Linear Operators and Spectral Theory
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Topics in the Theory of Linear Operators in Hilbert Spaces

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1 Preliminaries

For simplicity we will always assume that the Hilbert spaces considered in this manuscript are separable and complex (although most results extend to nonseparable complex Hilbert spaces).

Let $\mathcal{H}_1$, $\mathcal{H}_2$ be separable Hilbert spaces and A be a linear operator $A : D(A) \subset \mathcal{H}_1 \to \mathcal{H}_2$.

We denote by $B(\mathcal{H}_1, \mathcal{H}_2)$ the set of all *bounded* linear operators from $\mathcal{H}_1$ into $\mathcal{H}_2$ and write $B(\mathcal{H}, \mathcal{H}) = B(\mathcal{H})$ for simplicity.

We recall that $A = B$ if $D(A) = D(B) = D$ and $Ax = Bx$ for all $x \in D$.

Next, let $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}$.

Definition 1.1. (i) Let T be densely defined in $\mathcal{H}$. Then T^* is called the *adjoint* of T if,

$$\begin{aligned} Dom(T^*) = \{g \in \mathcal{H} \,|\, &\text{there exists an } h_g \in \mathcal{H} \text{ such that } (h_g, f) = (g, Tf) \text{ for} \\ &\text{all } f \in Dom(T)\}, \\ T^* g = h_g&. \end{aligned}$$

(ii) An operator A in $\mathcal{H}$ is called *symmetric* if A is densely defined and $A \subseteq A^*$.
(iii) A densely defined operator B in $\mathcal{H}$ is called *self-adjoint* if $B = B^*$.
(iv) A densely defined operator S in $\mathcal{H}$ is called *normal* if $SS^* = S^*S$.

We note that for every self-adjoint operator A in $\mathcal{H}$ one has $\overline{D(A)} = \mathcal{H}$. For every bounded operator A we will assume $D(A) = \mathcal{H}$ unless explicitly stated otherwise.

Definition 1.2. (i) $z \in \mathbb{C}$ lies in the *resolvent set* of A if $(A - zI)^{-1}$ exists and is bounded. The resolvent set of A is denoted by $\rho(A)$.
(ii) If $z \in \rho(A)$, then $(A - zI)^{-1}$ is called the *resolvent* of A at the point z.
(iii) $\sigma(A) = \mathbb{C} \setminus \rho(A)$ is called the *spectrum* of A.

We will use the notation,

$$R(z, A) = (A - zI)^{-1}, \quad z \in \rho(A).$$

Fact 1.3. $\overline{\sigma(A)} = \sigma(A)$.

Fact 1.4. $A = A^* \Rightarrow \sigma(A) \subseteq \mathbb{R}$.

Fact 1.5. If A is a bounded operator, then $\sigma(A)$ is a bounded subset of $\mathbb{C}$.

Fact 1.6. If A is a bounded self-adjoint operator, then $\sigma(A) \subset \mathbb{R}$ is compact.

Fact 1.7. If A is a bounded self-adjoint operator, then $\|A\| = \sup_{\lambda \in \sigma(A)} |\lambda|$.

Fact 1.8. If A is a self-adjoint operator, then $R(z, A)$ is a normal operator for all $z \in \rho(A)$.

2 The spectral theorem for bounded self-adjoint operators

Let $\mathcal{H}$ be a separable Hilbert space and $A = A^* \in B(\mathcal{H})$. We recall that $\sigma(A) \subset \mathbb{R}$ is compact in this case.

Theorem 2.1. *([3], Thm. VII.1; the continuous functional calculus.)*
There is a unique map $\varphi_A : C(\sigma(A)) \to B(\mathcal{H})$ such that for all $f, g \in C(\sigma(A))$:

(i)
$$\varphi_A(fg) = \varphi_A(f)\varphi_A(g),$$
$$\varphi_A(\lambda f) = \lambda \varphi_A(f),$$
$$\varphi_A(1) = I,$$
$$\varphi_A(\overline{f}) = \varphi_A(f)^*.$$

*(These four conditions mean that φ_A is an algebraic *-homomorphism).*

(ii) $\varphi_A(f + g) = \varphi_A(f) + \varphi_A(g)$ *(linearity).*

(iii) $\|\varphi_A(f)\|_{B(\mathcal{H})} \le C \|f\|_\infty$ *(continuity).*

(iv) If $f(x) = x$, *then* $\varphi_A(f) = A$.

Moreover, φ_A has the following additional properties:

(v) If $A\psi = \lambda\psi$, *then* $\varphi_A(f)\psi = f(\lambda)\psi$.

(vi) $\sigma(\varphi_A(f)) = f(\sigma(A)) = \{f(\lambda) \mid \lambda \in \sigma(A)\}$ *(the spectral mapping theorem).*

(vii) If $f \ge 0$, *then* $\varphi_A(f) \ge 0$.

(viii) $\|\varphi_A(f)\|_{B(\mathcal{H})} = \|f\|_\infty$ *(this strengthens (iii)).*

In other words, $\varphi_A(f) = f(A)$.

Proof. (i), (ii) and (iv) uniquely determine $\varphi_A(p)$ for any polynomial p. Since polynomials are dense in $C(\sigma(A))$ (by the Stone–Weierstrass theorem), one only has to show that

$$\|p(A)\|_{B(\mathcal{H})} \leq C \sup_{\lambda \in \sigma(A)} |p(\lambda)| \,. \tag{2.1}$$

Then φ_A can be uniquely extended to the whole $C(\sigma(A))$ with the same bound and the first part of the theorem will be proven. Equation(2.1) follows from the subsequent two lemmas.

Now (viii) is obvious and properties (v), (vi) and (vii) follow easily as well. □

Lemma 2.2. $\sigma(p(A)) = p(\sigma(A)) = \{p(\lambda) \,|\, \lambda \in \sigma(A)\}$.

Lemma 2.3. $\|p(A)\| = \sup_{\lambda \in \sigma(A)} |p(\lambda)|$.

Proof. Using property (i), Fact 1.7, and Lemma 2.2, one gets

$$\begin{aligned} \|p(A)\|^2 = \|p(A)^* p(A)\| = \|(\overline{p}p)(A)\| = \sup_{\lambda \in \sigma((\overline{p}p)(A))} |\lambda| \\ = \Big(\sup_{\lambda \in \sigma(A)} |p(\lambda)| \Big)^2 . \end{aligned}$$

□

Since it is not sufficient to have a functional calculus only for continuous functions (the main goal of this construction is to define spectral projections of the operator A which are characteristic functions of A), we have to extend it to the space of bounded Borel functions, denoted by $Bor(\mathbb{R})$.

Definition 2.4. $f \in Bor(\mathbb{R})$ if f is a measurable function with respect to the Borel measure on $\mathbb{R}$ and $\sup_{x \in \mathbb{R}} |f(x)| < \infty$.

Theorem 2.5. *([3], Thm. VII.2.)*
Let $A = A^* \in B(\mathcal{H})$. Then there is a unique map $\widehat{\varphi}_A : Bor(\mathbb{R}) \to B(\mathcal{H})$ such that for all $f, g \in Bor(\mathbb{R})$ the following statements hold:

*(i) $\widehat{\varphi}_A$ is an algebraic *-homomorphism.*

(ii) $\widehat{\varphi}_A(f+g) = \widehat{\varphi}_A(f) + \widehat{\varphi}_A(g)$ *(linearity).*

(iii) $\|\widehat{\varphi}_A(f)\|_{B(\mathcal{H})} \leq \|f\|_\infty$ *(continuity).*

(iv) *If* $f(x) = x$*, then* $\widehat{\varphi}_A(f) = A$*.*

(v) *If* $f_n(x) \underset{n\to\infty}{\to} f(x)$ *for all* $x \in \mathbb{R}$*, and* $f_n(x)$ *are uniformly bounded w.r.t.* (x, n)*, then* $\widehat{\varphi}_A(f_n) \underset{n\to\infty}{\to} \widehat{\varphi}_A(f)$ *strongly.*

Moreover, $\widehat{\varphi}_A$ *has the following additional properties:*

(vi) *If* $A\psi = \lambda\psi$*, then* $\widehat{\varphi}_A(f)\psi = f(\lambda)\psi$*.*

(vii) *If* $f \geq 0$*, then* $\widehat{\varphi}_A(f) \geq 0$*.*

(viii) *If* $BA = AB$*, then* $B\widehat{\varphi}_A(f) = \widehat{\varphi}_A(f)B$*.*

Again, formally, $\widehat{\varphi}_A(f) = f(A)$*.*

Proof. This theorem can be proven by extending the previous theorem. (One has to invoke that the closure of $C(\mathbb{R})$ under the limits of the form (v) is precisely $Bor(\mathbb{R})$.) □

3 Spectral projections

Let $\mathcal{B}_\mathbb{R}$ denote the set of all Borel subsets of $\mathbb{R}$.

Definition 3.1. The family $\{P_\Omega\}_{\Omega\in\mathcal{B}_\mathbb{R}}$ of bounded operators in $\mathcal{H}$ is called a *projection-valued measure (p.v.m.) of bounded support* if the following conditions (i)–(iv) hold:

(i) P_Ω is an orthogonal projection for all $\Omega \in \mathcal{B}_\mathbb{R}$.

(ii) $P_\emptyset = 0$, there exist $a, b \in \mathbb{R}$, $a < b$ such that $P_{(a,b)} = I$ (the bounded support property).

(iii) If $\Omega = \cup_{k=1}^\infty \Omega_k$, $\Omega_i \cap \Omega_j = \emptyset$ for $i \neq j$, then $P_\Omega = \mathrm{s} - \lim_{N\to\infty} \sum_{k=1}^N P_{\Omega_k}$.

(iv) $P_{\Omega_1} P_{\Omega_2} = P_{\Omega_1 \cap \Omega_2}$.

Next, let $A = A^* \in B(\mathcal{H})$, $\Omega \in \mathcal{B}_\mathbb{R}$.

Definition 3.2. $P_\Omega(A) = \chi_\Omega(A)$ are called the *spectral projections* of A.

We note that the family $\{P_\Omega(A) = \chi_\Omega(A)\}_{\Omega \in \mathcal{B}_\mathbb{R}}$ satisfies conditions (i)–(iv) of Definition 3.1.

Next, consider a p.v.m. $\{P_\Omega\}_{\Omega \in \mathcal{B}_\mathbb{R}}$. Then for any $h \in \mathcal{H}$, $(h, P_\Omega h)$ is a positive (scalar) measure since properties (i)–(iv) imply all the necessary properties of a positive measure. We will use the symbol $d(h, P_\lambda h)$ to denote the integration with respect to this measure.

By construction, the support of every $(h, P_\Omega(A)h)$ is a subset of $\sigma(A)$. Hence, if we integrate with respect to the measure $(h, P_\Omega h)$, we integrate over $\sigma(A)$. If we are dealing with an arbitrary p.v.m. we will denote the support of the corresponding measure by $\operatorname{supp}(P_\Omega)$.

Theorem 3.3. *([3], Thm. VII.7.)*
If $\{P_\Omega\}_{\Omega \in \mathcal{B}_\mathbb{R}}$ is a p.v.m. and f is a bounded Borel function on $\operatorname{supp}(P_\Omega)$, then there is a unique operator B, which we will denote by $\int_{\operatorname{supp}(P_\Omega)} f(\lambda)\, dP_\lambda$, such that

$$(h, Bh) = \int_{\operatorname{supp}(P_\Omega)} f(\lambda)\, d(h, P_\lambda h), \quad h \in \mathcal{H}. \tag{3.1}$$

Proof. A standard Riesz argument. □

Next, we will show that if $P_\Omega(A)$ is a p.v.m. associated with A, then

$$f(A) = \int_{\sigma(A)} f(\lambda)\, dP_\lambda(A). \tag{3.2}$$

First, assume $f(\lambda) = \chi_\Omega(\lambda)$. Then

$$\begin{aligned}\int_{\sigma(A)} \chi_\Omega(\lambda)\, d(h, P_\lambda(A)h) &= \int_{\sigma(A)\cap\Omega} d(h, P_\lambda(A)h) = (h, P_\Omega(A)h) \\ &= (h, \chi_\Omega(A)h).\end{aligned}$$

Hence, (3.2) holds for all simple functions. Next, approximate any measurable function $f(\lambda)$ by a sequence of simple functions to obtain (3.2) for bounded Borel functions on $\sigma(A)$.

The inverse statement also holds: If we start from any bounded p.v.m. $\{P_\Omega\}_{\Omega \in \mathcal{B}_\mathbb{R}}$ and form $A = \int_{\operatorname{supp}(P_\Omega)} \lambda dP_\lambda$, then $\chi_\Omega(A) = P_\Omega(A) = P_\Omega$. This follows from the fact that for such an A, the mapping $f \mapsto \int_{\text{supp}(P_\Omega)} f(\lambda) dP_\lambda$ forms a functional calculus for A. By uniqueness of the functional calculus one then gets

$$P_\Omega(A) = \chi_\Omega(A) = \int_{\text{supp}(P_\Omega)} \chi_\Omega(\lambda)\, dP_\lambda = P_\Omega.$$

Summarizing, one obtains the following result:

Theorem 3.4. *([3], Thm. VII.8; the spectral theorem in p.v.m. form.)*
There is a one-to-one correspondence between bounded self-adjoint operators A and projection-valued measures $\{P_\Omega\}_{\Omega \in \mathcal{B}_\mathbb{R}}$ in $\mathcal{H}$ of bounded support given by

$$A \to \{P_\Omega(A)\}_{\Omega\in\mathcal{B}_\mathbb{R}} = \{\chi_\Omega(A)\}_{\Omega\in\mathcal{B}_\mathbb{R}},$$
$$\{P_\Omega\}_{\Omega\in\mathcal{B}_\mathbb{R}} \to A = \int_{\text{supp}(P_\Omega)} \lambda\, dP_\lambda.$$

4 The spectral theorem for unbounded self-adjoint operators

The construction of the spectral decomposition for unbounded self-adjoint operators will be based on the following theorem.

Theorem 4.1. *([3], Thm. VIII.4.)*
Assume $A = A^*$. Then there is a measure space $(M_A, d\mu_A)$ with μ_A a finite measure, a unitary operator $U_A : \mathcal{H} \to L^2(M_A, d\mu_A)$, and a real-valued function f_A on M_A which is finite a.e., such that

(i) $\psi \in D(A) \Leftrightarrow f_A(\cdot)(U_A\psi)(\cdot) \in L^2(M_A, d\mu_A)$.

(ii) *If* $\varphi \in U[D(A)]$, *then* $(U_A A U_A^{-1}\varphi)(m) = f_A(m)\varphi(m)$.

To prove this theorem we need some additional constructions. First we will prove a similar result for bounded normal operators.

Definition 4.2. Let A be a bounded normal operator in $\mathcal{H}$. Then $\psi \in \mathcal{H}$ is a *star-cyclic vector* for A if

$$\overline{Lin.span\{A^n(A^*)^m\psi\}_{n,m\in\mathbb{N}_0}} = \mathcal{H}.$$

Lemma 4.3. *Let A be a bounded normal operator in $\mathcal{H}$ with a star-cyclic vector $\psi \in \mathcal{H}$. Then there is a measure μ_A on $\sigma(A)$, and a unitary operator U_A, such that $U_A : \mathcal{H} \to L^2(\sigma(A), d\mu_A)$ with*

$$(U_A A U_A^{-1} f)(\lambda) = \lambda f(\lambda).$$

This equality holds in the sense of equality of elements of $L^2(\sigma(A), d\mu_A)$.

Proof. Introduce $\overline{\mathcal{P}} = \{\sum_{i,j=0}^{n} c_{ij}\lambda^i \overline{\lambda}^j, c_{ij} \in \mathbb{C}, n \in \mathbb{N}\}$ and take any $p(\cdot) \in \overline{\mathcal{P}}$. Define U_A by $U_A p(A)\psi = p$. One can prove that for all $x, y \in \mathcal{H}$ there exists a measure $\mu_{x,y,A}$ on $\sigma(A)$ such that

$$(p(A)x, y) = \int_{\sigma(A)} p(\lambda)\, d\mu_{x,y,A}, \quad p \in \overline{\mathcal{P}}.$$

Then

$$\begin{aligned} \|p(A)\|^2 &= (p(A)^* p(A)\psi, \psi) = ((\overline{p}p)(A)\psi, \psi) = \int_{\sigma(A)} \overline{p}(\lambda) p(\lambda)\, d\mu_{\psi,\psi,A} \\ &= \|p\|^2_{L^2(\sigma(A), d\mu_{\psi,\psi,A})}. \end{aligned} \tag{4.1}$$

Next we choose $\mu_A = \mu_{\psi,\psi,A}$. Since ψ is star-cyclic, U_A is densely defined and equation (4.1) implies that U_A is bounded. Thus, U_A can be extended to an isometry

$$U_A : \mathcal{H} \to L^2(\sigma(A), d\mu_A).$$

Since $\overline{\mathcal{P}}(\sigma(A))$ is dense in $L^2(\sigma(A), d\mu_A)$, $Ran(U_A) = L^2(\sigma(A), d\mu_A)$ and U_A is invertible. Thus, U_A is unitary.
Finally, if $p \in \overline{\mathcal{P}}(\sigma(A))$, then

$$(U_A A U_A^{-1} p)(\lambda) = (U_A A p(A)\psi)(\lambda) = (U_A(\lambda \cdot p)(A)\psi)(\lambda) = \lambda p(\lambda).$$

By continuity, this can be extended from $\overline{\mathcal{P}}(\sigma(A))$ to $L^2(\sigma(A), d\mu_A)$. □

Lemma 4.4. *Let A be a bounded normal operator on a separable Hilbert space $\mathcal{H}$. Then there is an orthogonal direct sum decomposition $\mathcal{H} = \oplus_{j=1}^{N} \mathcal{H}_j$ ($N \leq \infty$) such that:*

(i) For all j: $AH_j \subseteq \mathcal{H}_j$.

(ii) For all j there exists an $x_j \in \mathcal{H}_j$ such that x_j is star-cyclic for $A|_{\mathcal{H}_j}$.

Proof. Take any $h_1 \neq 0 \in \mathcal{H}$. If $\overline{\{p(A)h_1, \quad p(\cdot) \in \overline{\mathcal{P}}\}} = \mathcal{H}$, then h_1 is star-cyclic and we are done. Otherwise, denote $\mathcal{H}_1 = \overline{\{p(A)h_1, \quad p(\cdot) \in \overline{\mathcal{P}}\}}$, take any $h_2 \perp \mathcal{H}_1$, consider $\mathcal{H}_2 = \overline{\{p(A)h_2, \quad p(\cdot) \in \overline{\mathcal{P}}\}}$, etc. Then (i) and (ii) are obvious. To show that $\{\mathcal{H}_j\}$ are orthogonal one computes

$$(p(A)h_j, q(A)h_k) = (q(A)^*p(A)h_j, h_k) = ((\overline{q}p)(A)h_j, h_k) = 0, \quad if \quad j \neq k.$$

□

Theorem 4.5. *Let A be a bounded normal operator on a separable Hilbert space $\mathcal{H}$. Then there is a measure space $(M_A, d\mu_A)$ with μ_A a finite measure, a unitary operator $U_A : \mathcal{H} \to L^2(M_A, d\mu_A)$, and a bounded continuous function f_A on M_A, such that*

$$(U_A A U_A^{-1}\varphi)(\lambda) = f_A(\lambda)\varphi(\lambda).$$

Proof. Based on Lemmas 4.3 and 4.4. □

Now we return to the principal objective of this section:

Proof of Theorem 4.1. Since $R(\lambda, A)$ is a bounded normal operator, we can apply Theorem 4.5 to $(A+i)^{-1}$ and get $(U_A(A+i)^{-1}U_A^{-1}\varphi)(m) = g_A(m)\varphi(m)$ for some g_A. Since $Ker(A+i)^{-1} = \{0\}$, then $g_A \neq 0$ μ_A-a.e., so g_A^{-1} is finite μ_A-a.e. Define $f_A(m) = g_A(m)^{-1} - i$.

First, we prove that (i) holds: ($\Rightarrow$) Let $\psi \in D(A)$. Then there exists a $\varphi \in \mathcal{H}$ such that $\psi = (A+i)^{-1}\varphi$ and $U_A\psi = g_A U_A\varphi$. Since fg is bounded, one obtains $f_A(U_A\psi) \in L^2(M_A, d\mu_A)$.
($\Leftarrow$) Let $f_A(U_A\psi) \in L^2(M_A, d\mu_A)$. Then $U_A\varphi = (f_A+i)U_A\psi$ for some $\varphi \in \mathcal{H}$. Thus, $g_A U_A\varphi = g_A(f_A+i)U_A\psi$ and hence $\psi = (A+i)^{-1}\varphi \in D(A)$.

Next, we show that (ii) holds: Take any $\psi \in D(A)$. Then $\psi = (A+i)^{-1}\varphi$ for some $\varphi \in \mathcal{H}$ and $A\psi = \varphi - i\psi$. Therefore,

$$\begin{aligned}(U_A A\psi)(m) &= (U_A\varphi)(m) - i(U_A\psi)(m) = (g_A(m)^{-1} - i)(U_A\psi)(m) \\ &= f_A(m)(U_A\psi)(m).\end{aligned}$$

It remains to show that f is real-valued. We will prove this by contradiction. W.l.o.g. we suppose that $Im(f) > 0$ on a set of nonzero measure. Then there exists a bounded set $B \subset \{z \in \mathbb{C} \,|\, Im(z) > 0\}$ with

$S = \{x \in \mathbb{R} \,|\, f(x) \in B\}$, $\mu_A(S) \neq 0$. Hence, $Im((\chi_S, f\chi_S)) > 0$, implying that multiplication by f is not self-adjoint. □

Next, we can define functions of an operator A. Let $h \in Bor(\mathbb{R})$. Then

$$h(A) = U_A^{-1} T_{h(f_A)} U_A,$$

where

$$T_{h(f_A)} \colon \begin{cases} L^2(M_A, d\mu_A) \to L^2(M_A, d\mu_A) \\ \varphi \mapsto T_{h(f_A)}\varphi = h(f_A(m))\varphi(m). \end{cases} \tag{4.2}$$

Using (4.2), the next theorem follows from the previous facts.

Theorem 4.6. *Assume $A = A^*$. Then there is a unique map $\widetilde{\varphi}_A : Bor(\mathbb{R}) \to B(\mathcal{H})$ such that for all $f, g \in Bor(\mathbb{R})$ the following statements hold:*

(i) *$\widetilde{\varphi}_A$ is an algebraic *-homomorphism.*

(ii) *$\widetilde{\varphi}_A(f + g) = \widetilde{\varphi}_A(f) + \widetilde{\varphi}_A(g)$ (linearity).*

(iii) *$\|\widetilde{\varphi}_A(f)\|_{B(\mathcal{H})} \leq \|f\|_\infty$ (continuity).*

(iv) *If $\{f_n(x)\}_{n\in\mathbb{N}} \subset Bor(\mathbb{R})$, $f_n(x) \underset{n\to\infty}{\to} x$ for all $x \in \mathbb{R}$, and $|f_n(x)| \leq |x|$ for all $n \in \mathbb{N}$, then for any $\psi \in D(A)$, $\lim_{n\to\infty} \widetilde{\varphi}_A(f_n)\psi = A\psi$.*

(v) *If $f_n(x) \underset{n\to\infty}{\to} f(x)$ for all $x \in \mathbb{R}$ and $f_n(x)$ are uniformly bounded w.r.t. (x, n), then $\widetilde{\varphi}_A(f_n) \underset{n\to\infty}{\to} \widetilde{\varphi}_A(f)$ strongly.*

Moreover, $\widetilde{\varphi}_A$ has the following additional properties:

(vi) *If $A\psi = \lambda\psi$, then $\widetilde{\varphi}_A(f)\psi = f(\lambda)\psi$.*

(vii) *If $f \geq 0$, then $\widetilde{\varphi}_A(f) \geq 0$.*

Again, formally, $\widetilde{\varphi}_A(f) = f(A)$.

Now we are in position to introduce the spectral decomposition for unbounded self-adjoint operators.

Definition 4.7. The family $\{P_\Omega\}_{\Omega\in\mathcal{B}_\mathbb{R}}$ of bounded operators in $\mathcal{H}$ is called a *projection-valued measure (p.v.m.)* if the following conditions (i)–(iv) hold:

(i) P_Ω is an orthogonal projection for all $\Omega \in \mathcal{B}_\mathbb{R}$.

(ii) $P_\emptyset = 0$, $P_{(-\infty,\infty)} = I$.

(iii) If $\Omega = \cup_{k=1}^\infty \Omega_k$, $\Omega_i \cap \Omega_j = \emptyset$ for $i \neq j$, then $P_\Omega = \mathrm{s} - \lim_{N\to\infty} \sum_{k=1}^N P_{\Omega_k}$.

(iv) $P_{\Omega_1} P_{\Omega_2} = P_{\Omega_1 \cap \Omega_2}$.

It is easy to see that $\{\chi_\Omega(A)\}$ is a p.v.m. From now on $\{P_\Omega(A)\}$ will always denote $\{\chi_\Omega(A)\}$. In analogy to the case of bounded operators we then define $g(A)$ for any $g \in Bor(\mathbb{R})$ by

$$(h, g(A)h) = \int_{-\infty}^{\infty} g(\lambda)\, d(h, P_\lambda(A)h), \quad h \in \mathcal{H}, \tag{4.3}$$

where $d(h, P_\lambda(A)h)$ in (4.3) denotes integration with respect to the measure $(h, P_\Omega(A)h)$. One can show that the map $g \mapsto g(A)$ coincides with the map $g \mapsto \widetilde{\varphi}_A(g)$ in Theorem 4.6.

At this point we are ready to define $g(A)$ for unbounded functions g. First we introduce the domain of the operator $g(A)$ as follows:

$$D(g(A)) = \left\{ h \in \mathcal{H} \,\middle|\, \int_{-\infty}^{\infty} |g(\lambda)|^2\, d(h, P_\lambda(A)h) < \infty \right\}.$$

One observes that $\overline{D(g(A))} = \mathcal{H}$. Then $g(A)$ is defined by

$$(h, g(A)h) = \int_{-\infty}^{\infty} g(\lambda)\, d(h, P_\lambda(A)h), \quad h \in D(g(A)).$$

We write symbolically,

$$g(A) = \int_{\sigma(A)} g(\lambda)\, dP_\lambda(A).$$

Summarizing, one has the following result:

Theorem 4.8. *([3], Thm. VII.6.)*
There is a one-to-one correspondence between self-adjoint operators A and projection-valued measures $\{P_\Omega\}_{\Omega \in \mathcal{B}_\mathbb{R}}$ in $\mathcal{H}$ given by

$$A = \int_{-\infty}^{\infty} \lambda\, dP_\lambda.$$

If g is a real-valued Borel function on $\mathbb{R}$, then

$$g(A) = \int_{-\infty}^{\infty} g(\lambda)\, dP_\lambda(A),$$
$$D(g(A)) = \left\{ h \in \mathcal{H} \,\middle|\, \int_{-\infty}^{\infty} |g(\lambda)|^2\, d(h, P_\lambda(A)h) < \infty \right\}$$

is self-adjoint. If g is bounded, $g(A)$ coincides with $\widetilde{\varphi}_A(g)$ in Theorem 4.6.

5 More about spectral projections

Definition 5.1. Let$\{P_\Omega\}_{\Omega\in\mathcal{B}_\mathbb{R}}$ be a p.v.m. in $\mathcal{H}$. One defines

$$P_\lambda = P_{(-\infty,\lambda]}, \quad \lambda \in \mathbb{R}. \tag{5.1}$$

If $\{P_\Omega(A)\}_{\Omega\in\mathcal{B}_\mathbb{R}}$ is a p.v.m. associated with the self-adjoint operator A, we will write

$$P_\lambda(A) = P_{(-\infty,\lambda]}(A).$$

Definition 5.2. Assume $A = A^*$. Then $\{P_\lambda(A)\}_{\lambda\in\mathbb{R}}$ is called the *spectral family* of A.

P_λ in (5.1) has the following properties:

(i) $P_\lambda P_\mu = P_{\min(\lambda,\mu)}$, implying $P_\lambda \le P_\mu$ if $\lambda \le \mu$.

(ii) $\mathrm{s}-\lim_{\varepsilon\downarrow 0} P_{\lambda+\varepsilon} = P_\lambda$ (right continuity).

(iii) $\mathrm{s}-\lim_{\lambda\downarrow -\infty} P_\lambda = 0$, $\mathrm{s}-\lim_{\lambda\uparrow\infty} P_\lambda = I$.

The following formula is useful. It provides a way of computing the spectral projections of a self-adjoint operator in terms of its resolvent:

Theorem 5.3. *([1], Thm. X.6.1 and Thm. XII.2.10.)*
Assume $A = A^*$ and let (a, b) be an open interval. Then, in the strong operator topology,

$$P_{(a,b)} = \mathrm{s}-\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0} \frac{1}{2\pi i} \int_{a+\delta}^{b-\delta} (R(\mu + i\varepsilon, A) - R(\mu - i\varepsilon, A))\, d\mu.$$

6 An illustrative example

Most of the material of this section is taken from [2], Sect. XVI.7.
We study the following operator A in $L^2(\mathbb{R})$:

$$\begin{aligned} D(A) &= \{g \in L^2(\mathbb{R}) \,|\, g \in AC_{loc}(\mathbb{R}),\, g' \in L^2(\mathbb{R})\} = H^{2,1}(\mathbb{R}), \\ Af &= if', \quad f \in D(A). \end{aligned}$$

Lemma 6.1. *A is self-adjoint, $A = A^*$, and $\sigma(A) = \mathbb{R}$.*

Lemma 6.2. *The map $\mathcal{F} : L^2(\mathbb{R}) \to L^2(\mathbb{R})$,*

$$\begin{aligned} (\mathcal{F}f)(t) &= \mathrm{s} - \lim_{R\to\infty} \frac{1}{\sqrt{2\pi}} \int_{-R}^{R} e^{-its} f(s)\, ds \\ &= \frac{d}{dt} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{e^{-its} - 1}{-is} f(s)\, ds \;\; a.e.,\; f \in L^2(\mathbb{R}) \end{aligned} \tag{6.1}$$

is unitary (the Fourier transform in $L^2(\mathbb{R})$). Moreover,

$$A = \mathcal{F} M \mathcal{F}^{-1},$$

where M is defined by

$$(Mf)(t) = tf(t), \quad f \in D(M) = \{g \in L^2(\mathbb{R}) \,|\, tg \in L^2(\mathbb{R})\}.$$

One can get an explicit formula for the spectral projections of this operator. (In Lemma 6.3, "$p.v. \int$" denotes the principal value of an integral.)

Lemma 6.3.

$$(P_\lambda(A)f)(t) = \frac{1}{2} f(t) + \frac{1}{2\pi i} p.v. \int_{\mathbb{R}} \frac{e^{i\lambda(s-t)}}{(s-t)} f(s)\, ds, \quad f \in C_0^\infty(\mathbb{R}),$$

or

$$(P_\lambda(A)f)(t) = \frac{1}{2} f(t) - \frac{1}{2\pi i} e^{-i\lambda t} \frac{d}{dt} \int_{\mathbb{R}} e^{i\lambda s} f(s) \ln\left|1 - \frac{t}{s}\right| ds \; a.e., \quad f \in L^2(\mathbb{R})$$

(the Hilbert transform in $L^2(\mathbb{R})$). Thus, for $-\infty < a < b < \infty$,

$$\begin{aligned} (P_{(a,b]}(A)f)(t) &= (P_{(a,b)}(A)f)(t) \\ &= \frac{1}{2\pi} \int_{\mathbb{R}} \frac{e^{i(s-t)b} - e^{i(s-t)a}}{i(s-t)} f(s)\, ds \; a.e., \quad f \in L^2(\mathbb{R}). \end{aligned}$$

Proof. Let

$$\chi_\lambda = \chi_{(-\infty,\lambda]}(t) = \begin{cases} 1, & t \in (-\infty, \lambda], \\ 0, & t \in (\lambda, \infty). \end{cases}$$

Since $P_\lambda(A) = \mathcal{F}\chi_\lambda(\cdot)\mathcal{F}^{-1}$, one obtains

$$(P_\lambda(A)f)(t) = \mathcal{F}(\chi_\lambda(\cdot)\mathcal{F}^{-1}f)(t) = (\mathcal{F}\chi_\lambda * f)(t).$$

A computation of the distribution $\mathcal{F}\chi_\lambda$ then yields,

$$(\mathcal{F}\chi_\lambda)(x) = e^{i\lambda x}\left[\frac{1}{2}\delta(x) - \frac{i}{2\pi}p.v.\frac{1}{x}\right].$$

Hence,

$$\begin{aligned} (P_\lambda(A)f)(t) &= \int_{\mathbb{R}} e^{i\lambda(s-t)}\left[\frac{1}{2}\delta(s-t) - \frac{i}{2\pi}p.v.\frac{1}{s-t}\right] f(s)\,ds \\ &= \frac{1}{2}f(t) + \frac{1}{2\pi}p.v.\int_{\mathbb{R}} \frac{e^{i\lambda(s-t)}}{i(s-t)} f(s)\,ds, \quad f \in C_0^\infty(\mathbb{R}), \end{aligned}$$

or

$$(P_\lambda(A)f)(t) = \frac{1}{2}f(t) - \frac{1}{2\pi i}e^{-i\lambda t}\frac{d}{dt}\int_{\mathbb{R}} e^{i\lambda s} f(s) \ln\left|1 - \frac{t}{s}\right| ds \quad a.e., \quad f \in L^2(\mathbb{R}).$$

□

One can also get an explicit formula for the resolvent of this operator.

Lemma 6.4. *Let* $t \in \mathbb{R}$. *Then*

$$((A - zI)^{-1}g)(t) = \begin{cases} i\int_t^\infty e^{-iz(t-s)} g(s)\,ds, & Im(z) > 0, \\ -i\int_{-\infty}^t e^{-iz(t-s)} g(s)\,ds, & Im(z) < 0, \end{cases} \quad g \in L^2(\mathbb{R}).$$

7 Spectra of self-adjoint operators

Now we will give some characterizations of spectra of self-adjoint operators in terms of their spectral families. Throughout this section we fix a separable complex Hilbert space $\mathcal{H}$.

Theorem 7.1. *([4], Thm. 7.22.)*
Assume $A = A^*$ and let $P_\lambda(A)$ be the spectral family of A. Then the following conditions (i)–(iii) are equivalent:

(i) $s \in \sigma(A)$.

(ii) *There exists a sequence* $\{f_n\}_{n\in\mathbb{N}} \subset D(A)$ *with* $\liminf_{n\to\infty} \|f_n\| > 0$ *and* $\mathrm{s}-\lim_{n\to\infty}(s-A)f_n = 0$.

(iii) $P_{s+\varepsilon}(A) - P_{s-\varepsilon}(A) \neq 0$ *for every* $\varepsilon > 0$.

Proof. The equivalence of (i) and (ii) is obvious if we recall that $z \in \rho(A)$ is equivalent to the existence of a $C > 0$ such that $\|(z-A)f\| \geq C\|f\|$ for all $f \in D(A)$.
(ii) $\Rightarrow$ (iii): Assume (iii) does not hold. Then there exists an $\varepsilon > 0$ such that $P_{s+\varepsilon}(A) - P_{s-\varepsilon}(A) = 0$. Hence,

$$\begin{aligned}\|(s-A)f_n\|^2 &= ((s-A)f_n, (s-A)f_n) = (f_n, (s-A)^2 f_n)\\ &= \int_{\sigma(A)} |s-\lambda|^2 \, d(f_n, P_\lambda(A)f_n) \geq \varepsilon^2 \int_{\sigma(A)} d(f_n, P_\lambda(A)f_n) = \varepsilon^2 \|f_n\|^2 .\end{aligned}$$

Thus,

$$(s-A)f_n \stackrel{s}{\not\to} 0 \ \text{ as } n \to \infty.$$

(iii) $\Rightarrow$ (ii): Choose $\{f_n\}_{n\in\mathbb{N}}$ such that $f_n \in Ran(P_{s+\frac{1}{n}}(A) - P_{s-\frac{1}{n}}(A))$ and $\|f_n\| = 1$. Then

$$\|(s-A)f_n\|^2 = \int_{\sigma(A)} |s-\lambda|^2 \, d(f_n, P_\lambda(A)f_n) \leq \frac{1}{n^2}\|f_n\|^2 \to 0 \ \ as \ \ n \to \infty.$$

□

Definition 7.2. Assume $A = A^*$. Then the *point spectrum* $\sigma_p(A)$ of A is the set of all eigenvalues of A.

(Actually, this definition does not require self-adjointness of A but works generally for densely defined, closed, linear operators.)

Theorem 7.3. *([4], Thm. 7.23.)*
Assume $A = A^*$ and let $P_\lambda(A)$ be the spectral family of A. Let A_0 be a restriction of A such that $\overline{A_0} = A$. Then the following conditions (i)–(iv) are equivalent:

(i) $s \in \sigma_p(A)$.

(ii) *There exists a Cauchy sequence* $\{f_n\}_{n\in\mathbb{N}} \subset D(A)$ *with* $\lim_{n\to\infty} \|f_n\| > 0$ *and* $\mathrm{s}-\lim_{n\to\infty}(s-A)f_n = 0$.

(iii) *There exists a Cauchy sequence* $\{g_n\}_{n\in\mathbb{N}} \subset D(A_0)$ *with* $\lim_{n\to\infty} \|g_n\| > 0$ *and* $\mathrm{s}-\lim_{n\to\infty}(s-A_0)g_n = 0$.

(iv) $P_s(A) - P_{s_-}(A) \neq 0$.

Proof. (i) $\Rightarrow$ (ii) is obvious.
(ii) $\Rightarrow$ (iii): Choose $\{g_n\}_{n\in\mathbb{N}} \subset D(A_0)$ such that $\|g_n - f_n\| < \frac{1}{n}$ and $\|A_0 g_n - Af_n\| < \frac{1}{n}$.
(iii) $\Rightarrow$ (i): Take $f = \lim_{n\to\infty} g_n \in D(A)$, then $(s-A)f = 0$.
(i) $\Rightarrow$ (iv):

$$0 = \|(s-A)f\|^2 = \int_{\sigma(A)} |s-\lambda|^2 \, d(f, P_\lambda(A)f).$$

Hence,

$$P_{s_-}(A)f = \lim_{\lambda\to-\infty} P_\lambda(A)f = 0, \quad P_s(A)f = \lim_{\lambda\to\infty} P_\lambda(A)f = f.$$

Thus,

$$(P_s(A) - P_{s_-}(A))f = f.$$

(iv) $\Rightarrow$ (i): Pick any $0 \neq f \in Ran(P_s(A) - P_{s_-}(A))$. Then

$$\|(s-A)f\|^2 = \int_{\sigma(A)} |s-\lambda|^2 \, d(f, P_\lambda(A)f) = 0.$$

$\square$

Definition 7.4. Assume $A = A^*$. Then the *essential spectrum* $\sigma_e(A)$ of A is the set of those points of $\sigma(A)$ that are either accumulation points of $\sigma(A)$ or isolated eigenvalues of infinite multiplicity. (We note that geometric multiplicities and algebraic multiplicities of eigenvalues coincide since A is self-adjoint (normal).)

