm

$$\|f\|_{\mathbf{E_H}} := \|f^{**}\|_{\mathbf{E}}\ \ ,\ \ f \in \mathbf{E_H}\ ,$$

provided that $\mathbf{E_H} \ne \{0\}$.

Notice that in the standard case $(\mathbf{\Omega},\mu) = (\mathbf{R}_+,\mathbf{m})$, the space $\mathbf{E_H}$ is the largest r.i. space, for which the Hardy operator

$$(Hf)(x) := \frac{1}{x}\int_0^x f(u)\,du \quad , \quad x \in (0,\infty)$$

is a positive contraction from $\mathbf{E_H}$ to $\mathbf{E}$.

It should be mentioned that for any r.i. space $\mathbf{E}$ and $T \in \mathcal{PAC}$

$$T(\mathbf{E_H}) \subseteq \mathbf{E_H}$$

and the restriction $T|_{\mathbf{E_H}}\colon \mathbf{E_H} \to \mathbf{E_H}$ is a contraction.

Indeed, by Calderon-Mityagin theorem

$$(Tf)^{**}(x) \le f^{**}(x)\,,\ 0 < x < \infty$$

for all $f \in \mathbf{L}_1 + \mathbf{L}_\infty$ and $T \in \mathcal{PAC}$ (see [5], [26] or [21], Ch.II, §3.4). Whence

$$\|Tf\|_{\mathbf{E_H}} := \|(Tf)^{**}\|_{\mathbf{E}} \le \|f^{**}\|_{\mathbf{E}} := \|f\|_{\mathbf{E_H}}\ .$$

Thus every r.i. space of the form $\mathbf{E_H}$, is an interpolation space with respect to the pair $(\mathbf{L}_1 \cap \mathbf{L}_\infty, \mathbf{L}_1 + \mathbf{L}_\infty)$.

On the other hand, r.i. spaces need not to be interpolational. There exist r.i. spaces $\mathbf{E}$ such that $T\mathbf{E} \not\subseteq \mathbf{E}$ for some $T \in \mathcal{PAC}$([21], Ch. II §5.7). Thus Tf and $A_{n,T}f$ do not *a priori* belong to $\mathbf{E}$ for $f \in \mathbf{E}$ and $T \in \mathcal{PAC}$.

The r.i. space $\mathcal{R}_0 = \mathcal{R}_0(\mathbf{\Omega}, \mu)$ can be defined by

$$\mathcal{R}_0 = \{f \in \mathbf{L}_1 + \mathbf{L}_\infty \colon f^*(+\infty) := \lim_{x \to +\infty} f(x) = 0\} \ .$$

It plays an important role in our exposition. This space may be described in many different ways:

$$\mathcal{R}_0 = \{f \in \mathbf{L}_1 + \mathbf{L}_\infty \colon \mathbf{n}_f(x) < +\infty \, , \, x > 0\} = cl_{\mathbf{L}_1 + \mathbf{L}_\infty}(\mathbf{L}_1 \cap \mathbf{L}_\infty) = cl_{\mathbf{L}_1 + \mathbf{L}_\infty}(\mathbf{L}_1) \ ,$$

and $\mathcal{R}_0$ is the heart of $\mathbf{L}_1 + \mathbf{L}_\infty$ considered as an Orlicz space.

Now we can formulate our main result (solving Problem 1):

Theorem 2.1. *Let $\mathbf{E}$ be an r.i. space. Then for all $f \in \mathbf{E_H} \cap \mathcal{R}_0$ and all $T \in \mathcal{PAC}$ the sequence of averages $\{A_{n,T}f\}_{n=1}^\infty$ is order convergent in $\mathbf{E}$.*

Condition $f \in \mathbf{E_H}$ implies that the sequence $\{A_{n,T}f\}_{n=1}^\infty$ is order bounded in $\mathbf{E}$, i.e., $B_T f \in \mathbf{E}$. Thus Dominated Ergodic Theorem ($\mathcal{DET}$) in $\mathbf{E}$ holds on Hardy core $\mathbf{E_H}$ of $\mathbf{E}$.

Condition $f \in \mathcal{R}_0$ implies that the sequence $\{A_{n,T}f\}_{n=1}^\infty$ is order convergent in $\mathbf{L}_0$, i.e., Individual Ergodic Theorem ($\mathcal{IET}$) holds on $\mathcal{R}_0$.

The converse is also true. Namely,

Theorem 2.2. *Let $\mathbf{E}$ be an r.i. space such that $\mathbf{E} \neq \mathbf{E_H} \cap \mathcal{R}_0$. Then there exist $f \in \mathbf{E}$ and $T \in \mathcal{PAC}$ such that the sequence $\{A_{n,T}f\}_{n=1}^\infty$ is not order convergent in $\mathbf{E}$.*

Both $\mathcal{DET}$ and $\mathcal{IET}$ parts in the converse theorem can be made more precise separately. Let θ be a measure preserving transformation on $(\mathbf{\Omega}, \mu)$ and $T = T_\theta \in \mathcal{PAC}$ is of the form $T_\theta f = f \circ \theta$. Evidently, $T_\theta \in \mathcal{PAC}$ and $T_\theta \mathbf{E} = \mathbf{E}$ for each r.i. space $\mathbf{E}$. Let $\mathcal{PAC}_0$ consists of all operators T_θ, where θ is an *conservative ergodic measure preserving transformation* on $(\mathbf{\Omega}, \mu)$.

Theorem 2.3. *Let $\mathbf{E}$ be an r.i. space and $T = T_\theta \in \mathcal{PAC}_0$. Then*

1) *If $B_T f \in \mathbf{E}$ then $f \in \mathbf{E_H}$.*
2) *If $\mathbf{E} \not\subseteq \mathcal{R}_0$ then the sequence $\{A_{n,T}f\}_{n=1}^\infty$ is not order convergent for some $f \in \mathbf{E}$.*

Turning to Problem 2, we have the following corollary of Theorems 2.1 and 2.2.

Theorem 2.4. *Let $\mathbf{E}$ be an r.i. space. The following conditions are equivalent:*

(i) *The sequence $\{A_{n,T}f\}_{n=1}^\infty$ is order convergent for all $f \in \mathbf{E}$ and $T \in \mathcal{PAC}$.*
(ii) $\mathbf{E} = \mathbf{E_H} \cap \mathcal{R}_0$.

Thus

- *An r.i. space* $\mathbf{E}$ *satisfies Order Ergodic Theorem* ($\mathbf{E} \in \mathcal{OET}$), *iff* $\mathbf{E_H} = \mathbf{E}$ *and* $\mathbf{E} \subseteq \mathcal{R}_0$.

Condition $\mathbf{E_H} = \mathbf{E}$ means that the Hardy operator H acts as a bounded operator on $\mathbf{E}$. To clarify the condition one can use the dilation group $\{D_t\,,\, 0 < t < +\infty\}$ and the lower and upper indexes $1 \le p_{\mathbf{E}} \le q_{\mathbf{E}} \le +\infty$ of an r.i. space $\mathbf{E}$, which are defined as follows.

Let for any $f \in \mathbf{L}_0 = \mathbf{L}_0(\mathbf{R}_+, \mathbf{m})$:

$$D_t f(x) := f(x/t)\ ,\ 0 < x, t < \infty.$$

Then $\{D_t\,,\, 0 < t < \infty\}$ is a group of bounded linear operators $D_t \colon \mathbf{E} \to \mathbf{E}$ on the standard r.i. space $\mathbf{E} = \mathbf{E}(\mathbf{R}_+, \mathbf{m})$, corresponding to $\mathbf{E}(\mathbf{\Omega}, \mu)$.

The function $d_{\mathbf{E}}(t) := \|D_t\|_{\mathbf{E}\to\mathbf{E}}$ is semi-multiplicative on $(0, \infty)$, i.e., $d_{\mathbf{E}}(s+t) \le d_{\mathbf{E}}(s)\, d_{\mathbf{E}}(t)$ for all s, t. Hence, there exist the limits

$$p_{\mathbf{E}} := \lim_{t\to\infty} \frac{\log t}{\log d_{\mathbf{E}}(t)} = \inf_{1<t} \frac{\log(t)}{\log d_{\mathbf{E}}(t)},\quad q_{\mathbf{E}} := \lim_{t\to 0} \frac{\log t}{\log d_{\mathbf{E}}(t)} = \inf_{0<t<1} \frac{\log t}{\log d_{\mathbf{E}}(t)}\ ,$$

and they are called *lower and upper Boyd indices* of the r.i. space $\mathbf{E}$ (see [3], [21], Ch. II, §4.3, [24], Ch. 2.b).

Proposition 2.5 ([21], Chap. II, §6.1). *Let* $\mathbf{E}$ *be an r.i. space and* $d_{\mathbf{E}}(t) = \|D_t\|_{\mathbf{E}\to\mathbf{E}}$ *and* $p_{\mathbf{E}}$ *be the lower Boyd index. Then the following conditions are equivalent:*

- $\mathbf{E_H} = \mathbf{E}$.
- $p_{\mathbf{E}} > 1$.
- $\int_0^1 d_{\mathbf{E}}(1/t)\, dt < \infty$.
- $d_{\mathbf{E}}(t) = o(t)$ *as* $t \to +\infty$.

The second condition $\mathbf{E} \subseteq \mathcal{R}_0$ is well verifiable since $\mathbf{E} \nsubseteq \mathcal{R}_0$ implies $\mathbf{1} \in \mathbf{E}$ and $\mathbf{E} \supseteq \mathbf{L}_\infty$

For instance, $p_{\mathbf{L}_p} = q_{\mathbf{L}_p} = p$ for each $1 \le p \le +\infty$, whence $(\mathbf{L}_p)_{\mathbf{H}} = \mathbf{L}_p$ for $p > 1$, while $(\mathbf{L}_1)_{\mathbf{H}} = \mathcal{Z}_1 \nsubseteq \mathbf{L}_1$ (see below). Thus

- $\mathbf{L}_p \in \mathcal{OET}$ iff $1 < p < +\infty$.

while

- $\mathbf{L}_p \in \mathcal{DET}$ iff $1 < p \le +\infty$.
- $\mathbf{L}_p \in \mathcal{IET}$ iff $1 \le p < +\infty$.

3. Dominated Ergodic Theorem

Let $T \in \mathcal{PAC}$ and let $A_{n,T} = \frac{1}{n}\sum_{k=1}^{n} T^{k-1}$ be the corresponding Cesáro averages. Consider the *dominant function*

$$B_T f(\omega) = \sup_{n\ge 1}(A_{n,T}|f|)(\omega), \quad \omega \in \mathbf{\Omega}.$$

Notice that $B_T f(\omega) < \infty$ for all $f \in \mathbf{L}_1 + \mathbf{L}_\infty$ ([9], Ch. VIII, §4). This fact also follows from Lemma 3.3 (below).

In this section we consider two following problems

- Let $\mathbf{E}$ be an r.i. Banach space and $T \in \mathcal{PAC}$. What is the subset
$$\mathbf{E}^T_{\mathcal{DET}} := \{ f \in \mathbf{E} : \ B_T f \in \mathbf{E} \} \ ?$$
- What is the subclass of all r.i. Banach spaces E such that $\mathbf{E}^T_{\mathcal{DET}} = \mathbf{E}$ for all $T \in \mathcal{PAC}$, i.e., sequences of Cesáro averages $\{A_{n,T} f\}_{n=1}^{\infty}$ are order bounded in $\mathbf{E}$ for every $T \in \mathcal{PAC}$?

Theorem 3.1 (Dominated Ergodic Theorem). *Let $\mathbf{E}(\mathbf{\Omega}, \mu)$ be an r.i. space and $T \in \mathcal{PAC}$. Then $f \in \mathbf{E_H}$ implies $B_T f \in \mathbf{E}$ and*
$$\|B_T f\|_{\mathbf{E}} \leqslant \|f\|_{\mathbf{E_H}}.$$

Theorem 3.1 follows from the following two lemmas.

Lemma 3.2. *Let functions $f, \ g \in (\mathbf{L}_1 + \mathbf{L}_\infty)(\mathbf{\Omega}, \mu)$, $f \geq 0$, $g \geq 0$, satisfy the following condition:*

1) $g^*(\infty) = 0$;
2) *For every* $t > 0$
$$\mu\{g > t\} \leqslant \frac{1}{t} \int\limits_{\{g>t\}} f \, d\mu.$$

Then $g^*(s) \leqslant f^{**}(s)$ for all $s > 0$.

Proof. We shall use the following "maximal" property of the function f^* ([21], Ch. II, §2),
$$\int\limits_0^s f^*(x) \, dx = \sup_{G: \mu G = s} \int\limits_G f \, d\mu.$$
Let $t > 0$ and $s = \mu\{g > t\}$. Then
$$s \leqslant \frac{1}{t} \int\limits_{\{g>t\}} f \, d\mu,$$
and hence
$$t \leqslant \frac{1}{s} \int\limits_{\{g>t\}} f \, d\mu \leqslant \frac{1}{s} \sup_{G: \mu G = s} \int\limits_G f \, d\mu = \frac{1}{s} \int\limits_0^s f^*(x) \, dx = f^{**}(s).$$
Thus
$$t \leqslant f^{**}(\mu\{g > t\}) = f^{**}(s).$$
Since $s = \mu\{g > t\} = \mathbf{m}\{g^* > t\}$, then $g^*(s) \leqslant t$ and, in addition, $g^*(s) = t$ in the case when g^* is continuous at the point s.

Consider the partition $(0, +\infty) = \mathcal{A} \cup \mathcal{B}$, where
$$\mathcal{A} = \{s \in (0, +\infty) : \ s = \mu\{g > t\}, \ \text{for some } t > 0\}$$
and
$$\mathcal{B} = (0, +\infty) \backslash \mathcal{A}.$$

Consider two cases.

1) *Let* $s_0 \in \mathcal{A}$. Then

$$\{t > 0 : \mu\{g > t\} = s_0\} \neq \emptyset.$$

Denote

$$t_0 = \sup\{t > 0 : \mu\{g > t\} = s_0\} = \sup\{t > 0 : \mathbf{m}\{g^* > t\} = s_0\}.$$

Since $g^*(s)$ is a non-increasing right continuous function, we have

$$t_0 = g^*(s_0 - 0) = \lim_{s \to s_0 - 0} g^*(s).$$

Further, the inequality $t \leqslant f^{**}(s_0)$ holds for all $t > 0$ such that

$$\mu\{g > t\} = s_0.$$

Hence $t_0 \leqslant f^{**}(s_0)$ and

$$g^*(s_0 - 0) \leqslant f^{**}(s_0),$$

whence

$$g^*(s_0) \leqslant g^*(s_0 - 0) \leqslant f^{**}(s_0).$$

2) *Let* $s \in \mathcal{B}$. Consider

$$s_0 = \sup\{u > s : g^*(u) = g^*(s)\}.$$

There are three possible subcases

2.1) *g^* is not continuous at s_0.* Then

$$\mathbf{m}\{g^* > t\} = s_0$$

for every $t \in [g^*(s_0), g^*(s_0 - 0)]$. Hence $s_0 \in \mathcal{A}$ and

$$g^*(s_0) = g^*(s_0 - 0) \leqslant f^{**}(s_0) \leqslant f^{**}(s).$$

2.2) *g^* is continuous at s_0.* Let $s_1 > s_0$ and the function g^* is strictly decreasing on $[s_0, s_1]$. Then for every $s' \in (s_0, s_1)$ there exists $t > 0$ such that

$$\mathbf{m}\{g^* > t\} = \mu\{g > t\} = s'.$$

Hence $s' \in \mathcal{A}$ and

$$g^*(s') \leqslant f^{**}(s').$$

By passing to the limit with $s' \to s_0 - 0$ we have

$$g^*(s) = g^*(s_0) = g^*(s_0 + 0) \leqslant f^{**}(s_0 + 0) \leqslant f^{**}(s_0) \leqslant f^{**}(s).$$

2.3) *$s_0 = +\infty$.*

Then for each $x \in [s, +\infty)$ we have

$$g^*(x) = g^*(s) = g^*(\infty) = 0,$$

and hence

$$g^*(s) = 0 \leqslant f^{**}(s). \qquad \square$$

Lemma 3.3. *Let $T \in \mathcal{PAC}$ and $f \in (\mathbf{L}_1 + \mathbf{L}_\infty)(\mathbf{\Omega}, \mu)$. Then*

$$(B_T f)^*(s) \leqslant f^{**}(s).$$

Proof. We may assume without loss of generality that $f = |f| \geqslant 0$.

1) First consider the case $f^*(\infty) = 0$. Then $f^{**}(\infty) = 0$. It is not hard to show, that

$$(B_T f)^*(\infty) = 0.$$

We use Maximal Ergodic Inequality for $T \in \mathcal{PAC}$ ([22], Ch. 1, §1.6):

$$\mu\{B_T f > t\} \leqslant \frac{1}{t} \int\limits_{\{B_T f > t\}} f \, d\mu, \quad t > 0$$

and put $g = B_T f$.

The functions f and g satisfy the conditions of Lemma 3.2 and hence

$$g^*(s) = (B_T f)^* \leqslant f^{**}(s), \quad s > 0.$$

2) Let now $f^*(\infty) = \lambda > 0$. Then $f = f_\lambda + \lambda$, where $f_\lambda^*(\infty) = 0$. Since

$$(f_\lambda + \lambda)^*(t) = f_\lambda^*(t) + \lambda$$

and

$$\begin{aligned}(f_\lambda + \lambda)^{**}(t) &= \frac{1}{t} \int\limits_0^t (f_\lambda + \lambda)^*(s) \, ds = \frac{1}{t} \int\limits_0^t (f_\lambda^* + \lambda)(s) \, ds \\ &= \frac{1}{t} \int\limits_0^t f_\lambda^*(s) \, ds + \lambda = f_\lambda^{**}(t) + \lambda,\end{aligned}$$

we have

$$\begin{aligned}(B_T f)^*(s) = [B_T(f_\lambda + \lambda)]^*(s) &\leqslant [B_T(f_\lambda)]^*(s) + \lambda \\ &\leqslant f_\lambda^{**}(s) + \lambda = (f_\lambda + \lambda)^{**}(s) = f^{**}(s),\end{aligned}$$

i.e.,

$$(B_T f)^*(s) \leqslant f^{**}(s). \qquad \square$$

Proof of Theorem 3.1. Let $f \in \mathbf{E_H}$, then $f \in (\mathbf{L}_1 + \mathbf{L}_\infty)(\mathbf{\Omega}, \mu)$ and $f^{**} \in \mathbf{E}(\mathbf{R}_+, \mathbf{m})$.