Theorem 7.5. *([4], Thm. 7.24.)*
Assume $A = A^*$ *and let* $P_\lambda(A)$ *be the spectral family of* A*. Let* A_0 *be a restriction of* A *such that* $\overline{A_0} = A$*. Then the following conditions (i)–(iv) are equivalent:*

(i) $s \in \sigma_e(A)$.

(ii) *There exists a sequence* $\{f_n\}_{n\in\mathbb{N}} \subset D(A)$ *with* $\liminf_{n\to\infty} \|f_n\| > 0$, $\mathrm{w}-\lim_{n\to\infty} f_n = 0$, *and* $\mathrm{s}-\lim_{n\to\infty}(s-A)f_n = 0$.

(iii) *There exists a sequence* $\{g_n\}_{n\in\mathbb{N}} \subset D(A_0)$ *with* $\liminf_{n\to\infty} \|g_n\| > 0$, $\mathrm{w}-\lim_{n\to\infty} g_n = 0$, *and* $\mathrm{s}-\lim_{n\to\infty}(s-A_0)g_n = 0$.

(iv) $\dim(Ran(P_{s+\varepsilon}(A) - P_{s-\varepsilon}(A))) = \infty$ *for every* $\varepsilon > 0$.

8 One-parameter unitary groups

In the following let $\mathcal{H}$ be a complex separable Hilbert space.

Definition 8.1. A family of operators $\{B(t)\}_{t\in\mathbb{R}} \subset B(\mathcal{H})$ is called a *one-parameter group* if the following two conditions hold:

(i) $B(0) = I$.

(ii) $B(s)B(t) = B(s+t)$ for all $s, t \in \mathbb{R}$.

$\{B(t)\}_{t\in\mathbb{R}}$ is called a *unitary group* if, in addition to conditions (i) and (ii), $B(t)$ is a unitary operator for all $t \in \mathbb{R}$.
Moreover, $\{B(t)\}_{t\in\mathbb{R}}$ is called *strongly continuous* if $t \mapsto B(t)f$ is continuous in $\|\cdot\|_H$ for all $f \in \mathcal{H}$.

Definition 8.2. Let $\{B(t)\}_{t\in\mathbb{R}}$ be a one-parameter group. The operator A defined by

$$D(A) = \left\{ g \in \mathcal{H} \,\middle|\, \mathrm{s}-\lim_{t\to 0}\frac{1}{t}(B(t)-I)g \quad exists \right\},$$
$$Af = \mathrm{s}-\lim_{t\to 0}\frac{1}{t}(B(t)-I)f, \quad f \in D(A)$$

is called the *infinitesimal generator* of $\{B(t)\}_{t\in\mathbb{R}}$.

The following theorems show a connection between self-adjoint operators and strongly continuous one-parameter unitary groups.

Theorem 8.3. *([4], Thm. 7.37.)*
Assume $A = A^*$ and let $P_\lambda(A)$ be the spectral family of A. Define

$$U(t) = e^{itA} = \int_{\sigma(A)} e^{it\lambda}\, dP_\lambda(A), \quad t \in \mathbb{R}.$$

Then $\{U(t)\}_{t\in\mathbb{R}}$ is a strongly continuous unitary group with infinitesimal generator iA. Moreover, $U(t)f \in D(A)$ holds for all $f \in D(A)$, $t \in \mathbb{R}$.

Theorem 8.4. *([4], Thm. 7.38; Stone's theorem.)*
Let $\{U(t)\}_{t\in\mathbb{R}}$ be a strongly continuous unitary group. Then there exists a uniquely determined self-adjoint operator A such that $U(t) = e^{itA}$ for all $t \in \mathbb{R}$.
In the case where $\mathcal{H}$ is separable (as assumed throughout this section for simplicity), the assumption of strong continuity can be replaced by weak measurability, that is, it suffices to require that for all $f, g \in \mathcal{H}$, the function

$$(f, U(\cdot)g) : \mathbb{R} \to \mathbb{C}, \quad t \mapsto (f, U(t)g)$$

is measurable (with respect to Lebesgue measure on $\mathbb{R}$).

9 Trace class and Hilbert–Schmidt operators

Definition 9.1. $T : H_1 \to H_2$ is *compact* if for all bounded sequences $\{f_n\}_{n\in\mathbb{N}} \subset D(T)$ there exists a subsequence $\{f_{n_k}\}_{k\in\mathbb{N}} \subseteq \{f_n\}_{n\in\mathbb{N}}$ for which $\{Tf_{n_k}\}$ converges in H_2 as $k \to \infty$. The linear space of compact operators from $\mathcal{H}_1$ into $\mathcal{H}_2$ is denoted by $B_\infty(\mathcal{H}_1, \mathcal{H}_2)$ (and by $B_\infty(\mathcal{H})$ if $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}$).

One has, $B_\infty(\mathcal{H}_1, \mathcal{H}_2) \subseteq B(\mathcal{H}_1, \mathcal{H}_2)$. If T is compact, then T^*T is compact, self-adjoint, and non-negative in H_1.

In the following we denote

$$|T| = \sqrt{T^*T}.$$

(One chooses the square root branch such that $\sqrt{x} > 0$ for $x > 0$.)

Definition 9.2. Let T be a compact operator. Then the non-zero eigenvalues of $|T|$ are called the *singular values (singular numbers, s-numbers)* of T.

Notation: $\{s_j(T)\}_{j\in J}$, $J \subseteq \mathbb{N}$ an appropriate (finite or countably infinite) index set, denotes the non-increasing sequence of s-numbers of T. This sequence is built by taking multiplicities of the eigenvalues $s_j(T)$ of $|T|$ into account. (Since $|T|$ is self-adjoint, algebraic and geometric multiplicites of all its eigenvalues coincide.)

Definition 9.3. Let $B_p(\mathcal{H}_1, \mathcal{H}_2)$ denote the following subset of the set of compact operators from $\mathcal{H}_1$ into $\mathcal{H}_2$,

$$B_p(\mathcal{H}_1, \mathcal{H}_2) = \left\{ T \in B_\infty(\mathcal{H}_1, \mathcal{H}_2) \,\middle|\, \sum_{j\in J} (s_j(T))^p < \infty \right\}, \quad p \in (0, \infty).$$

(If $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}$, we write $B_p(\mathcal{H})$ for simplicity.)

Definition 9.4. $B_2(\mathcal{H}_1, \mathcal{H}_2)$ is called the *Hilbert–Schmidt class.*

One introduces the norm,

$$\|T\|_{B_2(\mathcal{H}_1,\mathcal{H}_2)} = \left(\sum_{j\in J} (s_j(T))^2 \right)^{\frac{1}{2}} = \|T\|_2\,, \quad T \in B_2(\mathcal{H}_1, \mathcal{H}_2).$$

Definition 9.5. $B_1(\mathcal{H}_1, \mathcal{H}_2)$ is called the *trace class.*

One introduces the norm,

$$\|T\|_{B_1(\mathcal{H}_1,\mathcal{H}_2)} = \sum_{j\in J} s_j(T) = \|T\|_1\,, \quad T \in B_1(\mathcal{H}_1, \mathcal{H}_2).$$

Lemma 9.6. *([4], Thm. 7.10(a).)*
$T \in B_2(\mathcal{H}_1, \mathcal{H}_2)$ if and only if there exists an orthonormal basis $\{e_\alpha\}_{\alpha\in\mathcal{A}}$ in $\mathcal{H}_1$ such that $\sum_{\alpha\in\mathcal{A}} \|Te_\alpha\|^2 < \infty$.

Proof. Let $\{f_j\}_{j\in J}$ be the orthonormal eigenelements of $|T|$ that correspond to the non-zero eigenvalues $s_j(T)$ and let $\{g_\alpha\}_{\alpha\in\mathcal{A}}$ be an o.n.b. in $Ker(T)$. Then $\{f_j\}_{j\in J} \cup \{g_\alpha\}_{\alpha\in\mathcal{A}}$ is an o.n.b. in $\mathcal{H}$ and

$$\sum_{j\in J} \|Tf_j\|^2 + \sum_{\alpha\in\mathcal{A}} \|Tg_\alpha\|^2 = \sum_{j\in J} \||T|\, f_j\|^2 = \sum_{j\in J} (s_j(T))^2 < \infty.$$

□

If $T \in B_2(\mathcal{H}_1, \mathcal{H}_2)$ one can show ([4], Thm. 7.10(a) and [4], p. 136) that

$$\|T\|_2 = \left(\sum_{\alpha \in \mathcal{A}} \|Te_\alpha\|^2 \right)^{1/2} \tag{9.1}$$

is independent of the choice of the orthonormal basis $\{e_\alpha\}_{\alpha \in \mathcal{A}}$ in H_1.

The following two results will permit us to define the trace of a trace class operator.

Theorem 9.7. *([4], Thm. 7.9.)*
Let $p, q, r > 0$ with $\frac{1}{p} + \frac{1}{q} = \frac{1}{r}$. Then $T \in B_r(\mathcal{H}, \mathcal{H}_1)$ if and only if there exist $T_1 \in B_p(\mathcal{H}, \mathcal{H}_2)$ and $T_2 \in B_q(\mathcal{H}_2, \mathcal{H}_1)$ (with an arbitrary Hilbert space $\mathcal{H}_2$) for which $T = T_2 T_1$. The operators can be chosen such that $\|T\|_r = \|T_1\|_p \|T_2\|_q$.

Corollary 9.8. *$T \in B_1(\mathcal{H}, \mathcal{H}_1)$ if and only if there exist $T_1 \in B_2(\mathcal{H}, \mathcal{H}_2)$ and $T_2 \in B_2(\mathcal{H}_2, \mathcal{H}_1)$ such that $T = T_2 T_1$.*

In the following let $\{e_\alpha\}_{\alpha \in \mathcal{A}}$ be an o.n.b. in H. We will prove that $\sum_{\alpha \in \mathcal{A}} (e_\alpha, Te_\alpha)$ converges absolutely if $T \in B_1(\mathcal{H})$. Since T can be decomposed into $T = T_2 T_1$ with $T_1, T_2 \in B_2(\mathcal{H})$, one obtains

$$\begin{aligned} \sum_{\alpha \in \mathcal{A}} |(e_\alpha, Te_\alpha)| &= \sum_{\alpha \in \mathcal{A}} |(e_\alpha, T_2 T_1 e_\alpha)| \\ &= \sum_{\alpha \in \mathcal{A}} |(T_2^* e_\alpha, T_1 e_\alpha)| \le \left(\sum_{\alpha \in \mathcal{A}} \|T_2^* e_\alpha\|^2 \right)^{1/2} \left(\sum_{\alpha \in \mathcal{A}} \|T_1 e_\alpha\|^2 \right)^{1/2} < \infty. \end{aligned} \tag{9.2}$$

Next, we will prove that $\sum_{\alpha \in \mathcal{A}} (e_\alpha, Te_\alpha)$ is well-defined in the sense that it does not depend on the choice of the o.n.b. $\{e_\alpha\}_{\alpha \in \mathcal{A}}$. Take $T_1 \in B_2(\mathcal{H}, \mathcal{H}_2)$, $T_2 \in B_2(\mathcal{H}_2, \mathcal{H}_1)$ such that $T = T_2 T_1$. Let $\{e_\alpha\}_{\alpha \in \mathcal{A}} \subset \mathcal{H}$ be an o.n.b. in $\mathcal{H}$ and $\{f_\beta\}_{\beta \in \mathcal{B}} \subset \mathcal{H}_2$ be an o.n.b. in $\mathcal{H}_2$.

Using the fact that $T_2^* e_\alpha = \sum_{\beta \in \mathcal{B}} (T_2^* e_\alpha, f_\beta) f_\beta$, one obtains

$$\begin{aligned} \sum_{\alpha \in \mathcal{A}} (e_\alpha, Te_\alpha) &= \sum_{\alpha \in \mathcal{A}} (T_2^* e_\alpha, T_1 e_\alpha) = \sum_{\alpha \in \mathcal{A}} \sum_{\beta \in \mathcal{B}} (T_2^* e_\alpha, f_\beta)(f_\beta, T_1 e_\alpha) \\ &= \sum_{\beta \in \mathcal{B}} \sum_{\alpha \in \mathcal{A}} (T_1^* f_\beta, e_\alpha)(e_\alpha, T_2 f_\beta) = \sum_{\beta \in \mathcal{B}} (T_1^* f_\beta, T_2 f_\beta) = \sum_{\beta \in \mathcal{B}} (f_\beta, T_1 T_2 f_\beta) \\ &= \sum_{\beta \in \mathcal{B}} (f_\beta, T f_\beta). \end{aligned} \tag{9.3}$$

Since we took arbitrary bases, the statement is proved.

These facts permit one to introduce the following definition.

Definition 9.9. Let $T \in B_1(\mathcal{H})$ and $\{e_\alpha\}_{\alpha\in\mathcal{A}}$ be an o.n.b. in $\mathcal{H}$. Then $tr(T) = \sum_{\alpha\in\mathcal{A}}(e_\alpha, Te_\alpha)$ is called the *trace* of T.

By (9.2) the trace of trace class operators is absolutely convergent and by (9.3) the definition of the trace is independent of the orthonormal basis chosen (cf. also (9.1)).

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Von Neumann's Theory of Self-Adjoint Extensions of Symmetric Operators and some of its Refinements due to Friedrichs and Krein

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- Self-adjoint extensions of symmetric operators in a Hilbert space

- The Friedrichs extension of semibounded operators in a Hilbert space

- Krein's formula for self-adjoint extensions in the case of finite deficiency indices

1 Self-adjoint extensions of symmetric operators in a Hilbert space

In the following, $\mathcal{H}$ denotes a separable complex Hilbert space with scalar product $(\cdot,\cdot)$ linear in the second entry. The Banach space of all bounded linear operators on $\mathcal{H}$ will be denoted by $B(\mathcal{H})$.

Definition 1.1. $T : Dom(T) \to \mathcal{H},\ Dom(T) \subseteq \mathcal{H}$ is called *closed* if the following holds: If $\{f_n\}_{n\in\mathbb{N}}$ is a sequence in $Dom(T)$ that is convergent in $\mathcal{H}$ as $n \to \infty$ and the sequence $\{Tf_n\}_{n\in\mathbb{N}}$ is convergent in $\mathcal{H}$ as $n \to \infty$ then we have

$$\lim_{n\to\infty} f_n \in Dom(T) \ \ and \ \ T(\lim_{n\to\infty} f_n) = \lim_{n\to\infty} Tf_n.$$

An operator S is called *closable* if it has a closed extension.

Every closable operator S has a unique smallest closed extension which is called the *closure* of S and denoted by $\overline{S}$. In fact, if S is densely defined, S is closable if and only if S^* is densely defined (in which case one obtains $\overline{S} = S^{**}$, where, in obvious notation, $S^{**} = (S^*)^*$).

Definition 1.2. (i) Let T be densely defined in $\mathcal{H}$. Then T^* is called the *adjoint* of T if

$$\begin{aligned} Dom(T^*) = \{g \in \mathcal{H} \,|\, &\text{there exists an } h_g \in \mathcal{H} \text{ such that } (h_g, f) = (g, Tf) \text{ for} \\ &\text{all } f \in Dom(T)\}, \\ T^*g = h_g&. \end{aligned}$$

(ii) An operator A in $\mathcal{H}$ is called *symmetric* if A is densely defined and $A \subseteq A^*$.
(iii) A densely defined operator B in $\mathcal{H}$ is called *self-adjoint* if $B = B^*$.

In particular, A is symmetric if

$$(Af, g) = (f, Ag) \ \text{ for all } f, g \in Dom(A).$$

Since the adjoint T^* of any densely defined operator T is closed, any symmetric operator A is closable and its closure $\overline{A}$ is still a symmetric operator. In particular,

$$A \subseteq \overline{A} = A^{**} \subseteq A^* = (\overline{A})^*.$$

Thus, in the context of this manuscript, one can without loss of generality restrict one's attention to closed symmetric operators.

Theorem 1.3. *([4], Thm. VIII.3; the basic criterion for self-adjointness) Let A be a symmetric operator in $\mathcal{H}$. Then the following statements (a)–(c) are equivalent:*

(i) A is self-adjoint.

(ii) A is closed and $Ker(A^* \pm iI) = \{0\}$.

(iii) $Ran(A \pm iI) = \mathcal{H}$.

Proof. (i) implies (ii): Since A is self-adjoint it is of course a closed operator. Next, suppose that there is a $\varphi \in Dom(A^*) = Dom(A)$ so that $A^*\varphi = i\varphi$. Then $A\varphi = i\varphi$ and

$$-i(\varphi, \varphi) = (i\varphi, \varphi) = (A\varphi, \varphi) = (\varphi, A^*\varphi) = (\varphi, A\varphi) = i(\varphi, \varphi).$$

Thus, $\varphi = 0$. A similar proof shows that the equation $A^*\varphi = -i\varphi$ can have no nontrivial solutions.
(ii) implies (iii): Suppose that (ii) holds. Since $A^*\varphi = -i\varphi$ has no nontrivial solutions, $Ran(A - iI)$ must be dense. Otherwise, if $\psi \in Ran(A - iI)^\perp$, we would have $((A - iI)\varphi, \psi) = 0$ for all $\varphi \in Dom(A)$, so $\psi \in Dom(A^*)$ and $(A - iI)^*\psi = (A^* + iI)\psi = 0$, which is impossible since $A^*\psi = -i\psi$ has no nontrivial solutions. (Reversing this last argument we can show that if $Ran(A-iI)$ is dense, then $Ker(A^*+iI) = \{0\}$.) Since $Ran(A-iI)$ is dense, we only need to prove it is closed to conclude that $Ran(A - iI) = \mathcal{H}$. But for all $\varphi \in Dom(A)$

$$\|(A - iI)\varphi\|^2 = \|A\varphi\|^2 + \|\varphi\|^2 .$$

Thus, if $\varphi_n \in Dom(A)$ and $(A - iI)\varphi_n \to \psi_0$, we conclude that φ_n converges to some vector φ_0 and $A\varphi_n$ converges too. Since A is closed, $\varphi_0 \in Dom(A)$ and $(A - iI)\varphi_0 = \psi_0$. Thus, $Ran(A - iI)$ is closed, so $Ran(A - iI) = \mathcal{H}$. Similarly, one proves that $Ran(A + iI) = \mathcal{H}$.
(iii) implies (i): Let $\varphi \in Dom(A^*)$. Since $Ran(A - iI) = \mathcal{H}$, there is an $\eta \in Dom(A)$ so that $(A - iI)\eta = (A^* - iI)\varphi$. $Dom(A) \subset Dom(A^*)$, so $\varphi - \eta \in Dom(A^*)$ and

$$(A^* - iI)(\varphi - \eta) = 0.$$

Since $Ran(A + iI) = \mathcal{H}$, $Ker(A^* - iI) = \{0\}$, so $\varphi = \eta \in Dom(A)$. This proves that $Dom(A^*) = Dom(A)$, so A is self-adjoint. □

Next, we recall the definition of the field of regularity, the resolvent set, and the spectrum of a closed operator T in $\mathcal{H}$.

Definition 1.4. (i) Let T be a closed operator with a dense domain $Dom(T)$ in the Hilbert space $\mathcal{H}$. The complex number z is called a *regular-type point* of the operator T, if the following inequality is satisfied for all $f \in Dom(T)$,

$$\|(T - zI)f\| > k_z\|f\|, \tag{1.1}$$

where $k_z > 0$ and independent of f. The set of all points of regular-type of T is called the *field of regularity* of T and denoted by $\pi(T)$.
(ii) If for a given $z \in \pi(T)$ one has $(T - zI)Dom(T) = \mathcal{H}$, then z is called a *regularity point* of the operator T. The set of all regularity points of the operator T is called the *resolvent set* and denoted by $\rho(T)$.
(iii) The *spectrum* $\sigma(T)$ of a densely defined closed operator T is defined by

$$\sigma(T) = \{\lambda \in \mathbb{C} | (T - \lambda I)^{-1} \notin B(\mathcal{H})\}. \tag{1.2}$$

One then has the following:

$$\begin{aligned} &\rho(T) \subseteq \pi(T) \textit{ and both sets are open.} \\ &z \in \pi(T) \text{ implies that } Ran(T - zI) \textit{ is closed.} \\ &z \in \rho(T) \text{ implies that } Ran(T - zI) = \mathcal{H}. \\ &\sigma(T) = \mathbb{C} \backslash \rho(T). \end{aligned}$$

Theorem 1.5. *([5], Thm. X.1.)*
Let A be a closed symmetric operator in a Hilbert space $\mathcal{H}$. Then

(i)
- *(a) (a) $n_+(A) = dim\ [Ker(A^* - zI)]$ is constant throughout the open upper complex half-plane.*
- *(b) $n_-(A) = dim\ [Ker(A^* - zI)]$ is constant throughout the open lower complex half-plane.*

(ii) The spectrum of A is one of the following:
- *(a) the closed upper complex half-plane if $n_+(A) = 0$, $n_-(A) > 0$,*
- *(b) the closed lower complex half-plane if $n_-(A) = 0$, $n_+(A) > 0$,*
- *(c) the entire complex plane if $n_\pm(A) > 0$,*
- *(d) a subset of the real axis if $n_\pm(A) = 0$.*

(iii) A is self-adjoint if and only if case(2d) holds.

(iv) A is self-adjoint if and only if $n_{\pm}(A) = 0$*.*

Proof. Let $z = x + iy$, $y \neq 0$. Since A is symmetric,

$$\|(A - zI)\varphi\|^2 \geq y^2 \|\varphi\|^2 \tag{1.3}$$

for all $\varphi \in Dom(A)$. From this inequality and the fact that A is closed, it follows that $Ran(A - zI)$ is a closed subspace of $\mathcal{H}$. Moreover,

$$Ker(A^* - zI) = Ran(A - \overline{z}I)^{\perp}. \tag{1.4}$$

We will show that if $\eta \in \mathbb{C}$ with $|\eta|$ sufficiently small, $Ker(A^* - zI)$ and $Ker(A^* - (z + \eta)I)$ have the same dimension. Let $u \in Dom(A^*)$ be in $Ker(A^* - (z+\eta)I)$ with $\|u\| = 1$. Suppose $(u, v) = 0$ for all $v \in Ker(A^* - zI)$. Then by (1.4), $u \in Ran(A - \overline{z}I)$, so there is a $\varphi \in Dom(A)$ with $(A - \overline{z})\varphi = u$. Thus,

$$\begin{aligned} 0 = ((A^* - (z + y)I)u, \varphi) &= (u, (A - \overline{z}I)\varphi) - \bar{y}(u, \varphi) \\ &= \|u\|^2 - \bar{y}(u, \varphi). \end{aligned}$$

This is a contradiction if $|\eta| < |y|$ since by (1.3), $\|\varphi\| \leq \|u\| / |y|$. Thus, for $|\eta| < |y|$, there is no $u \in Ker(A^* - (z + \eta)I)$ which is in $[Ker(A^* - zI)]^{\perp}$. A short argument shows that

$$dim[Ker(A^* - (z + \eta)I)] \leq dim[Ker(A^* - zI)].$$

The same argument shows that if $|\eta| < |y|/2$, then $dim[Ker(A^* - zI)] \leq dim[Ker(A^* - (z + \eta)I)]$, so we conclude that

$$dim[Ker(A^* - zI)] = dim[Ker(A^* - (z + \eta)I)] \quad if \ |\eta| < |y|/2.$$

Since $dim[Ker(A^* - zI)]$ is locally constant, it equals a constant in the upper complex half-plane and equals a (possibly different) constant in the lower complex half-plane. This proves (i).
It follows from (1.3) that if $z \neq 0$, $A - zI$ always has a bounded left inverse and from (1.4) that $(A - zI)^{-1}$ is defined on all of $\mathcal{H}$ if and only if $dim[Ker(A^* - \bar{z}I)] = 0$. Thus, it follows from part (i) that each of the open upper and lower

half-planes is either entirely in the spectrum of A or entirely in the resolvent set. Next, suppose, for instance, that $n_+(A) = 0$. Then

$$\{0\} = Ker(A^* - zI) = Ran(A - \bar{z}I)^\perp, \quad z \in \mathbb{C},\ \mathrm{Im}(z) > 0,$$

implies

$$Ran(A - zI) = \mathcal{H}, \quad z \in \mathbb{C},\ \mathrm{Im}(z) < 0.$$

By the closed graph theorem, this implies that $(A - zI)^{-1}$ exists and is a bounded operator defined on all of $\mathcal{H}$ for $z \in \mathbb{C}$, $\mathrm{Im}(z) < 0$. Hence, the open lower complex half-plane belongs to the resolvent set of A. By exactly the same arguments, if $n_-(A) = 0$, then the open upper complex half-plane belongs to the resolvent set of A. This, and the fact that $\sigma(A)$ is closed proves (ii).
(iii) and (iv) are restatements of Theorem 1.3. □

Corollary 1.6. *([5], p. 137.)*
If A is a closed symmetric operator that is bounded from below, that is, for some $\gamma \in \mathbb{R}$, $(A\varphi, \varphi) \geq \gamma\|\varphi\|^2$ for all $\varphi \in Dom(A)$, then dim $[Ker(A^* - zI)]$ is constant for $z \in \mathbb{C} \setminus [\gamma, \infty)$. The analogous statement holds if A is bounded from above.

Corollary 1.7. *([5], p. 137.)*
If a closed symmetric operator has at least one real number in its resolvent set, then it is self-adjoint.

Proof. Since the resolvent set is open and contains a point in the real axis, it must contain points in both lower and upper complex half-planes. The corollary now follows from part (3) of Theorem 1.5. □

The following result is a refinement of Theorem 1.5.

Theorem 1.8. *([1], p. 92, [6], p. 230.)*
If Γ is a connected subset of the field of regularity $\pi(T)$ of a densely defined closed operator T, then the dimension of the subspace $\mathcal{H} \ominus Ran(T - zI)$ is constant (i.e., independent of z) for each $z \in \Gamma$.

Since the dimensions of the kernels of $A^* - iI$ and $A^* + iI$ play an important role, it is customary to give them names.

Definition 1.9. Suppose that A is a symmetric operator in a Hilbert space $\mathcal{H}$. Let

$$K_+(A) = Ker(A^* - iI) = Ran(A + iI)^\perp,$$
$$K_-(A) = Ker(A^* + iI) = Ran(A - iI)^\perp.$$

$K_+(A)$ and $K_-(A)$ are called the *deficiency subspaces* of A. The numbers $n_\pm(A)$, given by $n_+(A) = dim(K_+(A))$ *and* $n_-(A) = dim(K_-(A))$, are called the *deficiency indices* of A.

Remark 1.10. It is possible for the deficiency indices to be any pair of nonnegative integers, and further it is possible for n_+, or n_-, or both, to be equal to infinity.

Remark 1.11. The basic idea behind the construction of self-adjoint extensions of a closed symmetric but not self-adjoint operator A is the following: Suppose B is a (proper) closed symmetric extension of A. Then,

$$A \subset B \text{ implies } A \subset B \subset B^* \subset A^*.$$

Continuing this process, one can hope to arrive at a situation where

$$A \subset B \subset C = C^* \subset B^* \subset A^*,$$

and hence C is a self-adjoint extension of A. The precise conditions under which such a construction is possible will be discussed in the remainder of this section.

Next, let $\mathcal{D}_1$ and $\mathcal{D}_2$ be two linear subspaces of $\mathcal{H}$. We will denote by $\mathcal{D}_1 + \mathcal{D}_2$ the sum of $\mathcal{D}_1$ and $\mathcal{D}_2$,

$$\mathcal{D}_1 + \mathcal{D}_2 = \{f + g \,|\, f \in \mathcal{D}_1,\, g \in \mathcal{D}_2\}.$$

If in addition $\mathcal{D}_1 \cap \mathcal{D}_2 = \{0\}$, this results in the direct sum of $\mathcal{D}_1$ and $\mathcal{D}_2$, denoted by $\mathcal{D}_1 \dotplus \mathcal{D}_2$,

$$\mathcal{D}_1 \dotplus \mathcal{D}_2 = \{f + g \,|\, f \in \mathcal{D}_1,\, g \in \mathcal{D}_2\}, \quad \mathcal{D}_1 \cap \mathcal{D}_2 = \{0\}.$$

Finally, if the two subspaces $\mathcal{D}_1$ and $\mathcal{D}_2$ are orthogonal, $\mathcal{D}_1 \perp \mathcal{D}_2$, then clearly $\mathcal{D}_1 \cap \mathcal{D}_2 = \{0\}$. In this case the direct sum of $\mathcal{D}_1$ and $\mathcal{D}_2$ is called the orthogonal direct sum of $\mathcal{D}_1$ and $\mathcal{D}_2$ and denoted by $\mathcal{D}_1 \oplus \mathcal{D}_2$,

$$\mathcal{D}_1 \oplus \mathcal{D}_2 = \{f + g \,|\, f \in \mathcal{D}_1,\, g \in \mathcal{D}_2\}, \quad \mathcal{D}_1 \perp \mathcal{D}_2.$$

Definition 1.12. Let A be a symmetric operator in a Hilbert space $\mathcal{H}$. The *Cayley transform* of A is defined by

$$V = (A - iI)(A + iI)^{-1}.$$

V is a linear operator from $Ran(A + iI)$ onto $Ran(A - iI)$.

Definition 1.13. Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be separable complex Hilbert spaces.
(i) An operator $U : \mathcal{H}_1 \to \mathcal{H}_2$ such that $Dom(U) = \mathcal{H}_1,\ Ran(U) = \mathcal{H}_2$ is called *unitary* if $\|Uf\| = \|f\|$ for all $f \in \mathcal{H}_1$.
(ii) An operator $V : \mathcal{D}_1 \to \mathcal{H}_2$ with $Dom(V) = \mathcal{D}_1$ dense in $\mathcal{H}_1$ is called *isometric* if $\|Vf\| = \|f\|$ for all $f \in \mathcal{D}_1$.

We note that U is unitary if and only if

$$U^*U = I_{\mathcal{H}_1} \text{ and } UU^* = I_{\mathcal{H}_2}, \text{ that is, if and only if } U^* = U^{-1}.$$

Similarly, V is isometric if and only if

$$V^*V = I_{\mathcal{D}_1}.$$

Moreover, the closure $\overline{V}$ of V is then also an isometric operator with domain $\mathcal{H}_1$.

Theorem 1.14. *([6], Thm. 8.2.)*
Let A be a symmetric operator in $\mathcal{H}$. Then the Cayley transform V of A is an isometric mapping from $Ran(A + iI)$ onto $Ran(A - iI)$. The range $Ran(I - V)$ is dense in $\mathcal{H}$, and $A = i(I + V)(I - V)^{-1}$. In particular, A is uniquely determined by V.

Proof. For every $g = (A + iI)f \in Ran(A + iI) = Dom(V)$ one has

$$\begin{aligned} \|Vg\|^2 &= \left\|(A - iI)(A + iI)^{-1}g\right\|^2 = \|(A - iI)f\|^2 \\ &= \|f\|^2 + \|Af\|^2 = \|(A + iI)f\|^2 = \|g\|^2 . \end{aligned}$$

Consequently, V is isometric. It is clear that $Ran(V) = Ran(A - iI)$, since $(A + iI)^{-1}$ maps $Dom(V) = Ran(A + iI)$ onto $Dom(A)$ and $(A - iI)$ maps $Dom(A)$ onto $Ran(A - iI)$. Moreover,

$$\begin{aligned} I - V &= I - (A - iI)(A + iI)^{-1} = [(A + iI) - (A - iI)](A + iI)^{-1} \\ &= 2i(A + iI)^{-1}, \\ I + V &= I + (A - iI)(A + iI)^{-1} = 2A(A + iI)^{-1}. \end{aligned}$$

In particular, $Ran(I-V) = Dom(A)$ is dense, $I-V$ is injective, and

$$A = i(I+V)(I-V)^{-1}.$$

$\square$

Theorem 1.15. *([6], Thm. 8.3.)*
An operator V on the complex Hilbert space $\mathcal{H}$ is the Cayley transform of a symmetric operator A if and only if V has the following properties:

(i) V is an isometric mapping of $Dom(V)$ onto $Ran(V)$.

(ii) $Ran(I-V)$ is dense in $\mathcal{H}$.

The symmetric operator A is given by the equality

$$A = i(I+V)(I-V)^{-1}.$$

Proof. If V is the Cayley transform of A, then V has properties (i) and (ii) by Theorem 1.14. We also infer that $A = i(I+V)(I-V)^{-1}$. Let V now be an operator with properties (i) and (ii). Then $I-V$ is injective, since the equality $Vg = g$ implies that

$$\begin{aligned}(g, f - Vf) &= (g,f) - (g, Vf) = (g,f) - (Vg, Vf)\\ &= (g,f) - (g,f) = 0 \quad \textit{for all } f \in Dom(V).\end{aligned}$$

Thus, $g \in Ran(I-V)^{\perp}$ and hence $g = 0$. Therefore, we can define an operator A by the equality

$$A = i(I+V)(I-V)^{-1}.$$

By hypothesis, $Dom(A) = Ran(I-V)$ is dense. For all $f = (I-V)f_1$ and $g = (I-V)g_1$ in $Dom(A) = Ran(I-V)$ one obtains

$$\begin{aligned}(Af, g) &= -i((I+V)(I-V)^{-1}f, g) = -i((I+V)f_1, (I-V)g_1)\\ &= -i[(f_1, g_1) + (Vf_1, g_1) - (f_1, Vg_1) - (Vf_1, Vg_1)]\\ &= -i[(Vf_1, Vg_1) + (Vf_1, g_1) - (f_1, Vg_1) - (f_1, g_1)]\\ &= i((I-V)f_1, (I+V)g_1) = i(f, (I+V)(I-V)^{-1}g)\\ &= (f, Ag).\end{aligned}$$

Thus, A is symmetric.

It remains to prove that V is the Cayley transform of A. This follows from

$$\begin{aligned}(A-iI) &= -iI + i(I+V)(I-V)^{-1} = -i[(I-V)-(I+V)](I-V)^{-1} \\ &= 2iV(I-V)^{-1}, \\ (A+iI) &= i[(I-V)+(I+V)](I-V)^{-1} = 2i(I-V)^{-1}.\end{aligned}$$

□

Theorem 1.16. *([6], Thm. 8.4.)*
Let A be a symmetric operator in a Hilbert space $\mathcal{H}$ and denote by V its Cayley transform. Then

(i) The following statements (a)–(d) are equivalent:

- *(a) A is closed.*
- *(b) V is closed.*
- *(c) $Dom(V) = Ran(A+iI)$ is closed.*
- *(d) $Ran(V) = Ran(A-iI)$ is closed.*

(ii) A is self-adjoint if and only if V is unitary.

Proof. (i): (a) is equivalent to (c) and (d): A is closed if and only if $(A \pm iI)^{-1}$ is closed and the bounded operator $(A \pm iI)^{-1}$ is closed if and only if $Dom((A-iI)^{-1}) = Ran(A-iI) = Ran(V)$ is closed or $Dom((A+iI)^{-1}) = Ran(A+iI) = Dom(V)$ is closed.
(b) is equivalent to (c): The bounded operator V is closed if and only if its domain is closed.

(ii): A is self-adjoint if and only if $Ran(A-iI) = Ran(A+iI) = \mathcal{H}$ (i.e., $Dom(V) = Ran(V) = \mathcal{H}$). This is equivalent to the statement that V is unitary. □

Theorem 1.17. *([6], Thm. 8.5.)*
Let A_1 and A_2 be symmetric operators in a Hilbert space $\mathcal{H}$ and let V_1 and V_2 denote their Cayley transforms. Then $A_1 \subseteq A_2$ if and only if $V_1 \subseteq V_2$.

Proof. This follows from Theorem 1.15 and in particular from $A_j = i(I + V_j)(I - V_j)^{-1}, \ j = 1, 2$. □

Consequently, we can obtain all self-adjoint extensions (provided that such exist) if we determine all unitary extensions V' of the Cayley transform V of A.

In particular, A has self-adjoint extensions if and only if V has unitary extensions. The following theorem makes it possible to explicitly construct the extensions V' of V.

Theorem 1.18. *([6], Thm. 8.6.)*
Let A be a closed symmetric operator in a Hilbert space $\mathcal{H}$ and let V denote its Cayley transform.

(i) V' is the Cayley transform of a closed symmetric extension A' of A if and only if the following holds:

There exist closed subspaces F_+ of $K_+(A) = Ran(A+iI)^\perp$ and F_- of $K_-(A) = Ran(A-iI)^\perp$ and an isometric mapping $\widetilde{V}$ of F_+ onto F_- for which

$$Dom(V') = Ran(A' + iI) = Ran(A + iI) \oplus F_+,$$
$$V'(f+g) = Vf + \widetilde{V}g, \quad f \in Ran(A+iI),\ g \in F_+,$$
$$Ran(V') = Ran(A' - iI) = Ran(A - iI) \oplus F_-, \quad dim(F_-) = dim(F_+).$$

(ii) The operator V' in part (i) is unitary (i.e., A' is self-adjoint) if and only if $F_- = K_-(A)$ and $F_+ = K_+(A)$.

(iii) A possesses self-adjoint extensions if and only if its deficiency indices are equal, $n_+(A) = n_-(A)$.

Proof. (i): If V' has the given form, then V' is an isometric mapping of $Ran(A+iI)\oplus F_+$ onto $Ran(A-iI)\oplus F_-$. Consequently, V' satisfies assumption (i) of Theorem 1.15. Since $Ran(I-V)$ is dense, $Ran(I-V')$ is also dense, so that V' also satisfies (ii) of Theorem 1.15. Therefore, V' is the Cayley transform of a symmetric extension A' of A. Since $\widetilde{V}$ is an isomorphism of F_+ onto F_-, we have $dim\ F_+ = dim\ F_-$. If V' is the Cayley transform of a symmetric extension A' of A, then put $F_- = Ran(A' - iI) \ominus Ran(A - iI)$, $F_+ = Ran(A' + iI) \ominus Ran(A + iI)$, and $\widetilde{V} = V'|_{F_+}$.

(ii): V' is unitary if and only if $Dom(V') = \mathcal{H} = Ran(V')$, that is, if and only if $F_+ = Ran(A+iI)^\perp = K_+(A)$ and $F_- = Ran(A-iI)^\perp = K_-(A)$.

(iii): By (i) and (ii), V possesses a unitary extension if and only if there exists an isometric mapping $\widetilde{V}$ of $Ran(A+iI)^{\perp}$ onto $Ran(A-iI)^{\perp}$. This happens if and only if

$$dim[Ran(A+iI)^{\perp}] = dim[Ran(A-iI)^{\perp}].$$

□

Corollary 1.19. *([5], p. 141.)*
Let A be a closed symmetric operator with deficiency indices $n_+(A)$ and $n_-(A)$ in a Hilbert space $\mathcal{H}$. Then

(i) A is self-adjoint if and only if $n_+(A) = 0 = n_-(A)$.