By Lemma 3.3,

$$(B_T f)^*(s) \leqslant f^{**}(s), \ s > 0.$$

Therefore $(B_T f)^* \in \mathbf{E}(\mathbf{R}_+, \mathbf{m})$ and

$$\|(B_T f)^*\|_{\mathbf{E}(\mathbf{R}_+, \mathbf{m})} \leqslant \|f^{**}\|_{\mathbf{E}(\mathbf{R}_+, \mathbf{m})}.$$

Since $[(B_T f)^*]^* = (B_T f)^*$, we have also $B_T f \in \mathbf{E}$ and

$$\|B_T f\|_{\mathbf{E}} = \|(B_T f)^*\|_{\mathbf{E}(\mathbf{R}_+, \mathbf{m})} \leqslant \|f^{**}\|_{\mathbf{E}(\mathbf{R}_+, \mathbf{m})} = \|f\|_{\mathbf{E_H}}. \qquad \square$$

4. Converse Dominated Ergodic Theorem

Theorem 4.1 (Converse Dominated Ergodic Theorem). *Let $\mathbf{E}(\mathbf{\Omega},\mu)$ be an r.i. space, θ be an ergodic conservative measure preserving transformation on $(\mathbf{\Omega},\mu)$ and $T=T_\theta\in\mathcal{PAC}_0$ is of the form $T_\theta f=f\circ\theta$. Then $B_Tf\in\mathbf{E}$ implies $f\in\mathbf{E_H}$.*

In order to prove the theorem we need the following inequalities.

Proposition 4.2. *Let $f\in\mathbf{L}_1(\mathbf{\Omega},\mu)+\mathbf{L}_\infty(\mathbf{\Omega},\mu)$, $f\geqslant 0$ and $C>1$. Then*

$$(C-1)\mathbf{m}\{f^{**}\geqslant Ct\}\leqslant\frac{1}{t}\int\limits_{\{f>t\}}f\,d\mu\leqslant\mathbf{m}\{f^{**}>t\}$$

for all $t>f^*(\infty)$.

Proof. 1) *The first inequality.* Since $\mathbf{n}_f=\mathbf{n}_{f^*}$ we may suppose without loss of generality that $f=f^*$.

Let $s=\mathbf{m}\{f^{**}\geqslant Ct\}$. Since $t>f^*(\infty)$ and $C>1$, we have $Ct>f^*(\infty)$. For every $u>f^*(\infty)$

$$f^{**}(\mathbf{m}\{f^{**}>u\})=u,$$

therefore $f^{**}(s)=Ct$. Thus

$$\frac{1}{s}\int\limits_0^s f^*(\tau)\,d\tau=Ct,\quad\text{and}\quad s=\frac{1}{Ct}\int\limits_0^s f^*\,d\mathbf{m}.$$

If $s\leqslant\mathbf{m}\{f^*>t\}$, Then

$$s\leqslant\frac{1}{Ct}\int\limits_0^{\mathbf{m}\{f^*>t\}}f^*\,d\mathbf{m}=\frac{1}{Ct}\int\limits_{\{f^*>t\}}f^*\,d\mathbf{m}.$$

Whence

$$(C-1)s<Cs\leqslant\frac{1}{t}\int\limits_{\{f^*>t\}}f^*\,d\mathbf{m}=\int\limits_{\{f>t\}}f\,d\mu.$$

The function f^* is non-increasing, hence $s>\mathbf{m}\{f^*>t\}$ implies $f^*(s)\leqslant t$. Then

$$\frac{1}{Ct}\int\limits_{\mathbf{m}\{f^*>t\}}^s f^*\,d\mathbf{m}\leqslant\frac{1}{Ct}\int\limits_{\mathbf{m}\{f^*>t\}}^s t\,d\mathbf{m}\leqslant\frac{1}{Ct}st=\frac{s}{C}$$

and hence

$$s-\frac{s}{C}\leqslant\frac{1}{Ct}\int\limits_0^{\mathbf{m}\{f^*>t\}}f^*\,d\mathbf{m}.$$

Thus

$$(C-1)s\leqslant\frac{1}{t}\int\limits_{\{f^*>t\}}f^*\,d\mathbf{m}.$$

2) *The second inequality.* Let $u = \mathbf{m}\{f^{**} > t\}$. Since $t > f^{**}(\infty)$, we have $f^{**}(u) = t$ and

$$t = \frac{1}{u}\int\limits_0^u f^*(s)\,ds.$$

Whence

$$u = \frac{1}{t}\int\limits_0^u f^*(s)\,ds \geqslant \frac{1}{t}\int\limits_{\{f^*>f^*(u)\}} f^*\,d\mathbf{m}.$$

Since $t = f^{**}(u) \geqslant f^*(u)$, we have also

$$\frac{1}{t}\int\limits_{\{f^*>f^*(u)\}} f^*\,d\mathbf{m} \geqslant \frac{1}{t}\int\limits_{\{f^*>t\}} f^*\,d\mathbf{m},$$

i.e.,

$$\mathbf{m}\{f^{**} > t\} = u \geqslant \frac{1}{t}\int\limits_{\{f^*>t\}} f^*\,d\mathbf{m}. \qquad \square$$

Lemma 4.3. *Let θ be an ergodic conservative measure preserving transformation on $(\mathbf{\Omega}, \mu)$ and $T = T_\theta \in \mathcal{PAC}$ is of the form $T_\theta f = f \circ \theta$. Then*

$$f^{**}(s) \leqslant 2(B_T f)^*\left(\frac{s}{2}\right)$$

for all $s > 0$ and for every $f \in \mathcal{R}_0$.

Proof. We may suppose without loss of generality that $f = |f| \geqslant 0$.

By Proposition 4.2 with $C = 2$ we have

$$\mathbf{m}\{f^{**} \geqslant 2t\} \leqslant \frac{1}{t}\int\limits_{\{f>t\}} f\,d\mu$$

for all $t > f^*(\infty)$. Here $f^*(\infty) = 0$ since $f \in \mathcal{R}_0$. It is proved in [22], Lemma 6.7, that

$$\frac{1}{2t}\int\limits_{\{f>t\}} f\,d\mu \leqslant \frac{1}{2t}\int\limits_{\{B_T f>t\}} f\,d\mu \leqslant \mu\{B_T f > t\}.$$

Thus

$$\mathbf{m}\{f^{**} \geqslant 2t\} \leqslant 2\mu\{B_T f > t\}$$

for all $t > 0$. This inequality holds for every $T \in \mathcal{PAC}$ of the form $T = T_\theta$, where θ is an ergodic conservative measure preserving transformation of $(\mathbf{\Omega}, \mu)$.

For every $s > 0$ we have now

$$\begin{aligned}(B_T f)^*\left(\frac{s}{2}\right) &= \inf\left\{t > 0:\ \mu\{B_T f > t\} \leqslant \frac{s}{2}\right\}\\ &\geqslant \inf\{t > 0:\ \mathbf{m}\{f^{**} \geqslant 2t\} \leqslant s\} \geqslant \inf\{t > 0:\ \mathbf{m}\{f^{**} > 2t\} \leqslant s\}\\ &= \frac{1}{2}\inf\{2t > 0 : \mathbf{m}\{f^{**} > 2t\} \leqslant s\} = \frac{1}{2}(f^{**})^*(s) = \frac{1}{2}f^{**}(s). \qquad \square\end{aligned}$$

Proof of Theorem 4.1. Let $B_T f \in \mathbf{E}$. By using the dilation operator D_t with $t = 2$,

$$(D_2 g)(t) = g\left(\frac{t}{2}\right), \quad t > 0,$$

and putting $g = B_T f$, we can write the inequality in Lemma 4.3 as $f^{**} \leq 2D_2(B_T f)^*$. It is known ([21], Ch. II, §4.3, [24], Ch. 2.b) that the dilation operator D_t act as a bounded liner operator in each of standard rearrangement invariant space $\mathbf{E}(\mathbf{R}_+, \mathbf{m})$. Hence,

$$B_T f \in \mathbf{E}(\mathbf{\Omega}, \mu) \;\Leftrightarrow\; (B_T f)^* \in \mathbf{E}(\mathbf{R}_+, \mathbf{m}) \;\Leftrightarrow\; D_2(B_T f)^* \in \mathbf{E}(\mathbf{R}_+, \mathbf{m}).$$

Therefore

$$B_T f \in \mathbf{E}(\mathbf{\Omega}, \mu) \;\Rightarrow\; f^{**} \in \mathbf{E}(\mathbf{R}_+, \mathbf{m}) \;\Leftrightarrow\; f \in \mathbf{E}_{\mathbf{H}}(\mathbf{\Omega}, \mu)\ . \qquad \square$$

We shall say that an r.i. space $\mathbf{E}$ has Hardy-Littlewood property ($\mathbf{E} \in \mathcal{HLP}$) if $\mathbf{E}_{\mathbf{H}} = \mathbf{E}$, that is $f \in \mathbf{E} \;\Leftrightarrow\; f^{**} \in \mathbf{E}$. We shall write $\mathbf{E} \in \mathcal{DET}$ if $B_T f \in \mathbf{E}$ for all $f \in \mathbf{E}$ and $T \in \mathcal{PAC}$.

Corollary 4.4. $\mathbf{E} \in \mathcal{DET} \;\Leftrightarrow\; \mathbf{E} \in \mathcal{HLP}$.

5. Pointwise Ergodic Theorem

Recall that $\mathcal{R}_0 = cl_{\mathbf{L}_1+\mathbf{L}_\infty}(\mathbf{L}_1 \cap \mathbf{L}_\infty)$ is the minimal part of the space $\mathbf{L}_1 + \mathbf{L}_\infty$. It consists of all $f \in \mathbf{L}_1 + \mathbf{L}_\infty$ such that $f^*(\infty) = 0$, or (an equivalent condition) $\mathbf{n}_f(x) < \infty$ for all $x > 0$.

Theorem 5.1. *Let $T \in \mathcal{PAC}$ and $f \in \mathcal{R}_0$, then $\{A_{n,T} f\}_{n=1}^{\infty}$ converges almost everywhere on $(\mathbf{\Omega}, \mu)$. Conversely, let θ be an ergodic conservative measure preserving transformation on $(\mathbf{\Omega}, \mu)$ and $T = T_\theta$ is of the form $T_\theta f = f \circ \theta$. Then there exists $f \in \mathbf{L}_\infty$ such that $\{A_{n,T} f\}_{n=1}^{\infty}$ is not a.e. convergent on $(\mathbf{\Omega}, \mu)$.*

Proof. The first part of the theorem is an improved version of Dunford-Schwartz Pointwise Ergodic Theorem (see, for example, [10], Ch. 8, §8.2.6 and §8.6.11).

In order to prove the "converse" part we suppose that θ be an ergodic conservative μ-preserving transformation on $\mathbf{\Omega}$ and $T = T_\theta$ satisfies the condition:

$$\{A_{n,T} f\}_{n=1}^{\infty} \text{ converges almost everywhere on } (\mathbf{\Omega}, \mu) \text{ for every } f \in \mathbf{L}_\infty. \qquad (*)$$

Then for any probability measure $\nu \sim \mu$ and all measurable sets A there exist limits

$$\widetilde{\nu}(A) = \lim_{n\to\infty} \int\limits_{\mathbf{\Omega}} A_{n,T}\chi_A \, d\nu = \lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} \nu(\theta^{-k} A). \qquad (**)$$

It can be shown by means Theorems 4.3.1–4.3.3 from [22], that the weak convergence

$$\frac{1}{n} \sum_{k=0}^{n-1} \nu \circ \theta^{-k} \to \widetilde{\nu} \qquad (***)$$

in $(**)$ yields in fact convergence in norm.

Indeed, let $h = \frac{d\nu}{d\mu} \in \mathbf{L_1}(\nu)$ be Radon-Nikodym derivative and

$$T_\theta^o: \quad \mathbf{L}_1(\nu) \ni g \to T_\theta^o g = g \circ \theta^{-1} \frac{h \circ \theta^{-1}}{h} \in \mathbf{L}_1(\nu).$$

Then

$$\int_{\mathbf{\Omega}} (T_\theta^o g)(\omega)\, d\nu(\omega) = \int_{\mathbf{\Omega}} g(\theta^{-1} w) \frac{h(\theta^{-1} w)}{h(\omega)}\, d\nu(\omega) = \int_{\mathbf{\Omega}} g(\theta^{-1} w) h(\theta^{-1} w)\, d\mu(\omega)$$

$$= \int_{\mathbf{\Omega}} g(\omega) h(\omega)\, d\mu(\omega) = \int_{\mathbf{\Omega}} g(\omega)\, d\nu(\omega),$$

i.e., the operator T_θ^o is a positive isometry in $\mathbf{L}_1(\nu)$ as well as its dual T_θ is a positive isometry in $\mathbf{L}_\infty(\nu) = \mathbf{L}_\infty(\widetilde{\nu})$. Setting $g = \mathbf{1} \in \mathbf{L}_1(\nu)$ and using Mean Ergodic Theorem ([22], Theorem 2.1.1), we get that the weak convergence of $\frac{1}{n}\sum_{k=0}^{n-1} T_\theta^o \mathbf{1}$ (provided by $(*)$) implies the strong convergence to a function $\widetilde{h} \in \mathbf{L}_1(\nu)$, which is nothing more than $\frac{d\widetilde{\nu}}{d\nu}$.

Thus $\widetilde{\nu} = \frac{d\widetilde{\nu}}{d\nu}\nu$ is a θ-invariant measure on $\mathbf{\Omega}$ such that $\widetilde{\nu} \sim \mu$ and $\widetilde{\nu}(\mathbf{\Omega}) = 1$. Since θ is ergodic and conservative, every such θ-invariant measure is of the form $c\mu$ with a constant $c > 0$, i.e., $\widetilde{\nu}(\mathbf{\Omega}) = \infty$. The contradiction shows that $(*)$ does not hold. $\square$

6. Consequences for Orlicz and Lorentz spaces

Orlicz spaces

Let $\Phi\colon [0, +\infty) \to [0, +\infty]$ be an Orlicz function, i.e., $\Phi(0) = 0$, Φ is increasing left-continuous and convex. Assume also that Φ is nontrivial, i.e., $\Phi(x) > 0$ and $\Phi(y) < \infty$ for some $x, y > 0$. The derivative Φ' exists a.e., and it is assumed to be left-continuous with $\Phi'(x) = +\infty$ iff $\Phi(x) = +\infty$.

The corresponding conjugate Orlicz function Ψ is defined by its derivative Ψ', which is the left-continuous inverse of Φ'.

The *Orlicz space* $\mathbf{L}_\Phi = \mathbf{L}_\Phi(\mathbf{\Omega}, \mu)$ is the set defined as follows

$$\mathbf{L}_\Phi := \left\{ f \in \mathbf{L}_0 \colon \int_{\mathbf{\Omega}} \Phi(f/a)\, d\mu < \infty \text{ for some } a > 0 \right\},$$

equipped with the norm

$$\|f\|_{\mathbf{L}_\Phi} := \inf \left\{ a > 0 \colon \int_{\mathbf{\Omega}} \Phi(|f|/a)\, d\mu \le 1 \right\}, \ f \in \mathbf{L}_0,$$

where $\inf \emptyset := \infty$.

Notice that this “slightly generalized” definition includes the spaces $\mathbf{L}_1$, $\mathbf{L}_\infty$ and also $\mathbf{L}_1 \cap \mathbf{L}_\infty$, $\mathbf{L}_1 + \mathbf{L}_\infty$ as the smallest and largest Orlicz spaces (see [19], Ch. 2, [10], Ch. 2, §2.1 and also [35], [36]).

We use also the heart $\mathbf{H}_\Phi = \mathbf{H}_\Phi(\boldsymbol{\Omega}, \mu)$ of the Orlicz space $\mathbf{L}_\Phi$,

$$\mathbf{H}_\Phi := \left\{ f \in \mathbf{L}_0 \colon \int_{\boldsymbol{\Omega}} \Phi(|f|/a)\, d\mu < \infty \text{ for all } a > 0 \right\} ,$$

which is a closed subspace of $\mathbf{L}_\Phi$. If $\Phi(x) < +\infty$ for all $x > 0$, the heart $\mathbf{H}_\Phi$ coincides with the closure $cl_{\mathbf{L}_\Phi}(\mathbf{L}_1 \cap \mathbf{L}_\infty)$ of $\mathbf{L}_\Phi$. If $\mathbf{L}_\Phi(x) = +\infty$ for some $x > 0$ then $\mathbf{H}_\Phi = \{0\}$.

For any Orlicz function Φ we use the function ξ_Φ defined by

$$\xi_\Phi(x) = \Psi(\Phi'(x)) .$$

If $y = \Phi'(x) < +\infty$, there is equality $xy = \Phi(x) + \Psi(y)$ in the Young's inequality $xy \leq \Phi(x) + \Psi(y)$, i.e.,

$$\xi_\Phi(x) = x\Phi'(x) - \Phi(x) .$$

In many important cases (but not always) ξ_Φ is an Orlicz function.

A converse question thus arises: Does there exist an Orlicz function Φ_H such that $\xi_{\Phi_H} = \Phi$, for a given Orlicz function Φ? It is easy to show, for instance, that $\xi_{\Phi_H} = \Phi$ for

$$\Phi_H(x) = x \int_0^x \frac{\Phi'(u)}{u}\, du - \Phi(x) ,$$

provided that the integral exists for some $x > 0$ small enough.

Proposition 6.1. *Let Φ and Φ_H be two Orlicz functions such that $\xi_{\Phi_H} = \Phi$. Then*

$$(\mathbf{L}_\Phi)_\mathbf{H} = \mathbf{L}_{\Phi_H} \quad \textit{and} \quad (\mathbf{H}_\Phi)_\mathbf{H} = \mathbf{H}_{\Phi_H} .$$

The Boyd indexes $p_{\mathbf{L}_\phi}$ and $q_{\mathbf{L}_\phi}$ of Orlicz spaces can be computed by the function Φ. They coincide with the dilation indexes of Φ,

$$p_{\mathbf{L}_\Phi} = \lim_{x \to \infty} \frac{\log M_\Phi(x)}{\log x} \quad , \text{ where } M_\Phi(x) = \sup_{0<y<\infty} \frac{\Phi(xy)}{\Phi(y)}.$$

To check condition $(\mathbf{L}_\Phi)_\mathbf{H} = \mathbf{L}_\Phi$, (which is equivalent to $p_{\mathbf{L}_\Phi} > 1$), one can also use

$$p(\Phi) := \sup \left\{ p > 0 \colon \inf_{x>0, y>1} \frac{\Phi(xy)}{x^p \Phi(x)} > 0 \right\} .$$

Note that the index $p(\Phi)$ was studied in [4] in the case $\mu(\boldsymbol{\Omega}) < +\infty$, and in [11] under additional Δ_2-conditions.

Proposition 6.2. *Let Φ be an Orlicz function. Then*

1) $(\mathbf{L}_\Phi)_\mathbf{H} = \mathbf{L}_\Phi \iff p(\Phi) > 1 \iff (\mathbf{H}_\Phi)_\mathbf{H} = \mathbf{H}_\Phi$.
2) a) $\mathbf{L}_\Phi \subseteq \mathcal{R}_0 \iff \Phi(x) > 0$ *for all* $x > 0$.
   b) $\mathbf{H}_\Phi \subseteq \mathcal{R}_0$

These results together with Theorems 2.1 and 2.4 solve Problems 1 and 2 for Orlicz spaces and their hearts.

- *The sequence of averages $\{A_{n,T} f\}_{n=1}^\infty$ is order convergent in $\mathbf{L}_\Phi$ if $f \in \mathbf{L}_{\Phi_H}$ and $f^*(+\infty) = 0$.*
- *The sequence of averages $\{A_{n,T} f\}_{n=1}^\infty$ is order convergent in $\mathbf{H}_\Phi$ if $f \in \mathbf{H}_{\Phi_H}$.*

- *An Orlicz space* $\mathbf{L}_\Phi$ *satisfies Order Ergodic Theorem* ($\mathbf{L}_\Phi \in \mathcal{OET}$) *iff* $p(\Phi) > 1$ *and* $\Phi(x) > 0$ *for all* $x > 0$.
- *An Orlicz heart* $\mathbf{H}_\Phi$ *satisfies Order Ergodic Theorem* ($\mathbf{L}_\Phi \in \mathcal{OET}$) *iff* $p(\Phi) > 1$.

Zygmund classes

$\mathcal{Z}_r = \mathbf{L}\log^r \mathbf{L}\,,\ 0 \le r < +\infty$.

This important class of Orlicz spaces $\mathcal{Z}_r = \mathcal{Z}_r(\boldsymbol{\Omega}, \mu)$ is defined by the following Orlicz functions:

$$\Phi_r(x) := \begin{cases} 0 & , \quad 0 \le x \le 1 \\ x\log^r x & , \quad 1 < x < \infty \end{cases} \quad , \quad 0 < r < +\infty\,.$$

We set

$$\mathcal{Z}_r := \mathbf{L}_{\Phi_r} \ \ , \ \ \mathcal{R}_r := \mathbf{H}_{\Phi_r} \ \ , \ \ 0 < r < \infty\,,$$

and also $\mathcal{Z}_0 = \mathbf{L}_1 + \mathbf{L}_\infty$, having the heart $\mathcal{R}_0$.

Proposition 6.3. *For all* $0 \le r < +\infty$*:*

1) $(\mathcal{Z}_r)_\mathbf{H} = \mathcal{Z}_{r+1}$ *and* $(\mathcal{R}_r)_\mathbf{H} = \mathcal{R}_{r+1}$.
2) $\mathcal{Z}_r \cap \mathcal{R}_0 = \mathcal{R}_r = cl_{\mathcal{Z}_r}(\mathbf{L}_1 \cap \mathbf{L}_\infty)$.

Thus for all $0 \le r < +\infty$:

- *The sequence of averages* $\{A_{n,T}f\}_{n=1}^\infty$ *is order bounded in* $\mathcal{Z}_r$ *if* $f \in \mathcal{Z}_{r+1}$.
- *The sequence of averages* $\{A_{n,T}f\}_{n=1}^\infty$ *is order convergent in* $\mathcal{Z}_r$ *if* $f \in \mathcal{R}_{r+1}$.

Lorentz spaces

Let W be an increasing function on $[0, +\infty)$ such that: $W(0) = 0$, W is concave on $(0, +\infty)$, and $W(x) > 0$ for some $x > 0$. Then W is absolutely continuous on the open interval $(0, \infty)$ with the decreasing density function $W'(x)\,,\ x > 0$, while $W(0+)$ may be positive.

The Lorentz space $\boldsymbol{\Lambda}_W = \boldsymbol{\Lambda}_W(\boldsymbol{\Omega}, \mu)$ is defined as

$$\boldsymbol{\Lambda}_W := \{f \in \mathbf{L}_0 \colon \|f\|_{\boldsymbol{\Lambda}_W} < +\infty\}$$

with the norm

$$\|f\|_{\boldsymbol{\Lambda}_W} := \int_0^\infty f^*(x)\,d\,W(x) = f^*(0)W(0+) + \int_0^\infty f^*(x)\,W'(x)\,dx < \infty\,,$$

where $+\infty \cdot 0 = 0$ (see [21], Ch. II, §5.1, and also [24], Ch. 2, [25] and references therein).

The Stieltjes integral $\int\limits_0^\infty f^*(x)\,d\,W(x)$ has an atomic part $f^*(0)\,W(0+)$ in the case $W(0+) > 0$. The Lorentz spaces are maximal r.i. spaces with respect to the norm $\|\cdot\|_{\boldsymbol{\Lambda}_W}$.

By this definition $\boldsymbol{\Lambda}_W \subseteq \mathbf{L}_\infty$ if $W(0+) > 0$, and $\boldsymbol{\Lambda}_W \supseteq \mathbf{L}_\infty$ if $W(+\infty) := \lim\limits_{x\to\infty} W(x) < +\infty$. Whence $\boldsymbol{\Lambda}_W = \mathbf{L}_\infty$ if both the conditions $W(0+) > 0$ and $W(+\infty) < +\infty$ hold.

The Hardy core $(\boldsymbol{\Lambda}_W)_\mathbf{H}$ of the Lorentz space $\boldsymbol{\Lambda}_W$ and its lower index $p_{\boldsymbol{\Lambda}_W}$ are easily computed by the weight function W.

Proposition 6.4.

1) *Let $\mathbf{\Lambda}_{W_H} = \mathbf{\Lambda}_{W_H}(\mathbf{\Omega}, \mu)$ be the Lorentz space, where its weight function W_H is uniquely defined by the conditions: $W_H(0) = W(0) = 0$, $W_H(0+) = W(0+)$ and*
$$W'_H(x) = \int_x^{+\infty} \frac{W'(u)}{u}\, du < +\infty \quad , \quad x \in (0, +\infty) \ .$$
Then $(\mathbf{\Lambda}_W)_{\mathbf{H}} = \mathbf{\Lambda}_{W_H}$. (If $\int\limits_1^{+\infty} \frac{W'(x)}{x}\, dx = +\infty$ then $(\mathbf{\Lambda}_W)_{\mathbf{H}} = \{0\}$.)

2) *The index $p_{\mathbf{\Lambda}_w}$ is equal to $(\beta_W)^{-1}$, where the dilation index β_W of W is defined by*
$$\beta_W = \lim_{x\to\infty} \frac{\log M_W(x)}{\log x} \quad , \quad \textit{where } M_W(x) = \sup_{0<y<\infty} \frac{W(xy)}{W(y)} \ .$$

3) $\mathbf{\Lambda}_W \subseteq \mathcal{R}_0$ *iff* $W(+\infty) := \lim\limits_{x\to+\infty} W(x) = +\infty$.

Thus for any Lorentz space $\mathbf{\Lambda}_W$,

- The sequence of averages $\{A_{n,T}f\}_{n=1}^{\infty}$ is order convergent in $\mathbf{\Lambda}_W$ if $f \in \mathbf{\Lambda}_{W_H}$ and $f^*(+\infty) = 0$.
- A Lorentz space $\mathbf{\Lambda}_W$ satisfies the Order Ergodic Theorem ($\mathbf{\Lambda}_W \in \mathcal{OET}$) iff $\beta_W < 1$ and $W(+\infty) = +\infty$.

More general Lorentz spaces $\mathbf{\Lambda}_{W,\,q} = \mathbf{\Lambda}_{W,\,q}(\mathbf{\Omega}, \mu)$ are defined by
$$\mathbf{\Lambda}_{W,\,q} := \left\{ f \in \mathcal{S}_0 \colon \|f\|_{\mathbf{L}_{W,\,q}} := \left(\int_0^{\infty} (f^*(x))^q \, dW(x) \right)^{1/q} < \infty \right\}$$
for $1 \le q < \infty$, where $\mathbf{\Lambda}_{W,\,1} = \mathbf{\Lambda}_W$.

The classical Lorentz spaces are defined as $\mathbf{L}_{p,q} := \mathbf{\Lambda}_{W,\,q}$ with $W(x) = x^{q/p}$, and for $1 \le q \le p \le \infty$,
$$\mathbf{L}_{p,\infty} := \left\{ f \in \mathbf{L}_0 \colon \|f\|_{\mathbf{L}_{p,\,\infty}} := \sup_{0<x<\infty} \left(x^{1/p} f^*(x) \right) < \infty \right\} \ .$$
The cases when $q > p$ (i.e., W is not concave) are relevant as well, while $\|\cdot\|_{\mathbf{L}_{W,\,q}}$ is not a norm there (see [37], Ch. V, §3).

Order Ergodic Theorems in the spaces $\mathbf{\Lambda}_{W,q}$ with $1 < q < +\infty$ are quite similar to the case of $\mathbf{\Lambda}_W$. Roughly speaking, the second index q has no influence on the order convergence in $\mathbf{\Lambda}_{W,q}$.

7. Additional comments and remarks

Orlicz-Lorentz spaces

The situation becomes more intricate if we turn to general Orlicz-Lorentz spaces.

These r.i. spaces $\mathbf{\Lambda}_{W,\Phi} = \mathbf{\Lambda}_{W,\Phi}(\mathbf{\Omega}, \mu)$, can be defined by
$$\mathbf{\Lambda}_{W,\Phi} := \{ f \in \mathcal{S}_0(\mathbf{\Omega}, \mu) \colon \mathcal{I}_{W,\Phi}(f/a) < \infty \text{ for some } a > 0 \} \ ,$$

with the norm

$$\|f\|_{\mathbf{\Lambda}_{W,\Phi}} := \inf\{a > 0 \colon \mathcal{I}_{W,\Phi}(f/a) \le 1\} ,$$

where

$$\mathcal{I}_{W,\Phi}(f) := \int_0^\infty \Phi(f^*(x))\, dW(x) , \ f \in \mathbf{L}_0 = \mathbf{L}_0(\mathbf{\Omega}, \mu).$$

The functions Φ and W in this definition are not usually assumed to be convex and concave.

This very wide class of r.i. spaces (including original Orlicz and Lorentz spaces) has been intensively studied for the last two décades. We can refer to [27], [28], [13], [14], [15], [16], [20] and to the references cited therein as well.

The computation of Boyd indexes $p_{\mathbf{E}}$, $q_{\mathbf{E}}$ and the description of Hardy core $\mathbf{E_H}$ for the spaces $\mathbf{E} = \mathbf{L}_{\Phi,W}$ is a hard partly open problem. (See, e.g., [6], [7], [14], [15], [23], [29].)

Any progress in this direction will imply new results on Problems 1 and 2.

Order convergence of conditional expectations

Order convergence results (similar to Theorems 2.1, 2.2, 2.4) can be proved for sequences of conditional expectations $T_n = E^{\mathcal{F}_n}$.

Let $\mathcal{F}$ denote the σ-algebra of all μ-measurable subsets of $\mathbf{\Omega}$ and $\mathcal{F}_1 \subseteq \mathcal{F}_2 \subseteq \mathcal{F}_3 \subseteq \cdots$ be an increasing sequence of σ-subalgebras $\mathcal{F}_n$ of $\mathcal{F}$. Since $\mu(\mathbf{\Omega}) = +\infty$, the conditional expectation operators $T_n = E^{\mathcal{F}_n}$ (with respect to $\mathcal{F}_n$) need not to be well defined. However, $T_n \in \mathcal{PAC}$ if the restriction $\mu|_{\mathcal{F}_n}$ of the measure μ on $\mathcal{F}_n$ is σ-finite.

Theorem 7.1. *Let $T_n = E^{\mathcal{F}_n}$, $n \ge 1$, be the conditional expectations with respect to $\mathcal{F}_n$ and assume that $T_n \in \mathcal{PAC}$ for all n. Let $\mathbf{E}$ be an r.i. space. Then the sequence of the conditional expectations $T_n = E^{\mathcal{F}_n} f$ is order convergent in $\mathbf{E}$ for all $f \in \mathbf{E_H} \cap \mathcal{R}_0$.*

Conversely, for every $f \notin \mathbf{E_H} \cap \mathcal{R}_0$ there exists a sequence of conditional expectations $T_n = E^{\mathcal{F}_n} \in \mathcal{PAC}$, $n \ge 1$, such that the sequence $\{T_n f\}_{n=1}^\infty$ is not order convergent in $\mathbf{E}$.

The proof is based on Lemmas 3.3 and 4.3 with the dominant function

$$g = Bf := \sup_{n \ge 1} E^{\mathcal{F}_n} f .$$

Suitable versions of Doob maximal inequality (adapted to the case of infinite measure) are used to this end. It should be mentioned that analogous estimates for $Bf = \sup\limits_{n\ge1} T_n f$ were obtained in [10], Ch. 3, in the case of Orlicz spaces $\mathbf{E} = \mathbf{L}_\Phi$. The mentioned above map $\Phi \to \xi_\Phi$ was introduced and treated therein to this end.

$\mathcal{OET}$ on finite measure spaces

Main Order convergence results (Theorems 2.1–2.4) hold if $\mathbf{m}(\mathbf{\Omega}) < +\infty$. The restriction that $f \in \mathcal{R}_0$ is evidently unnecessary in this case.

In other words, order boundedness in $\mathbf{E}$ of the Cesáro sums $\{A_{n,T}f\}_{n=1}^{\infty}$, $T \in \mathcal{PAC}$ implies their order convergence in the r.i. space $\mathbf{E}$. In particular, $\mathbf{E} \in \mathcal{DET}$ implies $\mathbf{E} \in \mathcal{OET}$.

Dominated Ergodic Theorems in r.i. spaces on finite measure spaces are studied in [4].

Convergence in norm

Statistical (Mean) Ergodic Theorems ($\mathcal{SET}$) deal with the norm convergence of Cesáro sums $\{A_{n,T}f\}_{n=1}^{\infty}$, where T is a bounded linear operator on a Banach space. The operator is assumed to be Cesáro bounded (see, e.g., [22], Ch. 2 §2.1).

For rearrangement invariant Banach spaces a natural related problem is: When does the sequence $\{A_{n,T}]_{n=1}^{\infty}$ converge in the norm $\|\cdot\|_{\mathbf{E}}$ of the r.i. space $\mathbf{E}$, for all $f \in \mathbf{E}$ and all $T \in \mathcal{PAC}$ ($\mathbf{E} \in \mathcal{SET}$)?

The following result can be proved in the case of finite measure ([38] and [39]):

Theorem 7.2. *Let $\mathbf{E} = \mathbf{E}(\mathbf{\Omega}, \mu)$ be an r.i. space and $\mu(\mathbf{\Omega}) < \infty$. Then $\mathbf{E} \in \mathcal{SET}$ iff $\mathbf{E}$ has order continuous norm, i.e.,*

$$0 \le f_n \in \mathbf{E} \;\;,\;\; f_n \downarrow 0 \quad , \quad \|f_n\|_{\mathbf{E}} \to 0\ .$$

The *order continuous norm* property can be described in some different ways (see [21], Ch. II, §4, [24], Ch. I).

Proposition 7.3. *Let $\mathbf{E} = \mathbf{E}(\mathbf{\Omega}, \mu)$ be an r.i. space. Then the following conditions are equivalent:*

1) *$\mathbf{E}$ has an order continuous norm.*
2) *$\mathbf{E}$ is minimal (i.e., $\mathbf{E} = cl_{\mathbf{E}}(\mathbf{L}_1 \cap \mathbf{L}_\infty)$) and $\varphi_{\mathbf{E}}(0+) = 0$, where $\varphi_{\mathbf{E}}$ is the fundamental function of $\mathbf{E}$.*
3) *$\mathbf{E}' = \mathbf{E}^*$, i.e., the associated (Köthe dual) space of $\mathbf{E}$ coincides with its dual space.*
4) *The standard r.i. space $\mathbf{E}(\mathbf{R}_+, \mathbf{m})$ corresponding to $\mathbf{E}$ is separable.*

It should be noted that there is no connection between the conditions $\mathbf{E} \in \mathcal{OET}$ and $\mathbf{E} \in \mathcal{SET}$. For instance, (provided that $\mu(\mathbf{\Omega}) < \infty$), one has:

- $\mathbf{L}_p \in \mathcal{OET}$ and $\mathbf{L}_p \in \mathcal{SET}$ for $1 < p < +\infty$.
- $\mathbf{L}_1 \notin \mathcal{OET}$ and $\mathbf{L}_1 \in \mathcal{SET}$.
- $\mathbf{L}_{p,\infty} \in \mathcal{OET}$ and $\mathbf{L}_{p,\infty} \notin \mathcal{SET}$ for $1 < p < +\infty$.

In the case $\mu(\mathbf{\Omega}) = \infty$ the space $\mathbf{L}_1$ has an order continuous norm, however $\mathbf{L}_1 \notin \mathcal{SET}$. While $\mathbf{L}_p \in \mathcal{SET}$ for $1 < p < \infty$, since the spaces are reflexive.

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Local Approximation of Observables and Commutator Bounds

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Abstract. We discuss conditional expectations that can be used as generalizations of the partial trace for quantum systems with an infinite-dimensional Hilbert space of states.