(ii) A has self-adjoint extensions if and only if $n_+(A) = n_-(A)$. There is a one-to-one correspondence between self-adjoint extensions of A and unitary maps from $K_+(A)$ onto $K_-(A)$.

(iii) If either $n_+(A) = 0 \neq n_-(A)$ or $n_-(A) = 0 \neq n_+(A)$, then A has no nontrivial symmetric extensions (in particular, it has no self-adjoint extensions) in $\mathcal{H}$ (such operators are called maximally symmetric).

Theorem 1.20. *([6], Thm. 8.11; von Neumann's first formula.)*
Let A be a closed symmetric operator on a complex Hilbert space $\mathcal{H}$. Then,

$$\begin{aligned} Dom(A^*) &= Dom(A) \dot{+} K_+(A) \dot{+} K_-(A) \\ A^*(f_0 + g_+ + g_-) &= Af_0 + ig_+ - ig_- \quad for\ f_0 \in Dom(A), g_+ \in K_+(A), \\ &\qquad\qquad\qquad\qquad g_- \in K_-(A). \end{aligned}$$

Proof. Since $K_+(A) \subset Dom(A^*)$ and $K_-(A) \subset Dom(A^*)$, we have

$$Dom(A) + K_+(A) + K_-(A) \subseteq Dom(A^*).$$

We show that we have equality here, that is, every $f \in Dom(A^*)$ can be written in the form $f = f_0 + g_+ + g_-$ with $f_0 \in Dom(A)$, $g_+ \in K_+(A)$, and $g_- \in K_-(A)$. To this end, let $f \in Dom(A^*)$. Then by the projection theorem we can decompose $(A^* + iI)f$ into its components in $K_+(A)$ and in $K_+(A)^{\perp} = Ran(A+iI)$,

$$(A^* + iI)f = (A+iI)f_0 + g, \quad (A+iI)f_0 \in Ran(A+iI), \ g \in K_+(A).$$

Since $A^* f_0 = Af_0$ and $A^* g = ig$, we have with $g_+ = -(i/2)g$

$$\begin{aligned} A^*(f - f_0 - g_+) &= A^* f - Af_0 - ig_+ = A^* f - Af_0 - (1/2)g \\ &= -if + if_0 + (1/2)g = -i(f - f_0) + ig_+ \\ &= -i(f - f_0 - g_+). \end{aligned}$$

If we set $g_- = f - f_0 - g_+$, then $g_- \in K_-(A)$ and $f = f_0 + g_+ + g_-$.

It remains to prove that the sum is direct, that is, $0 = f_0 + g_+ + g_-$, $f_0 \in Dom(A)$, $g_+ \in K_+(A)$, and $g_- \in K_-(A)$ imply $f_0 = g_+ = g_- = 0$. It follows from $0 = f_0 + g_+ + g_-$ that

$$0 = A^*(f_0 + g_+ + g_-) = Af_0 + ig_+ - ig_-.$$

We obtain from this that

$$(A - iI)f_0 = ig_- - ig_+ - if_0 = 2ig_- - i(g_- + g_+ + f_0) = 2ig_-$$

and analogously that

$$(A + iI)f_0 = -2ig_+.$$

Thus, $g_- \in K_-(A) \cap Ran(A - iI) = \{0\}$, $g_+ \in K_+(A) \cap Ran(A + iI) = \{0\}$. Therefore, $g_- = g_+ = 0$, and thus $f_0 = 0$. □

Theorem 1.21. *([6], Thm. 8.12; von Neumann's second formula.)* *Let A be a closed symmetric operator on a complex Hilbert space $\mathcal{H}$.*

(i) A' is a closed symmetric extension of A if and only if the following holds:
There are closed subspaces $F_+ \subseteq K_+(A)$ and $F_- \subseteq K_-(A)$ and an isometric mapping $\widehat{V}$ of F_+ onto F_- such that

$$Dom(A') = Dom(A) \dotplus (I + \widehat{V})F_+$$

and

$$\begin{aligned} A'(f_0 + g + \widehat{V}g) &= Af_0 + ig - i\widehat{V}g \\ &= A^*(f_0 + g + \widehat{V}g) \; for \; f_0 \in Dom(A), \; g \in F_+. \end{aligned}$$

(ii) A' is self-adjoint if and only if the subspaces $F_+ = K_+(A)$ and $F_- = K_-(A)$ satisfy property (i).

Proof. This theorem follows from Theorem 1.18 if we show that the operator A' of Theorem 1.18 can be represented in the above form. We have (with $\widetilde{V}$ as in Theorem 1.18)

$$\begin{aligned} Dom(A') &= Ran(I - V') = (I - V')Dom(V') = (I - V')(Dom(V) + F_+) \\ &= (I - V)Dom(V) + (I - \widetilde{V})F_+ \\ &= Dom(A) + \{g - \widetilde{V}g \mid g \in F_+\}. \end{aligned}$$

The sum is direct, as $\{g - \widetilde{V}g \mid g \in F_+\} \subseteq F_+ + F_- \subseteq K_+(A) + K_-(A)$. Since $A' \subseteq A^*$, we have in addition that

$$A'(f_0 + g - \widetilde{V}g) = A^*(f_0 + g - \widetilde{V}g) = Af_0 + ig + i\widetilde{V}g$$

for all $f_0 \in Dom(A)$ and $g \in F_+$. The assertion then follows by taking $\widehat{V} = -\widetilde{V}$. ☐

Remark 1.22. Since the set of unitary matrices $U(n)$ in $\mathbb{C}^n$, $n \in \mathbb{N}$, is parametrized by n^2 real parameters, the set of all self-adjoint extensions of a closed symmetric operator A with (finite) deficiency indices $n_\pm(A) = n$ is parametrized by n^2 real parameters according to Theorem 1.16 (b) and Theorem 1.21.

Example 1.23. Consider[1] the following operator A in $L^2((0,1);dx)$,

$$\begin{aligned} &(Af)(x) = if'(x), \\ &f \in Dom(A) = \{g \in L^2((0,1);dx) \mid g \in AC([0,1]);\ g(0) = 0 = g(1); \\ &\qquad\qquad\qquad\qquad g' \in L^2((0,1);dx)\}. \end{aligned}$$

Then

$$\begin{aligned} &(A^*f)(x) = if'(x), \\ &f \in Dom(A^*) = \{g \in L^2((0,1);dx) \mid g \in AC([0,1]);\ g' \in L^2((0,1);dx)\} \end{aligned}$$

and

$$Ker(A^* - iI) = \{ce^x \mid c \in \mathbb{C}\}, \quad Ker(A^* + iI) = \{ce^{-x} \mid c \in \mathbb{C}\}.$$

[1]Here $AC([a,b])$ denotes the set of absolutely continuous functions on $[a,b]$, $a, b \in \mathbb{R}$, $a < b$.

In particular,

$$n_{\pm}(A) = 1.$$

Since the unitary maps in the one-dimensional Hilbert space $\mathbb{C}$ are all of the form $e^{i\alpha}$, $\alpha \in \mathbb{R}$, all self-adjoint extensions of A in $L^2((0,1);dx)$ are given by the following one-parameter family A_α,

$$\begin{aligned} &(A_\alpha f)(x) = if'(x), \\ f \in Dom(A_\alpha) = \{&g \in L^2((0,1);dx) \,|\, g \in AC([0,1]);\ g(0) = e^{i\alpha} g(1); \\ &g' \in L^2((0,1);dx)\}, \quad \alpha \in \mathbb{R}. \end{aligned}$$

Definition 1.24. Let T be a densely defined operator in $\mathcal{H}$. Then T is called *essentially self-adjoint* if the closure $\overline{T}$ of T is self-adjoint.

Theorem 1.25. *([6], Thm. 8.7.)*
Let A be a symmetric operator in a Hilbert space $\mathcal{H}$. The operator A is essentially self-adjoint if and only if A has precisely one self-adjoint extension.

Proof. If A is essentially self-adjoint, then $\overline{A}$ is the only self-adjoint extension of A, since self-adjoint operators have no closed symmetric extensions. We show that if A is not essentially self-adjoint (i.e., $\overline{A}$ is not self-adjoint) then A has either no or infinitely many self-adjoint extensions. If the deficiency indices of $\overline{A}$ are different, then $\overline{A}$ and thus A have no self-adjoint extensions. If the deficiency indices are equal (and hence strictly positive, as $\overline{A}$ is not self-adjoint) then there are infinitely many unitary mappings

$$\widetilde{V} : Ran(A + iI)^{\perp} \to Ran(A - iI)^{\perp}$$

and therefore there are infinitely many self-adjoint extensions of A. ☐

Theorem 1.26. *([6], Thm. 8.8.)*
Let A be a symmetric operator in a Hilbert space $\mathcal{H}$.

(i) If $\pi(A) \cap \mathbb{R} \neq \emptyset$, where $\pi(A)$ denotes the field of regularity of A introduced in Definition 1.4, then A has self-adjoint extensions.

(ii) If A is bounded from below or bounded from above, then A has self-adjoint extensions.

Proof. (i) $\pi(A)$ is connected, since $\pi(A) \cap \mathbb{R} \neq \emptyset$. Then $n_+(A) = n_-(A)$ and therefore, A has self-adjoint extensions.
(ii) Let A be bounded from below and let γ be a lower bound of A. Then

$$\|(A - \lambda I)f\| \geq (f, (A - \lambda)f)\ \|f\|^{-1} \geq (\gamma - \lambda)\|f\|$$

for $\lambda < \gamma$ and all $f \in Dom(A)$, $f \neq 0$. Defining $k(\lambda) = \gamma - \lambda$, then $\pi(A) \cap \mathbb{R} \neq \emptyset$ and hence (ii) follows from (i). ☐

Theorem 1.27. *([6], p. 247.)*
If A is bounded from below with lower bound $\gamma \in \mathbb{R}$ and A has finite deficiency indices (m, m), then each of its self-adjoint extensions has only a finite number of eigenvalues in $(-\infty, \gamma)$ and the sum of the multiplicities of these eigenvalues does not exceed m.

For additional results of this type, see [6], Sect. 8.3.

Theorem 1.28. *([1], Sect. 85, Thm. 2)*
An operator A bounded from below with lower bound γ has a self-adjoint extension $\widetilde{A}$ with lower bound not smaller than an arbitrarily pre-assigned number $\gamma' < \gamma$.

The above result will be improved in Section 2.

Theorem 1.29. *([5], Thm. X.26.)*
Let A be a strictly positive symmetric operator, that is, $(Af, f) \geq \gamma(f, f)$ for all $f \in Dom(A)$ and some $\gamma > 0$. Then the following are equivalent:

(i) *A is essentially self-adjoint.*

(ii) *$Ran(A)$ is dense.*

(iii) *$Ker(A^*) = \{0\}$.*

(iv) *A has precisely one self-adjoint extension bounded from below.*

2 The Friedrichs extension of semibounded operators in a Hilbert space

Let $\mathcal{L}$ be a vector space over the field $\mathbb{C}$.

Definition 2.1. A mapping $s : \mathcal{L} \times \mathcal{L} \to \mathbb{C}$ is called a *sesquilinear form* on $\mathcal{L}$, if for all $f, g, h \in \mathcal{L}$ and $a, b \in \mathbb{C}$ we have

$$s(f, ag + bh) = a\ s(f, g) + b\ s(f, h),$$
$$s(af + bg, h) = \bar{a}\ s(f, h) + \bar{b}\ s(g, h).$$

where $\bar{a}$ and $\bar{b}$ represent the complex conjugates of a and b.

Definition 2.2. A sesquilinear form s on $\mathcal{H}$ is said to be *bounded*, if there exists a $C \geq 0$ such that

$$|s(f, g)| \leq C\|f\|\|g\| \ for\ all\ f, g \in \mathcal{H}.$$

The smallest C is called the *norm* of s and denoted by $\|s\|$.

If $T \in B(\mathcal{H})$ then the equality $t(f, g) = (Tf, g)$ defines a bounded sesquilinear form on $\mathcal{H}$ and $\|t\| = \|T\|$. Conversely, every bounded sesquilinear form induces an operator on $B(\mathcal{H})$.

Theorem 2.3. *([6], Thm. 5.35.)*
If t is a bounded sesquilinear form on $\mathcal{H}$, then there exists precisely one $T \in B(\mathcal{H})$ such that $t(f, g) = (Tf, g)$ for all $f, g \in \mathcal{H}$. We then have $\|T\| = \|t\|$.

Proof. For every $f \in \mathcal{H}$ the function $g \mapsto t(f, g)$ is a continuous linear functional on $\mathcal{H}$, since we have $|t(f, g)| \leq \|t\|\|f\|\|g\|$. Therefore for each $f \in \mathcal{H}$ there exists exactly one $\tilde{f} \in \mathcal{H}$ such that $t(f, g) = (\tilde{f}, g)$. The mapping $f \mapsto \tilde{f}$ is obviously linear. Let us define T by the equality $Tf = \tilde{f}$ for all $f \in \mathcal{H}$. The operator T is bounded with norm

$$\begin{aligned}\|T\| &= \sup\{|(Tf, g)| \mid f, g \in \mathcal{H},\ \|f\| = \|g\| = 1\} \\ &= \sup\{|t(f, g)| \mid f, g \in \mathcal{H},\ \|f\| = \|g\| = 1\} = \|t\|.\end{aligned}$$

If T_1 and T_2 are in $B(\mathcal{H})$ and $(T_1 f, g) = t(f, g) = (T_2 f, g)$ for all $f, g \in \mathcal{H}$, then one concludes that $T_1 = T_2$, that is, T is uniquely determined. ☐

For unbounded sesquilinear forms the situation is more complicated. We consider only a special case.

Theorem 2.4. *([6], Thm. 5.36.)*
Let $(\mathcal{H}, (\cdot,\cdot))$ be a Hilbert space and let $\mathcal{H}_1$ be a dense subspace of $\mathcal{H}$. Assume that a scalar product $(\cdot,\cdot)_1$ is defined on $\mathcal{H}_1$ in such a way that $(\mathcal{H}_1, (\cdot,\cdot)_1)$ is a Hilbert space and with some $\kappa > 0$ we have $\kappa\|f\|^2 \leq \|f\|_1^2$ for all $f \in \mathcal{H}_1$. Then there exists exactly one self-adjoint operator T on $\mathcal{H}$ such that

$$Dom(T) \subseteq \mathcal{H}_1 \text{ and } (Tf, g) = (f, g)_1 \; for \; f \in Dom(T), \; g \in \mathcal{H}_1.$$

Moreover, T is bounded from below with lower bound κ. The operator T is defined by

$$\begin{aligned} Dom(T) = \{f \in \mathcal{H}_1 \mid & \text{ there exists an } \tilde{f} \in \mathcal{H} \text{ such that } (f,g)_1 = (\tilde{f}, g) \\ & for \; all \; g \in \mathcal{H}_1\}, \\ Tf = \tilde{f}. & \end{aligned}$$

In what follows let $\mathcal{D}$ be a dense subspace of $\mathcal{H}$.

Definition 2.5. Let s be a sesquilinear form on $\mathcal{D} \subseteq \mathcal{H}$. Then s is called *bounded from below* if there exists a $\gamma \in \mathbb{R}$ such that for all $f \in \mathcal{D}$,

$$s(f,f) \geq \gamma\|f\|^2.$$

Let s be a sesquilinear form on $\mathcal{D}$ bounded from below. Then the equality $(f,g)_s = (1-\gamma)(f,g) + s(f,g)$ defines a scalar product on $\mathcal{D}$ such that $\|f\|_s \geq \|f\|$ for all $f \in \mathcal{D}$. Moreover, we assume that $\|\cdot\|_s$ is compatible with $\|\cdot\|$ in the following sense:

$$\begin{aligned} &\text{If } \{f_n\} \text{ is a } \|\cdot\|_s\text{-Cauchy sequence in } \mathcal{D} \text{ and } \|f_n\| \to 0, \\ &\text{then we also have } \|f_n\|_s \to 0. \end{aligned} \tag{2.1}$$

Next, let $\mathcal{H}_s$ be the $\|\cdot\|_s$-completion of $\mathcal{D}$. It follows from the compatibility assumption that $\mathcal{H}_s$ may be considered as a subspace of $\mathcal{H}$ if the embedding of $\mathcal{H}_s$ into $\mathcal{H}$ is defined as follows: Let $\{f_n\}_{n\in\mathbb{N}}$ be a $\|\cdot\|_s$-Cauchy sequence in $\mathcal{D}$. Then $\{f_n\}_{n\in\mathbb{N}}$ is a Cauchy sequence in $\mathcal{H}$. Let the element $\lim_{n\to\infty} f_n$ in $\mathcal{H}$ correspond to the element $[\{f_n\}_{n\in\mathbb{N}}]$ of $\mathcal{H}_s$. By the compatibility assumption (2.1), this correspondence is injective and the embedding is continuous. The spaces $\mathcal{H}$ and $\mathcal{H}_s$ are related the same way as $\mathcal{H}$ and $\mathcal{H}_1$ were in Theorem 2.4 (with $\kappa = 1$). Let

$$\bar{s}(f,g) = (f,g)_s - (1-\gamma)(f,g) \; for \; f, g \in \mathcal{H}_s.$$

Therefore, $\bar{s}(f,g) = s(f,g)$ for $f, g \in \mathcal{D}$. The sesquilinear form $\bar{s}$ is called the closure of s.

Theorem 2.6. *([6], Thm. 5.37.)*
Assume that $\mathcal{H}$ is a Hilbert space, $\mathcal{D}$ is a dense subspace of $\mathcal{H}$, and s is a symmetric sesquilinear form on $\mathcal{D}$ bounded from below with lower bound γ. Let $\|\cdot\|_s$ be compatible with $\|\cdot\|$. Then there exists precisely one self-adjoint operator T bounded from below with lower bound γ such that

$$Dom(T) \subseteq \mathcal{H}_s \text{ and } (Tf, g) = s(f, g) \text{ for all } f \in \mathcal{D} \cap Dom(T),\ g \in \mathcal{D}. \tag{2.2}$$

In particular, one has

$$\begin{aligned} Dom(T) = \{f \in \mathcal{H}_s \mid & \text{ there exists an } \hat{f} \in \mathcal{H} \text{ such that } s(f, g) = (\hat{f}, g) \\ & \text{for all } g \in \mathcal{D}\}, \\ Tf = \hat{f} & \text{ for } f \in Dom(T). \end{aligned} \tag{2.3}$$

Proof. If we replace $(\mathcal{H}_1, (\cdot,\cdot)_1)$ by $(\mathcal{H}_s, (\cdot,\cdot)_s)$ in Theorem 2.4, then we obtain precisely one self-adjoint operator T_0 such that $Dom(T_0) \subseteq \mathcal{H}_s$ and

$$(T_0 f, g) = (f, g)_s \text{ for all } f \in Dom(T_0),\ g \in \mathcal{H}_s.$$

T_0 is bounded from below with lower bound 1. The operator $T = T_0 - (1-\gamma)$ obviously possesses the required properties. The uniqueness follows from the uniqueness of T_0. Formula (2.2) implies (2.3), since $\mathcal{D}$ is dense (in $\mathcal{H}_s$ and in $\mathcal{H}$). □

If S is a symmetric operator bounded from below with lower bound γ, then the equality

$$s(f, g) = (Sf, g),\ f, g, \in Dom(S)$$

defines a sesquilinear form s on $Dom(S)$ bounded from below with lower bound γ. In this case

$$(f, g)_s = (Sf, g) + (1-\gamma)(f, g) \text{ and } \|f\|_s^2 = (Sf, f) + (1-\gamma)\|f\|^2$$

for all $f, g \in Dom(S)$. The norm $\|\cdot\|_s$ is compatible with $\|\cdot\|$: Let $\{f_n\}_{n\in\mathbb{N}}$ be a $\|\cdot\|_s$-Cauchy sequence in $Dom(S)$ such that $f_n \to 0$ as $n \to \infty$. Then for all $n, m \in \mathbb{N}$ we have

$$\begin{aligned} \|f_n\|_s^2 = (f_n, f_n)_s &= |(f_n, f_n - f_m)_s + (f_n, f_m)_s| \\ &\leq \|f_n\|_s \|f_n - f_m\|_s + \|(S + 1 - \gamma) f_n\| \|f_m\|. \end{aligned}$$

The sequence $\{\|f_n\|_s\}_{n\in\mathbb{N}}$ is bounded, $\|f_n - f_m\|_s$ is small for large n and m and for any fixed n we have $\|(S+1-\gamma)f_n\|\,\|f_m\| \to 0$ as $m \to \infty$. Consequently, it follows that $\|f_n\|_s \to 0$ as $n \to \infty$. This fact permits the construction of a self-adjoint extension (the *Friedrichs extension*) of a symmetric operator bounded from below in such a way that the lower bound remains unchanged.

A symmetric operator T bounded from below has equal deficiency indices, hence such an operator always has self-adjoint extensions. There is a distinguished extension, called the Friedrichs extension, which is obtained from the sesquilinear form associated with T.

Theorem 2.7. *([6], Thm. 5.38.)*
Let S be a symmetric operator bounded from below with lower bound γ. Then there exists a self-adjoint extension of S bounded from below with lower bound γ. In particular, if one defines $s(f,g) = (Sf,g)$ for $f,g \in Dom(S)$, and with $\mathcal{H}_s$ as above, then the operator S_F defined by

$$Dom(S_F) = Dom(S^*) \cap \mathcal{H}_s \text{ and } S_F f = S^* f \text{ for } f \in Dom(S_F)$$

is a self-adjoint extension of S with lower bound γ. The operator S_F is the only self-adjoint extension of S having the property $Dom(S_F) \subseteq \mathcal{H}_s$.

Proof. By Theorem 2.6 there exists precisely one self-adjoint operator S_F with $Dom(S_F) \subset \mathcal{H}_s$ and

$$(S_F f, g) = s(f,g) = (Sf,g) \text{ for } f \in Dom(S) \cap Dom(S_F),\ g \in Dom(S).$$

Moreover, γ is a lower bound for S_F. By (2.3) we have

$$\begin{aligned} Dom(S_F) = \{f \in \mathcal{H}_s \mid & \text{ there exists an } \hat{f} \in \mathcal{H} \text{ with } \bar{s}(f,g) = (\hat{f},g) \\ & \text{ for all } g \in Dom(S)\}, \\ S_F f = \hat{f} & \text{ for } f \in Dom(S_F). \end{aligned} \tag{2.4}$$

We can replace $\bar{s}(f,g)$ by (f,Sg) in (2.4): If we choose a sequence $\{f_n\}_{n\in\mathbb{N}} \subset Dom(S)$ such that $\|f_n - f\|_s \to 0$ as $n \to \infty$, then we obtain

$$\bar{s}(f,g) = \lim_{n\to\infty} \bar{s}(f_n,g) = \lim_{n\to\infty} (f_n, Sg) = (f,Sg).$$

Consequently, it follows that

$$Dom(S_F) = Dom(S^*) \cap \mathcal{H}_s \text{ and } S_F = S^*|_{Dom(S_F)}.$$

Because of the inclusions $S \subseteq S^*$ and $Dom(S) \subseteq \mathcal{H}_s$ one concludes that S_F is an extension of S. Let T be an arbitrary self-adjoint extension of S such that $Dom(T) \subseteq \mathcal{H}_s$. Then $T \subseteq S^*$ and $Dom(S_F) = Dom(S^*) \cap \mathcal{H}_s$ imply that $T \subseteq S_F$, and consequently, $T = S_F$. □

The operator S_F in Theorem 2.7 is called the Friedrichs extension of S.

Theorem 2.8. *([5], Thm. X.24.)*
Let A be a symmetric operator bounded from below. If the Friedrichs extension $\widehat{A}$ is the only self-adjoint extension of A that is bounded from below, then A is essentially self-adjoint.

Proof. If the deficiency indices of $\overline{A}$ are finite, then any self-adjoint extension of $\overline{A}$ is bounded below (possibly with a smaller lower bound). Therefore, we only need to consider the case where the deficiency indices of $\overline{A}$ equal infinity. Suppose $\widehat{A}$ is the Friedrichs extension of $\overline{A}$ and let $\widetilde{A}$ be a symmetric extension of $\overline{A}$ contained in $\widehat{A}$ which has deficiency indices equal to 1. Then $\widetilde{A}$ is bounded from below, so all its self-adjoint extensions will be bounded from below. Hence A has more than one self-adjoint extension bounded from below unless its deficiency indices are equal to 0. □

Analogous results apply of course to operators and sesquilinear forms bounded from above.

Our arguments thus far enable us to study the operator product A^*A as well. If $A \in B(\mathcal{H}_1, \mathcal{H}_2)$, where $B(\mathcal{H}_1, \mathcal{H}_2)$ represents the set of bounded operators from $\mathcal{H}_1$ into $\mathcal{H}_2$ (where $\mathcal{H}_j,\ j = 1, 2$, are separable complex Hilbert spaces), then A^*A is self-adjoint in $\mathcal{H}_1$.

Definition 2.9. Let T be a closed operator. A subspace $\mathcal{D}$ of $Dom(T)$ is called a *core* of T provided $S = T|_D$ implies $\overline{S} = T$.

Theorem 2.10. *([6], Thm. 5.39.)*
Let $(\mathcal{H}_1, (\cdot,\cdot)_1)$ and $(\mathcal{H}_2, (\cdot,\cdot)_2)$ be Hilbert spaces and let A be a densely defined closed operator from $\mathcal{H}_1$ into $\mathcal{H}_2$. Then A^*A is a self-adjoint operator on $\mathcal{H}_1$ with lower bound 0 (i.e., $A^*A \geq 0$). $Dom(A^*A)$ is a core of A and $Ker(A^*A) = Ker(A)$, where

$$Dom(A^*A) = \{f \in Dom(A) \,|\, Af \in Dom(A^*)\}.$$

Proof. As A is closed, $Dom(A)$ is a Hilbert space with the scalar product $(f,g)_A = (Af, Ag)_2 + (f,g)_1$, and $\|f\|_A \geq \|f\|_1$ for all $f \in Dom(A)$. Therefore, by Theorem 2.4 there exists a self-adjoint operator T with lower bound 1 for which

$$\begin{aligned} Dom(T) = \{f \in Dom(A) \,|\, & \text{ there exists an } \hat{f} \in \mathcal{H}_1 \text{ such that} \\ & (f,g)_A = (\hat{f}, g)_1 \text{ for all } g \in Dom(A)\}, \\ Tf = \hat{f} & \text{ for } f \in Dom(T). \end{aligned}$$

On account of the equality $(f,g)_A = (Af, Ag)_2 + (f,g)_1$, this implies that $f \in Dom(T)$ if and only if $Af \in Dom(A^*)$ (i.e., $f \in Dom(A^*A)$) and $Tf = \hat{f} = A^*Af + f$. Hence it follows that $T = A^*A + I$, $A^*A = T - I$, that is, A^*A is self-adjoint and non-negative. From Theorem 2.4 it follows that $Dom(A^*A)$ is dense in $Dom(A)$ with respect to $\|\cdot\|_A$, that is, $Dom(A^*A)$ is a core of A. If $f \in Ker(A)$, then $Af = 0 \in Dom(A^*)$ and hence $A^*Af = 0$. Therefore, $Ker(A) \subseteq Ker(A^*A)$. If $f \in Ker(A^*A)$, then $\|Af\|^2 = (A^*Af, f) = 0$. Hence, $Ker(A^*A) \subseteq Ker(A)$, and thus $Ker(A^*A) = Ker(A)$. □

Corollary 2.11. *([5], p. 181.)*
If A is symmetric and A^2 is densely defined, then A^*A is the Friedrichs extension of A^2.

Theorem 2.12. *([6], Thm. 5.40.)*
Let A_1 and A_2 be densely defined closed operators from $\mathcal{H}$ into $\mathcal{H}_1$ and from $\mathcal{H}$ into $\mathcal{H}_2$, respectively. Then $A_1^*A_1 = A_2^*A_2$ if and only if $Dom(A_1) = Dom(A_2)$ and $\|A_1 f\| = \|A_2 f\|$ for all $f \in Dom(A_1) = Dom(A_2)$.

Proof. Assume that $Dom(A_1) = Dom(A_2)$ and $\|A_1 f\| = \|A_2 f\|$ for all $f \in Dom(A_1)$. It follows from the polarization identity that

$$(A_1 f, A_1 g) = (A_2 f, A_2 g) \text{ for all } f, g \in Dom(A_1) = Dom(A_2).$$

Then the construction of Theorem 2.10 provides the same operator for $A = A_1$ and $A = A_2$, and consequently, $A_1^*A_1 = A_2^*A_2$. If this equality holds, then

$$\begin{aligned} & \|A_1 f\|^2 = (A_1^*A_1 f, f) = (A_2^*A_2 f, f) = \|A_2 f\|^2 \\ & \text{for all } f \in Dom(A_1^*A_1) = Dom(A_2^*A_2) \end{aligned}$$

(here we have used the inclusions $Dom(A_1^*A_1) \subseteq Dom(A_1)$ and $Dom(A_2^*A_2) \subseteq Dom(A_2)$). By Theorem 2.10 the subspace $Dom(A_1^*A_1) = Dom(A_2^*A_2)$

is a core of A_1 and A_2. As the A_1-norm and the A_2-norm coincide on $Dom(A_1^*A_1) = Dom(A_2^*A_2)$, it follows finally that $Dom(A_1) = Dom(A_2)$ and $\|A_1 f\| = \|A_2 f\|$ for all $f \in Dom(A_1) = Dom(A_2)$. □

3 Krein's formula for self-adjoint extensions in the case of finite deficiency indices

In this part we consider a closed symmetric operator A_0 with finite and equal deficiency indices (m, m), $m \in \mathbb{N}$.

Let A_1 and A_2 be two self-adjoint extensions of A_0,

$$A_1 \supset A_0, \ A_2 \supset A_0.$$

It is natural to call a closed operator C which satisfies

$$A_1 \supset C, \ A_2 \supset C$$

a *common part* of A_1 and A_2. Moreover, there exists a closed operator A which satisfies

$$A_1 \supset A, \ A_2 \supset A \tag{3.1}$$

and which is an extension of every common part of A_1 and A_2.

Definition 3.1. (i) The operator A in (3.1) which extends any common part of A_1 and A_2 is called the *maximal common part* of A_1 and A_2.
(ii) Two extensions A_1 and A_2 of A_0 are called *relatively prime* if

$$h \in Dom(A_1) \cap Dom(A_2) \ \textit{implies} \ h \in Dom(A_0). \tag{3.2}$$

The maximal common part A either is an extension of A_0 or it coincides with A_0. (In the latter case A_1 and A_2 are relatively prime.)

If the maximal number of vectors which are linearly independent modulo $Dom(A_0)$ and which satisfy conditions (3.2) is equal to p $(0 \le p \le m-1)$, then the maximal common part A of A_1 and A_2 has deficiency indices (n, n), $n = m - p$. In this case, A_1 and A_2 can be considered as relatively prime self-adjoint extensions of A. The problem of the present section is the derivation of a formula which relates the resolvents of two self-adjoint extensions A_1 and A_2 of A.

Let $M_n(\mathbb{C})$ be the set of $n \times n$ matrices with entries in $\mathbb{C}$, I_n the identity matrix in $\mathbb{C}^n$, and abbreviate $Re(M) = (M + M^*)/2$, $Im(M) = (M - M^*)/2i$, $M \in M_n(\mathbb{C})$.

Theorem 3.2. *([1], Sect. 84 and [3]; Krein's formula.)*
Let A_1 and A_2 be two self-adjoint extensions of the closed symmetric operator A_0 with deficiency indices $n_\pm(A_0) = m$, $m \in \mathbb{N}$. Moreover, let $A \supseteq A_0$ be the maximal common part of A_1 and A_2 with deficiency indices $n_\pm(A) = n \leq m$. Then there exists an $n \times n$ matrix $P(z) = (P_{j,k}(z))_{1\leq j,k\leq n} \in M_n(\mathbb{C})$, $z \in \rho(A_2) \cap \rho(A_1)$, such that

$$\begin{aligned}
&det(P(z)) \neq 0, \;\; z \in \rho(A_2) \cap \rho(A_1),\\
&P(z)^{-1} = P(z_0)^{-1} - (z - z_0)((u_{1,j}(\bar{z}), u_{1,k}(z_0)))_{1\leq j,k\leq n}, \;\; z, z_0 \in \rho(A_1),\\
&Im(P(i)^{-1}) = -I_n,\\
&(A_2 - z)^{-1} = (A_1 - z)^{-1} + \sum_{j,k=1}^{n} P_{j,k}(z)(u_{1,k}(\bar{z}), \cdot)u_{1,j}(z), \;\; z \in \rho(A_2) \cap \rho(A_1).
\end{aligned}$$

Here

$$u_{1,j}(z) = U_{1,z,i}u_j(i), \;\; 1 \leq j \leq n, \;\; z \in \rho(A_1)$$

such that $\{u_j(i)\}_{1\leq j\leq n}$ is an orthonormal basis for $Ker(A^* - i)$ and hence $\{u_{1,j}(z)\}_{1\leq j\leq n}$ is a basis for $Ker(A^* - z)$, $z \in \rho(A_1)$ and

$$U_{1,z,z_0} = I + (z - z_0)(A_1 - z)^{-1} = (A_1 - z_0)(A_1 - z)^{-1}, \;\; z, z_0 \in \rho(A_1).$$

Proof. Let $z \in \pi(A)$, $h \in Ker(A^* - \bar{z}I)$. Then

$$\begin{aligned}
([(A_1 - z)^{-1} - (A_2 - z)^{-1}]f, h) &= (f, [(A_1 - z)^{-1} - (A_2 - z)^{-1}]^* h)\\
&= (f, [(A_1 - \bar{z})^{-1} - (A_2 - \bar{z})^{-1}]h)\\
&= (f, (A_1 - \bar{z})^{-1}h - (A_2 - \bar{z})^{-1}h)\\
&= (f, 0) = 0.
\end{aligned}$$

Therefore,

$$[(A_1 - z)^{-1} - (A_2 - z)^{-1}]f \begin{cases} = 0 & for \;\; f \in Ran(A - zI) \\ \in Ker(A^* - \bar{z}I) & for \;\; f \in Ker(A^* - zI). \end{cases} \tag{3.3}$$

Next, we choose n linearly independent vectors $u_{1,1}(\bar{z}), \ldots, u_{1,n}(\bar{z})$ in $Ker(A^* - zI)$ as well as n linearly independent vectors $u_{1,1}(z), \ldots, u_{1,n}(z)$ in $Ker(A^* - \bar{z}I)$. It follows from (3.3) that for each $f \in \mathcal{H}$,

$$[(A_1 - z)^{-1} - (A_2 - z)^{-1}]f = \sum_{k=1}^{n} c_k(f)u_{1,k}(z), \tag{3.4}$$

where $c_k(f)$ are linear functionals of f. Hence, by the Riesz representation theorem, there exist vectors $h_k(z)$ such that

$$c_k(f) = (f, h_k(z)),\ k = 1, \ldots, n.$$

Since $u_{1,1}(z), \ldots, u_{1,n}(z)$ are linearly independent for each $f \perp Ker(A^* - zI)$,

$$(f, h_k(z)) = 0,\ k = 1, \ldots, n.$$

Therefore, $h_k(z) \in Ker(A^* - zI),\ k = 1, \ldots, n$, so that

$$h_k(z) = \sum_{j=1}^{n} \overline{P_{j,k}(z)} u_{1,j}(\bar{z}), \quad k = 1, \ldots, n$$

and (3.4) can be represented as

$$[(A_1 - z)^{-1} - (A_2 - z)^{-1}]f = \sum_{j,k=1}^{n} P_{j,k}(z)(u_{1,k}(\bar{z}), f)u_{1,j}(z). \tag{3.5}$$

The matrix function $P(z) = (P_{j,k}(z))_{1 \le j,k \le n}$, which is defined on the set of all common regular points of A_1 and A_2, is nonsingular. Indeed, if $\det((P_{j,k}(z_0))_{1 \le j,k \le n}) = 0$, then $h_k(z_0),\ k = 1, \ldots, n$ would be linearly dependent and this would imply the existence of a vector $0 \ne h \in \mathcal{H}$ such that

$$h \perp h_k(z_0),\ h \in Ker(A^* - z_0 I), \quad k = 1, \ldots, n.$$

Then it follows from (3.4) that

$$[(A_1 - z)^{-1} - (A_2 - z)^{-1}]h = 0.$$

This would contradict the fact that A_1 and A_2 are relatively prime extensions of A.

In (3.5), we now omit f and consider the expressions $(u_{1,k}(\bar{z}), \cdot)u_{1,j}(z)$, $j, k = 1, \ldots, n$ as operators in $\mathcal{H}$ to obtain Krein's formula

$$(A_2 - z)^{-1} = (A_1 - z)^{-1} + \sum_{j,k=1}^{n} P_{j,k}(z)(u_{1,k}(\bar{z}), \cdot)u_{1,j}(z) \tag{3.6}$$

for each common regular point z of A_1 and A_2. $\square$

Here, the choice of the vector functions $u_{1.j}(z)$ and $u_{1,k}(\bar{z})$, $j,k = 1,\dots,n$ has been arbitrary. At the same time, the left-hand side and hence the right-hand side of (3.5) is a regular analytic vector function of z. Actually, $u_{1,j}(z)$, $j = 1,\dots,n$ can be defined as a regular analytic function of z and then we obtain a formula for the matrix function $P(z) = (P_{j,k}(z))_{1\le i,j\le n}$ which corresponds to this choice.

Theorem 3.2 summarizes the treatment of Krein's formula (3.6) in Akhiezer and Glazman [1] (see also [3] for an extension of these results to the case of infinite deficiency indices). Krein's formula has been used in a great variety of problems in mathematical physics (see, e.g., the list of references in [3]).

We conclude with a simple illustration.