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1. Introduction

We denote by $\mathcal{B}(\mathcal{H})$ the bounded linear operators on a complex Hilbert space $\mathcal{H}$, equipped with the operator norm, and for $A, B \in \mathcal{B}(\mathcal{H})$, $[A, B] = AB - BA$ is the commutator of A and B. Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Hilbert spaces and $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ their tensor product. In this note we consider the following situation. Suppose $A \in \mathcal{B}(\mathcal{H})$ and $\epsilon \geq 0$ are such that

$$\big|\big| [A, \quad \otimes B] \big|\big| \leq \epsilon \|A\| \|B\| \quad \text{ for all } B \in \mathcal{B}(\mathcal{H}_2). \tag{1.1}$$

We will prove that there exists $A' \in \mathcal{B}(\mathcal{H}_1)$ such that $\|A - A' \otimes \quad \| \leq \epsilon \|A\|$. The case $\epsilon = 0$ is trivial, since in that case we have $A \in (\quad \otimes \mathcal{B}(\mathcal{H}_2))' = \mathcal{B}(\mathcal{H}_1) \otimes \quad$, and therefore there exists $A' \in \mathcal{B}(\mathcal{H}_1)$ such that $A = A' \otimes \quad$. If $\mathcal{H}_2$ is finite dimensional, the result is also well known. In that case one can take for A' the normalized partial trace of A:

$$A' = \frac{1}{\dim \mathcal{H}_2} \mathrm{Tr}_{\mathcal{H}_2} A.$$

To see that this choice for A' does the job, it suffices to note that

$$A' \otimes \quad = \int_{\mathcal{U}(\mathcal{H}_2)} dU \, (\quad \otimes U^*) A (\quad \otimes U),$$

where dU is the normalized Haar measure on the unitary group, $\mathcal{U}(\mathcal{H}_2)$, of $\mathcal{H}_2$.

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Then, by the assumption (1.1) one has

$$\|A' \otimes \quad - A\| \leq \int_{\mathcal{U}(\mathcal{H}_2)} dU \, \big|\big| (\quad \otimes U^*)[A, (\quad \otimes U)] \, \big|\big| \leq \epsilon \|A\| \, . \tag{1.2}$$

Our direct motivation for extending this result to the general case, in which $\mathcal{H}_2$ is allowed to be infinite dimensional, stems from the recent applications of Lieb-Robinson bounds [8] to obtaining local approximations of time-evolved observables in quantum mechanics in the works [1, 2, 9, 10].

2. The main lemma

The existence of an approximation $A' \in \mathcal{B}(\mathcal{H}_1)$ satisfying the same error bound $\epsilon\|A\|$ as in (1.2) is shown in the following lemma. The lemma shows that, as in the finite-dimensional case, one can take A' to given by a completely positive linear map $\quad : \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2) \to \mathcal{B}(\mathcal{H}_1)$ which has the defining properties of a conditional expectation.

Lemma 2.1. *Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces. Then there is a completely positive linear map $\quad : \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2) \to \mathcal{B}(\mathcal{H}_1)$ with the following properties:*

1. *For all $A \in \mathcal{B}(\mathcal{H}_1)$, $\quad (A \otimes \quad) = A$;*
2. *Whenever $A \in \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ satisfies the commutator bound*
$$\big|\big| [A, \quad \otimes B] \, \big|\big| \leq \epsilon \|A\| \|B\| \text{ for all } B \in \mathcal{B}(\mathcal{H}_2),$$
$\quad (A) \in \mathcal{B}(\mathcal{H}_1)$ *satisfies the estimate*
$$\| \quad (A) \otimes \quad - A\| \leq \epsilon \|A\|;$$
3. *For all $C, D \in \mathcal{B}(\mathcal{H}_1)$ and $A \in \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$, we have*
$$\quad ((C \otimes \quad)A(D \otimes \quad)) = C \quad (A)D.$$

Proof. For any finite-dimensional projection $P \in \mathcal{B}(\mathcal{H}_2)$ denote by $\mathcal{U}(P)$ the compact group of unitary operators of the form $U = (\quad - P) + PUP$, and by $\quad_P$ the averaging operator with the normalized Haar measure dU on $\mathcal{U}(P)$:

$$\quad_P(A) = \int_{\mathcal{U}(P)} dU \; (\quad \otimes U^*) A (\quad \otimes U). \tag{2.1}$$

By the argument given in the introduction we have $\|A - \quad_P(A)\| \leq \epsilon\|A\|$ and for $C, D \in \mathcal{B}(\mathcal{H}_1)$ and $A \in \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$, we have $\quad_P((C \otimes \quad)A(D \otimes \quad)) = C \quad_P(A)D$. Moreover, if $P \geq Q$, we have $\mathcal{U}(P) \supset \mathcal{U}(Q)$, and hence

$$[\quad \otimes U, \quad_P(A)] = 0 \quad \text{for } P \geq Q \text{ and } U \in \mathcal{U}(Q). \tag{2.2}$$

Now let $(P(\alpha))_{\alpha \in I}$ be a universal subnet of the net of finite-dimensional projections over some directed index set I. Then since $\| \quad_{P(\alpha)}(A)\| \leq \|A\|$, the universal subnet is bounded and therefore must be weak-*-convergent. We call the limit $\quad_\infty(A)$. Clearly then, $\quad_\infty$ is linear, completely positive, leaves every operator $A \otimes \quad$ fixed, and also satisfies the property 3 of the statement of the lemma, since it is defined as a weak limit of a map with these properties. Moreover, if A satisfies the commutator bound each ${}_P(A)$ lies in the compact $(\epsilon\|A\|)$-ball around A and so does the limit.

It remains to prove that we can write ${}_\infty(A) = \ (A) \otimes \ $, i.e., that $[\ \otimes B, {}_\infty(A)] = 0$ for all $B \in \mathcal{B}(\mathcal{H}_2)$. By taking the limit of Eq. (2.2) over P along the chosen net, we find that this is true for any $B \in \mathcal{U}(Q)$ for any finite-dimensional Q. But these sets generate a weakly dense subalgebra of $\mathcal{B}(\mathcal{H}_2)$, which concludes the proof. □

Note that the map of Lemma 2.1 is completely positive and unit preserving and therefore bounded (with $\|\ \| = 1$) and hence norm-continuous. Norm-continuity is however not always sufficient in applications. It is sometimes important that the map $A \mapsto A'$ is continuous with respect to a different, more suitable topology. In [1], e.g., the local approximations appear in an integral and continuity is relied on to insure the integrability of the integrand. Since in Lemma 2.1 A' is obtained as a weak cluster point, its continuity properties are not obvious. Therefore, we consider other maps with the properties of a conditional expectation, namely 1 and 3 of Lemma 2.1, but with a slightly worse approximation property (to be precise, with the ϵ in property 2 of Lemma 2.1 replaced by 2ϵ) and which is continuous with respect to the weak (and σ-weak) operator topology.

Proposition 2.2. *Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces and let ρ be a normal state on $\mathcal{B}(\mathcal{H}_2)$. Define the map ${}_\rho = \mathrm{id} \otimes \rho$ by ${}_\rho(A \otimes B) = \rho(B)A$ for all $A \in \mathcal{B}(\mathcal{H}_1)$ and $B \in \mathcal{B}(\mathcal{H}_2)$. Then, ${}_\rho$ has the properties* 1 *and* 3 *of Lemma* 2.1 *and, whenever $A \in \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ satisfies the commutator bound*

$$\|[A, \ \otimes B]\| \leq \epsilon\|A\|\|B\| \quad \textit{for all } B \in \mathcal{B}(\mathcal{H}_2).$$

we have

$$\|\ {}_\rho(A) - A\| \leq 2\epsilon\|A\|. \tag{2.3}$$

Proof. By Lemma 2.1 we have

$$\|\ (A) - \ {}_\rho(A)\| = \|\ {}_\rho\Big(\ (A) \otimes \ - A\Big)\| \leq \|\ (A) \otimes \ - A\| \leq \epsilon\|A\|.$$

Therefore, it follows that

$$\|\ {}_\rho(A) \otimes \ - A\| \leq \|(\ (A) - \ {}_\rho(A)) \otimes \ \| + \|\ (A) \otimes \ - A\| \leq 2\epsilon\|A\|. \quad \square$$

It is unclear whether the factor 2 in equation (2.3) is really needed. Numerical evidence suggests that maybe it is even true with the same bound as in the Lemma. By an approximation argument it would suffice to show this in finite dimension. We tried low-dimensional (21×21) random matrices A, choosing for ρ the state farthest removed from the tracial state, namely a pure one. The random matrices were drawn from the unitarily invariant ensemble. Then $\delta = \|\ {}_\rho(A) - A\|$ is readily computed, and in all cases we found unitary operators $U \in \mathcal{B}(\mathcal{H}_2)$ such that $\|A - (\ \otimes U^*)A(\ \otimes U)\| \geq \delta$. We are, of course aware, that this is far from conclusive, since by measure concentration random matrices in high dimension might easily avoid the regions of counterexample with high probability. That is, for most of the cases with respect to the unitarily invariant measure the factor 2 is not needed, but counterexamples nevertheless might exist.

3. Application to infinite systems

So far, we have discussed two-component systems with a Hilbert space of the form $\mathcal{H}_1 \otimes \mathcal{H}_2$. In applications the decomposition into two components often corresponds to selecting a finite subsystem of an infinite system [1].

Consider a collection of systems labeled by a countable set Γ (e.g., Γ is often taken to be the d-dimensional hypercubic lattice $\mathbb{Z}^d$.) Associated with each site $x \in \Gamma$, there is a quantum system with a Hilbert space $\mathcal{H}_x$. For finite $\Lambda \subset \Gamma$, we define

$$\mathcal{H}_\Lambda = \bigotimes_{x\in\Lambda} \mathcal{H}_x \quad \text{and} \quad \mathcal{A}_\Lambda = \bigotimes_{x\in\Lambda} \mathcal{B}(\mathcal{H}_x) \tag{3.1}$$

where $\mathcal{B}(\mathcal{H}_x)$ denotes the bounded linear operators on $\mathcal{H}_x$. For $\Lambda_0 \subset \Lambda \subset \Gamma$, $\mathcal{A}_{\Lambda_0}$ can be identified in the natural way with $\mathcal{A}_{\Lambda_0} \otimes \quad {}_{\Lambda\setminus\Lambda_0} \subset \mathcal{A}_\Lambda$. One then defines

$$\mathcal{A}_{\mathrm{loc}} = \bigcup_{\Lambda\subset\Gamma} \mathcal{A}_\Lambda \tag{3.2}$$

as an inductive limit taken over the net of all finite subsets of Γ. The completion of $\mathcal{A}_{\mathrm{loc}}$ with respect to the operator norm is a C^*-algebra, which we will denote by $\mathcal{A}_\Gamma$.

The strategy of Proposition 2.2 now allows us to define a family of maps ${}_\Lambda$, for finite $\Lambda \subset \Gamma$, such that ${}_\Lambda : \mathcal{A}_\Gamma \to \mathcal{A}_\Lambda$, in a way compatible with the embeddings $\mathcal{A}_{\Lambda_0} \subset \mathcal{A}_\Lambda$, for $\Lambda_0 \subset \Lambda$, i.e., such that

$$ {}_{\Lambda_0} = \quad {}_{\Lambda_0} \circ \quad {}_\Lambda, \text{ if } \Lambda_0 \subset \Lambda. \tag{3.3}$$

We will therefore choose a family of normal states on $\mathcal{B}(\mathcal{H}_x)$, or equivalently, a family of density matrices, $(\rho_x)_{x\in\Gamma}$ and let ρ_Γ be the corresponding a product state on $\mathcal{A}_\Gamma$. For each $\Lambda \subset \Gamma$, let ρ_{Λ^c} denote the restriction of ρ_Γ to $\mathcal{A}_{\Gamma\setminus\Lambda}$. On $\mathcal{A}_{\mathrm{loc}}$, ${}_\Lambda$ is then defined by setting

$$ {}_\Lambda = \mathrm{id}_{\mathcal{A}_\Lambda} \otimes \rho_{\Lambda^c} \,. \tag{3.4}$$

and it is straightforward to see that the ${}_\Lambda$ defined in this way satisfy the compatibility property (3.3). All these maps are contractions and extend uniquely to $\mathcal{A}_\Gamma$ by continuous extension, with preservation of the compatibility property. Clearly, ${}_\Lambda$ can be considered as a map $\mathcal{A}_\Gamma \to \mathcal{A}_\Gamma$ with ran ${}_\Lambda = \mathcal{A}_\Lambda \subset \mathcal{A}_\Gamma$. Note that the maps ${}_\Lambda$ depend on the choice of normal states ρ_x. Since the properties we are interested in here do not explicitly depend on this choice, we suppress it in the notation. The following property is a direct consequence of the construction of the ${}_\Lambda$ and Proposition 2.2.

Corollary 3.1. *Let $\Lambda \subset \Gamma$ be finite. Suppose $\epsilon \geq 0$ and $A \in \mathcal{A}_\Gamma$ are such that*

$$\big|\big|\, [A, \quad \otimes B] \,\big|\big| \leq \epsilon \|A\| \|B\| \text{ for all } B \in \mathcal{A}_{\Gamma\setminus\Lambda}.$$

Then, with ${}_\Lambda$ the map defined in (3.4), *we have ${}_\Lambda(A) \in \mathcal{A}_\Lambda$ and*

$$\| \quad {}_\Lambda(A) - A\| \leq 2\epsilon \|A\|. \tag{3.5}$$

We remark that if $\dim \mathcal{H}_x < \infty$, for all $x \in \Gamma$, i.e., when $\mathcal{A}_\Gamma$ is a UHF algebra, we can take the normalized partial trace (maximally mixed state) for each of the ρ_x and replace 2ϵ by ϵ by the argument given in the introduction. In any case, it is easy to construct representations of $\mathcal{A}_\Gamma$ in which the maps $\ _\Lambda$ are represented by weakly continuous maps. Again, it is an interesting question whether the replacement of the 'error' ϵ by 2ϵ is really necessary in order to be able to treat the situation with infinite-dimensional component systems.

In the next section we discuss the relation of our construction of a conditional expectations , with the property P introduced by Schwartz almost fifty years ago [12].

4. Extension to general von Neumann algebras

The ideas in Lemma 2.1 can be extended to the wider setting of von Neumann algebras, when we replace the algebra $\mathcal{B}(\mathcal{H}_2)$ by a general von Neumann algebra $\mathcal{M}$ on the Hilbert space $\mathcal{H}$, which replaces $\mathcal{H}_1 \otimes \mathcal{H}_2$. As usual, $\mathcal{M}'$ denotes the commutant of $\mathcal{M}$, i.e., the von Neumann algebra of bounded operators commuting with $\mathcal{M}$.

Some of the following equivalences are known deep results. Our addition is the last item. Let us mention that while some implications in the following proposition are only valid in the case of $\mathcal{H}$ being separable, the others do not depend on this assumption. This will be made clear in the proof.

Proposition 4.1. *Let $\mathcal{M} \subset \mathcal{B}(\mathcal{H})$ be a von Neumann algebra with trivial center. Then the following properties are equivalent:*

1. *$\mathcal{M}$ is hyperfinite, i.e., the weak closure of an increasing family of matrix algebras all sharing the same identity.*
2. *$\mathcal{M}$ has property P* [11]*, i.e., for every $X \in \mathcal{B}(\mathcal{H})$ the weak*-closed convex hull of $\{U^*XU \mid U \in \mathcal{M} \text{ unitary}\}$ contains an element of $\mathcal{M}'$.*
3. *$\mathcal{M}'$ is injective, i.e., there is a linear map $\ : \mathcal{B}(\mathcal{H}) \to \mathcal{M}'$ such that $\| \ (X)\| \le \|X\|$, and $\ (A) = A$ for $A \in \mathcal{M}'$.*
4. *There is a linear map $\ : \mathcal{B}(\mathcal{H}) \to \mathcal{M}'$ such that for all $X \in \mathcal{B}(\mathcal{H})$*
$$\| \ (X) - X\| \le \sup\Big\{ \|[X, U]\| \,\Big|\, U \in \mathcal{M} \text{ unitary}\Big\}.$$
Furthermore we have that   is completely positive with norm 1 and fulfills
$$\ (AXB) = A \ (X)B \text{ for } A, B \in \ (\mathcal{M}).$$

Proof. The next three implications also apply to the case where $\mathcal{H}$ is not separable.

(1) implies (2) follows by an easy application of the fact that $\mathcal{M}$ is the weak closure of matrix algebras $\mathcal{M}_\alpha$, and each of these algebras obviously has property P. But then $\mathcal{M}$ has property P since its commutant is the intersection of the commutants $\mathcal{M}'_\alpha$, see also [11], Corollary 4.4.17.

That (1) implies the first equation in (4) is proven along the lines of the proof of Lemma 2.1, using again the fact that $\mathcal{M}$ is the weak closure of matrix algebras $\mathcal{M}_\alpha$, for which the bound is immediate. But if we choose $X \in \mathcal{M}'$ we find that $\| \ (X) - X\| = 0$. The second identity then follows from the fact that if $\ : \mathcal{N} \to \mathcal{N}$ is a projection on a von Neumann algebra such that the range $\ (\mathcal{N})$ is a von Neumann subalgebra containing the identity, then has to be completely positive with norm 1, and satisfies the identity $\ (AXB) = A \ (X)B$ for $A, B \in \ (\mathcal{N})$ [5, 14]. The implication (4) to (3) follows immediately from the last argument.

The last two implications do require a separable Hilbert space $\mathcal{H}$.

The equivalence of the notions of hyperfiniteness and injectivity is a deep result by Connes [4] (see [7] for a simpler proof). It is easily seen that $\mathcal{M}$ is injective if and only if $\mathcal{M}'$ is injective, see [13], Proposition XV.3.2. Hence, (3) also implies (1).

The missing implication, *i.e.*, (2) implies (3), was proven by Schwartz, in the same paper where he also defined property P [12]. □

In the above situation we have that, for $A \in \mathcal{M}$ and $B \in \mathcal{M}'$, we get $B \ (A) = \ (BA) = \ (AB) = \ (A)B$, i.e., $\ (A) \in \mathcal{M}' \cap \mathcal{M}'' = \mathbb{C}$. Hence there is a state ρ such that $\ (A) = \rho(A)$, and thus

$$\ (AB) = \rho(A)B \quad \text{for } A \in \mathcal{M},\ B \in \mathcal{M}'. \tag{4.1}$$

Since the linear hull of the set of elements AB is weak*-dense in $\mathcal{B}(\mathcal{H})$ it would seem that via this formula the state ρ determines . However, that is deceptive, because need not be normal (i.e., weak*-continuous). Indeed, the *only* case in which is normal, is the case described in Proposition 2.2. The state ρ is then obviously also normal. That $\mathcal{M}' = \ (\mathcal{B}(\mathcal{H})))$ must be type one follows from a general result of Tomiyama that the von Neumann type (I, II, or III) cannot increase under normal conditional expectations (see also [6, Example 1.1] and [15, Theorem IV.2.2]). Note also that by evaluating with a normal state σ we can obtain product states $AB \mapsto \rho(A)\sigma(\ (B))$ between $\mathcal{M}$ and $\mathcal{M}'$ when is normal, such product states could also be made normal, which also entails that $\mathcal{M}$ is type I [3].