Example 3.3. Let $\mathcal{H} = L^2((0,\infty);dx)$,

$$\begin{aligned}
&A = -\frac{d^2}{dx^2},\\
&Dom(A) = \{g \in L^2((0,\infty);dx)\,|\, g,g' \in AC([0,R]) \text{ for all } R>0;\\
&\qquad\qquad\qquad\qquad g(0_+) = g'(0_+) = 0;\ g'' \in L^2((0,\infty);dx)\},\\
&A^* = -\frac{d^2}{dx^2},\\
&Dom(A^*) = \{g \in L^2((0,\infty);dx)\,|\, g,g' \in AC([0,R]) \text{ for all } R>0;\\
&\qquad\qquad\qquad\qquad g'' \in L^2((0,\infty);dx)\},\\
&A_1 = A_F = -\frac{d^2}{dx^2}, \quad Dom(A_1) = \{g \in Dom(A^*)\ |\, g(0_+) = 0\},\\
&A_2 = -\frac{d^2}{dx^2},\\
&Dom(A_2) = \{g \in Dom(A^*)\ |\, g'(0_+) + 2^{-1/2}(1-\tan(\alpha))g(0_+) = 0\},\\
&\qquad\qquad\qquad\qquad \alpha \in [0,\pi)\backslash\{\pi/2\},
\end{aligned}$$

where A_F denotes the Friedrichs extension of A (corresponding to $\alpha = \pi/2$). One then verifies,

$$\begin{aligned}
&Ker(A^*-z) = \{ce^{i\sqrt{z}x}, c \in \mathbb{C}\},\ \mathrm{Im}\,(\sqrt{z}) > 0,\ z \in \mathbb{C}\setminus[0,\infty),\\
&n_\pm(A) = (1,1), \quad u_1(i,x) = 2^{1/4}e^{i\sqrt{i}x}, \quad u_{1,1}(-i,x) = 2^{1/4}e^{i\sqrt{-i}x},\\
&P(z) = -(1-\tan(\alpha)+i\sqrt{2z})^{-1},\ z \in \rho(A_2), \quad P(i)^{-1} = \tan(\alpha) - i.
\end{aligned}$$

Finally, Krein's formula relating A_1 and A_2 reads

$$(A_2 - z)^{-1} = (A_1 - z)^{-1} - (2^{-1/2}(1 - \tan(\alpha)) + i\sqrt{z})^{-1}(\overline{e^{i\sqrt{z}\cdot}}, \cdot)e^{i\sqrt{z}\cdot},$$
$$z \in \rho(A_2),\ \operatorname{Im}(\sqrt{z}) > 0.$$

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Trace Ideals and (Modified) Fredholm Determinants

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- Properties of singular values of compact operators

- Schatten–von Neumann ideals

- (Modified) Fredholm determinants

- Perturbation determinants

1 Preliminaries

The material in sections 1–5 of this manuscript can be found in the monographs [1]–[4], [6], [7].

For simplicity all Hilbert spaces in this manuscript are assumed to be separable and complex. (See, however, Remark 3.8.)

Definition 1.1. (i) The set of *bounded* operators from a Hilbert space $\mathcal{H}_1$ to a Hilbert space $\mathcal{H}_2$ is denoted by $B(\mathcal{H}_1, \mathcal{H}_2)$. (If $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}$ we write $B(\mathcal{H})$ for simplicity.)
(ii) The set of *compact* operators from a Hilbert space $\mathcal{H}_1$ to a Hilbert space $\mathcal{H}_2$ is denoted by $B_\infty(\mathcal{H}_1, \mathcal{H}_2)$. (If $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}$ we write $B_\infty(\mathcal{H})$ for simplicity.)
(iii) Let T be a compact operator. The non-zero eigenvalues of $|T| = (T^*T)^{\frac{1}{2}}$ are called the *singular values* (also *singular numbers* or *s-numbers*) of T. By $\{s_j(T)\}_{j\in\mathcal{J}}$, $\mathcal{J} \subseteq \mathbb{N}$ an appropriate index set, we denote the non-decreasing sequence[1] of the singular numbers of T. Every number is counted according to its multiplicity as an eigenvalue of $(T^*T)^{\frac{1}{2}}$.
(iv) Let $B_p(\mathcal{H}_1, \mathcal{H}_2)$ denote the following subset of $B_\infty(\mathcal{H}_1, \mathcal{H}_2)$,

$$B_p(\mathcal{H}_1, \mathcal{H}_2) = \left\{ T \in B_\infty(\mathcal{H}_1, \mathcal{H}_2) \,\middle|\, \sum_{j\in\mathcal{J}} (s_j(T))^p < \infty \right\}, \quad p \in (0, \infty). \tag{1.1}$$

(If $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}$, we write $B_p(\mathcal{H})$ for simplicity.) For $T \in B_p(\mathcal{H}, \mathcal{H}_1)$, $p \in (0, \infty)$, we define

$$\|T\|_p = \left(\sum_{j\in\mathcal{J}} |s_j(T)|^p \right)^{\frac{1}{p}}. \tag{1.2}$$

(v) For $T \in B_\infty(\mathcal{H})$, we denote the sum of the algebraic multiplicities of all the nonzero eigenvalues of T by $\nu(T)$ ($\nu(T) \in \mathbb{N} \cup \{\infty\}$).

We note that $B_\infty(\mathcal{H}_1, \mathcal{H}_2) \subseteq B(\mathcal{H}_1, \mathcal{H}_2)$.

2 Properties of singular values of compact operators and Schatten–von Neumann ideals

Theorem 2.1. *([9], Thm. 7.7.)*

[1] This sequence may be finite.

(i) Let S*,* $T \in B_\infty(\mathcal{H}_1, \mathcal{H}_2)$*. Then* $s_1(T) = \|T\|$ *and*

(a) For all[2] $j \in \mathbb{N}$*,*

$$s_{j+1}(T) = \inf_{g_1,\ldots g_j \in \mathcal{H}} \sup\{\|Tf\| \mid f \in h, f \perp \{g_1, ..., g_j\}, \|f\| = 1\}. \tag{2.1}$$

(b) For all $j, k \in \mathbb{N}_0$*,*

$$s_{j+k+1}(S + T) \leq s_{j+1}(S) + s_{k+1}(T). \tag{2.2}$$

(ii) Let $T \in B_\infty(\mathcal{H}, \mathcal{H}_1)$ *and* $S \in B_\infty(\mathcal{H}_1, \mathcal{H}_2)$*. Then for all* $j, k \in \mathbb{N}_0$*,*

$$s_{j+k+1}(ST) \leq s_{j+1}(S)s_{k+1}(T). \tag{2.3}$$

(iii) Let $T \in B_\infty(\mathcal{H}, \mathcal{H}_1)$ *and* $S \in B(\mathcal{H}_1, \mathcal{H}_2)$*. Then for all* $j \in \mathbb{N}$*,*

$$s_j(ST) = s_j(T^*S^*) \leq \|S\| \, s_j(T) = \|S^*\| \, s_j(T^*). \tag{2.4}$$

Corollary 2.2. *([1], Cor. XI.9.4.)*
(i) For $S, T \in B_\infty(\mathcal{H}_1, \mathcal{H}_2)$ *and for all* $j \in \mathbb{N}$*,*

$$|s_j(S) - s_j(T)| \leq \|S - T\| \, . \tag{2.5}$$

(ii) For $T \in B_\infty(\mathcal{H}, \mathcal{H}_1), S \in B(\mathcal{H}_1, \mathcal{H}_2)$*, and for all* $j \in \mathbb{N}$*,*

$$s_j(ST) \leq \|S\| \, s_j(T). \tag{2.6}$$

Corollary 2.3. *([1], Lemma XI.9.6., [4], Ch. II, Cor. 3.1.)*
Let $T \in B_\infty(\mathcal{H})$ *and denote the sequences of nonzero eigenvalues of* T *and s-numbers of* T *by* $\{\lambda_j(T)\}_{j=1}^{\nu(T)}$ *and* $\{s_j(T)\}_{j\in\mathcal{J}}$*, respectively.*
(i) For $p \in (0, \infty)$ *and* $1 \leq n \leq \nu(T)$ *we have*

$$|\lambda_1(T) \cdots \lambda_n(T)| \leq |s_1(T) \cdots s_n(T)|, \tag{2.7}$$

$$\sum_{j=1}^{n} |\lambda_j(T)|^p \leq \sum_{j=1}^{n} s_j(T)^p, \tag{2.8}$$

$$s_j(T) = s_j(T^*), \quad j \in \mathcal{J}. \tag{2.9}$$

(ii) For $1 \leq n \leq \nu(T)$ *and* r *any positive number we have*

$$\prod_{j=1}^{n}(1 + r|\lambda_j(T)|) \leq \prod_{j=1}^{n}(1 + rs_j(T)). \tag{2.10}$$

[2] If the sequence of singular numbers is finite, that is, $|\mathcal{J}| < \infty$, we have $s_j(T) = 0$, $j > |\mathcal{J}|$.

Theorem 2.4. *([9], Thm. 7.8.)*
(i) If $S, T \in B_p(\mathcal{H}, \mathcal{H}_1)$, $0 < p < \infty$, *then* $S + T$ *also belongs to* $B_p(\mathcal{H}, \mathcal{H}_1)$ *and*

$$\|S + T\|_p \leq (\|S\|_p + \|T\|_p), \quad p \geq 1, \tag{2.11}$$

$$\|S + T\|_p^p \leq 2\left(\|S\|_p^p + \|T\|_p^p\right), \quad p \leq 1. \tag{2.12}$$

The sets $B_p(\mathcal{H}, \mathcal{H}_1)$, $p \in (0, \infty)$, *are therefore vector spaces.*
(ii) If $T \in B_p(\mathcal{H}, \mathcal{H}_1)$, $S \in B_q(\mathcal{H}_1, \mathcal{H}_2)$, $p, q \in (0, \infty)$, *and* $\frac{1}{r} = \frac{1}{p} + \frac{1}{q}$, *then* $ST \in B_r(\mathcal{H}, \mathcal{H}_2)$ *and*

$$\|ST\|_r \leq 2^{\frac{1}{r}} \|S\|_q \|T\|_p. \tag{2.13}$$

(iii) If $T \in B_p(\mathcal{H}, \mathcal{H}_1)$, $p \in (0, \infty)$, *and* $S \in B(\mathcal{H}_1, \mathcal{H}_2)$, *then* $ST \in B_p(\mathcal{H}, \mathcal{H}_2)$ *and*

$$\|ST\|_p \leq \|S\| \|T\|_p. \tag{2.14}$$

The corresponding results hold for $T \in B(\mathcal{H}, \mathcal{H}_1)$ *and* $S \in B_p(\mathcal{H}_1, \mathcal{H}_2)$, $p \in (0, \infty)$.

Proof. (i) We recall from (2.2) that for all $j, k \in \mathbb{N}_0$ we have $s_{j+k+1}(S+T) \leq s_{j+1}(T) + s_{k+1}(T)$. Thus,

$$\begin{aligned} \|S + T\|_p^p &= \sum_j s_j(S + T)^p = \sum_j \{s_{2j-1}(S + T)^p + s_{2j}(S + T)^p\} \\ &= \sum_j \{s_{(j-1)+(j-1)+1}(S + T)^p + s_{(j-1)+j+1}(S + T)^p\} \\ &\leq \sum_j \{[s_j(S) + s_j(T)]^p + [s_j(S) + s_{j+1}(T)]^p\}. \end{aligned}$$

If $p \geq 1$: By Minkowski's inequality for the l_p norm, the above estimate implies that

$$\begin{aligned}
\|S+T\|_p^p &\leq \left[\left(\sum_j s_j(S)^p\right)^{\frac{1}{p}} + \left(\sum_j s_j(T)^p\right)^{\frac{1}{p}}\right]^p \\
&\quad + \left[\left(\sum_j s_j(S)^p\right)^{\frac{1}{p}} + \left(\sum_j s_{j+1}(T)^p\right)^{\frac{1}{p}}\right]^p \\
&\leq 2\left[\|S\|_p + \|T\|_p\right]^p .
\end{aligned}$$

If $p \leq 1$: We use the fact that $|\alpha|^p + |\beta|^p \geq |\alpha+\beta|^p$. Then,

$$\begin{aligned}
\|S+T\|_p^p &\leq \sum_j \{[s_j(S)+s_j(T)]^p + [s_j(S)+s_{j+1}(T)]^p\} \\
&\leq \sum_j [s_j(S)^p + s_j(T)^p + s_j(S)^p + s_{j+1}(T)^p] \\
&\leq \sum_j 2\left[s_j(S)^p + s_j(T)^p\right] \\
&= 2\left(\|S\|_p^p + \|T\|_p^p\right).
\end{aligned}$$

(ii) Note that $\frac{1}{r} = \frac{1}{p} + \frac{1}{q}$ implies that $\frac{r}{p} + \frac{r}{q} = 1$. We recall from (2.3) that for all $j, k \in \mathbb{N}_0$ we have $s_{j+k+1}(ST) \le s_{j+1}(S)s_{k+1}(T)$. Thus,

$$\begin{aligned}
\|ST\|_r &= \left(\sum_j s_j(ST)^r\right)^{\frac{1}{r}} \\
&= \left(\sum_j s_{2j-1}(ST)^r + s_{2j}(ST)^r\right)^{\frac{1}{r}} \\
&\le \left(\sum_j s_j(S)^r s_j(T)^r + \sum_j s_j(S)^r s_{j+1}(T)^r\right)^{\frac{1}{r}} \\
&\le \Bigg(\Big(\sum_j s_j(S)^q\Big)^{\frac{r}{q}} \Big(\sum_j s_j(T)^p\Big)^{\frac{r}{p}} \\
&\quad + \Big(\sum_j s_j(S)^q\Big)^{\frac{r}{q}} \Big(\sum_j s_{j+1}(T)^p\Big)^{\frac{r}{p}}\Bigg)^{\frac{1}{r}} \\
&= \left(2\left(\sum_j s_j(S)^q\right)^{\frac{r}{q}} \left(\sum_j s_j(T)^p\right)^{\frac{r}{p}}\right)^{\frac{1}{r}} \\
&= 2^{\frac{1}{r}} \|S\|_q \|T\|_p .
\end{aligned}$$

(iii) We recall from (2.4) that for $T \in B_\infty(\mathcal{H}, \mathcal{H}_1)$ and $S \in B(\mathcal{H}_1, \mathcal{H}_2)$ we have

$$s_j(ST) = s_j(T^*S^*) \le \|S\| \, s_j(T) = \|S^*\| \, s_j(T^*), \quad j \in \mathbb{N}.$$

Thus,

$$\begin{aligned}
\|ST\|_p &= \left(\sum_j s_j(ST)^p\right)^{\frac{1}{p}} \le \left(\sum_j \left(\|S\|^p s_j(T)^p\right)\right)^{\frac{1}{p}} \\
&= \left(\|S\|^p \sum_j s_j(T)^p\right)^{\frac{1}{p}} = \|S\| \left(\sum_j s_j(T)^p\right)^{\frac{1}{p}} .
\end{aligned}$$

□

Remark 2.5. *i*) and *iii*) above imply that the linear spaces $B_p(\mathcal{H})$, $p \in (0,\infty]$, are two-sided ideals of $B(\mathcal{H})$ and that for $S \in B(\mathcal{H})$ and $T \in B_p(\mathcal{H})$ we have $\|ST\|_p \leq \|S\| \, \|T\|_p$ and $\|TS\|_p \leq \|T\| \, \|S\|_p$. One can show, in fact, that $B_\infty(\mathcal{H})$ is the maximal and only closed two-sided ideal of $B(\mathcal{H})$ (see [4], Ch. III, Thm. 1.1 and Cor. 1.1).

Definition 2.6. Given $T \in B(\mathcal{H})$ and $\lambda^{-1} \notin \sigma(T)$, the *Fredholm resolvent* $T(\lambda)$ is defined by

$$I + \lambda T(\lambda) = (I - \lambda T)^{-1}. \tag{2.15}$$

Lemma 2.7. *For $|\lambda| < |T|^{-1}$ the Fredholm resolvent $T(\lambda)$ has the expansion*

$$T(\lambda) = \sum_{j=0}^{\infty} \lambda^j T^{j+1}$$

which is convergent in operator norm. From (2.15) we have

$$(I + \lambda T(\lambda))(I - \lambda T) = (I - \lambda T)(I + \lambda T(\lambda)) = I$$

which implies

$$T(\lambda) = T + \lambda T T(\lambda) = T + \lambda T(\lambda) T.$$

Therefore, if $T \in B_p(\mathcal{H})$ for some $p \in (0,\infty)$, then its Fredholm resolvent $T(\lambda) \in B_p(\mathcal{H})$ as well.

Remark 2.8. (i) It can be verified that the object $\|T\|_p = \left(\sum_{j\in\mathcal{J}} |s_j(T)|^p\right)^{\frac{1}{p}}$ is a norm on the $B_p(\mathcal{H})$ spaces, $p \in [1,\infty)$ (see [4], Ch. 3, Thm. 7.1). For $p \in (0,1)$, $\|\cdot\|_p$ lacks the triangle inquality property of a norm.
(ii) If we regard sequences of singular numbers $\{s_j(T)\}_{j\in\mathcal{J}}$ as members of $l_p(\mathcal{J})$, then it follows that for $T \in B_{p_1}(\mathcal{H})$, $p_1 \in (0,\infty)$, if $0 < p_1 \leq p_2 < \infty$ then $\|T\|_{p_2} \leq \|T\|_{p_1}$. The inclusion $B_{p_1}(\mathcal{H}) \subseteq B_{p_2}(\mathcal{H})$, $0 < p_1 < p_2 < \infty$ follows. Indeed, we have

$$B_{p_1}(\mathcal{H}) \subseteq B_{p_2}(\mathcal{H}) \subseteq B_\infty(\mathcal{H}) \subseteq B(\mathcal{H}), \quad 0 < p_1 < p_2 < \infty.$$

Moreover, we have the following lemma regarding completeness of the B_p spaces:

Lemma 2.9. *([1], Lemma XI.9.10.)*
Let $T_n \in B_p(\mathcal{H})$ be a sequence of operators such that for some $p \in (0, \infty)$, $\|T_n - T_m\|_p \to 0$ as $m, n \to \infty$. Then there exists a compact operator $T \in B_p(\mathcal{H})$ such that $T_n \to T$ in the $B_p(\mathcal{H})$ topology as $n \to \infty$. In particular, the spaces $B_p(\mathcal{H})$, $p > 0$, are complete and in fact Banach spaces for $p \geq 1$.

Proof. Given T_n as above, there exists a compact operator $T \in B_\infty(\mathcal{H})$ such that $T_n \to T$ as $n \to \infty$ in the uniform topology. (We are using the facts that $B_{p_1} \subseteq B_{p_2} \subseteq B_\infty$, $p_1 \leq p_2$ and that compact operators are closed in the uniform topology of operators.) Then by (2.5), we have for fixed $j \in \mathcal{J}$

$$|s_j(T_m) - s_j(T)| \leq \|T_m - T\|,$$

which implies

$$\lim_{m\to\infty} s_j(T_m) = s_j(T),$$

which in turn implies that for fixed n, k

$$\lim_{m\to\infty} s_k(T_n - T_m) = s_k(T_n - T).$$

We then have

$$\begin{aligned} \left(\sum_{k=1}^{N} |s_k(T_n - T)|^p\right)^{\frac{1}{p}} &\leq \lim_{m\to\infty} \sup \left(\sum_{k=1}^{\infty} |s_k(T_n - T_m)|^p\right)^{\frac{1}{p}} \\ &= \lim_{m\to\infty} \sup \|T_n - T_m\|_p . \end{aligned}$$

Letting $N \to \infty$ so that

$$\left(\sum_{k=1}^{N} |s_k(T_n - T)|^p\right)^{\frac{1}{p}} \to \|T_n - T\|_p$$

implies

$$\|T_n - T\|_p \leq \lim_{m\to\infty} \sup \|T_n - T_m\|_p .$$

Finally, letting $n \to \infty$ yields

$$\lim_{n\to\infty} \|T_n - T\|_p \leq \lim_{n\to\infty} \left(\lim_{m\to\infty} \sup \|T_n - T_m\|_p\right) = 0.$$

□

Definition 2.10. An operator T in the set $B_1(\mathcal{H})$ (the trace class) has *trace* defined by

$$tr(T) = \sum_{\alpha \in \mathcal{A}} (e_\alpha, Te_\alpha), \tag{2.16}$$

where $\{e_\alpha\}_{\alpha \in \mathcal{A}}$ is an orthonormal basis of $\mathcal{H}$ and $\mathcal{A} \subseteq \mathbb{N}$ is an appropriate index set.

Definition 2.11. For operators $S, T \in B_2(\mathcal{H})$ (the set of Hilbert–Schmidt operators) we define a scalar product by

$$(S, T)_{B_2(\mathcal{H})} = tr(S^*T) = \sum_{\alpha \in \mathcal{A}} (e_\alpha, S^*Te_\alpha), \tag{2.17}$$

where $\{e_\alpha\}_{\alpha \in \mathcal{A}}$ is an orthonormal basis of $\mathcal{H}$ and $\mathcal{A} \subseteq \mathbb{N}$ is an appropriate index set.

Remark 2.12. One can verify that $\left((S, S)_{B_2(\mathcal{H})}\right)^{\frac{1}{2}} = \|S\|_2$ for $S \in B_2(\mathcal{H})$. Therefore, $B_2(\mathcal{H})$ is a Hilbert space.

3 Definition and properties of the determinant for trace class operators

Let $\widetilde{T}$ be an operator of finite rank in $\mathcal{H}$ with rank $\leq n$. Let Ω be an arbitrary finite-dimensional subspace which contains the ranges of the operators $\widetilde{T}$ and $\widetilde{T}^*$. Then Ω is an invariant subspace of $\widetilde{T}$ and $\widetilde{T}$ vanishes on the orthogonal complement of Ω. Let $\{e_\alpha\}_{\alpha=1}^m$, $m \leq n$, be an orthonormal basis for Ω. Then we denote by $\det(I + \widetilde{T})$ the determinant of the matrix $\left\| \delta_{jk} + (e_j, \widetilde{T}e_k) \right\|$, $1 \leq j, k \leq m$. This determinant does not depend on the choice of the subspace Ω or the basis for it since we have

$$\det(1 + \widetilde{T}) = \prod_{j=1}^{\nu(T)} (1 + \lambda_j(\widetilde{T})),$$

where $\{\lambda_j(\widetilde{T})\}_{j=1}^{\nu(T)}$ are the nonzero eigenvalues of $\widetilde{T}$ counted up to algebraic multiplicity. This suggests that the determinant of any operator $T \in B_1(\mathcal{H})$

should be defined by the formula

$$\det(1+T) = \prod_{n=1}^{\nu(T)} (1+\lambda_n(T)), \tag{3.1}$$

where $\{\lambda_n(T)\}_{n=1}^{\nu(T)}$ are the nonzero eigenvalues of T counted up to algebraic muliplicity. The product on the right-hand side of (3.1) converges absolutely, since, for any $T \in B_1(\mathcal{H})$,

$$\sum_{j=1}^{\nu(T)} |\lambda_j(T)| \leq \|T\|_1 . \tag{3.2}$$

Theorem 3.1. *([4], p. 157)*
For $T \in B_1(\mathcal{H})$, where $\{\lambda_n(T)\}_{n=1}^{\nu(T)}$ are the nonzero eigenvalues of T counted up to algebraic muliplicity, $\det(1+zT)$ *is an entire function and*

$$|\det(1+zT)| \leq \exp\left(|z| \, \|T\|_1\right) \tag{3.3}$$

Proof. Certainly, $\det(1+zT)$ is an entire function by the definition. Then

$$\begin{aligned} |\det(1+zT)| &\leq \prod_{n=1}^{\nu(T)} (1+|z||\lambda_n(T)|) \\ &\leq \prod_{n=1}^{\infty} (1+|z|s_n(T)), \end{aligned}$$

where $\{s_n(T)\}_{n=1}^{\infty}$ are the s-numbers of T. Here the second inequality follows from (2.10). Then, using $1+x \leq \exp x$, one infers

$$\prod_{n=1}^{\infty} (1+|z|s_n(T)) \leq \exp\left(|z| \sum_{n=1}^{\infty} s_n(T)\right) = \exp\left(|z| \, \|T\|_1\right).$$

□

Theorem 3.2. *([8],Thm. 3.4.)*
The map

$$B_1(\mathcal{H}) \to \mathbb{C} \colon \; T \mapsto \det(1+T)$$

is continuous. Explicitly, for $S, T \in B_1(\mathcal{H})$,

$$|\det(1+S) - \det(1+T)| \leq \|S-T\|_1 \exp\left(1+\max(\|S\|_1 , \|T\|_1)\right). \tag{3.4}$$

Remark 3.3. The above inequality is actually a refinement of the inequality found in the cited theorem (see [8], p. 66, for details).

Theorem 3.4. *([8], Thm. 3.5.)*
(i) For any $S, T \in B_1(\mathcal{H})$,

$$\det(1 + S + T + ST) = \det(1 + S)\det(1 + T). \tag{3.5}$$

(ii) For $T \in B_1(\mathcal{H}), \det(1 + T) \neq 0$ *if an only if* $1 + T$ *is invertible.*
(iii) For $T \in B_1(\mathcal{H})$ *and* $z_0 = -\lambda^{-1}$ *with* λ *an eigenvalue with algebraic multiplicity* $n, \det(1 + zT)$ *has a zero of order* n *at* z_0.

Theorem 3.5. *(Lidskii's equality, [4], Ch. III, Thm. 8.4, [8], Thm. 3.7.) For* $T \in B_1(\mathcal{H})$, *let* $\{\lambda_n(T)\}_{n=1}^{\nu(T)}$ *be its nonzero eigenvalues counted up to algebraic mulitiplicity. Then,*

$$\sum_{n=1}^{\nu(T)} \lambda_n(T) = tr(T).$$

Corollary 3.6. *Let* $S, T \in B(\mathcal{H})$ *so that* $ST \in B_1(\mathcal{H})$ *and* $TS \in B_1(\mathcal{H})$. *Then,* $tr(ST) = tr(TS)$.

Remark 3.7. The corollary follows from the fact that ST and TS have the same eigenvalues including algebraic multiplicity. Lidskii's equality then gives the desired result.

Remark 3.8. The determinant of a trace class operator $T \in B_1(\mathcal{H})$ can also be introduced as follows (cf. [4], Sect. IV.1, [7]): Let $\{\phi_k\}_{k\in\mathcal{K}}$, $\mathcal{K} \subseteq \mathbb{N}$ an appropriate index set, be an orthonormal basis in $\mathcal{H}$. Then,

$$\det(I - T) = \lim_{N\to\infty} \det\Big(\big(\delta_{j,k} - (\phi_j, T\phi_k)\big)_{1\leq j,k\leq N}\Big).$$

Moreover, assume $\{\psi_k\}_{k\in\mathcal{K}}$, $\mathcal{K} \subseteq \mathbb{N}$ an appropriate index set, be an orthonormal basis in $\overline{\text{Ran}(T)}$. Then,

$$\det(I - T) = \lim_{N\to\infty} \det\Big(\big(\delta_{j,k} - (\psi_j, T\psi_k)\big)_{1\leq j,k\leq N}\Big).$$

Since the range $\text{Ran}(T)$ of any compact operator in $\mathcal{H}$ is separable (cf. [9], Thm. 6.5; this extends to compact operators in Banach spaces, cf. the proof of Thm. III.4.10 in [6]), and hence $\overline{\text{Ran}(T)}$ is separable (cf. [9], Thm. 2.5 (a)), this yields a simple way to define the determinant of trace class operators in nonseparable complex Hilbert spaces.

4 (Modified) Fredholm determinants

We seek explicit formulae for $g(\mu) \equiv (1+\mu T)^{-1}$, $T \in B_\infty(\mathcal{H})$ which work for all μ such that $-\mu^{-1} \notin \sigma(T)$. $g(\mu)$ is not entire in general, but it is meromorphic and can be expressed as a ratio of entire functions:

$$g(\mu) = \frac{C(\mu)}{B(\mu)}.$$

$B(\mu)$ must have zeros where $g(\mu)$ has poles. These poles are where $(1+\mu T)$ is not invertible. By Theorem 3.4, these are the values of μ where $\det(1+\mu T) = 0$. $\det(1+\mu T)$ is then a candidate for $B(\mu)$.

Remark 4.1. Let T be an $n \times n$ matrix with complex-valued entries and I_n the identity in $\mathbb{C}^n$. Then Cramer's rule gives

$$(I_n + \mu T)^{-1} = \frac{M(\mu)}{\det(I_n + \mu T)},$$

where the entries of $M(\mu)_{n\times n}$ are polynomials in μ. Using $(I_n + \mu T)^{-1} = I_n - \mu T(I_n + \mu T)^{-1}$ we then have

$$(I_n + \mu T)^{-1} = I_n + \frac{\mu \widetilde{M}(\mu)}{\det(I_n + \mu T)}$$

with $\widetilde{M}(\mu)_{n\times n}$ having polynomial entries in μ.

Remark 4.2. Alternatively, for T an $n \times n$ matrix with complex-valued entries, notice that $(I_n + \mu T)$ satisfies the Hamilton–Cayley equation

$$\sum_{m=0}^{n} \alpha_m (I_n + \mu T)^m = 0, \quad \alpha_n = 1, \quad \alpha_0 = \pm \det(I_n + \mu T).$$

Then

$$(I_n + \mu T) \sum_{m=1}^{n} \alpha_m (I_n + \mu T)^{m-1} = \mp \det(I_n + \mu T) I_n$$

and so

$$\begin{aligned}
(I_n + \mu T)^{-1} &= \frac{\mp \sum_{m=1}^{n} \alpha_m (I_n + \mu T)}{\det(I_n + \mu T)} = \frac{N(\mu)}{\det(I_n + \mu T)} \\
&= I_n + \frac{\widetilde{N}(\mu)}{\det(I_n + \mu T)},
\end{aligned}$$

where $N(\mu), \widetilde{N}(\mu)$ are $n \times n$ matrices with entries being polynomials in μ.

Definition 4.3. Let X, Y be Banach spaces. A function $f : X \to Y$ is *finitely analytic* if and only if for all $\alpha_1, \ldots, \alpha_n \in X$, $\mu_1, \ldots, \mu_n \in \mathbb{C}$, $f(\mu_1\alpha_1 + \cdots + \mu_n\alpha_n)$ is an entire function from $\mathbb{C}^n$ to Y.

Definition 4.4. Let $f : X \to Y$ be a function between Banach spaces X, Y. Let $x_0 \in X$. $F \in B(X, Y)$ is the *Frechet derivative* of f at x_0 (denoted $F = (Df)(x_0)$) if and only if $\|f(x + x_0) - f(x_0) - F(x)\| = o(\|x\|)$.

Theorem 4.5. *([8], Thm. 5.1.) Let X, Y be Banach spaces. Let f be a finitely analytic function from X to Y satisfying $\|f(x)\| \leq G(\|x\|)$ for some monotone function G on $[0, \infty)$. Then f is Frechet differentiable for all $x \in X$ and Df is a finitely analytic function from X to $B(X, Y)$ with $\|(Df)(x)\| \leq G(\|x\| + 1)$.*

Corollary 4.6. *([8], Cor. 5.2.) For $S, T \in B_1(\mathcal{H})$, the function $f : B_1(\mathcal{H}) \to \mathbb{C}$ given by $f(T) = \det(I + T)$ is Frechet differentiable with derivative given by*

$$(Df)(T) = (I + T)^{-1} \det(I + T)$$

for those T with $-1 \notin \sigma(T)$. In particular, the function

$$D(T) \equiv -T(I + T)^{-1} \det(I + T) \tag{4.1}$$

(henceforth the first Fredholm minor) defines a finitely analytic function from $B_1(\mathcal{H})$ to itself satisfying:

$$\|D(T)\|_1 \leq \|T\|_1 \exp\left(\|T\|_1\right)$$

and

$$\|D(S) - D(T)\|_1 \leq \|S - T\|_1 \exp(1 + max(\|S\|_1, \|T\|_1)).$$

Remark 4.7. The two inequalities above are refinements of the actual inequalities listed in Cor. 4.6 (see [8], p. 67 for details).

By definition,

$$I + \frac{D(\mu T)}{det(I + \mu T)} = I + \frac{-\mu T(I + \mu T)^{-1} \det(I + \mu T)}{\det(I + \mu T)} = I - \mu T(I + \mu T)^{-1}.$$

But $(I + \mu T)^{-1} = I - \mu T(I + \mu T)^{-1}$ implies that

$$(I + \mu T)^{-1} = I + \frac{D(\mu T)}{\det(I + \mu T)}. \tag{4.2}$$

Remark 4.8. The estimates for $D(\mu T)$ above and for $\det(I+\mu T)$ in Theorem 3.1 allow one to control the rate of convergence for $D(\mu T)$ and $\det(I+\mu T)$ and to obtain explicit expressions on the errors obtained by truncating their Taylor series.Our original question of finding explicit formula for $(I+\mu T)^{-1}$ has now shifted to finding expressions for the Taylor coefficients of $D(\mu T)$ and $\det(I+\mu T)$.

Theorem 4.9. *([8], Thm. 5.4.) For $T \in B_1(\mathcal{H})$, define $\alpha_n(T), \beta_n(T)$ by*

$$\det(I+\mu T) = \sum_{n=0}^{\infty} \alpha_n(T) \frac{\mu^n}{n!}$$

and

$$D(\mu T) = \sum_{n=0}^{\infty} \beta_n(T) \frac{\mu^{n+1}}{n!}.$$

Then

$$\alpha_n(T) = \begin{vmatrix} tr(T) & (n-1) & 0 & \cdots & \cdots & \cdots & 0 \\ tr(T^2) & tr(T) & (n-2) & 0 & \cdots & \cdots & 0 \\ \vdots & tr(T^2) & tr(T) & (n-3) & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ tr(T^n) & tr(T^{n-1}) & \cdots & \cdots & \cdots & \cdots & tr(T) \end{vmatrix}_{n\times n}$$

and
$\beta_n(T) =$

$$\begin{vmatrix} T & n & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ T^2 & tr(T) & (n-1) & 0 & \cdots & \cdots & \cdots & 0 \\ \vdots & tr(T^2) & tr(T) & (n-2) & 0 & \cdots & \cdots & 0 \\ \vdots & \vdots & tr(T^2) & tr(T) & (n-3) & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ T^{n+1} & tr(T^n) & tr(T^{n-1}) & \cdots & \cdots & \cdots & \cdots & tr(T) \end{vmatrix}_{(n+1)\times(n+1)}.$$

As a concrete application, we now consider an integral operator $T \in B_1(L^2((a,b);dx))$ such that

$$(Tf)(x) = \int_a^b K(x,y) f(y) dy, \quad f \in L^2((a,b);dx)$$

with $-\infty < a < b < \infty$ and with K continuous on $[a,b]\times[a,b]$.

Theorem 4.10. *([8], Thm. 3.9.) Let $T \in B_1(L^2((a,b);dx))$ with $a, b \in \mathbb{R}$, $a < b$, and integral kernel $K(\cdot,\cdot)$ continuous on $[a,b] \times [a,b]$. Then,*

$$tr(T) = \int_a^b K(x,x)dx.$$

Definition 4.11.

$$\begin{aligned} K\begin{pmatrix} x_1, & \dots, & x_n \\ y_1, & \dots, & y_n \end{pmatrix} &= \det[(K(x_i,y_j))_{1 \le i,j \le n}] \\ &= \begin{vmatrix} K(x_1,y_1) & K(x_1,y_2) & \cdots & K(x_1,y_n) \\ K(x_2,y_1) & K(x_2,y_2) & \cdots & K(x_2,y_n) \\ \vdots & \vdots & \vdots & \vdots \\ K(x_n,y_1) & \cdots & \cdots & K(x_n,y_n) \end{vmatrix}. \end{aligned}$$

Theorem 4.12. *(Fredholm formula, [8], Thm. 5.5.)*
Let $T \in B_1(L^2((a,b);dx))$ with integral kernel $K(\cdot,\cdot)$ continuous on $[a,b] \times [a,b]$. Then

$$\det(I + \mu T) = \sum_{n=0}^{\infty} \alpha_n(T) \frac{\mu^n}{n!}$$

and

$$D(\mu T) = \sum_{n=0}^{\infty} \beta_n(T) \frac{\mu^{n+1}}{n!},$$

where

$$\alpha_n(T) = \int_a^b \cdots \int_a^b dx_1 \cdots dx_n K\begin{pmatrix} x_1, & \cdots, & x_n \\ y_1, & \cdots, & y_n \end{pmatrix}$$

and $\beta_n(T)$ are integral operators with integral kernels

$$K_n(s,t) = \int_a^b \cdots \int_a^b dx_1 \cdots dx_n K\begin{pmatrix} s, & x_1, & \cdots, & x_n \\ t, & y_1, & \cdots, & y_n \end{pmatrix}.$$

Remark 4.13. The above results are not unique to $T \in B_1(L^2((a,b);dx))$. One can extend the formulas above to $T \in B_n(L^2((a,b);dx))$, $n \in \mathbb{N}$.

Lemma 4.14. *([8], Lemma 9.1.) Let $T \in B(\mathcal{H})$. Define*

$$\mathcal{R}_n(T) \equiv (I+T)\exp\left(\sum_{j=1}^{n-1} \frac{(-1)^j}{j} T^j\right) - I, \quad n \in \mathbb{N}. \tag{4.3}$$

Then for any $T \in B_n(\mathcal{H})$, $n \in \mathbb{N}$, we have $\mathcal{R}_n(T) \in B_1(\mathcal{H})$ and $T \mapsto \mathcal{R}_n(T)$ is finitely analytic.

Definition 4.15. For $T \in B_n(\mathcal{H}), n \in \mathbb{N}$, we denote

$$\det{}_n(I+T) = \det(I + \mathcal{R}_n(T)). \tag{4.4}$$

Theorem 4.16. *([8], Thm. 9.2.) Let $S, T \in B_n(\mathcal{H})$, $n \in \mathbb{N}$, with nonzero eigenvalues $\{\lambda_k(T)\}_{k=1}^{\nu(T)}$ counted up to algebraic multiplicity. Then:*
(i) For $z \in \mathbb{C}$,

$$\det{}_n(I+zT) = \prod_{k=1}^{\nu(T)} \left[(1+z\lambda_k(T))\exp\left(\sum_{j=1}^{n-1} \frac{(-1)^j}{j}\lambda_k(T)^j z^j\right)\right]. \tag{4.5}$$

(ii)

$$|\det{}_n(I+T)| \le \exp(C_n \|T\|_n^n). \tag{4.6}$$

(iii)

$$|\det{}_n(I+S) - \det{}_n(I+T)| \le \|S-T\|_n \exp[C_n(\|S\|_n + \|T\|_n + 1)^n]. \tag{4.7}$$

(iv) If $T \in B_{n-1}(\mathcal{H})$, then

$$\det{}_n(I+T) = \det{}_{n-1}(I+T)\exp\left[(-1)^{n-1}\frac{tr(T^{n-1})}{n-1}\right]. \tag{4.8}$$

In particular, if $T \in B_1(\mathcal{H})$, then

$$\det{}_n(I+T) = \det(I+T)\exp\left[\sum_{j=1}^{n-1} \frac{(-1)^j tr(T^j)}{j}\right]. \tag{4.9}$$

(v) $(I+T)^{-1}$ exists if and only if $\det_n(I+T) \neq 0$.
(vi) For $T \in B_n(\mathcal{H})$, $n \in \mathbb{N}$, and $z_0 = -\lambda^{-1}$ with λ an eigenvalue of algebraic multiplicity m, $\det_n(I+zT)$ has a zero of order m at z_0.
(vii) For $S, T \in B_2(\mathcal{H})$,

$$\det{}_2((I+S)(I+T)) = \det{}_2(I+S)\det{}_2(I+T)\exp(-tr(ST)). \tag{4.10}$$

Definition 4.17. For $T \in B_n(\mathcal{H}), n \in \mathbb{N}$, the *nth Fredholm minor* is

$$D_n(T) \equiv -Td(\mathcal{R}_1(T)) \exp\left(\sum_{j=1}^{n-1} \frac{(-1)^j T^j)}{j}\right), \tag{4.11}$$

where

$$d(T) = (I+T)^{-1} \det(I+T).$$

Theorem 4.18. *(Plemej-Smithies formula for $B_n(\mathcal{H})$, [8], Thm. 9.3.)*
Let $T \in B_n(\mathcal{H})$. Define $\alpha_m^{(n)}(T), \beta_m^{(n)}(T)$ by

$$\det{}_n(1+\mu T) = \sum_{m=0}^{\infty} \alpha_m^{(n)}(T) \frac{\mu^m}{m!}$$

and

$$D_n(\mu T) = \sum_{m=0}^{\infty} \beta_m^{(n)}(T) \frac{\mu^{m+1}}{m!}.$$

Then the formulae for $\alpha_m^{(n)}(T), \beta_m^{(n)}(T)$ are the same as those for $\alpha_m(T), \beta_m(T)$, repectively, in Theorem 4.9 after replacing $tr(T), \ldots, tr(T^{n-1})$ with zeros.

Theorem 4.19. *(Hilbert–Fredholm formula, [8], Thm. 9.4.)*
Let $T \in B_2(L^2((a,b); d\sigma))$, $(a,b) \subseteq \mathbb{R}$, σ any positive measure on (a,b), be an operator with square integrable kernel over $(a,b) \times (a,b)$, that is,

$$\int_a^b \int_a^b |K(x,y)|^2 d\sigma|x| d\sigma|y| < \infty.$$

Then

$$\det{}_2(I+\mu T) = \sum_{n=0}^{\infty} \alpha_n^{(2)} \frac{\mu^n}{n!}, \tag{4.12}$$

where

$$\alpha_n^{(2)}(T) = \int_a^b \cdots \int_a^b dx_1 \cdots dx_n \tilde{K} \begin{pmatrix} x_1, & \cdots, & x_n \\ y_1, & \cdots, & y_n \end{pmatrix}$$

and

$$\tilde{K}\begin{pmatrix} x_1, & \dots, & x_n \\ y_1, & \dots, & y_n \end{pmatrix} = \det[(K(x_i, y_j))(1-\delta_{ij}]$$
$$= \begin{vmatrix} 0 & K(x_1,y_2) & \cdots & K(x_1,y_n) \\ K(x_2,y_1) & 0 & \cdots & K(x_2,y_n) \\ \vdots & \vdots & \vdots & \vdots \\ K(x_n,y_1) & \cdots & \cdots & 0 \end{vmatrix}.$$

Theorem 4.20. *For $T \in B_1(\mathcal{H}), -\mu^{-1} \notin \sigma(T)$,*

$$(I+\mu T)^{-1} = I + \frac{\mu \widetilde{D}(\mu)}{\det(I+\mu T)},$$

where $\widetilde{D}(\mu) = \sum_{n=0}^{\infty} \mu^n \widetilde{D}_n$ is an entire operator function with $\widetilde{D}_n \in B_1(\mathcal{H})$, $n \geq 1$, and the $\widetilde{D}_n$ are given by the recurrence relation,

$$\widetilde{D}_0 = T, \widetilde{D}_n = \widetilde{D}_{n-1}T - \frac{1}{n}(tr(\widetilde{D}_{n-1}))T, \quad n \geq 1. \tag{4.13}$$

5 Perturbation determinants

Let $S, T \in B(\mathcal{H})$ with $S - T \in B_1(\mathcal{H})$. If $\mu^{-1} \notin \sigma(S)$, then

$$(I-\mu T)(I-\mu S)^{-1} = I - \mu(T-S)(I-\mu S)^{-1}$$

with $\mu(T-S)(I-\mu S)^{-1} \in B_1(\mathcal{H})$.

Definition 5.1. $D_{T/S}(\mu) = \det[(I-\mu T)(I-\mu S)^{-1}]$ is the *perturbation determinant* of the operator S by the operator $T - S$.

Remark 5.2. By definition, we have for $S, T \in B_1(\mathcal{H}), \mu^{-1} \notin \sigma(S)$,

$$D_{T/S}(\mu) = \frac{\det(I-\mu T)}{\det(I-\mu S)}.$$

Theorem 5.3. *If $S, T \in B_2(\mathcal{H}), S - T \in B_1(\mathcal{H})$, and $\mu^{-1} \notin \sigma(S)$, then*

$$D_{T/S}(\mu) = \frac{\det_2(I-\mu T)}{\det_2(I-\mu S)} \exp\left[\mu\, tr(S-T)\right].$$

Corollary 5.4. *Let $R, S, T \in B(\mathcal{H})$. If $\mu^{-1} \notin \sigma(R)$, $\mu^{-1} \notin \sigma(S)$, and $S - R, T - S \in B_1(\mathcal{H})$, then*

$$D_{T/S}(\mu)D_{S/R}(\mu) = D_{T/R}(\mu).$$

Corollary 5.5. *Let $S, T \in B(\mathcal{H})$. If $\mu^{-1} \notin \sigma(S)$, $\mu^{-1} \notin \sigma(T)$, and $S - T \in B_1(\mathcal{H})$, then*

$$D_{S/T}(\mu) = [D_{T/S}(\mu)]^{-1}.$$

Theorem 5.6. *Let $S, T \in B(\mathcal{H})$. If $\mu^{-1} \notin \sigma(S)$, $\mu^{-1} \notin \sigma(T)$, and $S - T \in B_1(\mathcal{H})$, then*

$$\begin{aligned} \frac{d}{d\mu} ln[D_{T/S}(\mu)] &= tr[S(\mu) - T(\mu)] \\ &= tr[(I - \mu T)^{-1}(S - T)(I - \mu S)^{-1}], \end{aligned}$$

where $S(\mu), T(\mu)$ are the Fredholm resolvents of S and T, respectively, as defined in (2.15). In particular, for $|\mu|$ sufficiently small, we have

$$\frac{d}{d\mu} ln[D_{T/S}(\mu)] = \sum_{j=0}^{\infty} \mu^j tr(S^{j+1} - T^{j+1}).$$

6 An example

The material of this section is taken from [5], p. 299 – 301.
Let T be an operator acting on $L^2((0,1); dx)$, defined as follows: Let

$$\begin{aligned} &K(\cdot, \cdot) \in L^2((0,1) \times (0,1); dx\, dy), \\ &K(x, y) = 0, \ y > x. \end{aligned}$$

Given $K(\cdot, \cdot)$, the Volterra integral operator T is then defined by

$$(Tf)(x) = \int_0^x K(x, y) f(y) dy, \quad x \in (0,1), \ f \in L^2((0,1); dx).$$

Consider the eigenvalue problem $Tf = \lambda f$, $0 \neq f \in L^2((0,1); dx)$. Let $g(x)$ be defined by $g(x) = \int_0^x |f(y)|^2 dy$. Then $g(x)$ is monotone and differentiable with $g'(x) = |f(x)|^2$ a.e. Let a be the infimum of the support of g, that is, $g(a) = 0$ and $g(x) > 0$ for $a < x \leq 1$. We note that $0 < g(1) < \infty$.

$$\lambda f(x) = Tf(x) = \int_0^x K(x,y)f(y)dy \quad a.e.,$$

so that

$$|\lambda|^2|f(x)| \leq \int_0^x |K(x,y)|^2 dy \int_0^x |f(y)|^2 dy \quad a.e.,$$

which implies that

$$|\lambda|^2 \frac{g'(x)}{g(x)} \leq \int_0^x |K(x,y)|^2 dy \quad a.e. \quad in \quad (0,1).$$

Integrate to get

$$|\lambda|^2 \log\left(g(x)\right)|_a^1 = \int_a^1 |\lambda|^2 \frac{g'(y)}{g(y)} dy \leq \int_0^1 \int_0^x |K(x,y)|^2 dy\, dx = \|K\|_2^2 .$$

But $0 < g(1) < \infty$ and $g(a) = 0$ imply that $|\lambda|^2 \log g(x)|_a^1$ is unbounded for non-zero λ. The only possible eigenvalue of the operator T is thus 0.

Theorem 6.1. *(The Fredholm alternative.)*
For $T \in B_\infty(\mathcal{H})$, if $\mu \neq 0$, then either:
(i) $(T - \mu I)f = g$ and $(T^* - \mu^* I)h = k$ are uniquely solvable for all $g, k \in \mathcal{H}$, or
(ii) $(T - \mu I)f = 0$ and $(T^* - \mu^* I)h = 0$ have nontrivial solutions.

Since T is compact, the Fredholm alternative implies that 0 is the only number in the spectrum of T. Therefore, every Volterra operator is quasinilpotent.

Next, let $K(x,y)$ be the characteristic function of the triangle $\{(x,y)|0 \leq y \leq x \leq 1\}$ (this is then a Volterra kernel). The induced operator is then

$$(Sf)(x) = \int_0^x f(y)dy, \quad x \in (0,1),\ f \in L^2((0,1);dx).$$

To find the norm of S, we recall that $\|S\| = s_1(S)$, that is, $\|S\|$ equals the largest non-zero eigenvalue of $(S^*S)^{\frac{1}{2}}$.

$$(S^*f)(x) = \int_x^1 f(y)dy \quad x \in (0,1),\ f \in L^2((0,1);dx).$$

We can find the integral kernel $S^*S(x,y)$ of S^*S to be

$$S^*S(x,y) = 1 - \max(x,y) = \begin{cases} 1-x, & 0 \le y \le x \le 1, \\ 1-y, & 0 \le x \le y \le 1. \end{cases}$$

Then, for $f \in L^2((0,1);dy)$,

$$(S^*Sf)(x) = \int_0^1 f(y)dy - x\int_0^x f(y)dy - \int_x^1 yf(y)dy \quad a.e.$$

Differentiating the equation $(S^*Sf)(x) = \lambda f(x)$ twice with respect to x then yields $-f(x) = \lambda f''(x)$. Solving this differential equation yields the eigenvalues

$$\lambda_k = \frac{1}{(k+\frac{1}{2})^2\pi^2}, \quad k \in \mathbb{N}_0 = \mathbb{N} \cup \{0\},$$

with corresponding orthonormal eigenvectors

$$f_k(x) = \sqrt{2}\cos[\pi(k+(1/2))x], \quad k \in \mathbb{N}_0.$$

The largest eigenvalue of $|S^*S|^{\frac{1}{2}}$ then occurs when $k=0$. Therefore,

$$\|S\| = \frac{2}{\pi}.$$

The singular values of T are

$$s_k(T) = \frac{2}{(2k+1)\pi}, \quad k \in \mathbb{N}_0.$$

One can then show that $S \in B_2((L^2(0,1));dy)$ but $S \notin B_1((L^2(0,1));dy)$. Specifically,

$$\begin{aligned} \|S\|_2 &= \left(\sum_{k\in\mathbb{N}_0} |s_k(S)|^2\right)^{\frac{1}{2}} \\ &= \frac{2}{\pi}\left(\sum_{k\in\mathbb{N}_0} \frac{1}{(2k+1)^2}\right)^{\frac{1}{2}} \\ &= \frac{2}{\pi}\left(\frac{\pi^2}{8}\right)^{\frac{1}{2}} = 2^{-\frac{1}{2}} \end{aligned}$$

and

$$\begin{aligned}\|S\|_1 &= \sum_{k\in\mathbb{N}_0} |s_k(S)| \\ &= \frac{2}{\pi}\sum_{k\in\mathbb{N}_0}\frac{1}{2k+1} \\ &= \infty.\end{aligned}$$

Since S is Hilbert-Schmidt and quasinilpotent, it can be approximated in the Hilbert-Schmidt norm by nilpotent operators S_n of finite rank. One then obtains,

$$\begin{aligned}\det_2(I+S) &= \lim_{n\to\infty}\det_2(I+S_n) \\ &= \lim_{n\to\infty}\det(I+S_n)\exp\left(\sum_{j=1}^{n-1}\frac{(-1)^j tr(S_n^j)}{j}\right).\end{aligned}$$

But $tr(S_n^j)=0$, $j\geq 1$ and

$$\det(I+S_n)=\prod_{k\in\mathbb{N}_0}(1+\lambda_k(S_n))=\prod_{k\in\mathbb{N}_0}(1+0)=1$$

implies that

$$\det_2(I+S)=1.$$

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(MODIFIED) FREDHOLM DETERMINANTS FOR OPERATORS WITH MATRIX-VALUED SEMI-SEPARABLE INTEGRAL KERNELS REVISITED

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Dedicated with great pleasure to Eduard R. Tsekanovskii on the occasion of his 65th birthday.

Abstract. We revisit the computation of (2-modified) Fredholm determinants for operators with matrix-valued semi-separable integral kernels. The latter occur, for instance, in the form of Green's functions associated with closed ordinary differential operators on arbitrary intervals on the real line. Our approach determines the (2-modified) Fredholm determinants in terms of solutions of closely associated Volterra integral equations, and as a result offers a natural way to compute such determinants.

We illustrate our approach by identifying classical objects such as the Jost function for half-line Schrödinger operators and the inverse transmission coefficient for Schrödinger operators on the real line as Fredholm determinants, and rederiving the well-known expressions for them in due course. We also apply our formalism to Floquet theory of Schrödinger operators, and upon identifying the connection between the Floquet discriminant and underlying Fredholm determinants, we derive new representations of the Floquet discriminant.

Finally, we rederive the explicit formula for the 2-modified Fredholm determinant corresponding to a convolution integral operator, whose kernel is associated with a symbol given by a rational function, in a straghtforward manner. This determinant formula represents a Wiener–Hopf analog of Day's formula for the determinant associated with finite Toeplitz matrices generated by the Laurent expansion of a rational function.

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To appaear in *Integral Equations and Operator Theory.*

1. Introduction

We offer a self-contained and elementary approach to the computation of Fredholm and 2-modified Fredholm determinants associated with $m\times m$ matrix-valued, semi-separable integral kernels on arbitrary intervals $(a,b)\subseteq\mathbb{R}$ of the type

$$K(x,x')=\begin{cases} f_1(x)g_1(x'), & a<x'<x<b,\\ f_2(x)g_2(x'), & a<x<x'<b,\end{cases} \tag{1.1}$$

associated with the Hilbert–Schmidt operator K in $L^2((a,b);dx)^m$, $m\in\mathbb{N}$,

$$(Kf)(x)=\int_a^b dx'\,K(x,x')f(x'),\quad f\in L^2((a,b);dx)^m, \tag{1.2}$$

assuming

$$f_j\in L^2((a,b);dx)^{m\times n_j},\ g_j\in L^2((a,b);dx)^{n_j\times m},\quad n_j\in\mathbb{N},\ j=1,2. \tag{1.3}$$

We emphasize that Green's matrices and resolvent operators associated with closed ordinary differential operators on arbitrary intervals (finite or infinite) on the real line are always of the form (1.1)–(1.3) (cf. [11, Sect. XIV.3]), as are certain classes of convolution operators (cf. [11, Sect. XIII.10]).

To describe the approach of this paper we briefly recall the principal ideas of the approach to $m\times m$ matrix-valued semi-separable integral kernels in the monographs by Gohberg, Goldberg, and Kaashoek [11, Ch. IX] and Gohberg, Goldberg, and Krupnik [14, Ch. XIII]. It consists in decomposing K in (1.2) into a Volterra operator H_a and a finite-rank operator QR

$$K=H_a+QR, \tag{1.4}$$

where

$$(H_af)(x)=\int_a^x dx'\,H(x,x')f(x'),\quad f\in L^2((a,b);dx)^m, \tag{1.5}$$

$$H(x,x')=f_1(x)g_1(x')-f_2(x)g_2(x'),\quad a<x'<x<b \tag{1.6}$$

and

$$Q\colon \mathbb{C}^{n_2}\mapsto L^2((a,b);dx)^m,\quad (Q\underline{u})(x)=f_2(x)\underline{u},\quad \underline{u}\in\mathbb{C}^{n_2}, \tag{1.7}$$

$$R\colon L^2((a,b);dx)^m\mapsto\mathbb{C}^{n_2},\quad (Rf)=\int_a^b dx'\,g_2(x')f(x'), \tag{1.8}$$
$$f\in L^2((a,b);dx)^m.$$

Moreover, introducing

$$C(x) = (f_1(x) \;\; f_2(x)), \quad B(x) = (g_1(x) \;\; -g_2(x))^\top \tag{1.9}$$

and the $n \times n$ matrix A $(n = n_1 + n_2)$

$$A(x) = \begin{pmatrix} g_1(x)f_1(x) & g_1(x)f_2(x) \\ -g_2(x)f_1(x) & -g_2(x)f_2(x) \end{pmatrix}, \tag{1.10}$$

one considers a particular nonsingular solution $U(\cdot, \alpha)$ of the following first-order system of differential equations

$$U'(x, \alpha) = \alpha A(x)U(x, \alpha) \text{ for a.e. } x \in (a, b) \text{ and } \alpha \in \mathbb{C} \tag{1.11}$$

and obtains

$$(I - \alpha H_a)^{-1} = I + \alpha J_a(\alpha) \text{ for all } \alpha \in \mathbb{C}, \tag{1.12}$$

$$(J_a(\alpha)f)(x) = \int_a^x dx' \, J(x, x', \alpha)f(x'), \quad f \in L^2((a, b); dx)^m, \tag{1.13}$$

$$J(x, x', \alpha) = C(x)U(x, \alpha)U(x', \alpha)^{-1}B(x'), \quad a < x' < x < b. \tag{1.14}$$

Next, observing

$$I - \alpha K = (I - \alpha H_a)[I - \alpha(I - \alpha H_a)^{-1}QR] \tag{1.15}$$

and assuming that K is a trace class operator,

$$K \in \mathcal{B}_1(L^2((a, b); dx)^m), \tag{1.16}$$

one computes,

$$\begin{aligned} \det(I - \alpha K) &= \det(I - \alpha H_a)\det(I - \alpha(I - \alpha H_a)^{-1}QR) \\ &= \det(I - \alpha(I - \alpha H_a)^{-1}QR) \\ &= \det_{\mathbb{C}^{n_2}}(I_{n_2} - \alpha R(I - \alpha H_a)^{-1}Q). \end{aligned} \tag{1.17}$$

In particular, the Fredholm determinant of $I - \alpha K$ is reduced to a finite-dimensional determinant induced by the finite rank operator QR in (1.4). Up to this point we followed the treatment in [11, Ch. IX]). Now we will depart from the presentation in [11, Ch. IX] and [14, Ch. XIII] that focuses on a solution $U(\cdot, \alpha)$ of (1.11) normalized by $U(a, \alpha) = I_n$. The latter normalization is in general not satisfied for Schrödinger operators on a half-line or on the whole real line possessing eigenvalues as discussed in Section 4.

To describe our contribution to this circle of ideas we now introduce the Volterra integral equations

$$\begin{aligned}\hat{f}_1(x,\alpha) &= f_1(x) - \alpha \int_x^b dx'\, H(x,x')\hat{f}_1(x',\alpha),\\ \hat{f}_2(x,\alpha) &= f_2(x) + \alpha \int_a^x dx'\, H(x,x')\hat{f}_2(x',\alpha), \quad \alpha\in\mathbb{C}\end{aligned} \tag{1.18}$$

with solutions $\hat{f}_j(\cdot,\alpha)\in L^2((a,b);dx)^{m\times n_j}$, $j=1,2$, and note that the first-order $n\times n$ system of differential equations (1.11) then permits the explicit particular solution

$$\begin{aligned}&U(x,\alpha)\\ &\quad = \begin{pmatrix} I_{n_1} - \alpha\int_x^b dx'\, g_1(x')\hat{f}_1(x',\alpha) & \alpha\int_a^x dx'\, g_1(x')\hat{f}_2(x',\alpha) \\ \alpha\int_x^b dx'\, g_2(x')\hat{f}_1(x',\alpha) & I_{n_2} - \alpha\int_a^x dx'\, g_2(x')\hat{f}_2(x',\alpha)\end{pmatrix},\\ &\qquad\qquad x\in(a,b).\end{aligned} \tag{1.19}$$

Given (1.19), one can supplement (1.17) by

$$\begin{aligned}\det(I-\alpha K) &= \det_{\mathbb{C}^{n_2}}(I_{n_2} - \alpha R(I-\alpha H_a)^{-1}Q)\\ &= \det_{\mathbb{C}^{n_2}}\bigg(I_{n_2} - \alpha\int_a^b dx\, g_2(x)\hat{f}_2(x,\alpha)\bigg)\\ &= \det_{\mathbb{C}^{n}}(U(b,\alpha)),\end{aligned} \tag{1.20}$$

our principal result. A similar set of results can of course be obtained by introducing the corresponding Volterra operator H_b in (2.5). Moreover, analogous results hold for 2-modified Fredholm determinants in the case where K is only assumed to be a Hilbert–Schmidt operator.

Equations (1.17) and (1.20) summarize this approach based on decomposing K into a Volterra operator plus finite rank operator in (1.4), as advocated in [11, Ch. IX] and [14, Ch. XIII], and our additional twist of relating this formalism to the underlying Volterra integral equations (1.18) and the explicit solution (1.19) of (1.11).

In Section 2 we set up the basic formalism leading up to the solution U in (1.19) of the first-order system of differential equations (1.11). In Section 3 we derive the set of formulas (1.17), (1.20), if K is a trace class operator, and their counterparts for 2-modified Fredholm determinants, assuming K to be a Hilbert–Schmidt operator only. Section 4 then treats four particular applications: First we treat the case of half-line Schrödinger operators in which we identify the Jost function as a Fredholm determinant (a well-known, in fact, classical result due to Jost and Pais [23]). Next, we study the case of Schrödinger operators on the real line in which we characterize the inverse of the transmission coefficient as a Fredholm determinant (also a well-known result, see, e.g., [31, Appendix A], [36, Proposition 5.7]). We also revisit this problem by replacing the second-order Schrödinger equation by the equivalent first-order 2×2 system and determine the associated 2-modified Fredholm determinant. The case of periodic Schrödinger operators in which we derive a new one-parameter family of representations of the Floquet discriminant and relate it to underlying Fredholm determinants is discussed next. Apparently, this is a new result. In our final Section 5, we rederive the explicit formula for the 2-modified Fredholm determinant corresponding to a convolution integral operator whose kernel is associated with a symbol given by a rational function. The latter represents a Wiener–Hopf analog of Day's formula [7] for the determinant of finite Toeplitz matrices generated by the Laurent expansion of a rational function. The approach to (2-modified) Fredholm determinants of semi-separable kernels advocated in this paper permits a remarkably elementary derivation of this formula compared to the current ones in the literature (cf. the references provided at the end of Section 5).

The effectiveness of the approach pursued in this paper is demonstrated by the ease of the computations involved and by the unifying character it takes on when applied to differential and convolution-type operators in several different settings.

2. Hilbert–Schmidt operators with semi-separable integral kernels

In this section we consider Hilbert-Schmidt operators with matrix-valued semi-separable integral kernels following Gohberg, Goldberg, and Kaashoek [11, Ch. IX] and Gohberg, Goldberg, and Krupnik [14, Ch. XIII] (see also [15]). To set up the basic formalism we introduce the following hypothesis assumed throughout this section.

Hypothesis 2.1. *Let $-\infty \leq a < b \leq \infty$ and $m, n_1, n_2 \in \mathbb{N}$. Suppose that f_j are $m \times n_j$ matrices and g_j are $n_j \times m$ matrices, $j = 1, 2$, with (Lebesgue) measurable entries on (a, b) such that*

$$f_j \in L^2((a,b); dx)^{m \times n_j}, \ g_j \in L^2((a,b); dx)^{n_j \times m}, \quad j = 1, 2. \tag{2.1}$$

Given Hypothesis 2.1, we introduce the Hilbert–Schmidt operator

$$\begin{aligned} &K \in \mathcal{B}_2(L^2((a,b); dx)^m), \\ &(Kf)(x) = \int_a^b dx'\, K(x,x') f(x'), \quad f \in L^2((a,b); dx)^m \end{aligned} \tag{2.2}$$

in $L^2((a,b);dx)^m$ with $m\times m$ matrix-valued integral kernel $K(\cdot,\cdot)$ defined by

$$K(x,x') = \begin{cases} f_1(x)g_1(x'), & a<x'<x<b, \\ f_2(x)g_2(x'), & a<x<x'<b. \end{cases} \tag{2.3}$$

One verifies that K is a finite rank operator in $L^2((a,b);dx)^m$ if $f_1=f_2$ and $g_1=g_2$ a.e. Conversely, any finite rank operator in $L^2((a,b));dx)^m$ is of the form (2.2), (2.3) with $f_1=f_2$ and $g_1=g_2$ (cf. [11, p. 150]).

Associated with K we also introduce the Volterra operators H_a and H_b in $L^2((a,b);dx)^m$ defined by

$$(H_af)(x) = \int_a^x dx'\, H(x,x')f(x'), \tag{2.4}$$

$$(H_bf)(x) = -\int_x^b dx'\, H(x,x')f(x'); \quad f\in L^2((a,b);dx)^m, \tag{2.5}$$

with $m\times m$ matrix-valued (triangular) integral kernel

$$H(x,x') = f_1(x)g_1(x') - f_2(x)g_2(x'). \tag{2.6}$$

Moreover, introducing the matrices[1]

$$C(x) = (f_1(x) \;\; f_2(x)), \tag{2.7}$$

$$B(x) = (g_1(x) \;\; -g_2(x))^\top, \tag{2.8}$$

one verifies

$$H(x,x') = C(x)B(x'), \;\text{ where } \begin{cases} a<x'<x<b & \text{for } H_a, \\ a<x<x'<b & \text{for } H_b \end{cases} \tag{2.9}$$

and[2]

$$K(x,x') = \begin{cases} C(x)(I_n-P_0)B(x'), & a<x'<x<b, \\ -C(x)P_0B(x'), & a<x<x'<b \end{cases} \tag{2.10}$$

with

$$P_0 = \begin{pmatrix} 0 & 0 \\ 0 & I_{n_2} \end{pmatrix}. \tag{2.11}$$

[1] $M^\top$ denotes the transpose of the matrix M.
[2] I_k denotes the identity matrix in $\mathbb{C}^k$, $k\in\mathbb{N}$.

Next, introducing the linear maps

$$Q\colon \mathbb{C}^{n_2} \mapsto L^2((a,b);dx)^m, \quad (Q\underline{u})(x) = f_2(x)\underline{u}, \quad \underline{u} \in \mathbb{C}^{n_2}, \tag{2.12}$$

$$R\colon L^2((a,b);dx)^m \mapsto \mathbb{C}^{n_2}, \quad (Rf) = \int_a^b dx'\, g_2(x')f(x'), \quad f \in L^2((a,b);dx)^m, \tag{2.13}$$

$$S\colon \mathbb{C}^{n_1} \mapsto L^2((a,b);dx)^m, \quad (S\underline{v})(x) = f_1(x)\underline{v}, \quad \underline{v} \in \mathbb{C}^{n_1}, \tag{2.14}$$

$$T\colon L^2((a,b);dx)^m \mapsto \mathbb{C}^{n_1}, \quad (Tf) = \int_a^b dx'\, g_1(x')f(x'), \quad f \in L^2((a,b);dx)^m, \tag{2.15}$$

one easily verifies the following elementary yet significant result.

Lemma 2.2 ([11], Sect. IX.2; [14], Sect. XIII.6)**.** *Assume Hypothesis* 2.1. *Then*

$$K = H_a + QR \tag{2.16}$$

$$= H_b + ST. \tag{2.17}$$

In particular, since R and T are of finite rank, so are $K - H_a$ and $K - H_b$.

Remark 2.3. *The decompositions* (2.16) *and* (2.17) *of K are significant since they prove that K is the sum of a Volterra and a finite rank operator. As a consequence, the* (2*-modified) determinants corresponding to $I - \alpha K$ can be reduced to determinants of finite-dimensional matrices, as will be further discussed in Sections* 3 *and* 4*.*

To describe the inverse[3] of $I - \alpha H_a$ and $I - \alpha H_b$, $\alpha \in \mathbb{C}$, one introduces the $n \times n$ matrix A ($n = n_1 + n_2$)

$$A(x) = \begin{pmatrix} g_1(x)f_1(x) & g_1(x)f_2(x) \\ -g_2(x)f_1(x) & -g_2(x)f_2(x) \end{pmatrix} \tag{2.18}$$

$$= B(x)C(x) \text{ for a.e. } x \in (a,b) \tag{2.19}$$

and considers a particular nonsingular solution $U = U(x,\alpha)$ of the first-order $n \times n$ system of differential equations

$$U'(x,\alpha) = \alpha A(x)U(x,\alpha) \text{ for a.e. } x \in (a,b) \text{ and } \alpha \in \mathbb{C}. \tag{2.20}$$

[3] I denotes the identity operator in $L^2((a,b);dx)^m$.

Since $A \in L^1((a,b))^{n\times n}$, the general solution V of (2.20) is an $n\times n$ matrix with locally absolutely continuous entries on (a,b) of the form $V = UD$ for any constant $n\times n$ matrix D (cf. [11, Lemma IX.2.1])[4].

Theorem 2.4 ([11], Sect. IX.2; [14], Sects. XIII.5, XIII.6)**.**
Assume Hypothesis 2.1 *and let* $U(\cdot,\alpha)$ *denote a nonsingular solution of* (2.20). *Then,*
(i) $I-\alpha H_a$ *and* $I-\alpha H_b$ *are invertible for all* $\alpha\in\mathbb{C}$ *and*

$$(I-\alpha H_a)^{-1} = I + \alpha J_a(\alpha), \tag{2.21}$$

$$(I-\alpha H_b)^{-1} = I + \alpha J_b(\alpha), \tag{2.22}$$

$$(J_a(\alpha)f)(x) = \int_a^x dx'\, J(x,x',\alpha)f(x'), \tag{2.23}$$

$$(J_b(\alpha)f)(x) = -\int_x^b dx'\, J(x,x',\alpha)f(x'); \quad f\in L^2((a,b);dx)^m, \tag{2.24}$$

$$J(x,x',\alpha) = C(x)U(x,\alpha)U(x',\alpha)^{-1}B(x'), \tag{2.25}$$

$$\text{where } \begin{cases} a < x' < x < b & \text{for } J_a, \\ a < x < x' < b & \text{for } J_b. \end{cases}$$

(ii) Let $\alpha\in\mathbb{C}$. *Then* $I-\alpha K$ *is invertible if and only if the* $n_2\times n_2$ *matrix* $I_{n_2} - \alpha R(I-\alpha H_a)^{-1}Q$ *is. Similarly,* $I-\alpha K$ *is invertible if and only if the* $n_1\times n_1$ *matrix* $I_{n_1}-\alpha T(I-\alpha H_b)^{-1}S$ *is. In particular,*

$$(I-\alpha K)^{-1} = (I-\alpha H_a)^{-1} + \alpha(I-\alpha H_a)^{-1}QR(I-\alpha K)^{-1} \tag{2.26}$$

$$= (I-\alpha H_a)^{-1} \tag{2.27}$$

$$\quad + \alpha(I-\alpha H_a)^{-1}Q[I_{n_2} - \alpha R(I-\alpha H_a)^{-1}Q]^{-1}R(I-\alpha H_a)^{-1}$$

$$= (I-\alpha H_b)^{-1} + \alpha(I-\alpha H_b)^{-1}ST(I-\alpha K)^{-1} \tag{2.28}$$

$$= (I-\alpha H_b)^{-1} \tag{2.29}$$

$$\quad + \alpha(I-\alpha H_b)^{-1}S[I_{n_1} - \alpha T(I-\alpha H_b)^{-1}S]^{-1}T(I-\alpha H_b)^{-1}.$$

[4] If $a > -\infty$, V extends to an absolutely continuous $n\times n$ matrix on all intervals of the type $[a,c)$, $c<b$. The analogous consideration applies to the endpoint b if $b<\infty$.

Moreover,

$$(I - \alpha K)^{-1} = I + \alpha L(\alpha), \tag{2.30}$$

$$(L(\alpha)f)(x) = \int_a^b dx'\, L(x, x', \alpha) f(x'), \tag{2.31}$$

$$L(x, x', \alpha) \tag{2.32}$$
$$= \begin{cases} C(x)U(x,\alpha)(I - P(\alpha))U(x',\alpha)^{-1}B(x'), & a < x' < x < b, \\ -C(x)U(x,\alpha)P(\alpha)U(x',\alpha)^{-1}B(x'), & a < x < x' < b, \end{cases}$$

where $P(\alpha)$ *satisfies*

$$P_0 U(b,\alpha)(I - P(\alpha)) = (I - P_0)U(a,\alpha)P(\alpha), \quad P_0 = \begin{pmatrix} 0 & 0 \\ 0 & I_{n_2} \end{pmatrix}. \tag{2.33}$$

Remark 2.5. (*i*) *The results* (2.21)–(2.25) *and* (2.30)–(2.33) *are easily verified by computing* $(I - \alpha H_a)(I + \alpha J_a)$ *and* $(I + \alpha J_a)(I - \alpha H_a)$*, etc., using an integration by parts. Relations* (2.26)–(2.29) *are clear from* (2.16) *and* (2.17)*, a standard resolvent identity, and the fact that* $K - H_a$ *and* $K - H_b$ *factor into* QR *and* ST*, respectively.*
(*ii*) *The discussion in* [11, Sect. IX.2], [14, Sects. XIII.5, XIII.6] *starts from the particular normalization*

$$U(a, \alpha) = I_n \tag{2.34}$$

of a solution U *satisfying* (2.20)*. In this case the explicit solution for* $P(\alpha)$ *in* (2.33) *is given by*

$$P(\alpha) = \begin{pmatrix} 0 & 0 \\ U_{2,2}(b,\alpha)^{-1}U_{2,1}(b,\alpha) & I_{n_2} \end{pmatrix}. \tag{2.35}$$

However, for concrete applications to differential operators to be discussed in Section 4*, the normalization* (2.34) *is not necessarily possible.*

Rather than solving the basic first-order system of differential equations $U' = \alpha AU$ in (2.20) with the fixed initial condition $U(a,\alpha) = I_n$ in (2.34), we now derive an explicit particular solution of (2.20) in terms of closely associated solutions of Volterra integral equations involving the integral kernel $H(\cdot,\cdot)$ in (2.6). This approach is most naturally suited for the applications to Jost functions, transmission coefficients, and Floquet discriminants we discuss in Section 4 and to the class of Wiener–Hopf operators we study in Section 5.

Still assuming Hypothesis 2.1, we now introduce the Volterra integral equations

$$\hat{f}_1(x,\alpha) = f_1(x) - \alpha \int_x^b dx'\, H(x,x')\hat{f}_1(x',\alpha), \tag{2.36}$$

$$\hat{f}_2(x,\alpha) = f_2(x) + \alpha \int_a^x dx'\, H(x,x')\hat{f}_2(x',\alpha); \quad \alpha \in \mathbb{C}, \tag{2.37}$$

with solutions $\hat{f}_j(\cdot,\alpha) \in L^2((a,b);dx)^{m\times n_j}$, $j = 1,2$.

Lemma 2.6. *Assume Hypothesis* 2.1 *and let* $\alpha \in \mathbb{C}$.
(*i*) *The first-order* $n\times n$ *system of differential equations* $U' = \alpha AU$ *a.e. on* (a,b) *in* (2.20) *permits the explicit particular solution*

$$U(x,\alpha) = \begin{pmatrix} I_{n_1} - \alpha \int_x^b dx'\, g_1(x')\hat{f}_1(x',\alpha) & \alpha \int_a^x dx'\, g_1(x')\hat{f}_2(x',\alpha) \\ \alpha \int_x^b dx'\, g_2(x')\hat{f}_1(x',\alpha) & I_{n_2} - \alpha \int_a^x dx'\, g_2(x')\hat{f}_2(x',\alpha) \end{pmatrix}, \quad x \in (a,b). \tag{2.38}$$

As long as[5]

$$\det_{\mathbb{C}^{n_1}}\left(I_{n_1} - \alpha \int_a^b dx\, g_1(x)\hat{f}_1(x,\alpha)\right) \neq 0, \tag{2.39}$$

or equivalently,

$$\det_{\mathbb{C}^{n_2}}\left(I_{n_2} - \alpha \int_a^b dx\, g_2(x)\hat{f}_2(x,\alpha)\right) \neq 0, \tag{2.40}$$

U *is nonsingular for all* $x \in (a,b)$ *and the general solution* V *of* (2.20) *is then of the form* $V = UD$ *for any constant* $n\times n$ *matrix* D.
(*ii*) *Choosing* (2.38) *as the particular solution* U *in* (2.30)–(2.33), $P(\alpha)$ *in* (2.33) *simplifies to*

$$P(\alpha) = P_0 = \begin{pmatrix} 0 & 0 \\ 0 & I_{n_2} \end{pmatrix}. \tag{2.41}$$

Proof. Differentiating the right-hand side of (2.38) with respect to x and using the Volterra integral equations (2.36), (2.37) readily proves that U satisfies $U' = \alpha AU$ a.e. on (a,b).

[5] $\det_{\mathbb{C}^k}(M)$ and $\operatorname{tr}_{\mathbb{C}^k}(M)$ denote the determinant and trace of a $k\times k$ matrix M with complex-valued entries, respectively.

By Liouville's formula (cf., e.g., [21, Theorem IV.1.2]) one infers

$$\det_{\mathbb{C}^n}(U(x,\alpha)) = \det_{\mathbb{C}^n}(U(x_0,\alpha)) \exp\left(\alpha \int_{x_0}^{x} dx' \operatorname{tr}_{\mathbb{C}^n}(A(x'))\right), \quad x, x_0 \in (a,b). \tag{2.42}$$

Since $\operatorname{tr}_{\mathbb{C}^n}(A) \in L^1((a,b);dx)$ by (2.1),

$$\lim_{x\downarrow a} \det_{\mathbb{C}^n}(U(x,\alpha)) \text{ and } \lim_{x\uparrow b} \det_{\mathbb{C}^n}(U(x,\alpha)) \text{ exist.} \tag{2.43}$$

Hence, if (2.39) holds, $U(x,\alpha)$ is nonsingular for x in a neighborhood (a,c), $a < c$, of a, and similarly, if (2.40) holds, $U(x,\alpha)$ is nonsingular for x in a neighborhood (c,b), $c < b$, of b. In either case, (2.42) then proves that $U(x,\alpha)$ is nonsingular for all $x \in (a,b)$.

Finally, since $U_{2,1}(b,\alpha) = 0$, (2.41) follows from (2.35). □

Remark 2.7. *In concrete applications* (*e.g., to Schrödinger operators on a half-line or on the whole real axis as discussed in Section* 4), *it may happen that* $\det_{\mathbb{C}^n}(U(x,\alpha))$ *vanishes for certain values of intrinsic parameters* (*such as the energy parameter*). *Hence, a normalization of the type* $U(a,\alpha) = I_n$ *is impossible in the case of such parameter values and the normalization of* U *is best left open as illustrated in Section* 4. *One also observes that in general our explicit particular solution* U *in* (2.38) *satisfies* $U(a,\alpha) \neq I_n$, $U(b,\alpha) \neq I_n$.