It follows from this discussion that one can, in general, not use (4.1) to define with a normal state ρ taking the place of the partial trace: the map densely defined by (4.1) cannot have a continuous extension to $\mathcal{B}(\mathcal{H})$, except in the type I case.

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The Spectra of Selfadjoint Extensions of Entire Operators with Deficiency Indices (1,1)

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Abstract. We give necessary and sufficient conditions for real sequences to be the spectra of selfadjoint extensions of an entire operator whose domain may be non-dense. For this spectral characterization we use de Branges space techniques and a generalization of Krein's functional model for simple, regular, closed, symmetric operators with deficiency indices (1,1). This is an extension of our previous work in which similar results were obtained for densely defined operators.

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1. Introduction

The aim of this work is to present a generalization of the spectral characterization of entire operators given in [18]. This generalization is realized by extending the notion of entire operators to a subclass of symmetric operators with deficiency indices $(1, 1)$ that may have non-dense domain. The spectral characterization of a given operator in the class is based on the distribution of the spectra of its selfadjoint extensions within the Hilbert space. More concretely, for a given simple, regular, closed symmetric (possibly not densely defined) operator with deficiency indices $(1, 1)$ to be entire it is necessary and sufficient that the spectra of two of its selfadjoint extensions satisfy conditions which reduce to the convergence of certain series (the precise statement is Proposition 5.2).

The class of entire operators was concocted by M.G. Krein as a tool for treating in a unified way several classical problems in analysis [10, 11, 12, 14]. The

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entire operators form a subclass of the closed, densely defined, symmetric, regular operators with equal deficiency indices. They have many remarkable properties as is accounted for in the review book [7]. Krein's definition of entire operators hinges on his functional model for symmetric operators and it requires the existence of an element of the Hilbert space with very peculiar properties. As first discussed in [18] it is possible to determine whether an operator is entire by conditions that rely exclusively on the distribution of the spectra of selfadjoint extensions of the operator.

Although Krein's original work considers only densely defined symmetric operators, it is clear that the definition of entire operators can be extended to the case of not necessarily dense domain with no formal changes (see Definition 2.5). Since non-densely and densely defined symmetric operators share certain properties, the machinery developed in [18] carries over with some mild modifications.

One ingredient of our discussion is an extension of the functional model developed in [18]. This functional model associates a de Branges space to every simple, regular, closed symmetric operator with deficiency indices (1,1). It is worth remarking that functional models for this and for related classes of operators have been implemented before; see for instance [5, 20]. However, the functional model proposed in [18] has shown to be particularly suitable for us. Here we deem appropriate to mention [16] for a related kind of results.

This paper is organized as follows. In Section 2 we recall some of the properties held by operators that are closed, simple, symmetric with deficiency indices $(1,1)$; the notion of entire operator is also introduced here. Section 3 provides a short review on the theory of de Branges Hilbert spaces, including those results relevant to this work, in particular, a slightly modified version of a theorem due to Woracek (Proposition 3.1). In Section 4 we introduce a functional model for any operator of the class under consideration so that the model space is always a de Branges space. Finally, in Section 5 we single out the class of de Branges spaces corresponding to entire operators and provide necessary and sufficient conditions on the spectra of two selfadjoint extensions of an entire operator.

2. On symmetric operators with not necessarily dense domain

Let $\mathcal{H}$ be a separable Hilbert space whose inner product $\langle\cdot,\cdot\rangle$ is assumed antilinear in its first argument. In this space we consider a closed, symmetric operator A with deficiency indices $(1,1)$. It is not assumed that its domain is dense in $\mathcal{H}$, therefore one should deal with the case when the adjoint of A is a linear relation. That is, in general,

$$A^* := \{\{\eta,\omega\} \in \mathcal{H} \oplus \mathcal{H} : \langle\eta, A\varphi\rangle = \langle\omega,\varphi\rangle \text{ for all } \varphi \in \operatorname{dom}(A)\}\,. \tag{1}$$

Whenever the orthogonal complement of $\operatorname{dom}(A)$ is trivial, the set $A^*(0) := \{\omega \in \mathcal{H} : \{0,\omega\} \in A^*\}$ is also trivial, i.e. $A^*(0) = \{0\}$, so A^* is an operator; otherwise A^* is a proper closed linear relation.

For $z \in \mathbb{C}$ one has

$$A^* - zI := \{\{\eta, \omega - z\eta\} \in \mathcal{H} \oplus \mathcal{H} : \{\eta, \omega\} \in A^*\}, \tag{2}$$

so accordingly

$$\ker(A^* - zI) := \{\eta \in \mathcal{H} : \{\eta, 0\} \in A^* - zI\}. \tag{3}$$

Since $\ker(A^* - zI) = \mathcal{H} \ominus \operatorname{ran}(A - \overline{z}I)$, our assumption on the deficiency indices implies $\dim\ker(A^* - zI) = 1$ for all $z \in \mathbb{C} \setminus \mathbb{R}$. Also, since

$$A^*(0) = \{\omega \in \mathcal{H} : \langle \omega, \psi \rangle = 0 \text{ for all } \psi \in \operatorname{dom}(A)\},$$

it is obvious that $A^*(0) = \operatorname{dom}(A)^\perp$.

The selfadjoint extensions within $\mathcal{H}$ of a closed, non-densely defined symmetric operator A are the selfadjoint linear relations that extend the graph of A. We recall that a linear relation B is selfadjoint if $B = B^*$ (as subsets of $\mathcal{H} \oplus \mathcal{H}$).

The following assertion follows easily from [8, Section 1, Lemma 2.2 and Theorem 2.4].

Proposition 2.1. *Let A be a closed, non-densely defined, symmetric operator in $\mathcal{H}$ with deficiency indices $(1,1)$. Then:*

(i) *The codimension of* $\operatorname{dom}(A)$ *equals one.*
(ii) *All except one of the selfadjoint extensions of A within $\mathcal{H}$ are operators.*
(iii) *Let A_γ be one of the selfadjoint extensions of A within $\mathcal{H}$. Then the operator*

$$I + (z - w)(A_\gamma - zI)^{-1}, \quad z \in \mathbb{C} \setminus \operatorname{spec}(A_\gamma), \quad w \in \mathbb{C}$$

maps $\ker(A^* - wI)$ *injectively onto* $\ker(A^* - zI)$.

In connection with this proposition we remind the reader that the spectrum of a closed linear relation B is the complement of the set of all $z \in \mathbb{C}$ such that $(B - zI)^{-1}$ is a bounded operator defined on all $\mathcal{H}$. Moreover, $\operatorname{spec}(B) \subset \mathbb{R}$ when B is a selfadjoint linear relation [6].

Given $\psi_{w_0} \in \ker(A^* - w_0 I)$, with $w_0 \in \mathbb{C} \setminus \mathbb{R}$, let us define

$$\psi(z) := \left[I + (z - w_0)(A_\gamma - zI)^{-1}\right] \psi_{w_0}, \tag{4}$$

Note that $I + (z - w_0)(A_\gamma - zI)^{-1}$ is the generalized Cayley transform. Obviously, $\psi(w_0) = \psi_{w_0}$. Moreover, a computation involving the resolvent identity yields

$$\psi(z) = \left[I + (z - v)(A_\gamma - zI)^{-1}\right] \psi(v), \tag{5}$$

for any pair $z, v \in \mathbb{C} \setminus \mathbb{R}$. This identity will be used later on.

Let us now recall some concepts that will be used to single out a class of closed symmetric operators with deficiency indices $(1,1)$.

A closed, symmetric operator A is called *simple* if

$$\bigcap_{z \in \mathbb{C} \setminus \mathbb{R}} \operatorname{ran}(A - zI) = \{0\}.$$

Equivalently, A is simple if there exists no non-trivial subspace $\mathcal{L} \subset \mathcal{H}$ that reduces A and whose restriction to $\mathcal{L}$ yields a selfadjoint operator [15, Proposition 1.1].

There is one property specific to simple, closed symmetric operators with deficiency indices $(1,1)$, that is of interest to us. It concerns their commutativity with involutions. We say that an involution J commutes with a selfadjoint relation B if

$$J(B - zI)^{-1}\varphi = (B - \overline{z}I)^{-1}J\varphi,$$

for every $\varphi \in \mathcal{H}$ and $z \in \mathbb{C} \setminus \mathbb{R}$. If B is moreover an operator this is equivalent to the usual notion of commutativity, that is,

$$J\,\mathrm{dom}(B) \subset \mathrm{dom}(B), \qquad JB\varphi = BJ\varphi$$

for every $\varphi \in \mathrm{dom}(B)$.

Proposition 2.2. *Let A be a simple, closed symmetric operator with deficiency indices* $(1,1)$. *Then there exists an involution J that commutes with all its selfadjoint extensions within $\mathcal{H}$.*

Proof. Choose a selfadjoint extension A_γ and consider $\psi(z)$ as defined by (4). Recalling (5) along with the unitary character of the generalized Cayley transform, and applying the resolvent identity, one can verify that

$$\langle \psi(\overline{z}), \psi(\overline{v})\rangle = \langle \psi(v), \psi(z)\rangle \tag{6}$$

for every pair $z, v \in \mathbb{C} \setminus \mathbb{R}$.

Now define the action of J on the set $\{\psi(z) : z \in \mathbb{C} \setminus \mathbb{R}\}$ by the rule

$$J\psi(z) = \psi(\overline{z}),$$

and on the set $\mathcal{D}$ of finite linear combinations of such elements as

$$J\left(\sum_n c_n\psi(z_n)\right) := \sum_n \overline{c_n}\psi(\overline{z_n}).$$

Then, on one hand, (6) implies that J is an involution on $\mathcal{D}$ which can be extended to all $\mathcal{H}$ because of the simplicity of A. On the other hand, since by the resolvent identity

$$(A_\gamma - wI)^{-1}\psi(z) = \frac{\psi(z) - \psi(w)}{z - w},$$

one obtains the identity

$$J(A_\gamma - wI)^{-1}\psi(z) = (A_\gamma - \overline{w}I)^{-1}J\psi(z)$$

which by linearity holds on $\mathcal{D}$ and in turn it extends to all $\mathcal{H}$.

So far we know that J commutes with A_γ. By resorting to the well-known resolvent formula due to Krein (see [8, Theorem 3.2] for a generalized formulation), one immediately obtains the commutativity of J with all the selfadjoint extensions of A within $\mathcal{H}$. □

A closed, symmetric operator is called *regular* if for every $z \in \mathbb{C}$ there exists $d_z > 0$ such that

$$\|(A - zI)\psi\| \geq d_z \|\psi\|, \tag{7}$$

for all $\psi \in \operatorname{dom}(A)$. In other words, A is regular if every point of the complex plane is a point of regular type.

Definition 2.3. Let $\mathcal{S}(\mathcal{H})$ be the class of simple, regular, closed symmetric operator in $\mathcal{H}$, whose deficiency indices are $(1,1)$.

In [17, 18] we deal with the subclass of operators in $\mathcal{S}(\mathcal{H})$ that are densely defined. In the present work we extend the results of [18] to the larger class defined above. At this point it is convenient to touch upon some well-known properties shared by the operators in $\mathcal{S}(\mathcal{H})$ that are densely defined, and whose generalizations to the whole class is rather straightforward. The following statement is one of such generalizations which we believe may have been already proven, however, due to the lack of the proper reference, we provide the proof below.

Proposition 2.4. *For $A \in \mathcal{S}(\mathcal{H})$ the following assertions hold true:*

(i) *The spectrum of every selfadjoint extension of A within $\mathcal{H}$ consists solely of isolated eigenvalues of multiplicity one.*
(ii) *Every real number is part of the spectrum of one, and only one, selfadjoint extension of A within $\mathcal{H}$.*
(iii) *The spectra of the selfadjoint extensions of A within $\mathcal{H}$ are pairwise interlaced.*

Proof. Let us prove (i) in a way similar to the one used to prove [7, Propositions 3.1 and 3.2], but taking into account that the operator is not necessarily densely defined.

For $A \in \mathcal{S}(\mathcal{H})$ and any $r \in \mathbb{R}$ consider the constant d_r of (7). Thus, the symmetric operator $(A - rI)^{-1}$, defined on the subspace $\operatorname{ran}(A - rI)$, is such that $\left\|(A - rI)^{-1}\right\| \le d_r^{-1}$. By [13, Theorem 2] there is a selfadjoint extension B of $(A - rI)^{-1}$ defined on the whole space and such that $\|B\| \le d_r^{-1}$. Now, B^{-1} is a selfadjoint extension of $A - rI$ and $\left\|B^{-1}f\right\| \ge d_r \|f\|$ for any $f \in \operatorname{dom}(B^{-1})$, which implies that the interval $(-d_r, d_r) \cap \operatorname{spec}(B^{-1}) = \emptyset$. By shifting B^{-1} one obtains a selfadjoint extension of A with no spectrum in the spectral lacuna $(r - d_r, r + d_r)$. By perturbation theory any selfadjoint extension of A which is an operator has no points of the spectrum in this spectral lacuna other than one eigenvalue of multiplicity one. When $\overline{\operatorname{dom}(A)} \ne \mathcal{H}$, the same is also true for the spectrum of the selfadjoint extension which is not an operator. This follows from a generalization of the Aronzajn-Krein formula (see [8, Equation 3.17]) after noting that the Weyl function is Herglotz and meromorphic for any selfadjoint extension being an operator. Now, for proving (i) consider any closed interval of $\mathbb{R}$, cover it with spectral lacunae and take a finite subcover.

Once (i) has been proven, the assertions (ii) and (iii) follow from [8, Equation 3.17] and the properties of Herglotz meromorphic functions. □

Definition 2.5. An operator $A \in \mathcal{S}(\mathcal{H})$ is called *entire* if there exists $\mu \in \mathcal{H}$ such that

$$\mathcal{H} = \operatorname{ran}(A - zI) \dot{+} \operatorname{span}\{\mu\}$$

for all $z \in \mathbb{C}$. Such μ is called an *entire gauge.*

If $A \in \mathcal{S}(\mathcal{H})$ turns out to be densely defined, then Definition 2.5 reduces to Krein's [12, Section 1]. There are various densely defined operators known to be entire [7, Chapter 3], [12, Section 4]. On the other hand, for what will be explained in the subsequent sections, there are also entire operators with non-dense domain. Let us outline how one may construct an entire operator which is not densely defined. The details of this construction will be expounded in a further paper.

Consider the semi-infinite Jacobi matrix

$$\begin{pmatrix} q_1 & b_1 & 0 & 0 & \cdots \\ b_1 & q_2 & b_2 & 0 & \cdots \\ 0 & b_2 & q_3 & b_3 & \\ 0 & 0 & b_3 & q_4 & \ddots \\ \vdots & \vdots & & \ddots & \ddots \end{pmatrix}, \tag{8}$$

where $b_k > 0$ and $q_k \in \mathbb{R}$ for $k \in \mathbb{N}$. Fix an orthonormal basis $\{\delta_k\}_{k\in\mathbb{N}}$ in $\mathcal{H}$. Let B be the operator in $\mathcal{H}$ whose matrix representation with respect to $\{\delta_k\}_{k\in\mathbb{N}}$ is (8) (cf. [2, Section 47]). We assume that $B \neq B^*$, equivalently, that B has deficiency indices $(1,1)$ [1, Chapter 4, Section 1.2]. Let B_0 be the restriction of B to the set $\{\phi \in \operatorname{dom}(B) : \langle \phi, \delta_1\rangle = 0\}$. It follows from (1), (2) and (3) that $\eta \in \ker(B_0^* - zI)$ if and only if it satisfies the equation

$$\langle B\phi, \eta\rangle = \langle \phi, z\eta\rangle \qquad \forall \phi \in \operatorname{dom}(B_0)\,.$$

Thus $\ker(B_0^* - zI)$ is the set of η's in $\mathcal{H}$ that satisfy

$$b_{k-1}\langle \delta_{k-1}, \eta\rangle + q_k \langle \delta_k, \eta\rangle + b_k \langle \delta_{k+1}, \eta\rangle = z\langle \delta_k, \eta\rangle \quad \forall k > 1 \tag{9}$$

Hence $\dim\ker(B_0^* - zI) \le 2$. Now, let

$$\pi(z) := \sum_{k=1}^{\infty} P_{k-1}(z)\delta_k \qquad \theta(z) := \sum_{k=1}^{\infty} Q_{k-1}(z)\delta_k\,,$$

where $P_k(z)$, respectively $Q_k(z)$, is the kth polynomial of first, respectively second, kind associated to (8). By the definition of the polynomials $P_k(z)$ and $Q_k(z)$ [1, Chapter 1, Section 2.1], $\pi(z)$ and $\theta(z)$ are linearly independent solutions of (9) for every fixed $z \in \mathbb{C}$. Moreover, since $B \neq B^*$, $\pi(z)$ and $\theta(z)$ are in $\mathcal{H}$ for all $z \in \mathbb{C}$ [1, Theorems 1.3.1, 1.3.2], [19, Theorem 3]. So one arrives at the conclusion that, for every fixed $z \in \mathbb{C}$,

$$\ker(B_0^* - zI) = \operatorname{span}\{\pi(z), \theta(z)\}\,.$$

Any symmetric non-selfadjoint extension of B_0 has deficiency indices (1,1). Furthermore, if $\kappa(z)$ is a (z-dependent) linear combination of $\pi(z)$ and $\theta(z)$ such that $\langle \kappa(z), \theta(z)\rangle = 0$ for all $z \in \mathbb{C}\setminus\mathbb{R}$, then (by a parametrized version of [19, Theorem 2.4]) there corresponds to an appropriately chosen isometry from $\operatorname{span}\{\kappa(z)\}$ onto $\operatorname{span}\{\kappa(\overline{z})\}$ a non-selfadjoint symmetric extension $\widetilde{B}$ of B_0 such that $\operatorname{dom}(\widetilde{B})$ is not dense and $\ker(\widetilde{B}^* - zI) = \operatorname{span}\{\theta(z)\}$. We claim that $\widetilde{B}$ is a non-densely defined entire operator. Indeed, $\widetilde{B} \in \mathcal{S}(\mathcal{H})$ (the simplicity follows from the properties of the associated polynomials [1, Chapter 1, Addenda and Problems 7]). Moreover, since

$$\langle \theta(z), \delta_2 \rangle = b_1^{-1}, \qquad \forall z \in \mathbb{C},$$

δ_2 is an entire gauge.

3. A review on de Branges spaces with zero-free functions

Let $\mathcal{B}$ denote a nontrivial Hilbert space of entire functions with inner product $\langle \cdot, \cdot \rangle_{\mathcal{B}}$. $\mathcal{B}$ is a de Branges space when, for every function $f(z)$ in $\mathcal{B}$, the following conditions holds:

(A1) For every $w \in \mathbb{C} \setminus \mathbb{R}$, the linear functional $f(\cdot) \mapsto f(w)$ is continuous;

(A2) for every non-real zero w of $f(z)$, the function $f(z)(z - \overline{w})(z - w)^{-1}$ belongs to $\mathcal{B}$ and has the same norm as $f(z)$;

(A3) the function $f^{\#}(z) := \overline{f(\overline{z})}$ also belongs to $\mathcal{B}$ and has the same norm as $f(z)$.

It follows from (A1) that for every non-real w there is a function $k(z, w)$ in $\mathcal{B}$ such that $\langle k(\cdot, w), f(\cdot) \rangle_{\mathcal{B}} = f(w)$ for every $f(z) \in \mathcal{B}$. Moreover, $k(w, w) = \langle k(\cdot, w), k(\cdot, w) \rangle_{\mathcal{B}} \geq 0$ where, as a consequence of (A2), the positivity is strict for every non-real w unless $\mathcal{B}$ is $\mathbb{C}$; see the proof of Theorem 23 in [4]. Note that $k(z, w) = \langle k(\cdot, z), k(\cdot, w) \rangle_{\mathcal{B}}$ whenever z and w are both non-real, therefore $k(w, z) = \overline{k(z, w)}$. Furthermore, due to (A3) it can be shown that $\overline{k(\overline{z}, w)} = k(z, \overline{w})$ for every non-real w; we refer again to the proof of Theorem 23 in [4]. Also note that $k(z, w)$ is entire with respect to its first argument and, by (A3), it is anti-entire with respect to the second one (once $k(z, w)$, as a function of its second argument, has been extended to the whole complex plane [4, Problem 52]).

There is another way of defining a de Branges space. One starts by considering an entire function $e(z)$ of the Hermite-Biehler class, that is, an entire function without zeros in the upper half-plane $\mathbb{C}^+$ that satisfies the inequality $|e(z)| > \left|e^{\#}(z)\right|$ for $z \in \mathbb{C}^+$. Then, the de Branges space $\mathcal{B}(e)$ associated to $e(z)$ is the linear manifold of all entire functions $f(z)$ such that both $f(z)/e(z)$ and $f^{\#}(z)/e(z)$ belong to the Hardy space $H^2(\mathbb{C}^+)$, and equipped with the inner product

$$\langle f(\cdot), g(\cdot) \rangle_{\mathcal{B}(e)} := \int_{-\infty}^{\infty} \frac{\overline{f(x)} g(x)}{|e(x)|^2} dx.$$

It turns out that $\mathcal{B}(e)$ is complete.

Both definitions of de Branges spaces are equivalent, viz., every space $\mathcal{B}(e)$ obeys (A1–A3); conversely, given a space $\mathcal{B}$ there exists an Hermite-Biehler function $e(z)$ such that $\mathcal{B}$ coincides with $\mathcal{B}(e)$ as sets and the respective norms satisfy the equality $\|f(\cdot)\|_{\mathcal{B}} = \|f(\cdot)\|_{\mathcal{B}(e)}$ [4, Chapter 2]. The function $e(z)$ is not unique; a choice for it is

$$e(z) = -i \sqrt{\frac{\pi}{k(w_0, w_0)\, \operatorname{im}(w_0)}}\, (z - \overline{w_0})\, k(z, w_0),$$

where w_0 is some fixed complex number in $\mathbb{C}^+$.

An entire function $g(z)$ is said to be associated to a de Branges space $\mathcal{B}$ if for every $f(z) \in \mathcal{B}$ and $w \in \mathbb{C}$,

$$\frac{g(z)f(w) - g(w)f(z)}{z - w} \in \mathcal{B}.$$

The set of associated functions is denoted $\operatorname{assoc}\mathcal{B}$. It is well known that

$$\operatorname{assoc}\mathcal{B} = \mathcal{B} + z\mathcal{B};$$

see [4, Theorem 25] and [9, Lemma 4.5] for alternative characterizations. In passing, let us note that $e(z) \in \operatorname{assoc}\mathcal{B}(e) \setminus \mathcal{B}(e)$; this fact follows easily from [4, Theorem 25].

The space $\operatorname{assoc}\mathcal{B}(e)$ contains a distinctive family of entire functions. They are given by

$$s_\beta(z) := \frac{i}{2}\left[e^{i\beta}e(z) - e^{-i\beta}e^{\#}(z)\right], \quad \beta \in [0, \pi).$$

These real entire functions are related to the selfadjoint extensions of the multiplication operator S defined by

$$\operatorname{dom}(S) := \{f(z) \in \mathcal{B} : zf(z) \in \mathcal{B}\}, \quad (Sf)(z) = zf(z). \tag{10}$$

This is a simple, regular, closed symmetric operator with deficiency indices $(1,1)$ which is not necessarily densely defined [9, Proposition 4.2, Corollary 4.3, Corollary 4.7]. It turns out that $\overline{\operatorname{dom}(S)} \neq \mathcal{B}$ if and only if there exists $\gamma \in [0, \pi)$ such that $s_\gamma(z) \in \mathcal{B}$. Furthermore, $\operatorname{dom}(S)^\perp = \operatorname{span}\{s_\gamma(z)\}$ [4, Theorem 29] and [9, Corollary 6.3]; compare with (i) of Proposition 2.1.

For any selfadjoint extension $S_\sharp$ of S there exists a unique β in $[0, \pi)$ such that

$$(S_\sharp - wI)^{-1}f(z) = \frac{f(z) - \frac{s_\beta(z)}{s_\beta(w)}f(w)}{z - w}, \quad w \in \mathbb{C} \setminus \operatorname{spec}(S_\sharp), \quad f(z) \in \mathcal{B}. \tag{11}$$

Moreover, $\operatorname{spec}(S_\sharp) = \{x \in \mathbb{R} : s_\beta(x) = 0\}$. [9, Propositions 4.6 and 6.1]. If $S_\sharp$ is a selfadjoint operator extension of S, then (11) is equivalent to

$$\operatorname{dom}(S_\sharp) = \left\{g(z) = \frac{f(z) - \frac{s_\beta(z)}{s_\beta(z_0)}f(z_0)}{z - z_0}, \quad f(z) \in \mathcal{B}, \quad z_0 : s_\beta(z_0) \neq 0\right\},$$

$$(S_\sharp g)(z) = zg(z) + \frac{s_\beta(z)}{s_\beta(z_0)}f(z_0).$$

The eigenfunction g_x corresponding to $x \in \operatorname{spec}(S_\sharp)$ is given (up to normalization) by

$$g_x(z) = \frac{s_\beta(z)}{z - x}.$$

Thus, since S is regular and simple, every $s_\beta(z)$ has only real zeros of multiplicity one and the (sets of) zeros of any pair $s_\beta(z)$ and $s_{\beta'}(z)$ are always interlaced.

The proof of the following result can be found in [21] for a particular pair of selfadjoint extensions of S. Another proof, when the operator S is densely defined, is given in [18, Proposition 3.9].

Proposition 3.1. *Suppose $e(x) \neq 0$ for $x \in \mathbb{R}$ and $e(0) = (\sin\gamma)^{-1}$ for some fixed $\gamma \in (0,\pi)$. Let $\{x_n\}_{n\in\mathbb{N}}$ be the sequence of zeros of the function $s_\gamma(z)$. Also, let $\{x_n^+\}_{n\in\mathbb{N}}$ and $\{x_n^-\}_{n\in\mathbb{N}}$ be the sequences of positive, respectively negative, zeros of $s_\gamma(z)$, arranged according to increasing modulus. Then a zero-free, real entire function belongs to $\mathcal{B}(e)$ if and only if the following conditions hold true:*

(C1) *The limit* $\lim_{r\to\infty} \sum_{0<|x_n|\leq r} \frac{1}{x_n}$ *exists;*

(C2) $\lim_{n\to\infty} \frac{n}{x_n^+} = -\lim_{n\to\infty} \frac{n}{x_n^-} < \infty$*;*

(C3) *Assuming that $\{b_n\}_{n\in\mathbb{N}}$ are the zeros of $s_\beta(z)$, define*

$$h_\beta(z) := \begin{cases} \lim_{r\to\infty} \prod_{|b_n|\leq r} \left(1 - \frac{z}{b_n}\right) & \text{if } 0 \text{ is not a root of } s_\beta(z), \\ z \lim_{r\to\infty} \prod_{0<|b_n|\leq r} \left(1 - \frac{z}{b_n}\right) & \text{otherwise.} \end{cases}$$

The series $\sum_{n\in\mathbb{N}} \left| \frac{1}{h_0(x_n) h_\gamma'(x_n)} \right|$ *is convergent.*

Proof. Combine Theorem 3.2 of [21] with Lemmas 3.3 and 3.4 of [18]. □

4. A functional model for operators in $\mathcal{S}(\mathcal{H})$

The functional model given in this section follows the construction developed in [18], now adapted to include all the operators in the class $\mathcal{S}(\mathcal{H})$. This functional model is based on (the properties of) the operator mentioned in (iii) of Proposition 2.1 with the following addition.

Proposition 4.1. *Given $A \in \mathcal{S}(\mathcal{H})$, let J be an involution that commutes with one of its selfadjoint extensions within $\mathcal{H}$ (hence with all of them), say, A_γ. Choose $v \in \operatorname{spec}(A_\gamma)$. Then, there exists $\psi_v \in \ker(A^* - vI)$ such that $J\psi_v = \psi_v$.*

Proof. Let ϕ_v be an element of $\ker(A_\gamma - vI)$. Since J commutes with A_γ, one immediately obtains that $J\phi_v \in \ker(A_\gamma - vI)$. But, by our assumption on the deficiency indices of A and its regularity, $\ker(A^* - vI)$ is a one-dimensional space and it contains $\ker(A_\gamma - vI)$. So, in $\ker(A_\gamma - vI)$, J reduces to multiplication by a scalar α and the properties of the involution imply that $|\alpha| = 1$. Now, $\psi_v := (1+\alpha)\phi_v$ has the required properties. □

Given $A \in \mathcal{S}(\mathcal{H})$ and an involution J that commutes with its selfadjoint extensions within $\mathcal{H}$, define

$$\xi_{\gamma,v}(z) := h_\gamma(z) \left[I + (z - v)(A_\gamma - zI)^{-1} \right] \psi_v \,, \tag{12}$$

where v and ψ_v are chosen as in the previous proposition, and $h_\gamma(z)$ is a real entire function whose zero set is $\operatorname{spec}(A_\gamma)$ (see Proposition 2.4 (i)). Clearly, up to a zero-free real entire function, $\xi_{\gamma,v}(z)$ is completely determined by the choice of the selfadjoint extension A_γ and v. Actually, as it is stated more precisely below, $\xi_{\gamma,v}(z)$ does not depend on A_γ nor on v.

Proposition 4.2.

(i) *The vector-valued function $\xi_{\gamma,v}(z)$ is zero-free and entire. It lies in* $\ker(A^* - zI)$ *for every $z \in \mathbb{C}$.*
(ii) *$J\xi_{\gamma,v}(z) = \xi_{\gamma,v}(\overline{z})$ for all $z \in \mathbb{C}$.*
(iii) *Given $\xi_{\gamma_1,v_1}(z)$ and $\xi_{\gamma_2,v_2}(z)$, there exists a zero-free real entire function $g(z)$ such that $\xi_{\gamma_2,v_2}(z) = g(z)\xi_{\gamma_1,v_1}(z)$.*

Proof. Due to (iii) of Proposition 2.1, the proof of (i) is rather straightforward. In fact, one should only follow the first part of the proof of [18, Lemma 4.1]. The proof of (ii) also follows easily from our choice of ψ_w and $h_\gamma(z)$ in the definition of $\xi_{\gamma,w}(z)$. To prove (iii), one first uses (iii) of Proposition 2.1 and the fact that $\dim\ker(A^* - wI) = 1$ to obtain that $\xi_{\gamma_2,w_2}(z)$ and $\xi_{\gamma_1,w_1}(z)$ differ by a nonzero scalar complex function. Then the reality of this function follows from (ii). $\square$

For the reason already explained, from now on the function $\xi_{\gamma,v}(z)$ will be denoted by $\xi(z)$. Now define

$$(\Phi\varphi)(z) := \langle \xi(\overline{z}), \varphi \rangle , \qquad \varphi \in \mathcal{H}.$$

Φ maps $\mathcal{H}$ onto a certain linear manifold $\widehat{\mathcal{H}}$ of entire functions. Since A is simple, it follows that Φ is injective. A generic element of $\widehat{\mathcal{H}}$ will be denoted by $\widehat{\varphi}(z)$, as a reminder of the fact that it is the image under Φ of a unique element $\varphi \in \mathcal{H}$.

The linear space $\widehat{\mathcal{H}}$ is turned into a Hilbert space by defining

$$\langle \widehat{\eta}(\cdot), \widehat{\varphi}(\cdot) \rangle := \langle \eta, \varphi \rangle \ .$$

Clearly, Φ is an isometry from $\mathcal{H}$ onto $\widehat{\mathcal{H}}$.

Proposition 4.3. *$\widehat{\mathcal{H}}$ is a de Branges space.*

Proof. It suffices to show that the axioms given at the beginning of Section 3 holds for $\widehat{\mathcal{H}}$.

It is straightforward to verify that $k(z,w) := \langle \xi(\overline{z}), \xi(\overline{w}) \rangle$ is a reproducing kernel for $\widehat{\mathcal{H}}$. This accounts for (A1).

Suppose $\widehat{\varphi}(z) \in \widehat{\mathcal{H}}$ has a zero at $z = w$. Then its preimage $\varphi \in \mathcal{H}$ lies in $\operatorname{ran}(A - wI)$. This allows one to set $\eta \in \mathcal{H}$ by

$$\eta = (A - \overline{w}I)(A - wI)^{-1}\varphi = \varphi + (w - \overline{w})(A_\gamma - wI)^{-1}\varphi.$$

Now, recalling (12) and applying the resolvent identity one obtains

$$\langle \xi(\overline{z}), \eta \rangle = \frac{z - \overline{w}}{z - w} \langle \xi(\overline{z}), \varphi \rangle \, .$$

Since η and φ are related by a Cayley transform, the equality of norms follows. This proves (A2).

As for (A3), consider any $\widehat{\varphi}(z) = \langle \xi(\overline{z}), \varphi \rangle$. Then, as a consequence of (ii) of Proposition 4.2, one has $\widehat{\varphi}^{\#}(z) = \langle \xi(\overline{z}), J\varphi \rangle$. $\square$

It is worth remarking that the last part of the proof given above shows that $^{\#} = \Phi J \Phi^{-1}$.

The following obvious assertion is the key of (every) functional model; we state it for the sake of completeness.

Proposition 4.4. *Let S be the multiplication operator on $\widehat{\mathcal{H}}$ given by* (10)*.*

(i) $S = \Phi A \Phi^{-1}$ *and* $\operatorname{dom}(S) = \Phi \operatorname{dom}(A)$.

(ii) *The selfadjoint extensions of S within $\widehat{\mathcal{H}}$ are in one-one correspondence with the selfadjoint extensions of A within $\mathcal{H}$.*

Item (ii) above can be stated more succinctly by saying that

$$\Phi(A_\beta - zI)^{-1}\Phi^{-1} = (S_\beta - zI)^{-1}, \quad z \in \mathbb{C} \setminus \operatorname{spec}(A_\gamma),$$

for all β of a certain (common) parametrization of the selfadjoint extensions of both A and S. This expression is of course valid even for the exceptional (i.e., non-operator) selfadjoint extension of A. In passing we note that the exceptional selfadjoint extension of a non-densely defined operator in $\mathcal{S}(\mathcal{H})$ corresponds to the selfadjoint extension of the operator S whose associated function lies in $\widehat{\mathcal{H}}$.

5. Spectral characterization

In the previous section we constructed a functional model that associates a de Branges space to every operator A in $\mathcal{S}(\mathcal{H})$ in such a way that the operator of multiplication in the de Branges space is unitarily equivalent to A. The first task in this section is to single out the class of de Branges spaces corresponding to entire operators in our functional model. Having found this class, we use the theory of de Branges spaces to give a spectral characterization of the multiplication operator for the class we found. This is how we give necessary and sufficient conditions on the spectra of two selfadjoint extensions of an entire operator.

The following proposition gives a characterization of the class of de Branges spaces corresponding to entire operators in our functional model.

Proposition 5.1. *$A \in \mathcal{S}(\mathcal{H})$ is entire if and only if $\widehat{\mathcal{H}}$ contains a zero-free entire function.*

Proof. Let $g(z) \in \widehat{\mathcal{H}}$ be the function whose existence is assumed. Clearly there exists (a unique) $\mu \in \mathcal{H}$ such that $g(z) \equiv \langle \xi(\overline{z}), \mu \rangle$. Therefore, μ is never orthogonal to $\ker(A^* - zI)$ for all $z \in \mathbb{C}$. That is, μ is an entire gauge for the operator A.