Remark 2.8. *In applications to Schrödinger and Dirac-type systems,* A *is typically of the form*

$$A(x) = e^{-Mx} \widetilde{A}(x) e^{Mx}, \quad x \in (a,b) \tag{2.44}$$

where M *is an* x*-independent* $n \times n$ *matrix* (*in general depending on a spectral parameter*) *and* $\widetilde{A}$ *has a simple asymptotic behavior such that for some* $x_0 \in (a,b)$

$$\int_a^{x_0} w_a(x) dx \, |\widetilde{A}(x) - \widetilde{A}_-| + \int_{x_0}^{b} w_b(x) dx \, |\widetilde{A}(x) - \widetilde{A}_+| < \infty \tag{2.45}$$

for constant $n \times n$ *matrices* $\widetilde{A}_\pm$ *and appropriate weight functions* $w_a \geq 0$, $w_b \geq 0$. *Introducing* $W(x,\alpha) = e^{Mx} U(x,\alpha)$, *equation* (2.20) *reduces to*

$$W'(x,\alpha) = [M + \alpha \widetilde{A}(x)] W(x,\alpha), \quad x \in (a,b) \tag{2.46}$$

with

$$\det_{\mathbb{C}^n}(W(x,\alpha)) = \det_{\mathbb{C}^n}(U(x,\alpha)) e^{-\operatorname{tr}_{\mathbb{C}^n}(M)x}, \quad x \in (a,b). \tag{2.47}$$

The system (2.46) *then leads to operators H_a, H_b, and K. We will briefly illustrate this in connection with Schrödinger operators on the line in Remark* 4.8.

3. (Modified) Fredholm determinants for operators with semi-separable integral kernels

In the first part of this section we suppose that K is a trace class operator and consider the Fredholm determinant of $I - K$. In the second part we consider 2-modified Fredholm determinants in the case where K is a Hilbert–Schmidt operator.

In the context of trace class operators we assume the following hypothesis.

Hypothesis 3.1. *In addition to Hypothesis* 2.1*, we suppose that K is a trace class operator, $K \in \mathcal{B}_1(L^2((a,b);dx)^m)$.*

The following results can be found in Gohberg, Goldberg, and Kaashoek [11, Theorem 3.2] and in Gohberg, Goldberg, and Krupnik [14, Sects. XIII.5, XIII.6] under the additional assumptions that a, b are finite and U satisfies the normalization $U(a) = I_n$ (cf. (2.20), (2.34)). Here we present the general case where $(a,b) \subseteq \mathbb{R}$ is an arbitrary interval on the real line and U is not normalized but given by the particular solution (2.38).

In the course of the proof we use some of the standard properties of determinants, such as,

$$\det((I_{\mathcal{H}} - A)(I_{\mathcal{H}} - B)) = \det(I_{\mathcal{H}} - A)\det(I_{\mathcal{H}} - B), \quad A, B \in \mathcal{B}_1(\mathcal{H}), \tag{3.1}$$

$$\begin{aligned} &\det(I_{\mathcal{H}_1} - AB) = \det(I_{\mathcal{H}} - BA) \quad \text{for all } A \in \mathcal{B}_1(\mathcal{H}_1, \mathcal{H}), \\ &\quad B \in \mathcal{B}(\mathcal{H}, \mathcal{H}_1) \text{ such that } AB \in \mathcal{B}_1(\mathcal{H}_1),\, BA \in \mathcal{B}_1(\mathcal{H}), \end{aligned} \tag{3.2}$$

and

$$\det(I_{\mathcal{H}} - A) = \det_{\mathbb{C}^k}(I_k - D_k) \text{ for } A = \begin{pmatrix} 0 & C \\ 0 & D_k \end{pmatrix}, \ \mathcal{H} = \mathcal{K} \dotplus \mathbb{C}^k, \tag{3.3}$$

since

$$I_{\mathcal{H}} - A = \begin{pmatrix} I_{\mathcal{K}} & -C \\ 0 & I_k - D_k \end{pmatrix} = \begin{pmatrix} I_{\mathcal{K}} & 0 \\ 0 & I_k - D_k \end{pmatrix} \begin{pmatrix} I_{\mathcal{K}} & -C \\ 0 & I_k \end{pmatrix}. \tag{3.4}$$

Here $\mathcal{H}$ and $\mathcal{H}_1$ are complex separable Hilbert spaces, $\mathcal{B}(\mathcal{H})$ denotes the set of bounded linear operators on $\mathcal{H}$, $\mathcal{B}_p(\mathcal{H})$, $p \geq 1$, denote the usual trace ideals of $\mathcal{B}(\mathcal{H})$, and $I_{\mathcal{H}}$ denotes the identity operator in $\mathcal{H}$.

Moreover, $\det_p(I_{\mathcal{H}}-A)$, $A\in\mathcal{B}_p(\mathcal{H})$, denotes the ($p$-modified) Fredholm determinant of $I_{\mathcal{H}}-A$ with $\det_1(I_{\mathcal{H}}-A)=\det(I_{\mathcal{H}}-A)$, $A\in\mathcal{B}_1(\mathcal{H})$, the standard Fredholm determinant of a trace class operator, and $\operatorname{tr}(A)$, $A\in\mathcal{B}_1(\mathcal{H})$, the trace of a trace class operator. Finally, $\dotplus$ in (3.3) denotes a direct but not necessary orthogonal direct decomposition of $\mathcal{H}$ into $\mathcal{K}$ and the k-dimensional subspace $\mathbb{C}^k$. (We refer, e.g., to [12], [18, Sect. IV.1], [34, Ch. 17], [35], [36, Ch. 3] for these facts).

Theorem 3.2. *Suppose Hypothesis* 3.1 *and let* $\alpha\in\mathbb{C}$. *Then,*

$$\operatorname{tr}(H_a)=\operatorname{tr}(H_b)=0, \quad \det(I-\alpha H_a)=\det(I-\alpha H_b)=1, \tag{3.5}$$

$$\operatorname{tr}(K)=\int_a^b dx\,\operatorname{tr}_{\mathbb{C}^{n_1}}(g_1(x)f_1(x))=\int_a^b dx\,\operatorname{tr}_{\mathbb{C}^m}(f_1(x)g_1(x)) \tag{3.6}$$

$$=\int_a^b dx\,\operatorname{tr}_{\mathbb{C}^{n_2}}(g_2(x)f_2(x))=\int_a^b dx\,\operatorname{tr}_{\mathbb{C}^m}(f_2(x)g_2(x)). \tag{3.7}$$

Assume in addition that U *is given by* (2.38). *Then,*

$$\det(I-\alpha K)=\det_{\mathbb{C}^{n_1}}(I_{n_1}-\alpha T(I-\alpha H_b)^{-1}S) \tag{3.8}$$

$$=\det_{\mathbb{C}^{n_1}}\bigg(I_{n_1}-\alpha\int_a^b dx\,g_1(x)\hat f_1(x,\alpha)\bigg) \tag{3.9}$$

$$=\det_{\mathbb{C}^{n}}(U(a,\alpha)) \tag{3.10}$$

$$=\det_{\mathbb{C}^{n_2}}(I_{n_2}-\alpha R(I-\alpha H_a)^{-1}Q) \tag{3.11}$$

$$=\det_{\mathbb{C}^{n_2}}\bigg(I_{n_2}-\alpha\int_a^b dx\,g_2(x)\hat f_2(x,\alpha)\bigg) \tag{3.12}$$

$$=\det_{\mathbb{C}^{n}}(U(b,\alpha)). \tag{3.13}$$

Proof. We briefly sketch the argument following [11, Theorem 3.2] since we use a different solution U of $U'=\alpha AU$. Relations (3.5) are clear from Lidskii's theorem (cf., e.g., [11, Theorem VII.6.1], [18, Sect. III.8, Sect. IV.1], [36, Theorem 3.7]). Thus,

$$\operatorname{tr}(K)=\operatorname{tr}(QR)=\operatorname{tr}(RQ)=\operatorname{tr}(ST)=\operatorname{tr}(TS) \tag{3.14}$$

then proves (3.6) and (3.7). Next, one observes

$$I-\alpha K=(I-\alpha H_a)[I-\alpha(I-\alpha H_a)^{-1}QR] \tag{3.15}$$

$$=(I-\alpha H_b)[I-\alpha(I-H_b)^{-1}ST] \tag{3.16}$$

and hence,

$$\begin{aligned}\det(I-\alpha K) &= \det(I-\alpha H_a)\det(I-\alpha(I-\alpha H_a)^{-1}QR)\\ &= \det(I-\alpha(I-\alpha H_a)^{-1}QR)\\ &= \det(I-\alpha R(I-\alpha H_a)^{-1}Q)\\ &= \det_{\mathbb{C}^{n_2}}(I_{n_2}-\alpha R(I-\alpha H_a)^{-1}Q) \quad (3.17)\\ &= \det_{\mathbb{C}^n}(U(b,\alpha)). \quad (3.18)\end{aligned}$$

Similarly,

$$\begin{aligned}\det(I-\alpha K) &= \det(I-\alpha H_b)\det(I-\alpha(I-\alpha H_b)^{-1}ST)\\ &= \det(I-\alpha(I-\alpha H_b)^{-1}ST)\\ &= \det(I-\alpha T(I-\alpha H_b)^{-1}S)\\ &= \det_{\mathbb{C}^{n_1}}(I_{n_1}-\alpha T(I-\alpha H_b)^{-1}S) \quad (3.19)\\ &= \det_{\mathbb{C}^n}(U(a,\alpha)). \quad (3.20)\end{aligned}$$

Relations (3.18) and (3.20) follow directly from taking the limit $x \uparrow b$ and $x \downarrow a$ in (2.39). This proves (3.8)–(3.13). □

Equality of (3.18) and (3.20) also follows directly from (2.42) and

$$\int_a^b dx' \operatorname{tr}_{\mathbb{C}^n}(A(x')) = \int_a^b dx' [\operatorname{tr}_{\mathbb{C}^{n_1}}(g_1(x')f_1(x')) - \operatorname{tr}_{\mathbb{C}^{n_2}}(g_2(x')f_2(x'))] \quad (3.21)$$

$$= \operatorname{tr}(H_a) = \operatorname{tr}(H_b) = 0. \quad (3.22)$$

Finally, we treat the case of 2-modified Fredholm determinants in the case where K is only assumed to lie in the Hilbert-Schmidt class. In addition to (3.1)–(3.3) we will use the following standard facts for 2-modified Fredholm determinants $\det_2(I-A)$, $A \in \mathcal{B}_2(\mathcal{H})$ (cf. e,g., [13], [14, Ch. XIII], [18, Sect. IV.2], [35], [36, Ch. 3]),

$$\det_2(I-A) = \det((I-A)\exp(A)), \quad A \in \mathcal{B}_2(\mathcal{H}), \quad (3.23)$$

$$\det_2((I-A)(I-B)) = \det_2(I-A)\det_2(I-B)e^{-\operatorname{tr}(AB)}, \quad A, B \in \mathcal{B}_2(\mathcal{H}), \quad (3.24)$$

$$\det_2(I-A) = \det(I-A)e^{\operatorname{tr}(A)}, \quad A \in \mathcal{B}_1(\mathcal{H}). \quad (3.25)$$

Theorem 3.3. *Suppose Hypothesis* 2.1 *and let* $\alpha \in \mathbb{C}$. *Then,*

$$\det_2(I-\alpha H_a) = \det_2(I-\alpha H_b) = 1. \quad (3.26)$$

Assume in addition that U is given by (2.38)*. Then,*

$$\det_2(I-\alpha K) = \det_{\mathbb{C}^{n_1}}(I_{n_1} - \alpha T(I-\alpha H_b)^{-1}S)\exp(\alpha\,\mathrm{tr}_{\mathbb{C}^m}(ST)) \tag{3.27}$$

$$= \det_{\mathbb{C}^{n_1}}\left(I_{n_1} - \alpha\int_a^b dx\, g_1(x)\hat{f}_1(x,\alpha)\right) \times \exp\left(\alpha\int_a^b dx\,\mathrm{tr}_{\mathbb{C}^m}(f_1(x)g_1(x))\right) \tag{3.28}$$

$$= \det_{\mathbb{C}^n}(U(a,\alpha))\exp\left(\alpha\int_a^b dx\,\mathrm{tr}_{\mathbb{C}^m}(f_1(x)g_1(x))\right) \tag{3.29}$$

$$= \det_{\mathbb{C}^{n_2}}(I_{n_2} - \alpha R(I-\alpha H_a)^{-1}Q)\exp(\alpha\,\mathrm{tr}_{\mathbb{C}^m}(QR)) \tag{3.30}$$

$$= \det_{\mathbb{C}^{n_2}}\left(I_{n_2} - \alpha\int_a^b dx\, g_2(x)\hat{f}_2(x,\alpha)\right) \times \exp\left(\alpha\int_a^b dx\,\mathrm{tr}_{\mathbb{C}^m}(f_2(x)g_2(x))\right) \tag{3.31}$$

$$= \det_{\mathbb{C}^n}(U(b,\alpha))\exp\left(\alpha\int_a^b dx\,\mathrm{tr}_{\mathbb{C}^m}(f_2(x)g_2(x))\right). \tag{3.32}$$

Proof. Relations (3.26) follow since the Volterra operators H_a, H_b have no nonzero eigenvalues. Next, again using (3.15) and (3.16), one computes,

$$\begin{aligned}\det_2(I-\alpha K) &= \det_2(I-\alpha H_a)\det_2(I-\alpha(I-\alpha H_a)^{-1}QR) \\ &\quad\times\exp(-\mathrm{tr}(\alpha^2 H_a(I-\alpha H_a)^{-1}QR)) \\ &= \det(I-\alpha(I-\alpha H_a)^{-1}QR)\exp(\alpha\,\mathrm{tr}((I-\alpha H_a)^{-1}QR)) \\ &\quad\times\exp(-\mathrm{tr}(\alpha^2 H_a(I-\alpha H_a)^{-1}QR)) \\ &= \det_{\mathbb{C}^{n_2}}(I_{n_2}-\alpha R(I-\alpha H_a)^{-1}Q)\exp(\alpha\,\mathrm{tr}(QR)) \qquad (3.33) \\ &= \det_{\mathbb{C}^n}(U(b,\alpha))\exp\left(\alpha\int_a^b dx\,\mathrm{tr}_{\mathbb{C}^m}(f_1(x)g_1(x))\right). \qquad (3.34)\end{aligned}$$

Similarly,

$$\begin{aligned}
\det{}_2(I-\alpha K) &= \det{}_2(I-\alpha H_b)\det{}_2(I-\alpha(I-\alpha H_b)^{-1}ST) \\
&\qquad \times \exp(-\operatorname{tr}(\alpha^2 H_b(I-\alpha H_b)^{-1}ST)) \\
&= \det(I-\alpha(I-\alpha H_b)^{-1}ST)\exp(\alpha\operatorname{tr}((I-\alpha H_b)^{-1}ST)) \\
&\quad \times \exp(-\operatorname{tr}(\alpha^2 H_b(I-\alpha H_b)^{-1}ST)) \\
&= \det{}_{\mathbb{C}^{n_1}}(I_{n_1}-\alpha T(I-\alpha H_b)^{-1}S)\exp(\alpha\operatorname{tr}(ST)) \qquad (3.35) \\
&= \det{}_{\mathbb{C}^n}(U(a,\alpha))\exp\bigg(\alpha\int_a^b dx\operatorname{tr}_{\mathbb{C}^m}(f_2(x)g_2(x))\bigg). \qquad (3.36)
\end{aligned}$$

□

Equality of (3.34) and (3.36) also follows directly from (2.42) and (3.21).

4. Some applications to Jost functions, transmission coefficients, and Floquet discriminants of Schrödinger operators

In this section we illustrate the results of Section 3 in three particular cases: The case of Jost functions for half-line Schrödinger operators, the transmission coefficient for Schrödinger operators on the real line, and the case of Floquet discriminants associated with Schrödinger operators on a compact interval. The case of a the second-order Schrödinger operator on the line is also transformed into a first-order 2×2 system and its associated 2-modified Fredholm deteminant is identified with that of the Schrödinger operator on $\mathbb{R}$. For simplicity we will limit ourselves to scalar coefficients although the results for half-line Schrödinger operators and those on the full real line immediately extend to the matrix-valued situation.

We start with the case of half-line Schrödinger operators:
The case $(a,b)=(0,\infty)$: Assuming

$$V \in L^1((0,\infty);dx), \tag{4.1}$$

(we note that V is not necessarily assumed to be real-valued) we introduce the closed Dirichlet-type operators in $L^2((0,\infty);dx)$ defined by

$$\begin{aligned}
&H_+^{(0)} f = -f'',\\
&f \in \operatorname{dom}\big(H_+^{(0)}\big) = \{g \in L^2((0,\infty);dx) \,|\, g, g' \in AC_{\mathrm{loc}}([0,R]) \\
&\qquad\qquad \text{for all } R>0,\ f(0_+)=0,\ f'' \in L^2((0,\infty);dx)\},
\end{aligned} \tag{4.2}$$

$$\begin{aligned}
&H_+ f = -f'' + Vf,\\
&f \in \operatorname{dom}(H_+) = \{g \in L^2((0,\infty);dx) \,|\, g, g' \in AC_{\mathrm{loc}}([0,R]) \\
&\quad \text{for all } R>0,\ f(0_+)=0,\ (-f''+Vf) \in L^2((0,\infty);dx)\}.
\end{aligned} \tag{4.3}$$

We note that $H_+^{(0)}$ is self-adjoint and that H_+ is self-adjoint if and only if V is real-valued.

Next we introduce the regular solution $\phi(z,\cdot)$ and Jost solution $f(z,\cdot)$ of $-\psi''(z) + V\psi(z) = z\psi(z)$, $z \in \mathbb{C}\backslash\{0\}$, by

$$\phi(z,x) = z^{-1/2}\sin(z^{1/2}x) + \int_0^x dx' g_+^{(0)}(z,x,x')V(x')\phi(z,x'), \tag{4.4}$$

$$f(z,x) = e^{iz^{1/2}x} - \int_x^\infty dx' g_+^{(0)}(z,x,x')V(x')f(z,x'), \tag{4.5}$$

$$\operatorname{Im}(z^{1/2}) \geq 0,\ z \neq 0,\ x \geq 0,$$

where

$$g_+^{(0)}(z,x,x') = z^{-1/2}\sin(z^{1/2}(x-x')). \tag{4.6}$$

We also introduce the Green's function of $H_+^{(0)}$,

$$G_+^{(0)}(z,x,x') = \big(H_+^{(0)} - z\big)^{-1}(x,x') = \begin{cases} z^{-1/2}\sin(z^{1/2}x)e^{iz^{1/2}x'}, & x \leq x',\\ z^{-1/2}\sin(z^{1/2}x')e^{iz^{1/2}x}, & x \geq x'. \end{cases} \tag{4.7}$$

The Jost function $\mathcal{F}$ associated with the pair $\big(H_+, H_+^{(0)}\big)$ is given by

$$\mathcal{F}(z) = W(f(z),\phi(z)) = f(z,0) \tag{4.8}$$

$$= 1 + z^{-1/2}\int_0^\infty dx\, \sin(z^{1/2}x)V(x)f(z,x) \tag{4.9}$$

$$= 1 + \int_0^\infty dx\, e^{iz^{1/2}x}V(x)\phi(z,x); \quad \operatorname{Im}(z^{1/2}) \geq 0,\ z \neq 0, \tag{4.10}$$

where

$$W(f,g)(x) = f(x)g'(x) - f'(x)g(x), \quad x \geq 0, \tag{4.11}$$

denotes the Wronskian of f and g. Introducing the factorization

$$\begin{aligned} &V(x) = u(x)v(x), \\ &u(x) = |V(x)|^{1/2}\exp(i\arg(V(x))), \quad v(x) = |V(x)|^{1/2}, \end{aligned} \tag{4.12}$$

one verifies[6]

$$\begin{aligned} (H_+ - z)^{-1} &= \big(H_+^{(0)} - z\big)^{-1} \\ &\quad - \big(H_+^{(0)} - z\big)^{-1} v\Big[I + \overline{u\big(H_+^{(0)} - z\big)^{-1} v}\Big]^{-1} u\big(H_+^{(0)} - z\big)^{-1}, \\ &\qquad z \in \mathbb{C}\backslash\text{spec}(H_+). \end{aligned} \tag{4.13}$$

To establish the connection with the notation used in Sections 2 and 3, we introduce the operator $K(z)$ in $L^2((0,\infty);dx)$ (cf. (2.3)) by

$$K(z) = -\overline{u\big(H_+^{(0)} - z\big)^{-1} v}, \quad z \in \mathbb{C}\backslash\text{spec}\big(H_+^{(0)}\big) \tag{4.14}$$

with integral kernel

$$K(z,x,x') = -u(x)G_+^{(0)}(z,x,x')v(x'), \quad \text{Im}(z^{1/2}) \geq 0, \ x, x' \geq 0, \tag{4.15}$$

and the Volterra operators $H_0(z)$, $H_\infty(z)$ (cf. (2.4), (2.5)) with integral kernel

$$H(z,x,x') = u(x)g_+^{(0)}(z,x,x')v(x'). \tag{4.16}$$

Moreover, we introduce for a.e. $x > 0$,

$$\begin{aligned} &f_1(z,x) = -u(x)e^{iz^{1/2}x}, && g_1(z,x) = v(x)z^{-1/2}\sin(z^{1/2}x), \\ &f_2(z,x) = -u(x)z^{-1/2}\sin(z^{1/2}x), && g_2(z,x) = v(x)e^{iz^{1/2}x}. \end{aligned} \tag{4.17}$$

Assuming temporarily that

$$\text{supp}(V) \text{ is compact} \tag{4.18}$$

in addition to hypothesis (4.1), introducing $\hat{f}_j(z,x)$, $j = 1,2$, by

$$\hat{f}_1(z,x) = f_1(z,x) - \int_x^\infty dx'\, H(z,x,x')\hat{f}_1(z,x'), \tag{4.19}$$

$$\hat{f}_2(z,x) = f_2(z,x) + \int_0^x dx'\, H(z,x,x')\hat{f}_2(z,x'), \tag{4.20}$$

$$\text{Im}(z^{1/2}) \geq 0, \ z \neq 0, \ x \geq 0,$$

[6] $\overline{T}$ denotes the operator closure of T and spec$(\cdot)$ abbreviates the spectrum of a linear operator.

yields solutions $\hat{f}_j(z,\cdot) \in L^2((0,\infty);dx)$, $j = 1,2$. By comparison with (4.4), (4.5), one then identifies

$$\hat{f}_1(z,x) = -u(x)f(z,x), \tag{4.21}$$

$$\hat{f}_2(z,x) = -u(x)\phi(z,x). \tag{4.22}$$

We note that the temporary compact support assumption (4.18) on V has only been introduced to guarantee that

$$f_2(z,\cdot), \hat{f}_2(z,\cdot) \in L^2((0,\infty);dx). \tag{4.23}$$

This extra hypothesis will soon be removed.

We start with a well-known result.

Theorem 4.1 (Cf. [33], Theorem XI.20)**.** *Suppose $f, g \in L^q(\mathbb{R};dx)$ for some $2 \leq q < \infty$. Denote by $f(X)$ the maximally defined multiplication operator by f in $L^2(\mathbb{R};dx)$ and by $g(P)$ the maximal multiplication operator by g in Fourier space*[7] *$L^2(\mathbb{R};dp)$. Then*[8] *$f(X)g(P) \in \mathcal{B}_q(L^2(\mathbb{R};dx))$ and*

$$\|f(X)g(P)\|_{\mathcal{B}_q(L^2(\mathbb{R};dx))} \leq (2\pi)^{-1/q}\|f\|_{L^q(\mathbb{R};dx)}\|g\|_{L^q(\mathbb{R};dx)}. \tag{4.24}$$

We will use Theorem 4.1, to sketch a proof of the following known result:

Theorem 4.2. *Suppose $V \in L^1((0,\infty);dx)$ and $z \in \mathbb{C}$ with $\mathrm{Im}(z^{1/2}) > 0$. Then*

$$K(z) \in \mathcal{B}_1(L^2((0,\infty);dx)). \tag{4.25}$$

Proof. For $z < 0$ this is discussed in the proof of [33, Theorem XI.31]. For completeness we briefly sketch the principal arguments of a proof of Theorem 4.2. One possible approach consists of reducing Theorem 4.2 to Theorem 4.1 in the special case $q = 2$ by embedding the half-line problem on $(0,\infty)$ into a problem on $\mathbb{R}$ as follows. One introduces the decomposition

$$L^2(\mathbb{R};dx) = L^2((0,\infty);dx) \oplus L^2((-\infty,0);dx), \tag{4.26}$$

[7] That is, $P = -id/dx$ with domain $\mathrm{dom}(P) = H^{2,1}(\mathbb{R})$ the usual Sobolev space.

[8] $\mathcal{B}_q(\mathcal{H})$, $q \geq 1$ denote the usual trace ideals, cf. [18], [36].

and extends u, v, V to $(-\infty, 0)$ by putting u, v, V equal to zero on $(-\infty, 0)$, introducing

$$\tilde u(x) = \begin{cases} u(x), & x > 0, \\ 0, & x < 0, \end{cases} \quad \tilde v(x) = \begin{cases} v(x), & x > 0, \\ 0, & x < 0, \end{cases}$$
$$\widetilde V(x) = \begin{cases} V(x), & x > 0, \\ 0, & x < 0. \end{cases} \tag{4.27}$$

Moreover, consider the Dirichlet Laplace operator $H_D^{(0)}$ in $L^2(\mathbb{R}; dx)$ by

$$\begin{aligned} &H_D^{(0)} f = -f'', \\ &\operatorname{dom}\big(H_D^{(0)}\big) = \{g \in L^2(\mathbb{R}; dx) \,|\, g, g' \in AC_{\mathrm{loc}}([0, R]) \cap AC_{\mathrm{loc}}([-R, 0]) \\ &\qquad \text{for all } R > 0,\ f(0_\pm) = 0,\ f'' \in L^2(\mathbb{R}; dx)\} \end{aligned} \tag{4.28}$$

and introduce

$$\widetilde K(z) = -\overline{\tilde u\big(H_D^{(0)} - z\big)^{-1}\tilde v} = K(z) \oplus 0, \quad \operatorname{Im}(z^{1/2}) > 0. \tag{4.29}$$

By Krein's formula, the resolvents of the Dirichlet Laplace operator $H_D^{(0)}$ and that of the ordinary Laplacian $H^{(0)} = P^2 = -d^2/dx^2$ on $H^{2,2}(\mathbb{R})$ differ precisely by a rank one operator. Explicitly, one obtains

$$\begin{aligned} G_D^{(0)}(z, x, x') &= G^{(0)}(z, x, x') - G^{(0)}(z, x, 0) G^{(0)}(z, 0, 0)^{-1} G^{(0)}(z, 0, x') \\ &= G^{(0)}(z, x, x') - \frac{i}{2z^{1/2}} \exp(iz^{1/2}|x|) \exp(iz^{1/2}|x'|), \\ &\qquad \operatorname{Im}(z^{1/2}) > 0,\ x, x' \in \mathbb{R}, \end{aligned} \tag{4.30}$$

where we abbreviated the Green's functions of $H_D^{(0)}$ and $H^{(0)} = -d^2/dx^2$ by

$$G_D^{(0)}(z, x, x') = \big(H_D^{(0)} - z\big)^{-1}(x, x'), \tag{4.31}$$

$$G^{(0)}(z, x, x') = \big(H^{(0)} - z\big)^{-1}(x, x') = \frac{i}{2z^{1/2}} \exp(iz^{1/2}|x - x'|). \tag{4.32}$$

Thus,

$$\widetilde K(z) = -\overline{\tilde u\big(H^{(0)} - z\big)^{-1}\tilde v} - \frac{i}{2z^{1/2}}\big(\tilde v\, \overline{\exp(iz^{1/2}|\cdot|)}\,,\, \cdot\,\big)\tilde u \exp(iz^{1/2}|\cdot|). \tag{4.33}$$

By Theorem 4.1 for $q = 2$ one infers that

$$\big[\tilde u\big(H^{(0)} - z\big)^{-1/2}\big] \in \mathcal{B}_2(L^2(\mathbb{R}; dx)), \quad \operatorname{Im}(z^{1/2}) > 0 \tag{4.34}$$

and hence,

$$\big[\tilde{u}\big(H^{(0)}-z\big)^{-1/2}\big]\overline{\big[\big(H^{(0)}-z\big)^{-1/2}\tilde{v}\big]} \in \mathcal{B}_1(L^2(\mathbb{R};dx)), \quad \operatorname{Im}(z^{1/2})>0. \tag{4.35}$$

Since the second term on the right-hand side of (4.33) is a rank one operator one concludes

$$\widetilde{K}(z) \in \mathcal{B}_1(L^2(\mathbb{R};dx)), \quad \operatorname{Im}(z^{1/2})>0 \tag{4.36}$$

and hence (4.25) using (4.29). ∎

An application of Lemma 2.6 and Theorem 3.2 then yields the following well-known result identifying the Fredholm determinant of $I-K(z)$ and the Jost function $\mathcal{F}(z)$.

Theorem 4.3. *Suppose* $V \in L^1((0,\infty);dx)$ *and* $z\in\mathbb{C}$ *with* $\operatorname{Im}(z^{1/2})>0$. *Then*

$$\det(I-K(z)) = \mathcal{F}(z). \tag{4.37}$$

Proof. Assuming temporarily that $\operatorname{supp}(V)$ is compact (cf. (4.18)), Lemma 2.6 applies and one obtains from (2.38) and (4.17)–(4.22) that

$$\begin{aligned} U(z,x) &= \begin{pmatrix} 1-\int_x^\infty dx'\, g_1(z,x')\hat{f}_1(z,x') & \int_0^x dx'\, g_1(z,x')\hat{f}_2(z,x') \\ \int_x^\infty dx'\, g_2(z,x')\hat{f}_1(z,x') & 1-\int_0^x dx'\, g_2(z,x')\hat{f}_2(z,x') \end{pmatrix}, \\ &= \begin{pmatrix} 1+\int_x^\infty dx'\, \frac{\sin(z^{1/2}x')}{z^{1/2}} V(x')f(z,x') & -\int_0^x dx'\, \frac{\sin(z^{1/2}x')}{z^{1/2}} V(x')\phi(z,x') \\ -\int_x^\infty dx'\, e^{iz^{1/2}x'}V(x')f(z,x') & 1+\int_0^x dx'\, e^{iz^{1/2}x'}V(x')\phi(z,x') \end{pmatrix}, \\ &\qquad x>0. \end{aligned} \tag{4.38}$$

Relations (3.9) and (3.12) of Theorem 3.2 with $m=n_1=n_2=1$, $n=2$, then immediately yield

$$\begin{aligned} \det(I-K(z)) &= 1+z^{-1/2}\int_0^\infty dx\, \sin(z^{1/2}x)V(x)f(z,x) \\ &= 1+\int_0^\infty dx\, e^{iz^{1/2}x}V(x)\phi(z,x) \\ &= \mathcal{F}(z) \end{aligned} \tag{4.39}$$

and hence (4.37) is proved under the additional hypothesis (4.18). Removing the compact support hypothesis on V now follows by a standard argument. For completeness we sketch this argument next. Multiplying u,v,V by a smooth cutoff function χ_ε of compact support of the type

$$0\le\chi\le 1, \quad \chi(x)=\begin{cases} 1, & x\in[0,1], \\ 0, & |x|\ge 2, \end{cases} \quad \chi_\varepsilon(x)=\chi(\varepsilon x),\ \varepsilon>0, \tag{4.40}$$

denoting the results by $u_\varepsilon = u\chi_\varepsilon$, $v_\varepsilon = v\chi_\varepsilon$, $V_\varepsilon = V\chi_\varepsilon$, one introduces in analogy to (4.27),

$$\tilde u_\varepsilon(x) = \begin{cases} u_\varepsilon(x), & x>0, \\ 0, & x<0, \end{cases} \quad \tilde v_\varepsilon(x) = \begin{cases} v_\varepsilon(x), & x>0, \\ 0, & x<0, \end{cases}$$
$$\tilde V_\varepsilon(x) = \begin{cases} V_\varepsilon(x), & x>0, \\ 0, & x<0, \end{cases} \tag{4.41}$$

and similarly, in analogy to (4.14) and (4.29),

$$K_\varepsilon(z) = -\overline{u_\varepsilon\big(H_+^{(0)}-z\big)^{-1}v_\varepsilon}, \quad \operatorname{Im}(z^{1/2})>0, \tag{4.42}$$
$$\widetilde K_\varepsilon(z) = -\overline{\tilde u_\varepsilon\big(H_D^{(0)}-z\big)^{-1}\tilde v_\varepsilon} = K_\varepsilon(z)\oplus 0, \quad \operatorname{Im}(z^{1/2})>0. \tag{4.43}$$

One then estimates,

$$\begin{aligned}
&\big\|\widetilde K(z) - \widetilde K_\varepsilon(z)\big\|_{\mathcal B_1(L^2(\mathbb R;dx))} \\
&\quad\le \Big\| -\overline{\tilde u\big(H^{(0)}-z\big)^{-1}\tilde v} + \overline{\tilde u_\varepsilon\big(H^{(0)}-z\big)^{-1}\tilde v_\varepsilon}\Big\|_{\mathcal B_1(L^2(\mathbb R;dx))} \\
&\qquad + \frac{1}{2|z|^{1/2}}\Big\|\big(\tilde v\,\overline{\exp(iz^{1/2}|\cdot|)}\,,\,\cdot\,\big)\tilde u\exp(iz^{1/2}|\cdot|) \\
&\qquad\qquad - \big(\tilde v_\varepsilon\,\overline{\exp(iz^{1/2}|\cdot|)}\,,\,\cdot\,\big)\tilde u_\varepsilon\exp(iz^{1/2}|\cdot|)\Big\|_{\mathcal B_1(L^2(\mathbb R;dx))} \\
&\quad\le \Big\| -\overline{\tilde u\big(H^{(0)}-z\big)^{-1}\tilde v} + \overline{\tilde u_\varepsilon\big(H^{(0)}-z\big)^{-1}\tilde v} \\
&\qquad - \overline{\tilde u_\varepsilon\big(H^{(0)}-z\big)^{-1}\tilde v} + \overline{\tilde u_\varepsilon\big(H^{(0)}-z\big)^{-1}\tilde v_\varepsilon}\Big\|_{\mathcal B_1(L^2(\mathbb R;dx))} \\
&\qquad + \frac{1}{2|z|^{1/2}}\Big\|\big(\tilde v\,\overline{\exp(iz^{1/2}|\cdot|)}\,,\,\cdot\,\big)\tilde u\exp(iz^{1/2}|\cdot|) \\
&\qquad\qquad - \big(\tilde v\,\overline{\exp(iz^{1/2}|\cdot|)}\,,\,\cdot\,\big)\tilde u_\varepsilon\exp(iz^{1/2}|\cdot|) \\
&\qquad\qquad + \big(\tilde v\,\overline{\exp(iz^{1/2}|\cdot|)}\,,\,\cdot\,\big)\tilde u_\varepsilon\exp(iz^{1/2}|\cdot|) \\
&\qquad\qquad - \big(\tilde v_\varepsilon\,\overline{\exp(iz^{1/2}|\cdot|)}\,,\,\cdot\,\big)\tilde u_\varepsilon\exp(iz^{1/2}|\cdot|)\Big\|_{\mathcal B_1(L^2(\mathbb R;dx))} \\
&\quad\le \widetilde C(z)\big[\|\tilde u - \tilde u_\varepsilon\|_{L^2(\mathbb R;dx)} + \|\tilde v - \tilde v_\varepsilon\|_{L^2(\mathbb R;dx)}\big] \\
&\quad= C(z)\|\tilde v - \tilde v_\varepsilon\|_{L^2(\mathbb R;dx)} \\
&\quad\le C(z)\|v - v_\varepsilon\|_{L^2((0,\infty);dx)},
\end{aligned} \tag{4.44}$$

where $C(z) = 2\widetilde C(z) > 0$ is an appropriate constant. Thus, applying (4.29) and (4.43), one finally concludes

$$\lim_{\varepsilon\downarrow 0}\big\|K(z) - K_\varepsilon(z)\big\|_{\mathcal B_1(L^2((0,\infty);dx))} = 0. \tag{4.45}$$

Since V_ε has compact support, (4.39) applies to V_ε and one obtains,

$$\det(I - K_\varepsilon(z)) = \mathcal{F}_\varepsilon(z), \tag{4.46}$$

where, in obvious notation, we add the subscript ε to all quantities associated with V_ε resulting in ϕ_ε, f_ε, $\mathcal{F}_\varepsilon$, $f_{\varepsilon,j}$, $\hat{f}_{\varepsilon,j}$, $j = 1, 2$, etc. By (4.45), the left-hand side of (4.46) converges to $\det(I - K(z))$ as $\varepsilon \downarrow 0$. Since

$$\lim_{\varepsilon \downarrow 0} \|V_\varepsilon - V\|_{L^1((0,\infty);dx)} = 0, \tag{4.47}$$

the Jost function $\mathcal{F}_\varepsilon$ is well-known to converge to $\mathcal{F}$ pointwise as $\varepsilon \downarrow 0$ (cf. [5]). Indeed, fixing z and iterating the Volterra integral equation (4.5) for f_ε shows that $|z^{-1/2} \sin(z^{1/2}x) f_\varepsilon(z, x)|$ is uniformly bounded with respect to (x, ε) and hence the continuity of $\mathcal{F}_\varepsilon(z)$ with respect to ε follows from (4.47) and the analog of (4.9) for V_ε,

$$\mathcal{F}_\varepsilon(z) = 1 + z^{-1/2} \int_0^\infty dx\, \sin(z^{1/2}x) V_\varepsilon(x) f_\varepsilon(z, x), \tag{4.48}$$

applying the dominated convergence theorem. Hence, (4.46) yields (4.37) in the limit $\varepsilon \downarrow 0$. ☐

Remark 4.4. (i) *The result* (4.39) *explicitly shows that* $\det_{\mathbb{C}^n}(U(z,0))$ *vanishes for each eigenvalue* z (*one then necessarily has* $z < 0$) *of the Schrödinger operator* H. *Hence, a normalization of the type* $U(z, 0) = I_n$ *is clearly impossible in such a case.*
(ii) *The right-hand side* $\mathcal{F}$ *of* (4.37) (*and hence the Fredholm determinant on the left-hand side*) *admits a continuous extension to the positive real line. Imposing the additional exponential falloff of the potential of the type* $V \in L^1((0,\infty); \exp(ax)dx)$ *for some* $a > 0$, *then* $\mathcal{F}$ *and hence the Fredholm determinant on the left-hand side of* (4.37) *permit an analytic continuation through the essential spectrum of* H_+ *into a strip of width* $a/2$ (*w.r.t. the variable* $z^{1/2}$). *This is of particular relevance in the study of resonances of* H_+ (*cf.* [37]).

The result (4.37) is well-known, we refer, for instance, to [23], [29], [30], [32, p. 344–345], [37]. (Strictly speaking, these authors additionally assume V to be real-valued, but this is not essential in this context.) The current derivation presented appears to be by far the simplest available in the literature as it only involves the elementary manipulations leading to (3.8)–(3.13), followed by a standard approximation argument to remove the compact support hypothesis on V.

Since one is dealing with the Dirichlet Laplacian on $(0,\infty)$ in the half-line context, Theorem 4.2 extends to a larger potential class characterized by

$$\int_0^R dx\, x|V(x)| + \int_R^\infty dx\, |V(x)| < \infty \tag{4.49}$$

for some fixed $R > 0$. We omit the corresponding details but refer to [33, Theorem XI.31], which contains the necessary basic facts to make the transition from hypothesis (4.1) to (4.49).

Next we turn to Schrödinger operators on the real line:
The case $(a, b) = \mathbb{R}$: Assuming

$$V \in L^1(\mathbb{R}; dx), \tag{4.50}$$

we introduce the closed operators in $L^2(\mathbb{R}; dx)$ defined by

$$H^{(0)} f = -f'', \quad f \in \mathrm{dom}\big(H^{(0)}\big) = H^{2,2}(\mathbb{R}), \tag{4.51}$$

$$\begin{aligned} &Hf = -f'' + Vf, \\ &f \in \mathrm{dom}(H) = \{g \in L^2(\mathbb{R}; dx) \,|\, g, g' \in AC_{\mathrm{loc}}(\mathbb{R}); \\ &\qquad\qquad\qquad (-f'' + Vf) \in L^2(\mathbb{R}); dx)\}. \end{aligned} \tag{4.52}$$

Again, $H^{(0)}$ is self-adjoint. Moreover, H is self-adjoint if and only if V is real-valued.

Next we introduce the Jost solutions $f_\pm(z,\cdot)$ of $-\psi''(z) + V\psi(z) = z\psi(z)$, $z \in \mathbb{C}\backslash\{0\}$, by

$$\begin{aligned} f_\pm(z,x) = e^{\pm iz^{1/2}x} - \int_x^{\pm\infty} dx' g^{(0)}(z,x,x')V(x')f_\pm(z,x'), \\ \mathrm{Im}(z^{1/2}) \geq 0,\ z \neq 0,\ x \in \mathbb{R}, \end{aligned} \tag{4.53}$$

where $g^{(0)}(z,x,x')$ is still given by (4.6). We also introduce the Green's function of $H^{(0)}$,

$$\begin{aligned} G^{(0)}(z,x,x') = \big(H^{(0)} - z\big)^{-1}(x,x') = \frac{i}{2z^{1/2}} e^{iz^{1/2}|x-x'|}, \\ \mathrm{Im}(z^{1/2}) > 0,\ x, x' \in \mathbb{R}. \end{aligned} \tag{4.54}$$

The Jost function $\mathcal{F}$ associated with the pair $\big(H, H^{(0)}\big)$ is given by

$$\mathcal{F}(z) = \frac{W(f_-(z), f_+(z))}{2iz^{1/2}} \tag{4.55}$$

$$= 1 - \frac{1}{2iz^{1/2}} \int_{\mathbb{R}} dx\, e^{\mp iz^{1/2}x} V(x) f_\pm(z,x), \quad \mathrm{Im}(z^{1/2}) \geq 0,\ z \neq 0, \tag{4.56}$$

where $W(\cdot,\cdot)$ denotes the Wronskian defined in (4.11). We note that if $H^{(0)}$ and H are self-adjoint, then

$$T(\lambda) = \lim_{\varepsilon\downarrow 0} \mathcal{F}(\lambda + i\varepsilon)^{-1}, \quad \lambda > 0, \tag{4.57}$$

denotes the transmission coefficient corresponding to the pair $\big(H, H^{(0)}\big)$. Introducing again the factorization (4.12) of $V = uv$, one verifies as in (4.13) that

$$\begin{aligned}(H - z)^{-1} &= \big(H^{(0)} - z\big)^{-1} \\ &\quad - \big(H^{(0)} - z\big)^{-1} v \Big[I + \overline{u\big(H^{(0)} - z\big)^{-1} v}\Big]^{-1} u\big(H^{(0)} - z\big)^{-1}, \\ &\qquad z \in \mathbb{C}\backslash\text{spec}(H).\end{aligned} \tag{4.58}$$

To make contact with the notation used in Sections 2 and 3, we introduce the operator $K(z)$ in $L^2(\mathbb{R}; dx)$ (cf. (2.3), (4.14)) by

$$K(z) = -\overline{u\big(H^{(0)} - z\big)^{-1} v}, \quad z \in \mathbb{C}\backslash\text{spec}\big(H^{(0)}\big) \tag{4.59}$$

with integral kernel

$$K(z, x, x') = -u(x) G^{(0)}(z, x, x') v(x'), \quad \text{Im}(z^{1/2}) \geq 0,\ z \neq 0,\ x, x' \in \mathbb{R}, \tag{4.60}$$

and the Volterra operators $H_{-\infty}(z)$, $H_{\infty}(z)$ (cf. (2.4), (2.5)) with integral kernel

$$H(z, x, x') = u(x) g^{(0)}(z, x, x') v(x'). \tag{4.61}$$

Moreover, we introduce for a.e. $x \in \mathbb{R}$,

$$\begin{aligned} f_1(z, x) &= -u(x) e^{iz^{1/2}x}, \qquad g_1(z, x) = (i/2) z^{-1/2} v(x) e^{-iz^{1/2}x}, \\ f_2(z, x) &= -u(x) e^{-iz^{1/2}x}, \qquad g_2(z, x) = (i/2) z^{-1/2} v(x) e^{iz^{1/2}x}. \end{aligned} \tag{4.62}$$

Assuming temporarily that

$$\text{supp}(V) \text{ is compact} \tag{4.63}$$

in addition to hypothesis (4.50), introducing $\hat f_j(z, x)$, $j = 1, 2$, by

$$\hat f_1(z, x) = f_1(z, x) - \int_x^\infty dx'\, H(z, x, x') \hat f_1(z, x'), \tag{4.64}$$

$$\hat f_2(z, x) = f_2(z, x) + \int_{-\infty}^x dx'\, H(z, x, x') \hat f_2(z, x'), \tag{4.65}$$

$$\text{Im}(z^{1/2}) \geq 0,\ z \neq 0,\ x \in \mathbb{R},$$

yields solutions $\hat{f}_j(z,\cdot) \in L^2(\mathbb{R};dx)$, $j=1,2$. By comparison with (4.53), one then identifies

$$\hat{f}_1(z,x) = -u(x) f_+(z,x), \tag{4.66}$$

$$\hat{f}_2(z,x) = -u(x) f_-(z,x). \tag{4.67}$$

We note that the temporary compact support assumption (4.18) on V has only been introduced to guarantee that $f_j(z,\cdot), \hat{f}_j(z,\cdot) \in L^2(\mathbb{R};dx)$, $j=1,2$. This extra hypothesis will soon be removed.

We also recall the well-known result.

Theorem 4.5. *Suppose $V \in L^1(\mathbb{R};dx)$ and let $z \in \mathbb{C}$ with $\operatorname{Im}(z^{1/2}) > 0$. Then*

$$K(z) \in \mathcal{B}_1(L^2(\mathbb{R};dx)). \tag{4.68}$$

This is an immediate consequence of Theorem 4.1 with $q=2$.

An application of Lemma 2.6 and Theorem 3.2 then again yields the following well-known result identifying the Fredholm determinant of $I-K(z)$ and the Jost function $\mathcal{F}(z)$ (inverse transmission coefficient).

Theorem 4.6. *Suppose $V \in L^1(\mathbb{R};dx)$ and let $z \in \mathbb{C}$ with $\operatorname{Im}(z^{1/2}) > 0$. Then*

$$\det(I-K(z)) = \mathcal{F}(z). \tag{4.69}$$

Proof. Assuming temporarily that $\operatorname{supp}(V)$ is compact (cf. (4.18)), Lemma 2.6 applies and one infers from (2.38) and (4.62)–(4.67) that

$$U(z,x) = \begin{pmatrix} 1-\int_x^\infty dx'\, g_1(z,x')\hat{f}_1(z,x') & \int_{-\infty}^x dx'\, g_1(z,x')\hat{f}_2(z,x') \\ \int_x^\infty dx'\, g_2(z,x')\hat{f}_1(z,x') & 1-\int_{-\infty}^x dx'\, g_2(z,x')\hat{f}_2(z,x') \end{pmatrix}, \quad x \in \mathbb{R}, \tag{4.70}$$

becomes

$$U_{1,1}(z,x) = 1 + \frac{i}{2z^{1/2}} \int_x^\infty dx'\, e^{-iz^{1/2}x'} V(x') f_+(z,x'), \tag{4.71}$$

$$U_{1,2}(z,x) = -\frac{i}{2z^{1/2}} \int_{-\infty}^x dx'\, e^{-iz^{1/2}x'} V(x') f_-(z,x'), \tag{4.72}$$

$$U_{2,1}(z,x) = -\frac{i}{2z^{1/2}} \int_x^\infty dx'\, e^{iz^{1/2}x'} V(x') f_+(z,x'), \tag{4.73}$$

$$U_{2,2}(z,x) = 1 + \frac{i}{2z^{1/2}} \int_{-\infty}^x dx'\, e^{iz^{1/2}x'} V(x') f_-(z,x'). \tag{4.74}$$

Relations (3.9) and (3.12) of Theorem 3.2 with $m = n_1 = n_2 = 1$, $n = 2$, then immediately yield

$$\begin{aligned} \det(I - K(z)) &= 1 - \frac{1}{2iz^{1/2}} \int_{\mathbb{R}} dx\, e^{\mp iz^{1/2}x} V(x) f_{\pm}(z,x) \\ &= \mathcal{F}(z) \end{aligned} \tag{4.75}$$

and hence (4.69) is proved under the additional hypothesis (4.63). Removing the compact support hypothesis on V now follows line by line the approximation argument discussed in the proof of Theorem 4.3. □

Remark 4.4 applies again to the present case of Schrödinger operators on the line. In particular, if one imposes the additional exponential falloff of the potential V of the type $V \in L^1(\mathbb{R}; \exp(a|x|)dx)$ for some $a > 0$, then $\mathcal{F}$ and hence the Fredholm determinant on the left-hand side of (4.69) permit an analytic continuation through the essential spectrum of H into a strip of width $a/2$ (w.r.t. the variable $z^{1/2}$). This is of relevance to the study of resonances of H (cf., e.g., [8], [37], and the literature cited therein).

The result (4.69) is well-known (although, typically under the additional assumption that V be real-valued), see, for instance, [9], [31, Appendix A], [36, Proposition 5.7], [37]. Again, the derivation just presented appears to be the most streamlined available for the reasons outlined after Remark 4.4.

For an explicit expansion of Fredholm determinants of the type (4.15) and (4.60) (valid in the case of general Green's functions G of Schrödinger operators H, not just for $G^{(0)}$ associated with $H^{(0)}$) we refer to Proposition 2.8 in [35].

Next, we revisit the result (4.69) from a different and perhaps somewhat unusual perspective. We intend to rederive the analogous result in the context of 2-modified determinants $\det_2(\cdot)$ by rewriting the scalar second-order Schrödinger equation as a first-order 2×2 system, taking the latter as our point of departure.

Assuming hypothesis 4.50 for the rest of this example, the Schrödinger equation

$$-\psi''(z,x) + V(x)\psi(z,x) = z\psi(z,x), \tag{4.76}$$

is equivalent to the first-order system

$$\Psi'(z,x) = \begin{pmatrix} 0 & 1 \\ V(x) - z & 0 \end{pmatrix} \Psi(z,x), \quad \Psi(z,x) = \begin{pmatrix} \psi(z,x) \\ \psi'(z,x) \end{pmatrix}. \tag{4.77}$$

Since $\Phi^{(0)}$ defined by

$$\Phi^{(0)}(z,x) = \begin{pmatrix} \exp(-iz^{1/2}x) & \exp(iz^{1/2}x) \\ -iz^{1/2}\exp(-iz^{1/2}x) & iz^{1/2}\exp(iz^{1/2}x) \end{pmatrix}, \quad \operatorname{Im}(z^{1/2}) \geq 0 \tag{4.78}$$

with

$$\det_{\mathbb{C}^2}(\Phi^{(0)}(z,x)) = 1, \quad (z,x) \in \mathbb{C} \times \mathbb{R}, \tag{4.79}$$

is a fundamental matrix of the system (4.77) in the case $V = 0$ a.e., and since

$$\begin{aligned} &\Phi^{(0)}(z,x)\Phi^{(0)}(z,x')^{-1} \\ &\quad = \begin{pmatrix} \cos(z^{1/2}(x-x')) & z^{-1/2}\sin(z^{1/2}(x-x')) \\ -z^{1/2}\sin(z^{1/2}(x-x')) & \cos(z^{1/2}(x-x')) \end{pmatrix}, \end{aligned} \tag{4.80}$$

the system (4.77) has the following pair of linearly independent solutions for $z \neq 0$,

$$\begin{aligned} F_\pm(z,x) &= F_\pm^{(0)}(z,x) \\ &\quad - \int_x^{\pm\infty} dx' \begin{pmatrix} \cos(z^{1/2}(x-x')) & z^{-1/2}\sin(z^{1/2}(x-x')) \\ -z^{1/2}\sin(z^{1/2}(x-x')) & \cos(z^{1/2}(x-x')) \end{pmatrix} \\ &\qquad \times \begin{pmatrix} 0 & 0 \\ V(x') & 0 \end{pmatrix} F_\pm(z,x') \\ &= F_\pm^{(0)}(z,x) - \int_x^{\pm\infty} dx' \begin{pmatrix} z^{-1/2}\sin(z^{1/2}(x-x')) & 0 \\ \cos(z^{1/2}(x-x')) & 0 \end{pmatrix} V(x')F_\pm(z,x'), \\ &\qquad \operatorname{Im}(z^{1/2}) \geq 0, \ z \neq 0, \ x \in \mathbb{R}, \end{aligned} \tag{4.81}$$

where we abbreviated

$$F_\pm^{(0)}(z,x) = \begin{pmatrix} 1 \\ \pm iz^{1/2} \end{pmatrix} \exp(\pm iz^{1/2}x). \tag{4.82}$$

By inspection, the first component of (4.81) is equivalent to (4.53) and the second component to the x-derivative of (4.53), that is, one has

$$F_\pm(z,,x) = \begin{pmatrix} f_\pm(z,x) \\ f'_\pm(z,x) \end{pmatrix}, \quad \operatorname{Im}(z^{1/2}) \geq 0, \ z \neq 0, \ x \in \mathbb{R}. \tag{4.83}$$

Next, one introduces

$$\begin{aligned}
f_1(z,x) &= -u(x)\begin{pmatrix} 1 \\ iz^{1/2} \end{pmatrix}\exp(iz^{1/2}x), \\
f_2(z,x) &= -u(x)\begin{pmatrix} 1 \\ -iz^{1/2} \end{pmatrix}\exp(-iz^{1/2}x), \\
g_1(z,x) &= v(x)\begin{pmatrix} \frac{i}{2z^{1/2}}\exp(-iz^{1/2}x) & 0 \end{pmatrix}, \\
g_2(z,x) &= v(x)\begin{pmatrix} \frac{i}{2z^{1/2}}\exp(iz^{1/2}x) & 0 \end{pmatrix}
\end{aligned} \tag{4.84}$$

and hence

$$H(z,x,x') = f_1(z,x)g_1(z,x') - f_2(z,x)g_2(z,x') \tag{4.85}$$

$$= u(x)\begin{pmatrix} z^{-1/2}\sin(z^{1/2}(x-x')) & 0 \\ \cos(z^{1/2}(x-x')) & 0 \end{pmatrix} v(x') \tag{4.86}$$

and we introduce

$$\widetilde{K}(z,x,x') = \begin{cases} f_1(z,x)g_1(z,x'), & x' < x, \\ f_2(z,x)g_2(z,x'), & x < x', \end{cases} \tag{4.87}$$

$$= \begin{cases} -u(x)\frac{1}{2}\exp(iz^{1/2}(x-x'))\begin{pmatrix} iz^{-1/2} & 0 \\ -1 & 0 \end{pmatrix} v(x'), & x' < x, \\ -u(x)\frac{1}{2}\exp(-iz^{1/2}(x-x'))\begin{pmatrix} iz^{-1/2} & 0 \\ 1 & 0 \end{pmatrix} v(x'), & x < x', \end{cases}$$

$$\operatorname{Im}(z^{1/2}) \geq 0,\ z \neq 0,\ x,x' \in \mathbb{R}. \tag{4.88}$$

We note that $\widetilde{K}(z,\cdot,\cdot)$ is discontinuous on the diagonal $x = x'$. Since

$$\widetilde{K}(z,\cdot,\cdot) \in L^2(\mathbb{R}^2; dx\, dx'), \quad \operatorname{Im}(z^{1/2}) \geq 0,\ z \neq 0, \tag{4.89}$$

the associated operator $\widetilde{K}(z)$ with integral kernel (4.88) is Hilbert–Schmidt,

$$\widetilde{K}(z) \in \mathcal{B}_2(L^2(\mathbb{R}; dx)), \quad \operatorname{Im}(z^{1/2}) \geq 0,\ z \neq 0. \tag{4.90}$$

Next, assuming temporarily that

$$\operatorname{supp}(V) \text{ is compact}, \tag{4.91}$$

the integral equations defining $\hat f_j(z,x)$, $j=1,2$,

$$\hat f_1(z,x) = f_1(z,x) - \int_x^\infty dx'\, H(z,x,x')\hat f_1(z,x'), \tag{4.92}$$

$$\hat f_2(z,x) = f_2(z,x) + \int_{-\infty}^x dx'\, H(z,x,x')\hat f_2(z,x'), \tag{4.93}$$

$$\operatorname{Im}(z^{1/2}) \geq 0,\ z\neq 0,\ x\in\mathbb{R},$$

yield solutions $\hat f_j(z,\cdot) \in L^2(\mathbb{R};dx)$, $j=1,2$. By comparison with (4.81), one then identifies

$$\hat f_1(z,x) = -u(x)F_+(z,x), \tag{4.94}$$

$$\hat f_2(z,x) = -u(x)F_-(z,x). \tag{4.95}$$

We note that the temporary compact support assumption (4.91) on V has only been introduced to guarantee that

$$f_j(z,\cdot), \hat f_j(z,\cdot) \in L^2(\mathbb{R};dx)^2, \quad j=1,2. \tag{4.96}$$

This extra hypothesis will soon be removed.

An application of Lemma 2.6 and Theorem 3.3 then yields the following result.

Theorem 4.7. *Suppose $V\in L^1(\mathbb{R};dx)$ and let $z\in\mathbb{C}$ with $\operatorname{Im}(z^{1/2})\geq 0$, $z\neq 0$. Then*

$$\det{}_2(I-\widetilde K(z)) = \mathcal{F}(z)\exp\bigg(-\frac{i}{2z^{1/2}}\int_{\mathbb{R}} dx\, V(x)\bigg) \tag{4.97}$$

$$= \det{}_2(I-K(z)) \tag{4.98}$$

with $K(z)$ defined in (4.59).

Proof. Assuming temporarily that $\operatorname{supp}(V)$ is compact (cf. (4.91)), equation (4.97) directly follows from combining (3.28) (or (3.31)) with $a=-\infty$, $b=\infty$, (3.17) (or (3.19)), (4.69), and (4.84). Equation (4.98) then follows from (3.25), (3.6) (or (3.7)), and (4.84). To extend the result to general $V\in L^1(\mathbb{R};dx)$ one follows the approximation argument presented in Theorem 4.3. □

One concludes that the scalar second-order equation (4.76) and the first-order system (4.77) share the identical 2-modified Fredholm determinant.

Remark 4.8. *Let* $\operatorname{Im}(z^{1/2}) \geq 0$*,* $z \neq 0$*, and* $x \in \mathbb{R}$*. Then following up on Remark* 2.8*, one computes*

$$\begin{aligned} A(z,x) &= \begin{pmatrix} g_1(z,x)f_1(z,x) & g_1(z,x)f_2(z,x) \\ -g_2(z,x)f_1(z,x) & -g_2(z,x)f_2(z,x) \end{pmatrix} \\ &= -\frac{i}{2z^{1/2}} V(x) \begin{pmatrix} 1 & e^{-2iz^{1/2}x} \\ -e^{2iz^{1/2}x} & -1 \end{pmatrix} \qquad (4.99) \\ &= -\frac{i}{2z^{1/2}} V(x) \begin{pmatrix} e^{-iz^{1/2}x} & 0 \\ 0 & e^{iz^{1/2}x} \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \begin{pmatrix} e^{iz^{1/2}x} & 0 \\ 0 & e^{-iz^{1/2}x} \end{pmatrix}. \end{aligned}$$

Introducing

$$W(z,x) = e^{M(z)x}U(z,x), \quad M(z) = iz^{1/2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad (4.100)$$

and recalling

$$U'(z,x) = A(z,x)U(z,x), \qquad (4.101)$$

(*cf.* (2.20))*, equation* (4.101) *reduces to*

$$W'(z,x) = \left[iz^{1/2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \frac{i}{2z^{1/2}} V(x) \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \right] W(z,x). \qquad (4.102)$$

Moreover, introducing

$$T(z) = \begin{pmatrix} 1 & 1 \\ iz^{1/2} & -iz^{1/2} \end{pmatrix}, \quad \operatorname{Im}(z^{1/2}) \geq 0, \ z \neq 0, \qquad (4.103)$$

one obtains

$$\begin{aligned} &\left[iz^{1/2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \frac{i}{2z^{1/2}} V(x) \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \right] \qquad (4.104) \\ &\quad = T(z)^{-1} \begin{pmatrix} 0 & 1 \\ V(x) - z & 0 \end{pmatrix} T(z), \quad \operatorname{Im}(z^{1/2}) \geq 0, \ z \neq 0, \ x \in \mathbb{R}, \end{aligned}$$

which demonstrates the connection between (2.20)*,* (4.102)*, and* (4.77)*.*

Finally, we turn to the case of periodic Schrödinger operators of period $\omega > 0$:

The case $(\mathbf{a}, \mathbf{b}) = (\mathbf{0}, \omega)$**:** Assuming

$$V \in L^1((0,\omega); dx), \qquad (4.105)$$

we now introduce two one-parameter families of closed operators in $L^2((0,\omega);dx)$ defined by

$$\begin{aligned} &H_\theta^{(0)} f = -f'', \\ &f \in \mathrm{dom}\big(H_\theta^{(0)}\big) = \{g \in L^2((0,\omega);dx) \,|\, g, g' \in AC([0,\omega]); \\ &\qquad g(\omega) = e^{i\theta} g(0),\ g'(\omega) = e^{i\theta} g'(0),\ g'' \in L^2((0,\omega);dx)\}, \qquad (4.106) \\ &H_\theta f = -f'' + Vf, \\ &f \in \mathrm{dom}(H_\theta) = \{g \in L^2((0,\omega);dx) \,|\, g, g' \in AC([0,\omega]); \qquad (4.107) \\ &\quad g(\omega) = e^{i\theta} g(0),\ g'(\omega) = e^{i\theta} g'(0),\ (-g'' + Vg) \in L^2((0,\omega);dx)\}, \end{aligned}$$

where $\theta \in [0, 2\pi)$. As in the previous cases considered, $H_\theta^{(0)}$ is self-adjoint and H_θ is self-adjoint if and only if V is real-valued.

Introducing the fundamental system of solutions $c(z,\cdot)$ and $s(z,\cdot)$ of $-\psi''(z) + V\psi(z) = z\psi(z)$, $z \in \mathbb{C}$, by

$$c(z,0) = 1 = s'(z,0), \quad c'(z,0) = 0 = s(z,0), \qquad (4.108)$$

the associated fundamental matrix of solutions $\Phi(z,x)$ is defined by

$$\Phi(z,x) = \begin{pmatrix} c(z,x) & s(z,x) \\ c'(z,x) & s'(z,x) \end{pmatrix}. \qquad (4.109)$$

The monodromy matrix is then given by $\Phi(z,\omega)$, and the Floquet discriminant $\Delta(z)$ is defined as half of the trace of the latter,

$$\Delta(z) = \mathrm{tr}_{\mathbb{C}^2}(\Phi(z,\omega))/2 = [c(z,\omega) + s'(z,\omega)]/2. \qquad (4.110)$$

Thus, the eigenvalue equation for H_θ reads,

$$\Delta(z) = \cos(\theta). \qquad (4.111)$$

In the special case $V = 0$ a.e. one obtains

$$c^{(0)}(z,x) = \cos(z^{1/2}x), \quad s^{(0)}(z,x) = \sin(z^{1/2}x) \qquad (4.112)$$

and hence,

$$\Delta^{(0)}(z) = \cos(z^{1/2}\omega). \qquad (4.113)$$

Next we introduce additional solutions $\varphi_\pm(z,\cdot)$, $\psi_\pm(z,\cdot)$ of $-\psi''(z) + V\psi(z) = z\psi(z)$, $z \in \mathbb{C}$, by

$$\varphi_\pm(z,x) = e^{\pm iz^{1/2}x} + \int_0^x dx'\, g^{(0)}(z,x,x')V(x')\varphi_\pm(z,x'), \qquad (4.114)$$

$$\psi_\pm(z,x) = e^{\pm iz^{1/2}x} - \int_x^\omega dx'\, g^{(0)}(z,x,x')V(x')\psi_\pm(z,x'), \qquad (4.115)$$

$$\mathrm{Im}(z^{1/2}) \geq 0,\ x \in [0,\omega],$$

where $g^{(0)}(z,x,x')$ is still given by (4.6). We also introduce the Green's function of $H_\theta^{(0)}$,

$$\begin{aligned} G_\theta^{(0)}(z,x,x') &= \big(H_\theta^{(0)}-z\big)^{-1}(x,x') \\ &= \frac{i}{2z^{1/2}}\bigg[e^{iz^{1/2}|x-x'|} + \frac{e^{iz^{1/2}(x-x')}}{e^{i\theta}e^{-iz^{1/2}\omega}-1} + \frac{e^{-iz^{1/2}(x-x')}}{e^{-i\theta}e^{-iz^{1/2}\omega}-1}\bigg], \\ &\qquad \operatorname{Im}(z^{1/2})>0,\ x,x'\in(0,\omega). \end{aligned} \tag{4.116}$$

Introducing again the factorization (4.12) of $V=uv$, one verifies as in (4.13) that

$$\begin{aligned} (H_\theta - z)^{-1} &= \big(H_\theta^{(0)}-z\big)^{-1} \\ &\quad - \big(H_\theta^{(0)}-z\big)^{-1}v\Big[I+\overline{u\big(H_\theta^{(0)}-z\big)^{-1}v}\Big]^{-1}u\big(H_\theta^{(0)}-z\big)^{-1}, \\ &\qquad z\in\mathbb{C}\backslash\{\operatorname{spec}(H_\theta)\cup\operatorname{spec}(H_\theta^{(0)})\}. \end{aligned} \tag{4.117}$$

To establish the connection with the notation used in Sections 2 and 3, we introduce the operator $K_\theta(z)$ in $L^2((0,\omega);dx)$ (cf. (2.3), (4.14)) by

$$K_\theta(z) = -\overline{u\big(H_\theta^{(0)}-z\big)^{-1}v}, \quad z\in\mathbb{C}\backslash\operatorname{spec}\big(H_\theta^{(0)}\big) \tag{4.118}$$

with integral kernel

$$\begin{aligned} K_\theta(z,x,x') &= -u(x)G_\theta^{(0)}(z,x,x')v(x'), \\ &\quad z\in\mathbb{C}\backslash\operatorname{spec}\big(H_\theta^{(0)}\big),\ x,x'\in[0,\omega], \end{aligned} \tag{4.119}$$

and the Volterra operators $H_0(z)$, $H_\omega(z)$ (cf. (2.4), (2.5)) with integral kernel

$$H(z,x,x') = u(x)g^{(0)}(z,x,x')v(x'). \tag{4.120}$$

Moreover, we introduce for a.e. $x\in(0,\omega)$,

$$\begin{aligned} f_1(z,x) &= f_2(z,x) = f(z,x) = -u(x)(e^{iz^{1/2}x}\ \ e^{-iz^{1/2}x}), \\ g_1(z,x) &= \frac{i}{2z^{1/2}}v(x)\begin{pmatrix} \frac{\exp(i\theta)\exp(-iz^{1/2}\omega)\exp(-iz^{1/2}x)}{\exp(i\theta)\exp(-iz^{1/2}\omega)-1} \\ \frac{\exp(iz^{1/2}x)}{\exp(-i\theta)\exp(-iz^{1/2}\omega)-1} \end{pmatrix}, \\ g_2(z,x) &= \frac{i}{2z^{1/2}}v(x)\begin{pmatrix} \frac{\exp(-iz^{1/2}x)}{\exp(i\theta)\exp(-iz^{1/2}\omega)-1} \\ \frac{\exp(-i\theta)\exp(-iz^{1/2}\omega)\exp(iz^{1/2}x)}{\exp(-i\theta)\exp(-iz^{1/2}\omega)-1} \end{pmatrix}. \end{aligned} \tag{4.121}$$

Introducing $\hat{f}_j(z,x)$, $j=1,2$, by

$$\hat{f}_1(z,x) = f(z,x) - \int_x^\omega dx'\, H(z,x,x')\hat{f}_1(z,x'), \tag{4.122}$$

$$\hat{f}_2(z,x) = f(z,x) + \int_0^x dx'\, H(z,x,x')\hat{f}_2(z,x'), \tag{4.123}$$

$$\operatorname{Im}(z^{1/2}) \geq 0,\ z \neq 0,\ x \geq 0,$$

yields solutions $\hat{f}_j(z,\cdot) \in L^2((0,\omega);dx)$, $j=1,2$. By comparison with (4.4), (4.5), one then identifies

$$\hat{f}_1(z,x) = -u(x)(\psi_+(z,x)\ \ \psi_-(z,x)), \tag{4.124}$$

$$\hat{f}_2(z,x) = -u(x)(\varphi_+(z,x)\ \ \varphi_-(z,x)). \tag{4.125}$$

Next we mention the following result.

Theorem 4.9. *Suppose $V \in L^1((0,\omega);dx)$, let $\theta \in [0,2\pi)$, and $z \in \mathbb{C}\backslash\operatorname{spec}\big(H_\theta^{(0)}\big)$. Then*

$$K_\theta(z) \in \mathcal{B}_1(L^2((0,\omega);dx)) \tag{4.126}$$

and

$$\det(I - K_\theta(z)) = \frac{\Delta(z) - \cos(\theta)}{\cos(z^{1/2}\omega) - \cos(\theta)}. \tag{4.127}$$

Proof. Since the integral kernel of $K_\theta(z)$ is square integrable over the set $(0,\omega)\times(0,\omega)$, one has of course $K_\theta(z) \in \mathcal{B}_2(L^2((0,\omega);dx))$. To prove its trace class property one imbeds $(0,\omega)$ into $\mathbb{R}$ in analogy to the half-line case discussed in the proof of Theorem 4.2, introducing

$$L^2(\mathbb{R};dx) = L^2((0,\omega);dx) \oplus L^2(\mathbb{R}\backslash[0,\omega];dx) \tag{4.128}$$

and

$$\begin{aligned} &\tilde{u}(x) = \begin{cases} u(x), & x \in (0,\omega), \\ 0, & x \notin (0,\omega), \end{cases} \quad \tilde{v}(x) = \begin{cases} v(x), & x \in (0,\omega), \\ 0, & x \notin (0,\omega), \end{cases} \\ &\widetilde{V}(x) = \begin{cases} V(x), & x \in (0,\omega), \\ 0, & x \notin (0,\omega). \end{cases} \end{aligned} \tag{4.129}$$

At this point one can follow the proof of Theorem 4.2 line by line using (4.116) instead of (4.30) and noticing that the second and third term on the right-hand side of (4.116) generate rank one terms upon multiplying them by $\tilde{u}(x)$ from the left and $\tilde{v}(x')$ from the right.

By (4.111) and (4.113), and since

$$\det(I - K_\theta(z)) = \det\Big(\big(H_\theta^{(0)} - z\big)^{-1/2}(H_\theta - z)\big(H_\theta^{(0)} - z\big)^{-1/2}\Big), \tag{4.130}$$

$\det(I - K_\theta(z))$ and $[\Delta(z) - \cos(\theta)]/[\cos(z^{1/2}\omega) - \cos(\theta)]$ have the same set of zeros and poles. Moreover, since either expression satisfies the asymptotics $1 + o(1)$ as $z \downarrow -\infty$, one obtains (4.127). □

An application of Lemma 2.6 and Theorem 3.2 then yields the following result relating the Fredholm determinant of $I - K_\theta(z)$ and the Floquet discriminant $\Delta(z)$.

Theorem 4.10. *Suppose $V \in L^1((0,\omega); dx)$, let $\theta \in [0, 2\pi)$, and $z \in \mathbb{C}\backslash\mathrm{spec}\big(H_\theta^{(0)}\big)$. Then*

$$\begin{aligned}
\det(I - K_\theta(z)) &= \frac{\Delta(z) - \cos(\theta)}{\cos(z^{1/2}\omega) - \cos(\theta)} \\
&= \bigg[1 + \frac{i}{2z^{1/2}} \frac{e^{i\theta}e^{-iz^{1/2}\omega}}{e^{i\theta}e^{-iz^{1/2}\omega} - 1} \int_0^\omega dx\, e^{-iz^{1/2}x} V(x)\psi_+(z,x)\bigg] \\
&\quad \times \bigg[1 + \frac{i}{2z^{1/2}} \frac{1}{e^{-i\theta}e^{-iz^{1/2}\omega} - 1} \int_0^\omega dx\, e^{iz^{1/2}x} V(x)\psi_-(z,x)\bigg] \\
&\quad + \frac{1}{4z} \frac{e^{i\theta}e^{-iz^{1/2}\omega}}{\big[e^{i\theta}e^{-iz^{1/2}\omega} - 1\big]\big[e^{-i\theta}e^{-iz^{1/2}\omega} - 1\big]} \\
&\qquad \times \int_0^\omega dx\, e^{iz^{1/2}x} V(x)\psi_+(z,x) \int_0^\omega dx\, e^{-iz^{1/2}x} V(x)\psi_-(z,x)
\end{aligned} \tag{4.131}$$

$$\begin{aligned}
&= \bigg[1 + \frac{i}{2z^{1/2}} \frac{1}{e^{i\theta}e^{-iz^{1/2}\omega} - 1} \int_0^\omega dx\, e^{-iz^{1/2}x} V(x)\varphi_+(z,x)\bigg] \\
&\quad \times \bigg[1 + \frac{i}{2z^{1/2}} \frac{e^{-i\theta}e^{-iz^{1/2}\omega}}{e^{-i\theta}e^{-iz^{1/2}\omega} - 1} \int_0^\omega dx\, e^{iz^{1/2}x} V(x)\varphi_-(z,x)\bigg] \\
&\quad + \frac{1}{4z} \frac{e^{-i\theta}e^{-iz^{1/2}\omega}}{\big[e^{i\theta}e^{-iz^{1/2}\omega} - 1\big]\big[e^{-i\theta}e^{-iz^{1/2}\omega} - 1\big]} \\
&\qquad \times \int_0^\omega dx\, e^{iz^{1/2}x} V(x)\varphi_+(z,x) \int_0^\omega dx\, e^{-iz^{1/2}x} V(x)\varphi_-(z,x).
\end{aligned} \tag{4.132}$$

Proof. Again Lemma 2.6 applies and one infers from (2.38) and (4.121)–(4.125) that

$$U(z,x) = \begin{pmatrix} 1 - \int_x^\omega dx'\, g_1(z,x')\hat f(z,x') & \int_0^x dx'\, g_1(z,x')\hat f(z,x') \\ \int_x^\omega dx'\, g_2(z,x')\hat f(z,x') & 1 - \int_0^x dx'\, g_2(z,x')\hat f(z,x') \end{pmatrix}, \quad x \in [0,\omega], \tag{4.133}$$

becomes

$$U_{1,1}(z,x) = I_2 + \frac{i}{2z^{1/2}} \int_x^\omega dx' \begin{pmatrix} \frac{\exp(i\theta)\exp(-iz^{1/2}\omega)\exp(-iz^{1/2}x')}{\exp(i\theta)\exp(-iz^{1/2}\omega)-1} \\ \frac{e^{iz^{1/2}x'}}{\exp(-i\theta)\exp(-iz^{1/2}\omega)-1} \end{pmatrix} V(x') \times (\psi_+(z,x') \;\; \psi_-(z,x')), \tag{4.134}$$

$$U_{1,2}(z,x) = -\frac{i}{2z^{1/2}} \int_0^x dx' \begin{pmatrix} \frac{\exp(i\theta)\exp(-iz^{1/2}\omega)\exp(-iz^{1/2}x')}{\exp(i\theta)\exp(-iz^{1/2}\omega)-1} \\ \frac{\exp(iz^{1/2}x')}{\exp(-i\theta)\exp(-iz^{1/2}\omega)-1} \end{pmatrix} V(x') \times (\varphi_+(z,x') \;\; \varphi_-(z,x')), \tag{4.135}$$

$$U_{2,1}(z,x) = -\frac{i}{2z^{1/2}} \int_x^\omega dx' \begin{pmatrix} \frac{\exp(-iz^{1/2}x')}{\exp(i\theta)\exp(-iz^{1/2}\omega)-1} \\ \frac{\exp(-i\theta)\exp(-iz^{1/2}\omega)\exp(iz^{1/2}x')}{\exp(-i\theta)\exp(-iz^{1/2}\omega)-1} \end{pmatrix} V(x') \times (\psi_+(z,x') \;\; \psi_-(z,x')), \tag{4.136}$$

$$U_{2,2}(z,x) = I_2 + \frac{i}{2z^{1/2}} \int_0^x dx' \begin{pmatrix} \frac{\exp(-iz^{1/2}x')}{\exp(i\theta)\exp(-iz^{1/2}\omega)-1} \\ \frac{\exp(-i\theta)\exp(-iz^{1/2}\omega)\exp(iz^{1/2}x')}{\exp(-i\theta)\exp(-iz^{1/2}\omega)-1} \end{pmatrix} V(x') \times (\varphi_+(z,x') \;\; \varphi_-(z,x')). \tag{4.137}$$

Relations (3.9) and (3.12) of Theorem 3.2 with $m = 1$, $n_1 = n_2 = 2$, $n = 4$, then immediately yield (4.131) and (4.132). □

To the best of our knowledge, the representations (4.131) and (4.132) of $\Delta(z)$ appear to be new. They are the analogs of the well-known representations of Jost functions (4.9), (4.10) and (4.56) on the half-line and on the real line, respectively. That the Floquet discriminant $\Delta(z)$ is related to infinite determinants is well-known. However, the connection between $\Delta(z)$ and determinants of Hill-type discussed in the literature (cf., e.g., [27], [14, Ch. III, Sect. VI.2], [28, Sect. 2.3]) is of a different nature than the one in (4.127) and based on the Fourier expansion of the potential V. For different connections between Floquet theory and perturbation determinants we refer to [10].