The necessity is established by noting that the image of the entire gauge under Φ is a zero-free function. $\square$

Proposition 5.2. *For $A \in \mathcal{S}(\mathcal{H})$, consider the selfadjoint extensions* (*within $\mathcal{H}$*) A_0 *and A_γ, with $0 < \gamma < \pi$. Then A is entire with real entire gauge μ ($J\mu = \mu$) if and only if* $\operatorname{spec}(A_0)$ *and* $\operatorname{spec}(A_\gamma)$ *obey conditions* (C1)*,* (C2) *and* (C3) *of Proposition* 3.1*.*

Proof. Apply Proposition 3.1 along with Proposition 5.1. □

We remark that when A is an entire operator with non-dense domain, it may be that either A_0 or A_γ is not an operator (see Proposition 2.1 (ii)). Nevertheless, even in this case, $\operatorname{spec}(A_0)$ and $\operatorname{spec}(A_\gamma)$ satisfy (C1), (C2) and (C3).

The following proposition shows, among other things, that the original functional model by Krein is a particular case of our functional model.

Proposition 5.3. *Assume $1 \in \widehat{\mathcal{H}}$. Then there exists $\mu \in \mathcal{H}$ such that*

$$h_\gamma(z) = \left\langle \psi_v + (z - v)(A_\gamma - zI)^{-1}\psi_v, \mu \right\rangle^{-1}$$

and $J\mu = \mu$. Moreover, μ is the unique entire gauge of A modulo a real scalar factor.

Proof. Necessarily, $1 \equiv \langle \xi(\overline{z}), \mu \rangle$ for some $\mu \in \mathcal{H}$. By (12), and taking into account the occurrence of J, one obtains the stated expression for $h_\gamma(z)$. By the same token, the reality of μ is shown.

Suppose that there are two real entire gauges μ and μ'. The discussion in Paragraph 5.2 of [7] shows that $(\Phi_\mu \mu')(z) = ae^{ibz}$ with $a \in \mathbb{C}$ and $b \in \mathbb{R}$. Due to the assumed reality, one concludes that $b = 0$ and $a \in \mathbb{R}$. □

6. Concluding remarks

We would like to add some few comments concerning further extensions of the present work.

First, since there are de Branges spaces that contain the constant functions but whose multiplication operator is not densely defined, it follows that, apart from the example given in Section 2, there should be other operators in the class introduced in this work that are not comprised in the original Krein's notion of entire operators. The details of our example as well as other ones and applications of our results will be studied elsewhere.

Second, it is possible to define a notion of a (possibly non-densely defined) operator that is entire in a generalized sense, much in the same vein as the original definition by Krein for densely defined operators (see [7, Chapter 2, Section 9]). Following [18, Section 5], operators entire in this generalized sense could also be characterized by the spectra of their selfadjoint extensions.

Finally, it is known that the set of selfadjoint operator extensions within $\mathcal{H}$ of a non-densely defined operator are in one-one correspondence with a set of rank-one perturbations of one of these selfadjoint operator extensions [8, Section 2]. This set of rank-one perturbations is generated by elements in $\mathcal{H}$ so it seems interesting to study the relation (if any) between these elements and the gauges of operators in $\mathcal{S}(\mathcal{H})$. Ultimately, we believe that a suitable characterization of the rank-one perturbations could provide another necessary and sufficient condition for a non-densely defined operator in $\mathcal{S}(\mathcal{H})$ to be entire. This problem, as well as the previous one, will be discussed in a subsequent work.

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Asymptotics of Eigenvalues of an Energy Operator in a Problem of Quantum Physics

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Abstract. In this paper we consider eigenvalues asymptotics of the energy operator in one of the most interesting models of quantum physics, describing an interaction between two-level system and harmonic oscillator. The energy operator in this model can be reduced to a class of infinite Jacobi matrices. Discrete spectrum of this class of operators represents the perturbed spectrum of harmonic oscillator. The perturbation is an unbounded operator compact with respect to unperturbed one. We use slightly modified Janas-Naboko successive diagonalization approach and some new compactness criteria for infinite matrices. First two terms of eigenvalues asymptotics and the estimation of remainder are found.

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1. Introduction and main results

We consider the energy operator of the following form

$$\hat{\mathbf{H}} = \frac{\hbar\omega_0}{2}\,\hat{\sigma}_z + \hbar\omega\,\hat{\mathbf{a}}^+\,\hat{\mathbf{a}} + \hbar\lambda\,(\hat{\sigma}_+ + \hat{\sigma}_-)(\,\hat{\mathbf{a}} + \hat{\mathbf{a}}^+\,)\,,$$

where $\hat{\sigma}_z, \hat{\sigma}_+, \hat{\sigma}_-$ are the 2×2 matrices of form

$$\hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \hat{\sigma}_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \hat{\sigma}_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

$\hat{\mathbf{a}}$ and $\hat{\mathbf{a}}^+$ are the creation and annihilation operators of the harmonic oscillator, λ is the interaction constant, ω is the oscillator frequency, ω_0 is the transition frequency in the two-level system. These matrices and operators satisfy the following commutative relations

$$[\hat{\sigma}_+, \hat{\sigma}_-] = \hat{\sigma}_z\,, \quad [\hat{\sigma}_z, \hat{\sigma}_+] = 2\,\hat{\sigma}_+\,, \quad [\hat{\sigma}_z, \hat{\sigma}_-] = -2\,\hat{\sigma}_-\,, \quad [\hat{\mathbf{a}}, \hat{\mathbf{a}}^+] = 1$$

It was shown [13] that the hamiltonian of this model is represented by two Jacobi matrices. These matrices have the following general form

$$A = \begin{pmatrix} c_1 & g\sqrt{1} & 0 & 0 & 0 & \dots \\ g\sqrt{1} & 1+c_2 & g\sqrt{2} & 0 & 0 & \dots \\ 0 & g\sqrt{2} & 2+c_1 & g\sqrt{3} & 0 & \dots \\ 0 & 0 & g\sqrt{3} & 3+c_2 & g\sqrt{4} & \dots \\ 0 & 0 & 0 & g\sqrt{4} & 4+c_1 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix} \tag{1.1}$$

where g, c_1, c_2 are real parameters. It is well known [1, 2] that the matrix A defines a selfadjoint operator with simple spectrum and the domain $D(A)$ is dense in the space $l_2(\mathbb{N})$. Since the operator A can be considered as relatively compact perturbation of the main diagonal, its spectrum is discrete.

The main goal of this paper is the investigation of the eigenvalues $\lambda_n(A)$ behavior for large values of n with other parameters fixed. There are many articles concerning similar problems [3, 4, 5, 6, 7, 8, 9, 10, 11, 12].

The result of this paper is given by the following asymptotic formula (Theorem 3.3)

$$\lambda_n(A) = n - g^2 + \frac{c_1+c_2}{2} + O\left(\frac{1}{n^{1/16}}\right), \quad n \to \infty \quad (g \neq 0).$$

2. Selection of the main component in the asymptotics

Let us present the operator A in (1.1) in the form

$$A = A_0 + \frac{c_1+c_2}{2}\, I + \frac{c_1-c_2}{2}\, R, \tag{2.1}$$

where I is the identical matrix, A_0 and R are defined in the following way

$$A_0 = \begin{pmatrix} 0 & g\sqrt{1} & 0 & 0 & \dots \\ g\sqrt{1} & 1 & g\sqrt{2} & 0 & \dots \\ 0 & g\sqrt{2} & 2 & g\sqrt{3} & \dots \\ 0 & 0 & g\sqrt{3} & 3 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}, \quad R = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots \\ 0 & -1 & 0 & 0 & \dots \\ 0 & 0 & 1 & 0 & \dots \\ 0 & 0 & 0 & -1 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

The matrix A_0 represents so-called “shifted oscillator” operator: $a^+a + g\,(a + a^+)$, where a^+ and a are the creation and annihilation operators. If we use the matrix representation of a^+ and a, we obtain exactly the matrix A_0.

Eigenvalues problem for the operator A_0 has an exact solution. This solution can be obtained in different ways. For example, with the help of Bogolubov's transformation [14] or by using continued fractions [15, 16]. In the work [7] the operator A_0 was considered using the Bargmann space.

The solution of the eigenvalues problem for the operator A_0 has the form

$$A_0\, a_n = \mu_n\, a_n\,, \quad \mu_n = n - g^2\,, \quad n = 0, 1, 2, \dots \tag{2.2}$$

Here a_n are normalized eigenvectors of the operator A_0. Its expansion through the basis vectors e_n of the matrix representation (1.1) has the form

$$a_m = \sum_{n=0}^{\infty} U_{n,m}\, e_n\,,$$

$$U_{n,m} \equiv \begin{cases} \exp\{-g^2/2\}\sqrt{n!m!}\; g^{m-n} \\ \qquad \times \sum_{i=0}^{n} (-1)^i \dfrac{(g^2)^i}{i!\,(n-i)!\,(i+m-n)!}\,, & m \ge n \\ \exp\{-g^2/2\}\sqrt{n!m!}\; g^{n-m}\,(-1)^{n-m} \\ \qquad \times \sum_{i=0}^{m} (-1)^i \dfrac{(g^2)^i}{i!\,(m-i)!\,(i+n-m)!}\,, & n \ge m. \end{cases} \tag{2.3}$$

Using the definition of generalized Chebyshev-Laguerre polynomials $L_n^{(s)}(x)$ [19]

$$L_n^{(s)}(x) = \frac{(n+s)!}{n!} \sum_{i=0}^{n} C_n^i\,(-1)^i \frac{x^i}{(i+s)!}\,, \quad C_n^i = \frac{n!}{i!\,(n-i)!}\,, \quad (s \ge 0)$$

and its property

$$L_n^{(-s)}(x) = (-x)^s\,\frac{(n-s)!}{n!}\,L_{n-s}^{(s)}(x)\,, \quad (s \ge 0)\,, \tag{2.4}$$

we obtain

$$U_{n,m} \equiv U_{n,m}(g) = \exp\{-g^2/2\}\sqrt{\frac{n!}{m!}}\; g^{m-n}\,L_n^{(m-n)}(g^2). \tag{2.5}$$

The simplest way to obtain (2.2) is to use Bogolubov's transformation. Its idea is following. It is well known that the spectrum of harmonic oscillator can be obtained through the commutative property $[a, a^+] = 1$ of operators a and a^+ only. Assume that $a = b + C$ $(a^+ = b^+ + C)$, where C is some real constant. It is evident that $[b, b^+] = 1$, and the spectrum of b^+b is the spectrum of harmonic oscillator. On the other hand

$$A_0 = a^+a + g\,(a + a^+) = b^+b + (C+g)(b+b^+) + C^2 + 2gC.$$

If $C = -g$, $A_0 = b^+b - g^2$, i.e., A_0 is shifted oscillator. From that (2.2) follows at once.

To receive (2.3) let us notice that the transition $a \to (a-g)$ can be obtained by orthogonal transformation U

$$a - g = U^+aU\,, \quad U = e^{g(a-a^+)} = e^{-g^2/2}e^{-ga^+}e^{ga}.$$

This transformation is well known in the theory of coherent states (see for example [17]). Thus we have

$$U^+A_0U = a^+a - g^2\,, \quad a_m = Ue_m = e^{-g^2/2}e^{-ga^+}e^{ga}e_m.$$

Expanding exponents to the series and using relations

$$a e_m = \sqrt{m}\, e_{m-1}\,, \quad a^+ e_m = \sqrt{m+1}\, e_{m+1}\,, \quad m = 0, 1, 2, \dots\,,$$

after simple algebraic transformations, we obtain (2.3) and hence (2.5).

Let us note here that the completeness of the "shifted oscillator" eigenfunctions (in coordinate representation) for complex values of the parameter g is considered in [18].

Let us find the matrix of the operator R in the basis of the operator A_0 eigenvectors. Denoting the elements of the transformed matrix as $\tilde{R}_{k,m}$ and taking into account that $R_{n,m} = (-1)^n\, \delta_{n,m}$, we obtain

$$\tilde{R}_{k,m} = (R e_m, e_k) = (U^T R U)_{k,m} = \sum_{n=0}^{\infty} (-1)^n\, U_{n,k}\, U_{n,m}. \tag{2.6}$$

Let us represent matrix elements $U_{n,m} = U_{n,m}(g)$ as contour integral

$$U_{n,m}(g) = \exp\{-g^2/2\} \sqrt{\frac{m!}{n!}}\; g^{n-m}\, \frac{1}{2\pi i} \oint\limits_C x^{m-1} \left(\frac{1}{x} - 1\right)^n \exp\left\{\frac{g^2}{x}\right\} dx\,, \tag{2.7}$$

where C is a unit circle centered in the origin of the complex plane x (C is positively oriented). This expression can be easily checked by calculation of integral with the help of residues.

Substituting (2.7) in (2.6) and summing up over n, we find

$$\begin{aligned} \tilde{R}_{k,m} =\; & \exp\{-2g^2\} \sqrt{k!\, m!}\; g^{-m-k}\, \frac{1}{(2\pi i)^2} \\ & \times \oint\limits_C \oint\limits_C (x)^{m-1}\, (x')^{k-1} \exp\left\{ g^2 \left(\frac{2}{x} + \frac{2}{x'} - \frac{1}{x x'} \right) \right\} dx\, dx'. \end{aligned}$$

Contour integrals in this expression can be calculated consistently with the help of residues as before. As a result, using (2.5), we obtain

$$\tilde{R}_{k,m} = (-1)^k\, U_{k,m}(2g). \tag{2.8}$$

In spite of seeming asymmetry, the matrix $\tilde{R}_{k,m}$ is symmetric ($\tilde{R}_{k,m} = \tilde{R}_{m,k}$). It can be easily verified by means of the property (2.4).

Using the asymtotics of the generalized Chebyshev-Laguerre polynomials [19]

$$\begin{aligned} L_n^s(x) = \;& \pi^{-1/2}\, n^{s/2-1/4}\, x^{-s/2-1/4}\, e^{x/2} \\ & \times \left\{ \cos\left(2\sqrt{nx} - s\pi/2 - \pi/4\right) + O(n^{-1/2}) \right\}\,, \quad n \to \infty\,, \end{aligned} \tag{2.9}$$

we find

$$\lim_{n\to\infty} \tilde{R}_{n,n+p} = 0\,, \quad \forall p \in Z. \tag{2.10}$$

In what follows we will need the following result [5]

Lemma 2.1 (J. Janas-S. Naboko). *Let D be a selfadjoint operator in a Hilbert space H with simple discrete spectrum ($De_n = \mu_n e_n$), where $\{e_n\}$ is an orthonormal basis of eigenvectors in H and μ_n are simple eigenvalues ($\mu_n \to \infty$), ordered by $|\mu_i| \leq |\mu_{i+1}|$. Assume that $|\mu_i - \mu_k| \geq \epsilon_0 > 0$, $\forall i \neq k$. If R is a compact operator in H then the eigenvalues $\lambda_n(T)$ of the operator $T = D+R$ (with discrete spectrum too) become simple for large values of n and satisfy to the asymptotic formula*

$$\lambda_n(T) = \mu_n + O(\|R^* e_n\|)\,, \quad n \to \infty\,, \tag{2.11}$$

where R^* is the adjoint operator with respect to R.

Matrices R and $\tilde{R} = U^T R U$ represent bounded noncompact operator (projector) since $R^2 = I$. Therefore we can't apply here at once Lemma 2.1.

Let us prove the following theorem:

Theorem 2.2. *Let D be a selfadjoint operator in a Hilbert space H with eigenvalues $\mu_n = n$, ($n = 0, 1, 2, \ldots$) and complete system of corresponding eigenvectors in H. Let R be a bounded, selfadjoint, noncompact operator and its matrix $R_{n,k}$ in the basis of operator D eigenvectors satisfy to the condition*

$$\lim_{n\to\infty} R_{n,\,n+p} = 0\,, \quad \forall p \in Z. \tag{2.12}$$

Then the eigenvalues $\lambda_n(T)$ of the operator $T = D+R$ (having a discrete spectrum too) become simple for large values of n and satisfy to the following asymptotic estimation

$$\lambda_n(T) = n + R_{n,n} + O\left(s_n\right)\,, \quad n \to \infty\,, \tag{2.13}$$

where

$$s_n = \sqrt{\sum_{k\neq n} \frac{|R_{k,n}|^2}{(n-k)^2}}\,,$$

and $s_n \to 0$ at $n \to \infty$.

For the proof of this theorem we need the following compactness criteria for infinite matrices.

Lemma 2.3. *Let V be a bounded, noncompact operator in a Hilbert space H. Let its matrix $V_{i,j}$ $(i, j = 0, 1, \ldots)$ in some orthonormal basis satisfy to the condition*

$$\lim_{n\to\infty} V_{n,\,n+p} = 0\,, \quad \forall p \in Z. \tag{2.14}$$

Let $b = \{b_i\}_{i=-\infty}^{\infty}$ is an arbitrary l_2-sequence

$$\|b\|^2 = \sum_{i=-\infty}^{\infty} |b_i|^2 < \infty. \tag{2.15}$$

Then the operator K with matrix $K_{i,j} = b_{i-j} V_{i,j}$ $(i, j = 0, 1, \ldots)$ is compact in H.

Proof. Let us show at first that the operator K is bounded. For that we need to prove the estimates [20]

$$\sum_{j=0}^{\infty} |K_{i,j}| < A\,, \ \forall i\,; \qquad \sum_{i=0}^{\infty} |K_{i,j}| < A\,, \ \forall j\,, \tag{2.16}$$

where A is a constant independent of i and j ($\|K\| \le A$). Using Cauchy's inequality, we have

$$\sum_{j=0}^{\infty} |K_{i,j}| = \sum_{j=0}^{\infty} |b_{i-j} V_{i,j}| \le \left(\sum_{j=0}^{\infty} |b_{i-j}|^2\right)^{1/2} \left(\sum_{j=0}^{\infty} |V_{i,j}|^2\right)^{1/2}$$
$$\le \|b\| \sqrt{(VV^*)_{i,i}} \le \|b\| \cdot \|V\|$$

Due to (2.15) the first estimate in (2.16) is fulfilled. By the same way the validity of the second estimate in (2.16) is established. Thus the operator K is bounded. Let us prove now its compactness.

Let us define the cut-off function $b^{(n)} = \{b_i^{(n)}\}_{i=-\infty}^{\infty}$ of the sequence $\{b_i\}$

$$b_i^{(n)} = \begin{cases} 0\,, & |i| > n \\ b_i\,, & |i| \le n. \end{cases}$$

Let us define the sequence of operators $K^{(n)}$ by the formula $K_{i,j}^{(n)} = b_{i-j}^{(n)} V_{i,j}$. It follows from this definition and from (2.14) that $K^{(n)}$ is a compact operator for arbitrary n. We proceed further as in the proof of (2.16)

$$\|K - K^{(n)}\| \le \|b - b^{(n)}\| \cdot \|V\|.$$

Therefore

$$\|K - K^{(n)}\| \to 0\,, \quad n \to \infty\,,$$

and K is compact as a limit by norm of compact operators [20, 21].

Proof of Theorem 2.2. Keeping the same notations, let us associate each operator with a matrix in the basis of the operator D eigenvectors.

Following the main ideas of the work [5] let us show that there exist such anti-hermitian operator K ($K^* = -K$) that

$$(I + K)T - D_1(I + K) = B\,, \tag{2.17}$$

where B is compact operator and $D_1 = D + \operatorname{diag}\{R_{n,n}\}$. (So D_1 is the diagonal matrix with elements $(D_1)_{n,n} = n + R_{n,n}$.) Suppose that such operator K have found. The condition (2.17) means that

$$T = (I + K)^{-1}(D_1 + B(I + K)^{-1})(I + K).$$

(The existence of the inverse operator $(I+K)^{-1}$ follows from the anti-hermitianess of K.) Thus the operators T and $D_1 + B(I + K)^{-1}$ are similar and have the same spectrum. But the operator B is compact and the eigenvalues of D_1 due to (2.12) satisfy the requirements of Lemma 2.1. Applying Lemma 2.1 we obtain

$$\lambda_n(T) = n + R_{n,n} + O\left(\|B^* e_n\|\right). \tag{2.18}$$

Therefore for the proof of the theorem we should establish the existence of such the operator K and find the matrix of the compact operator B. Substituting the expressions for the matrices T and D_1 in (2.17) we obtain

$$(I + K)T - D_1(I + K) = R_1 - [D, K] + KR - \operatorname{diag}\{R_{n,n}\} K\,, \tag{2.19}$$

where $[\cdot, \cdot]$ is the commutator and R_1 is the matrix of the operator R with zero main diagonal ($R_1 = R - \operatorname{diag}\{R_{n,n}\}$).

This expression will be the matrix of compact operator if we can find such a compact operator K that the condition $[D, K] = R_1$ is valid, or in matrix form: $K_{i,j}\,(i - j) = (R_1)_{i,j}$. It follows from that

$$K_{i,j} = \frac{R_{i,j}}{i - j}\,, \quad i \neq j\,; \qquad K_{i,i} = 0\,,\;\; i = 0, 1, \ldots. \tag{2.20}$$

As the operator R is selfadjoint the corresponding to the matrix (2.20) operator K is anti-hermitian. Its compactness follows from Lemma 2.3. Actually, if we choose the sequence $\{b_i\}$ as $\{1/i\}$ $(i \neq 0)$ then from (2.12) it follows that all conditions of Lemma 2.3 are fulfilled.

Now from (2.19) we find the form of the compact operator B:

$$B = KR - \operatorname{diag}\{R_{n,n}\}\, K.$$

Since $\|B^* e_n\| \leq C\|K^* e_n\|$, where C is constant, we can replace in (2.18) $O\left(\|B^* e_n\|\right)$ on $O\left(\|K^* e_n\|\right)$. Taking into account (2.20) we obtain

$$O\left(\|K^* e_n\|\right) = O\left(\sqrt{\sum_{k \neq n} \frac{|R_{k,n}|^2}{(n - k)^2}}\right).$$

Substituting this estimate to (2.18), we obtain the formula (2.13). The theorem is proved. □

Due to (2.10), the condition (2.12) of Theorem 2.2 is fulfilled. Hence, applying Theorem 2.2 and taking into account (2.2), (2.1) and (2.8) we have the following result

$$\lambda_n(A) = n - g^2 + \frac{c_1 + c_2}{2} + O\left(s_n\right)\,, \quad n \to \infty\,,$$

where

$$s_n = \sqrt{\sum_{k \neq n} \frac{|\tilde{R}_{k,n}|^2}{(n - k)^2}} = \sqrt{\sum_{k \neq n} \frac{|\omega_k^{(n-k)}(4g^2)|^2}{(n - k)^2}}. \tag{2.21}$$

We use here the normalized Laguerre functions $\omega_n^{(s)}(x)$

$$\omega_n^{(s)}(x) = \sqrt{\frac{n!}{(n+s)!}}\; e^{-x/2}\, x^{s/2}\, L_n^{(s)}(x)\,, \qquad \int\limits_0^{+\infty} \omega_m^{(s)}(x)\,\omega_n^{(s)}(x)\,dx = \delta_{n,m}.$$

From (2.5) and (2.8) it follows that

$$|\tilde{R}_{k,n}| = |\omega_k^{(n-k)}(4g^2)|.$$

3. Estimation of the remainder

To estimate the decreasing rate of the sequence s_n we should have another estimation for Laguerre's functions $\omega_n^{(s)}(x)$ rather than the estimation following from (2.9) (in (2.9) the parameter s is fixed). We could not find this result among known one and therefore we provide here not only the formulation but also the proof of it.

Lemma 3.1. *Suppose that $x > 0$, $s \in Z_+$. Then the following estimate for the Bessel functions $J_s(x)$ is valid*

$$|J_s(x)| \le 2\sqrt{\frac{2}{\pi x}}\,\left(1+\frac{s}{x}\right)^s.$$

Proof. Let us use known representation [22]

$$J_s(x) = \sqrt{\frac{2}{\pi x}}\,\left(P(x,s)\,\cos(x - s\pi/2 - \pi/4) - Q(x,s)\,\sin(x - s\pi/2 - \pi/4)\right)\,,$$

where

$$P(x,s) = \frac{1}{2\,\Gamma(s+1/2)}\int\limits_0^\infty e^{-u}\,u^{s-1/2}\left\{\left(1+\frac{iu}{2x}\right)^{s-1/2} + \left(1-\frac{iu}{2x}\right)^{s-1/2}\right\}du$$

$$Q(x,s) = \frac{1}{2i\,\Gamma(s+1/2)}\int\limits_0^\infty e^{-u}\,u^{s-1/2}\left\{\left(1+\frac{iu}{2x}\right)^{s-1/2} - \left(1-\frac{iu}{2x}\right)^{s-1/2}\right\}du.$$

It is evident that

$$|J_s(x)| \le \sqrt{\frac{2}{\pi x}}\,\left(|P(x,s)| + |Q(x,s)|\right)\,, \tag{3.1}$$

and everything reduces to the estimation of the integrals $P(x,s)$ and $Q(x,s)$. Let us consider the integral for $P(x,s)$. The estimation for $Q(x,s)$ is the same. At $s=0$ we have $|P(x,s)| \le 1$, $|Q(x,s)| \le 1$ and the estimation (3.1) gives the required inequality. Suppose that $s \in N$. In this case we have

$$|P(x,s)| \le \frac{1}{\Gamma(s+1/2)}\int\limits_0^\infty e^{-u}\,u^{s-1/2}\,\left(1+\frac{u}{2x}\right)^{s-1/2}\,du.$$

Expanding the binomial in this integral in the series on $u/2x$

$$\left(1+\frac{u}{2x}\right)^{s-1/2} = 1+\sum_{k=1}^{p-1} \frac{(s-1/2)\cdot\ \cdots\ \cdot(s-1/2-(k-1))}{k!} \left(\frac{u}{2x}\right)^{k} + \frac{(s-1/2)\cdot\ \cdots\ \cdot(s-1/2-(p-1))}{k!}(1+\theta)^{s-p-1/2}\left(\frac{u}{2x}\right)^{p}, \quad \theta\in(0,u/2x)$$

and putting $p=s$ we have $(1+\theta)^{s-p-1/2}<1$ and therefore

$$\left(1+\frac{u}{2x}\right)^{s-1/2} < 1+\sum_{k=1}^{s} \frac{(s-1/2)\cdot\ \cdots\ \cdot(s-1/2-(k-1))}{k!} \left(\frac{u}{2x}\right)^{k}.$$

Integrating by terms we obtain

$$|P(x,s)| \le 1+\sum_{k=1}^{s}\frac{\Gamma(s+k+1/2)}{\Gamma(s+1/2)}\ \frac{(s-1/2)\cdot\ \cdots\ \cdot(s-1/2-(k-1))}{k!}\ \frac{1}{(2x)^k}$$
$$< 1+\sum_{k=1}^{s}(2s)^k\,\frac{s\cdot\ \cdots\ \cdot(s-(k-1))}{k!}\ \frac{1}{(2x)^k} = \left(1+\frac{s}{x}\right)^{s}.$$

For $Q(x,s)$ the same estimate is valid and the formula (3.1) leads again to the required inequality. The lemma is proved. □

Lemma 3.2. *If* $x>0$*;* $n,s\in Z_+$ *and* $s^{16}\le n$ *then*

$$\left|\omega_n^{(s)}(x)\right| \le \frac{C(x)}{(n+1)^{1/4}}, \tag{3.2}$$

where the constant $C(x)$ *depends on* x *only.*

Proof. Let us use Laguerre's functions integral representation through the Bessel functions [19]

$$\omega_n^{(s)}(x) = \frac{e^{x/2}}{\sqrt{n!\,(n+s)!}}\int_0^\infty e^{-t}\,t^{n+\frac{s}{2}}\,J_s(2\sqrt{tx})\,dt, \quad n,s\in Z_+.$$

Let us split this integral into two one

$$\omega_n^{(s)}(x) = \frac{e^{x/2}}{\sqrt{n!\,(n+s)!}}\left(\int_0^{t_0} + \int_{t_0}^{\infty}\right),$$

where $t_0\ge 0$ is an arbitrary now.

For estimation of the first integral let us use the known inequality [22]

$$|J_s(x)|\le 1, \quad s\in Z_+,\ x\in R.$$

For estimation of the second integral we use more precise estimate from Lemma 3.1

$$|J_s(x)| \le 2\sqrt{\frac{2}{\pi x}}\left(1+\frac{s}{x}\right)^{s} < 2e\sqrt{\frac{2}{\pi x}}, \quad x\ge s^2.$$

Putting $t_0 = s^4/4x$ (so that at $t \geq t_0$ one can use the last estimate) we have

$$|\omega_n^{(s)}(x)| \leq \frac{e^{x/2}}{\sqrt{n!\,(n+s)!}} \left[\int_0^{t_0} e^{-t}\, t^{n+\frac{s}{2}}\, dt + \frac{2e}{\sqrt{\pi\sqrt{x}}} \int_{t_0}^{\infty} e^{-t}\, t^{n+\frac{s}{2}-1/4}\, dt \right]$$
$$\leq \frac{e^{x/2}}{\sqrt{n!\,(n+s)!}} \left[t_0 \max_{t\geq 0} \left\{ e^{-t}\, t^{n+\frac{s}{2}} \right\} + \frac{2e}{\sqrt{\pi\sqrt{x}}}\, \Gamma(n+s/2+3/4) \right]$$
$$= e^{x/2} \left[\frac{s^4}{4x}\, \frac{e^{-(n+\frac{s}{2})}\,(n+s/2)^{n+\frac{s}{2}}}{\sqrt{n!\,(n+s)!}} + \frac{2e}{\sqrt{\pi\sqrt{x}}}\, \frac{\Gamma(n+s/2+3/4)}{\sqrt{n!\,(n+s)!}} \right].$$

Using known inequalities for Gamma-function following from Stirling's formula

$$C_1\, z^{z-1/2}\, e^{-z} \leq \Gamma(z) \leq C_2\, z^{z-1/2}\, e^{-z}\,, \quad z \geq \delta > 0\,,$$

where C_1, C_2 are some constants independent of z. Let us estimate each term in square brackets. We have

$$\frac{2e}{\sqrt{\pi\sqrt{x}}}\, \frac{\Gamma(n+s/2+3/4)}{\sqrt{n!\,(n+s)!}} \leq C(x)\, \frac{(n+s/2+3/4)^{n+s/2+1/4}}{(n+1)^{n/2+1/4}\,(n+s+1)^{n/2+s/2+1/4}}$$
$$\leq \frac{C(x)}{(n+1)^{1/4}}\, \frac{(1+\frac{s}{2(n+1)})^n}{(1+\frac{s}{n+1})^{n/2}} \leq \frac{C(x)}{(n+1)^{1/4}} \left(1+\frac{s^2}{4(n+1)^2}\right)^{n/2}$$
$$\leq \frac{C(x)}{(n+1)^{1/4}}\, \exp\left\{\frac{s^2}{8(n+1)}\right\}.$$

At last, if we put $n \geq s^2$ then

$$\frac{2e}{\sqrt{\pi\sqrt{x}}}\, \frac{\Gamma(n+s/2+3/4)}{\sqrt{n!\,(n+s)!}} \leq \frac{C(x)}{(n+1)^{1/4}}\,, \quad (n \geq s^2). \tag{3.3}$$

Similarly, we can estimate the second term

$$\frac{s^4}{4x}\, \frac{e^{-(n+\frac{s}{2})}\,(n+s/2)^{n+\frac{s}{2}}}{\sqrt{n!\,(n+s)!}} \leq C(x)\, \frac{s^4\,(n+s/2)^{n+s/2}}{(n+1)^{n/2+1/4}\,(n+s+1)^{n/2+s/2+1/4}}$$
$$\leq \frac{C(x)}{(n+1)^{1/4}}\, \frac{s^4}{(n+s+1)^{1/4}}\, \frac{(1+\frac{s}{2(n+1)})^n}{(1+\frac{s}{n+1})^{n/2}}$$
$$\leq \frac{C(x)}{(n+1)^{1/4}}\, \frac{s^4}{(n+s+1)^{1/4}}\, \exp\left\{\frac{s^2}{8(n+1)}\right\}.$$

If $n \geq s^{16}$ then

$$\frac{s^4}{4x}\, \frac{e^{-(n+\frac{s}{2})}\,(n+s/2)^{n+\frac{s}{2}}}{\sqrt{n!\,(n+s)!}} \leq \frac{C(x)}{(n+1)^{1/4}}\,, \quad (n \geq s^{16}). \tag{3.4}$$

From (3.3), (3.4) it follows that

$$\left|\omega_n^{(s)}(x)\right| \leq \frac{C(x)}{(n+1)^{1/4}}\,, \quad (n \geq s^{16})\,, \qquad \square$$

Having the estimate (3.2) and the orthogonality condition of the transformation U:

$$\sum_{k=0}^{\infty} |U_{k,n}|^2 = \sum_{k=0}^{\infty} \left|\omega_k^{(n-k)}\right|^2 = \sum_{k=0}^{n} \left|\omega_{n-k}^{(k)}\right|^2 + \sum_{k=1}^{\infty} \left|\omega_n^{(k)}\right|^2 = 1\,, \quad \forall n \in Z_+ \tag{3.5}$$

($|\omega_k^{(n-k)}| = |\omega_n^{(k-n)}|$) one can give the estimate of the remainder which is defined by the sum

$$\sum_{k\neq n} \frac{|\omega_k^{(n-k)}|^2}{(n-k)^2} = \sum_{k=1}^{n} \frac{|\omega_{n-k}^{(k)}|^2}{k^2} + \sum_{k=1}^{\infty} \frac{|\omega_n^{(k)}|^2}{k^2}. \tag{3.6}$$

From Lemma 3.2 it follows that

$$|\omega_{n-k}^{(k)}|^2 \le \frac{C}{(n-k+1)^{1/2}}\,, \quad n-k \ge k^{16} \quad (n \ge k^{16}+k)$$
$$|\omega_n^{(k)}|^2 \le \frac{C}{(n+1)^{1/2}}\,, \qquad n \ge k^{16} \quad (k \le n^{1/16}).$$

Let $k_n \ge 0$ be a maximal nonnegative integer of k, satisfying to the equation $n \ge k^{16}+k$. It is evident that $k_n \le n^{1/16}$. Hence

$$|\omega_{n-k}^{(k)}|^2 \le \frac{C}{(n-n^{1/8}+1)^{1/2}}\,, \quad k \le k_n$$
$$|\omega_n^{(k)}|^2 \le \frac{C}{(n+1)^{1/2}}\,, \qquad k \le k_n.$$

Let us present the sum (3.6) in the form

$$\sum_{k\neq n} \frac{|\omega_k^{(n-k)}|^2}{(n-k)^2} = \left[\sum_{k=1}^{k_n} \frac{|\omega_{n-k}^{(k)}|^2}{k^2} + \sum_{k=1}^{k_n} \frac{|\omega_n^{(k)}|^2}{k^2}\right] + \left[\sum_{k=k_n+1}^{n} \frac{|\omega_{n-k}^{(k)}|^2}{k^2} + \sum_{k=k_n+1}^{\infty} \frac{|\omega_n^{(k)}|^2}{k^2}\right].$$

Due to last inequalities we have

$$\left[\sum_{k=1}^{k_n} \frac{|\omega_{n-k}^{(k)}|^2}{k^2} + \sum_{k=1}^{k_n} \frac{|\omega_n^{(k)}|^2}{k^2}\right] \le \frac{2C}{(n-n^{1/8}+1)^{1/2}} \sum_{k=1}^{k_n} \frac{1}{k^2} = O\left(\frac{1}{n^{1/2}}\right).$$

Since $k_n \sim n^{1/16}$, we have using (3.5)

$$\left[\sum_{k=k_n+1}^{n} \frac{|\omega_{n-k}^{(k)}|^2}{k^2} + \sum_{k=k_n+1}^{\infty} \frac{|\omega_n^{(k)}|^2}{k^2}\right] \le \frac{1}{(k_n+1)^2} \left[\sum_{k=k_n+1}^{n} |\omega_{n-k}^{(k)}|^2 + \sum_{k=k_n+1}^{\infty} |\omega_n^{(k)}|^2\right]$$
$$\le \frac{1}{(k_n+1)^2} = O\left(\frac{1}{n^{1/8}}\right).$$

Combining both estimates, we obtain

$$\sum_{k\neq n}\frac{|\omega_k^{(n-k)}|^2}{(n-k)^2}=O\left(\frac{1}{n^{1/2}}\right)+O\left(\frac{1}{n^{1/8}}\right)=O\left(\frac{1}{n^{1/8}}\right).$$

Taking into account formula (2.21), we arrive at the following main result

Theorem 3.3. *The eigenvalues $\lambda_n(A)$ of the operator A (1.1) at $g\neq 0$ have the following asymptotics*

$$\lambda_n(A)=n-g^2+\frac{c_1+c_2}{2}+O\left(\frac{1}{n^{1/16}}\right),\quad n\to\infty.$$

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