5. Integral operators of convolution-type

WITH RATIONAL SYMBOLS

In our final section we rederive the explicit formula for the 2-modified Fredholm determinant corresponding to integral operators of convolution-type, whose integral kernel is associated with a symbol given by a rational function, in an elementary and straghtforward manner. This determinant formula represents a truncated Wiener–Hopf analog of Day's formula for the determinant associated with finite Toeplitz matrices generated by the Laurent expansion of a rational function.

Let $\tau > 0$. We are interested in truncated Wiener–Hopf-type operators K in $L^2((0,\tau);dx)$ of the form

$$(Kf)(x) = \int_0^\tau dx'\, k(x-x')f(x'), \quad f \in L^2((0,\tau);dx), \tag{5.1}$$

where $k(\cdot)$, extended from $[-\tau,\tau]$ to $\mathbb{R}\backslash\{0\}$, is defined by

$$k(t) = \begin{cases} \sum_{\ell\in\mathcal{L}} \alpha_\ell\, e^{-\lambda_\ell t}, & t > 0, \\ \sum_{m\in\mathcal{M}} \beta_m e^{\mu_m t}, & t < 0 \end{cases} \tag{5.2}$$

and

$$\begin{aligned} &\alpha_\ell \in \mathbb{C},\ \ell \in \mathcal{L} = \{1,\dots,L\},\ L \in \mathbb{N}, \\ &\beta_m \in \mathbb{C},\ m \in \mathcal{M} = \{1,\dots,M\},\ M \in \mathbb{N}, \\ &\lambda_\ell \in \mathbb{C},\ \mathrm{Re}(\lambda_\ell) > 0,\ \ell \in \mathcal{L}, \\ &\mu_m \in \mathbb{C},\ \mathrm{Re}(\mu_m) > 0,\ m \in \mathcal{M}. \end{aligned} \tag{5.3}$$

In terms of semi-separable integral kernels, k can be rewritten as,

$$k(x-x') = K(x,x') = \begin{cases} f_1(x)g_1(x'), & 0 < x' < x < \tau, \\ f_2(x)g_2(x'), & 0 < x < x' < \tau, \end{cases} \tag{5.4}$$

where

$$\begin{aligned} f_1(x) &= \big(\alpha_1 e^{-\lambda_1 x}, \dots, \alpha_L e^{-\lambda_L x}\big), \\ f_2(x) &= \big(\beta_1 e^{\mu_1 x}, \dots, \beta_M e^{\mu_M x}\big), \\ g_1(x) &= \big(e^{\lambda_1 x}, \dots, e^{\lambda_L x}\big)^\top, \\ g_2(x) &= \big(e^{-\mu_1 x}, \dots, e^{-\mu_M x}\big)^\top. \end{aligned} \tag{5.5}$$

Since $K(\cdot,\cdot) \in L^2((0,\tau)\times(0,\tau);dx\,dx')$, the operator K in (5.1) belongs to the Hilbert–Schmidt class,

$$K \in \mathcal{B}_2(L^2((0,\tau);dx)). \tag{5.6}$$

Associated with K we also introduce the Volterra operators H_0, H_τ (cf. (2.4), (2.5)) in $L^2((0,\tau);dx)$ with integral kernel

$$h(x-x') = H(x,x') = f_1(x)g_1(x') - f_2(x)g_2(x'), \tag{5.7}$$

such that

$$h(t) = \sum_{\ell\in\mathcal{L}} \alpha_\ell\, e^{-\lambda_\ell t} - \sum_{m\in\mathcal{M}} \beta_m e^{\mu_m t}. \tag{5.8}$$

In addition, we introduce the Volterra integral equation

$$\hat f_2(x) = f_2(x) + \int_0^x dx'\, h(x-x')\hat f_2(x'), \quad x\in(0,\tau) \tag{5.9}$$

with solution $\hat f_2 \in L^2((0,\tau);dx)$.

Next, we introduce the Laplace transform $\mathbb{F}$ of a function f by

$$\mathbb{F}(\zeta) = \int_0^\infty dt\, e^{-\zeta t} f(t), \tag{5.10}$$

where either $f\in L^r((0,\infty);dt)$, $r\in\{1,2\}$ and $\mathrm{Re}(\zeta)>0$, or, f satisfies an exponential bound of the type $|f(t)|\le C\exp(Dt)$ for some $C>0$, $D\ge 0$ and then $\mathrm{Re}(\zeta)>D$. Moreover, whenever possible, we subsequently meromorphically continue $\mathbb{F}$ into the half-plane $\mathrm{Re}(\zeta)<0$ and $\mathrm{Re}(\zeta)<D$, respectively, and for simplicity denote the result again by $\mathbb{F}$.

Taking the Laplace transform of equation (5.9), one obtains

$$\widehat{\mathbb{F}}_2(\zeta) = \mathbb{F}_2(\zeta) + \mathbb{H}(\zeta)\widehat{\mathbb{F}}_2(\zeta), \tag{5.11}$$

where

$$\mathbb{F}_2(\zeta) = \big(\beta_1(\zeta-\mu_1)^{-1},\dots,\beta_M(\zeta-\mu_M)^{-1}\big), \tag{5.12}$$

$$\mathbb{H}(\zeta) = \sum_{\ell\in\mathcal{L}} \alpha_\ell(\zeta+\lambda_\ell)^{-1} - \sum_{m\in\mathcal{M}} \beta_m(\zeta-\mu_m)^{-1} \tag{5.13}$$

and hence solving (5.11), yields

$$\widehat{\mathbb{F}}_2(\zeta) = (1-\mathbb{H}(\zeta))^{-1}\big(\beta_1(\zeta-\mu_1)^{-1},\dots,\beta_M(\zeta-\mu_M)^{-1}\big). \tag{5.14}$$

Introducing the Fourier transform $\mathcal{F}(k)$ of the kernel function k by

$$\mathcal{F}(k)(x) = \int_{\mathbb{R}} dt\, e^{ixt}k(t), \quad x\in\mathbb{R}, \tag{5.15}$$

one obtains the rational symbol

$$\mathcal{F}(k)(x) = \sum_{\ell\in\mathcal{L}} \alpha_\ell(\lambda_\ell - ix)^{-1} + \sum_{m\in\mathcal{M}} \beta_m(\mu_m+ix)^{-1}. \tag{5.16}$$

Thus,

$$
\begin{aligned}
1 - \mathbb{H}(-ix) &= 1 - \mathcal{F}(k)(x) \\
&= \prod_{n\in\mathcal{N}}(-ix + i\zeta_n)\prod_{\ell\in\mathcal{L}}(-ix+\lambda_\ell)^{-1}\prod_{m\in\mathcal{M}}(-ix-\mu_m)^{-1} \qquad (5.17)
\end{aligned}
$$

for some

$$
\zeta_n \in \mathbb{C},\ n\in\mathcal{N}=\{1,\dots,N\},\ N = L+M. \qquad (5.18)
$$

Consequently,

$$
1-\mathbb{H}(\zeta) = \prod_{n\in\mathcal{N}}(\zeta + i\zeta_n)\prod_{\ell\in\mathcal{L}}(\zeta+\lambda_\ell)^{-1}\prod_{m\in\mathcal{M}}(\zeta-\mu_m)^{-1}, \qquad (5.19)
$$

$$
(1-\mathbb{H}(\zeta))^{-1} = 1 + \sum_{n\in\mathcal{N}}\gamma_n(\zeta+i\zeta_n)^{-1}, \qquad (5.20)
$$

where

$$
\gamma_n = \prod_{\substack{n'\in\mathcal{N}\\ n'\neq n}}(i\zeta_n - i\zeta_{n'})^{-1}\prod_{\ell\in\mathcal{L}}(\lambda_\ell - i\zeta_n)\prod_{m\in\mathcal{M}}(-i\zeta_n-\mu_m), \quad n\in\mathcal{N}. \qquad (5.21)
$$

Moreover, one computes

$$
\beta_m = \prod_{\ell\in\mathcal{L}}(\mu_m+\lambda_\ell)^{-1}\prod_{\substack{m'\in\mathcal{M}\\ m'\neq m}}(\mu_m-\mu_{m'})^{-1}\prod_{n\in\mathcal{N}}(\mu_m+i\zeta_n), \quad m\in\mathcal{M}. \qquad (5.22)
$$

Combining (5.14) and (5.20) yields

$$
\widehat{\mathbb{F}}_2(\zeta) = \bigg(1+\sum_{n\in\mathcal{N}}\gamma_n(\zeta+i\zeta_n)^{-1}\bigg)\big(\beta_1(\zeta-\mu_1)^{-1},\dots,\beta_M(\zeta-\mu_M)^{-1}\big) \qquad (5.23)
$$

and hence

$$
\begin{aligned}
\hat f_2(x) = \bigg(&\beta_1\bigg[e^{\mu_1 x} - \sum_{n\in\mathcal{N}}\gamma_n\big(e^{-i\zeta_n x}-e^{\mu_1 x}\big)(\mu_1+i\zeta_n)^{-1}\bigg],\dots \\
&\dots,\beta_M\bigg[e^{\mu_M x} - \sum_{n\in\mathcal{N}}\gamma_n\big(e^{-i\zeta_n x}-e^{\mu_M x}\big)(\mu_M+i\zeta_n)^{-1}\bigg]\bigg).
\end{aligned} \qquad (5.24)
$$

In view of (3.31) we now introduce the $M\times M$ matrix

$$
G = \big(G_{m,m'}\big)_{m,m'\in\mathcal{M}} = \int_0^\tau dx\, g_2(x)\hat f_2(x). \qquad (5.25)
$$

Lemma 5.1. *One computes*

$$G_{m,m'} = \delta_{m,m'} + e^{-\mu_m \tau} \beta_{m'} \sum_{n\in\mathcal{N}} \gamma_n e^{-i\zeta_n \tau} (\mu_m + i\zeta_n)^{-1} (\mu_{m'} + i\zeta_n)^{-1}, \quad m, m' \in \mathcal{M}. \tag{5.26}$$

Proof. By (5.25),

$$\begin{aligned} G_{m,m'} &= \int_0^\tau dt\, e^{-\mu_m t} \beta_{m'} \bigg(e^{\mu_{m'} t} - \sum_{n\in\mathcal{N}} \gamma_n \big(e^{-i\zeta_n t} - e^{\mu_{m'} t} \big) (i\zeta_n + \mu_{m'})^{-1} \bigg) \\ &= \beta_{m'} \int_0^\tau dt\, e^{-(\mu_m - \mu_{m'})t} \bigg(1 + \sum_{n\in\mathcal{N}} \gamma_n (i\zeta_n + \mu_{m'})^{-1} \bigg) \\ &\quad - \beta_{m'} \int_0^\tau dt\, e^{-\mu_m t} \sum_{n\in\mathcal{N}} \gamma_n e^{-i\zeta_n t} (i\zeta_n + \mu_{m'})^{-1} \\ &= -\beta_{m'} \sum_{n\in\mathcal{N}} \gamma_n (i\zeta_n + \mu_{m'})^{-1} \int_0^\tau dt\, e^{-(i\zeta_n + \mu_m)t} \\ &= \beta_{m'} \sum_{n\in\mathcal{N}} \gamma_n \big[e^{-(i\zeta_n + \mu_m)t} - 1 \big] (i\zeta_n + \mu_m)^{-1} (i\zeta_n + \mu_{m'})^{-1}. \end{aligned} \tag{5.27}$$

Here we used the fact that

$$1 + \sum_{n\in\mathcal{N}} \gamma_n (i\zeta_n + \mu_{m'})^{-1} = 0, \tag{5.28}$$

which follows from

$$1 + \sum_{n\in\mathcal{N}} \gamma_n (i\zeta_n + \mu_{m'})^{-1} = (1 - \mathbb{H}(\mu_{m'}))^{-1} = 0, \tag{5.29}$$

using (5.19) and (5.20). Next, we claim that

$$-\beta_{m'} \sum_{n\in\mathcal{N}} \gamma_n (i\zeta_n + \mu_m)^{-1} (i\zeta_n + \mu_{m'})^{-1} = \delta_{m,m'}. \tag{5.30}$$

Indeed, if $m \neq m'$, then

$$\begin{aligned} &\sum_{n\in\mathcal{N}} \gamma_n (i\zeta_n + \mu_m)^{-1} (i\zeta_n + \mu_{m'})^{-1} \\ &\quad = -\sum_{n\in\mathcal{N}} \gamma_n (\mu_m - \mu_{m'})^{-1} \big[(i\zeta_n + \mu_m)^{-1} - (i\zeta_n + \mu_{m'})^{-1} \big] = 0, \end{aligned} \tag{5.31}$$

using (5.28). On the other hand, if $m = m'$, then

$$\begin{aligned}\beta_m \sum_{n\in\mathcal{N}} \gamma_n (i\zeta_n + \mu_m)^{-2} &= -\beta_m \frac{d}{d\zeta}(1 - \mathbb{H}(\zeta))^{-1}\Big|_{\zeta=\mu_m} \\ &= \operatorname*{Res}_{\zeta=\mu_m} \big(\mathbb{H}(\zeta)\big) \frac{d}{d\zeta}(1 - \mathbb{H}(\zeta))^{-1}\Big|_{\zeta=\mu_m} \\ &= -\operatorname*{Res}_{\zeta=\mu_m} \frac{d}{d\zeta} \log\big((1 - \mathbb{H}(\zeta))^{-1}\big) \\ &= -1, \end{aligned} \tag{5.32}$$

using (5.19). This proves (5.30). Combining (5.27) and (5.30) yields (5.26). □

Given Lemma 5.1, one can decompose $I_M - G$ as

$$I_M - G = \operatorname{diag}(e^{-\mu_1\tau}, \dots, e^{-\mu_M\tau})\, \Gamma \operatorname{diag}(\beta_1, \dots, \beta_M), \tag{5.33}$$

where $\operatorname{diag}(\cdot)$ denotes a diagonal matrix and the $M \times M$ matrix Γ is defined by

$$\begin{aligned}\Gamma &= \big(\Gamma_{m,m'}\big)_{m,m'\in\mathcal{M}} \\ &= \bigg(- \sum_{n\in\mathcal{N}} \gamma_n e^{-i\zeta_n\tau} (\mu_m + i\zeta_n)^{-1} (\mu_{m'} + i\zeta_n)^{-1} \bigg)_{m,m'\in\mathcal{M}}. \end{aligned} \tag{5.34}$$

The matrix Γ permits the factorization

$$\Gamma = A \operatorname{diag}(\gamma_1 e^{-i\zeta_1\tau}, \dots, \gamma_N e^{-i\zeta_N\tau})\, B, \tag{5.35}$$

where A is the $M \times N$ matrix

$$A = \big(A_{m,n}\big)_{m\in\mathcal{M}, n\in\mathcal{N}} = \big((\mu_m + i\zeta_n)^{-1}\big)_{m\in\mathcal{M}, n\in\mathcal{N}} \tag{5.36}$$

and B is the $N \times M$ matrix

$$B = \big(B_{n,m}\big)_{n\in\mathcal{N}, m\in\mathcal{M}} = \big(-(\mu_m + i\zeta_n)^{-1}\big)_{n\in\mathcal{N}, m\in\mathcal{M}}. \tag{5.37}$$

Next, we denote by Ψ the set of all monotone functions

$$\psi \colon \{1, \dots, M\} \to \{1, \dots, N\} \tag{5.38}$$

(we recall $N = L + M$) such that

$$\psi(1) < \cdots < \psi(M). \tag{5.39}$$

The set Ψ is in a one-to-one correspondence with all subsets $\widetilde{\mathcal{M}}^{\perp} = \{1, \dots, N\} \backslash \widetilde{\mathcal{M}}$ of $\{1, \dots, N\}$ which consist of L elements. Here $\widetilde{\mathcal{M}} \subseteq \{1, \dots, N\}$ with cardinality of $\mathcal{M}$ equal to M, $|\widetilde{\mathcal{M}}| = M$.

Moreover, denoting by A_ψ and B^ψ the $M\times M$ matrices

$$A_\psi = \big(A_{m,\psi(m')}\big)_{m,m'\in\mathcal{M}}, \quad \psi\in\Psi, \tag{5.40}$$

$$B^\psi = \big(B_{\psi(m),m'}\big)_{m,m'\in\mathcal{M}}, \quad \psi\in\Psi, \tag{5.41}$$

one notices that

$$A_\psi^\top = -B^\psi, \quad \psi\in\Psi. \tag{5.42}$$

The matrix A^ψ is of Cauchy-type and one infers (cf. [24, p. 36]) that

$$A_\psi^{-1} = D_1^\psi A_\psi^\top D_2^\psi, \tag{5.43}$$

where D_j^ψ, $j=1,2$, are diagonal matrices with diagonal entries given by

$$\big(D_1^\psi\big)_{m,m} = \prod_{m'\in\mathcal{M}} (\mu_{m'} + i\zeta_{\psi(m)}) \prod_{\substack{m''\in\mathcal{M}\\ m''\neq m}} (-i\zeta_{\psi(m'')} + i\zeta_{\psi(m)})^{-1}, \quad m\in\mathcal{M}, \tag{5.44}$$

$$\big(D_2^\psi\big)_{m,m} = \prod_{m'\in\mathcal{M}} (\mu_{m} + i\zeta_{\psi(m')}) \prod_{\substack{m''\in\mathcal{M}\\ m''\neq m}} (\mu_m - \mu_{m''})^{-1}, \quad m\in\mathcal{M}. \tag{5.45}$$

One then obtains the following result.

Lemma 5.2. *The determinant of $I_M - G$ is of the form*

$$\begin{aligned}
&\det_{\mathbb{C}^M}(I_M - G)\\
&\quad = (-1)^M \exp\bigg(-\tau\sum_{m\in\mathcal{M}}\mu_m\bigg)\bigg(\prod_{\ell\in\mathcal{L}}\beta_\ell\bigg)\sum_{\psi\in\Psi}\bigg(\prod_{\ell'\in\mathcal{L}}\gamma_{\psi(\ell')}\bigg)\\
&\qquad \times \exp\bigg(-i\tau\sum_{\ell''\in\mathcal{L}}\zeta_{\psi(\ell'')}\bigg)\big[\det_{\mathbb{C}^M}\big(D_1^\psi\big)\det_{\mathbb{C}^M}\big(D_2^\psi\big)\big]^{-1}.
\end{aligned} \tag{5.46}$$

Proof. Let $\psi\in\Psi$. Then

$$\begin{aligned}
\det_{\mathbb{C}^M}\big(A_\psi\big)\det_{\mathbb{C}^M}\big(B^\psi\big) &= (-1)^M\big[\det_{\mathbb{C}^M}\big(A_\psi\big)\big]^2\\
&= (-1)^M\big[\det_{\mathbb{C}^M}\big(D_1^\psi\big)\det_{\mathbb{C}^M}\big(D_2^\psi\big)\big]^{-1}.
\end{aligned} \tag{5.47}$$

An application of the Cauchy–Binet formula for determinants yields

$$\det_{\mathbb{C}^M}(\Gamma) = \sum_{\psi\in\Psi}\det_{\mathbb{C}^M}\big(A_\psi\big)\det_{\mathbb{C}^M}\big(B^\psi\big)\prod_{m\in\mathcal{M}}\gamma_{\psi(m)}e^{-i\tau\zeta_{\psi(m)}}. \tag{5.48}$$

Combining (5.33), (5.47), and (5.48) then yields (5.46). ☐

Applying Theorem 3.3 then yields the principal result of this section.

Theorem 5.3. *Let K be the Hilbert–Schmidt operator defined in* (5.1)–(5.3). *Then*

$$\det{}_2(I-K) = \exp\Bigg(\tau k(0_-) - \tau \sum_{m\in\mathcal{M}} \mu_m\Bigg) \sum_{\substack{\widetilde{\mathcal{L}}\subseteq\{1,\dots,N\} \\ |\widetilde{\mathcal{L}}|=L}} V_{\widetilde{\mathcal{L}}} \exp\big(-i\tau v_{\widetilde{\mathcal{L}}}\big) \tag{5.49}$$

$$= \exp\Bigg(\tau k(0_+) - \tau \sum_{\ell\in\mathcal{L}} \lambda_\ell\Bigg) \sum_{\substack{\widetilde{\mathcal{M}}\subseteq\{1,\dots,N\} \\ |\widetilde{\mathcal{M}}|=M}} W_{\widetilde{\mathcal{M}}} \exp\big(i\tau w_{\widetilde{\mathcal{M}}}\big). \tag{5.50}$$

Here $k(0_\pm) = \lim_{\varepsilon\downarrow 0} k(\pm\varepsilon)$, $|\mathcal{S}|$ denotes the cardinality of $\mathcal{S}\subset\mathbb{N}$, and

$$\begin{aligned} V_{\widetilde{\mathcal{L}}} = & \prod_{\ell\in\mathcal{L},\, m\in\widetilde{\mathcal{L}}^\perp} (\lambda_\ell - i\zeta_m) \prod_{\ell'\in\widetilde{\mathcal{L}}, m'\in\mathcal{M}} (\mu_{m'} + i\zeta_{\ell'}) \\ & \times \prod_{\ell''\in\mathcal{L}, m''\in\mathcal{M}} (\mu_{m''} + \lambda_{\ell''})^{-1} \prod_{\ell'''\in\widetilde{\mathcal{L}}, m'''\in\widetilde{\mathcal{L}}^\perp} (i\zeta_{m'''} - i\zeta_{\ell'''})^{-1}, \end{aligned} \tag{5.51}$$

$$\begin{aligned} W_{\widetilde{\mathcal{M}}} = & \prod_{\ell\in\mathcal{L},\, m\in\widetilde{\mathcal{M}}} (\lambda_\ell - i\zeta_m) \prod_{\ell'\in\widetilde{\mathcal{M}}^\perp, m'\in\mathcal{M}} (\mu_{m'} + i\zeta_{\ell'}) \\ & \times \prod_{\ell''\in\mathcal{L}, m''\in\mathcal{M}} (\mu_{m''} + \lambda_{\ell''})^{-1} \prod_{\ell'''\in\widetilde{\mathcal{M}}^\perp, m'''\in\widetilde{\mathcal{M}}} (i\zeta_{\ell'''} - i\zeta_{m'''})^{-1}, \end{aligned} \tag{5.52}$$

$$v_{\widetilde{\mathcal{L}}} = \sum_{m\in\widetilde{\mathcal{L}}^\perp} \zeta_m, \tag{5.53}$$

$$w_{\widetilde{\mathcal{M}}} = \sum_{\ell\in\widetilde{\mathcal{M}}^\perp} \zeta_\ell \tag{5.54}$$

with

$$\widetilde{\mathcal{L}}^\perp = \{1,\dots,N\}\backslash\widetilde{\mathcal{L}} \text{ for } \widetilde{\mathcal{L}}\subseteq\{1,\dots,N\},\ |\widetilde{\mathcal{L}}| = L, \tag{5.55}$$

$$\widetilde{\mathcal{M}}^\perp = \{1,\dots,N\}\backslash\widetilde{\mathcal{M}} \text{ for } \widetilde{\mathcal{M}}\subseteq\{1,\dots,N\},\ |\widetilde{\mathcal{M}}| = M. \tag{5.56}$$

Finally, if $\mathcal{L}=\emptyset$ or $\mathcal{M}=\emptyset$, then K is a Volterra operator and hence $\det_2(I-K) = 1$.

Proof. Combining (3.31), (5.44), (5.45), and (5.46) one obtains

$$\begin{aligned} \det_2(I-K) &= \det_{\mathbb{C}^M}(I_M - G)\exp\bigg(\int_0^\tau dx\, f_2(x)g_2(x)\bigg) \\ &= \det_{\mathbb{C}^M}(I_M - G)\exp\bigg(\tau\sum_{m\in\mathcal{M}}\beta_m\bigg) \\ &= \det_{\mathbb{C}^M}(I_M - G)\exp(\tau k(0_-)) \\ &= \exp\bigg(\tau k(0_-) - \tau\sum_{m\in\mathcal{M}}\mu_m\bigg) \\ &\quad\times\sum_{\substack{\widetilde{\mathcal{L}}\subseteq\{1,\dots,N\}\\ |\widetilde{\mathcal{L}}|=L}} V_{\widetilde{\mathcal{L}}}\exp\bigg(-i\tau\sum_{m\in\widetilde{\mathcal{L}}^\perp}\zeta_m\bigg), \end{aligned} \tag{5.57}$$

where

$$\begin{aligned} V_{\widetilde{\mathcal{L}}} &= (-1)^M\bigg(\prod_{m\in\widetilde{\mathcal{L}}^\perp}\beta_m\bigg)\bigg(\prod_{m'\in\widetilde{\mathcal{L}}^\perp}\gamma_{m'}\bigg)\prod_{m''\in\widetilde{\mathcal{L}}^\perp}\prod_{\substack{p\in\widetilde{\mathcal{L}}^\perp\\ p\neq m''}}(i\zeta_{m''}-i\zeta_p) \\ &\quad\times\prod_{p'\in\mathcal{M}}\prod_{\substack{p''\in\mathcal{M}\\ p''\neq p'}}(\mu_{p'}-\mu_{p''})\prod_{q\in\widetilde{\mathcal{L}}^\perp}\prod_{q'\in\mathcal{M}}(\mu_{q'}+i\zeta_q)^{-1} \\ &\quad\times\prod_{r\in\mathcal{M}}\prod_{\substack{r'\in\widetilde{\mathcal{L}}^\perp\\ r'\neq r}}(\mu_r+i\zeta_{r'})^{-1}. \end{aligned} \tag{5.58}$$

Elementary manipulations, using (5.21), (5.22), then reduce (5.58) to (5.51) and hence prove (5.49). To prove (5.50) one can argue as follows. Introducing

$$\widetilde{\mathcal{F}(k)}(x) = \mathcal{F}(k)(-x), \quad x\in\mathbb{R} \tag{5.59}$$

with associated kernel function

$$\tilde{k}(t) = k(-t), \quad t\in\mathbb{R}\backslash\{0\}, \tag{5.60}$$

equation (5.17) yields

$$1 - \widetilde{\mathcal{F}(k)}(x) = \prod_{n\in\mathcal{N}}(x+\zeta_n)\prod_{\ell\in\mathcal{L}}(x-i\lambda_\ell)^{-1}\prod_{m\in\mathcal{M}}(x+i\mu_m)^{-1}. \tag{5.61}$$

Denoting by $\widetilde{K}$ the truncated Wiener–Hopf operator in $L^2((0,\tau);dx)$ with convolution integral kernel $\tilde{k}$ (i.e., replacing k by $\tilde{k}$ in (5.1), and applying (5.49) yields

$$\det_2(I - \widetilde{K}) = \exp\left(\tau \tilde{k}(0_-) - \tau \sum_{\ell \in \mathcal{L}} \lambda_\ell\right) \sum_{\substack{\widetilde{\mathcal{M}} \subseteq \{1,\dots,N\} \\ |\widetilde{\mathcal{M}}| = M}} W_{\widetilde{\mathcal{M}}} \exp\big(i\tau \sum_{\ell \in \widetilde{\mathcal{M}}^\perp} \zeta_\ell\big). \tag{5.62}$$

Here $W_{\widetilde{\mathcal{M}}}$ is given by (5.52) (after interchanging the roles of λ_ℓ and μ_m and interchanging ζ_m and $-\zeta_\ell$, etc.) By (5.60), $\tilde{k}(0_-) = k(0_+)$. Since $\widetilde{K} = K^\top$, where $K^\top$ denotes the transpose integral operator of K (i.e., $K^\top$ has integral kernel $K(x', x)$ if $K(x, x')$ is the integral kernel of K), and hence

$$\det_2(I - \widetilde{K}) = \det_2(I - K^\top) = \det_2(I - K), \tag{5.63}$$

one arrives at (5.50).

Finally, if $\mathcal{L} = \emptyset$ then $k(0_+) = 0$ and one infers $\det_2(I - K) = 1$ by (5.50). Similarly, if $\mathcal{M} = \emptyset$, then $k(0_-) = 0$ and again $\det_2(I - K) = 1$ by (5.49). □

Remark 5.4. (*i*) *Theorem* 5.3 *permits some extensions. For instance, it extends to the case where* $\mathrm{Re}(\lambda_\ell) \geq 0$, $\mathrm{Re}(\mu_m) \geq 0$. *In this case the Fourier transform of k should be understood in the sense of distributions. One can also handle the case where $-i\lambda_\ell$ and $i\mu_m$ are higher order poles of $\mathcal{F}(k)$ by using a limiting argument.*
(*ii*) *The operator K is a trace class operator, $K \in \mathcal{B}_1(L^2((0,\tau); dx))$, if and only if k is continuous at $t = 0$* (*cf. equation* (2) *on p. 267 and Theorem 10.3 in* [12]).

Explicit formulas for determinants of Toeplitz operators with rational symbols are due to Day [7]. Different proofs of Day's formula can be found in [2, Theorem 6.29], [19], and [22]. Day's theorem requires that the degree of the numerator of the rational symbol be greater or equal to that of the denominator. An extension of Day's result avoiding such a restriction recently appeared in [6]. Determinants of rationally generated block operator matrices have also been studied in [38] and [39]. Explicit representations for determinants of the block-operator matrices of Toeplitz type with analytic symbol of a special form has been obtained in [20]. Textbook expositions of these results can be found in [2, Theorem 6.29] and [3, Theorem 10.45] (see also [4, Sect. 5.9]).

The explicit result (5.50), that is, an explicit representation of the 2-modified Fredholm determinant for truncated Wiener-Hopf operators on a finite interval, has first been obtained by Böttcher [1]. He succeeded in reducing the problem to that of Toeplitz operators combining a discretization approach and Day's formula. Theorem 5.3 should thus be viewed as a continuous analog of Day's formula. The method of proof presented in this paper based on (3.31) is remarkably elementary and direct. A new method for the computation of (2-modified) determinants for truncated Wiener-Hopf operators, based on the Nagy–Foias functional model, has recently been suggested in [26] (cf. also [25]), without, however, explicitly computing the right-hand sides of (5.49), (5.50). A detailed exposition of the theory of operators of convolution type with rational symbols on a finite interval, including representations for resolvents, eigenfunctions, and (modified) Fredholm determinants (different from the explicit one in Theorem 5.3), can be found in [11, Sect. XIII.10]. Finally, extensions of the classical Szegő–Kac–Achiezer formulas to the case of matrix-valued rational symbols can be found in [17] and [16].

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Spectral and Inverse Spectral Theory of Second-Order Difference (Jacobi) Operators on $\mathbb{N}$ and on $\mathbb{Z}$

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- Preliminaries
- Jacobi operators on $\mathbb{N}$
- Polynomials of the first kind
- The eigenfunction expansion
- Eigenfunction transforms
- The inverse spectral problem on $\mathbb{N}$
- Polynomials of the second kind
- Jacobi operators on $\mathbb{Z}$
- Examples

1 Preliminaries

The results on half-line Jacobi operators in this manuscript are taken from [2], Sect. VII.1 and [1], Ch. 4. The results on Jacobi operators on $\mathbb{Z}$ are based on [2], Sect. VII.3, [3], and [4].

Definition 1.1. We denote $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$. Let $l^2(\mathbb{N}_0)$ be the Hilbert space of all sequences $u = (u_0, u_1, \dots)$, $u_j \in \mathbb{C}$, $j \in \mathbb{N}_0$, such that $\sum_{j=0}^{\infty} |u_j|^2 < \infty$ with scalar product $(\cdot, \cdot)$ to be linear in the second argument. Let $l_0^2(\mathbb{N}_0) \subset l^2(\mathbb{N}_0)$ be the dense subspace of all sequences of finite support

$$u = (u_0, u_1, \dots, u_N, 0, 0, \dots),$$

where $N = N(u)$ depends on u.

Definition 1.2. Let L be the following *Jacobi* difference expression:

$$(Lu)_j = a_{j-1}u_{j-1} + b_j u_j + a_j u_{j+1}, \quad j \in \mathbb{Z},\ u \in l^\infty(\mathbb{Z}), \tag{1.1}$$

where a_j and b_j are given real-valued coefficients with $a_j > 0$, $j \in \mathbb{Z}$.

Remark 1.3. *A straigtforward calculation shows that the following version of Green's formula is valid for the difference expression* (1.1)

$$\sum_{j=k}^{l} \left[(Lu)_j \overline{v}_j - u_j \overline{(Lv)_j} \right] = a_l (u_{l+1}\overline{v}_l - u_l \overline{v}_{l+1}) - a_{k-1}(u_k \overline{v}_{k-1} - u_{k-1}\overline{v}_k), \quad k, l \in \mathbb{Z}. \tag{1.2}$$

2 Jacobi operators on $\mathbb{N}$

The results in this section are taken from [2], p. 501-503.

Definition 2.1. Let $H'_+ : l_0^2(\mathbb{N}_0) \to l_0^2(\mathbb{N}_0)$ be the linear operator defined as $(H'_+ u)_j = (Lu)_j$, $j \in \mathbb{N}_0$ with $u_{-1} = 0$ on the Hilbert space $l_0^2(\mathbb{N}_0)$.

Remark 2.2. *(i) The condition $u_{-1} = 0$ plays the role of a boundary condition.*
(ii) Using Green's formula (1.2) *it is easy to see that the operator H'_+ is symmetric.*

In the following we denote by $H_+ = \overline{H'_+}$ the closure of the operator H'_+.

Remark 2.3. *H_+ is symmetric because H'_+ defined on the dense subset of $l^2(\mathbb{N}_0)$ is symmetric and H_+ is the closure of H'_+.*

Lemma 2.4. $\mathrm{Dom}\left(H_+^*\right) = \{v \in l^2(\mathbb{N}_0) \,|\, Lv \in l^2(\mathbb{N}_0)\}$.

Proof. Using Green's formula (1.2) we have the following equality:

$$(H_+u, v) = (Lu, v) = (u, Lv) = (u, H_+^*v) \text{ for all } u \in l_0^2(\mathbb{N}_0), v \in l^2(\mathbb{N}_0).$$

Therefore, H_+^* acts in $l^2(\mathbb{N}_0)$ as the difference expression (1.1). The required statement then follows from the previous equality and the definition of the domain of an adjoint operator,

$$\begin{aligned}\mathrm{Dom}\left(H_+^*\right) = \{v \in l^2(\mathbb{N}_0) \,|\, &\text{For all } u \in \mathrm{Dom}\,(H_+)\,, \text{ there exists a unique} \\ & w \in l^2(\mathbb{N}_0) \text{ s.t. } (H_+u, v) = (u, w),\ w = H_+^*v\}.\end{aligned}$$

□

Remark 2.5. *In general, $H_+ \subsetneqq H_+^*$, that is, $\mathrm{Dom}\,(H_+) \subsetneqq \mathrm{Dom}\left(H_+^*\right)$. In the latter case, H_+ is symmetric but not self-adjoint and H_+^* is not symmetric.*

Definition 2.6. The deficiency indices of a symmetric operator A are the dimensions of the orthogonal complements of $\mathrm{Ran}\,(A - zI)$ and $\mathrm{Ran}\,(A + zI)$, respectively, for any nonreal z.

Lemma 2.7. *The deficiency indices of the operator H_+ are equal and hence independent of z.*

Proof. The deficiency index of the symmetric operator is known to be constant in the open upper and lower half-planes. Therefore, there are at most two different deficiency numbers of the operator H_+ corresponding to $\mathrm{Im}\,(z) \gtrless 0$. But because the coefficients of H_+ are real, H_+ is real, that is, the domain of H_+ is invariant under the involution $v \to \overline{v}$ and $H_+\overline{v} = \overline{H_+v}$. Therefore, for all $v \in \mathrm{Ran}\,(H - zI)$, there exists $u \in \mathrm{Dom}\,(H_+)$ such that $(H_+ - zI)u = v$. By the invariance of the domain of H_+ under the involution we get

$$\overline{u} \in \mathrm{Dom}\,(H_+) \text{ and } (H_+ - \overline{z}I)\overline{u} = \overline{(H_+ - zI)u} = \overline{v},$$

which implies $\overline{v} \in \mathrm{Ran}\,(H_+ - \overline{z}I)$. Therefore,

$$\overline{\mathrm{Ran}\,(H_+ - zI)} \subseteq \mathrm{Ran}\,(H_+ - \overline{z}I)$$

and by symmetry the converse also holds:

$$\overline{\mathrm{Ran}\,(H_+ - zI)} \supseteq \mathrm{Ran}\,(H_+ - \overline{z}I)\,.$$

The previous inclusions imply

$$\dim\left(\overline{\mathrm{Ran}\,(H_+ - zI)}\right) = \dim\left(\mathrm{Ran}\,(H_+ - \overline{z}I)\right),$$

which proves equality of the deficiency indices of H_+. □

Remark 2.8. *The action of the operator H_+ on $u \in l^2(\mathbb{N}_0)$ can be represented as the multiplication of the following matrix by the vector $u = (u_0, u_1, \dots)$ from the right*

$$J = \begin{Vmatrix} b_0 & a_0 & 0 & 0 & 0 & \dots \\ a_0 & b_1 & a_1 & 0 & 0 & \dots \\ 0 & a_1 & b_2 & a_2 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{Vmatrix}.$$

Matrices of this form are called Jacobi matrices and the corresponding operators H_+ are called Jacobi operators.

3 Polynomials of the first kind

The results in this section are taken from [2], p. 503-508.

Consider the equation

$$\begin{aligned} &(Lu)_j = a_{j-1}u_{j-1} + b_j u_j + a_j u_{j+1} = z u_j, \quad j \in \mathbb{N}_0, \\ &u_{-1} = 0, \quad u_0 = 1, \end{aligned} \tag{3.1}$$

where z is some complex number. It can be considered as a recursion relation for the determination of u_{j+1} from u_j and u_{j-1}. By the hypothesis $a_j \neq 0$, this relation is always solvable. Define $P_{+,j}(z)$ for $j \geq 1$ by (3.1). Clearly, $P_{+,j}(z)$ is a polynomial of degree j in z. Explicitly, one obtains

$$\begin{aligned} P_{+,0}(z) &= 1, \\ P_{+,1}(z) &= (z - b_0)/a_0, \\ P_{+,2}(z) &= [(z - b_1)(z - b_0)/a_0 - a_0]/a_1, \text{ etc.} \end{aligned}$$

Definition 3.1. The polynomials $P_{+,j}(z)$ are called *polynomials of the first kind*, generated by the difference expression L.

Theorem 3.2. *The operator H_+ has deficiency indices $(0,0)$ or $(1,1)$. The first case is characterized by the divergence of the series $\sum_{j=0}^{\infty} |P_{+,j}(z)|^2$ for all nonreal z, and the second case by the convergence of this series.*

In the second case, the deficiency subspace $N_{\overline{z}}$ is a one dimensional subspace, and is spanned by the vector

$$P_+(z) = (P_{+,0}(z), P_{+,1}(z), \dots). \tag{3.2}$$

Proof. Let $\mathrm{Im}\,(z) \neq 0$, and denote by $N_{\overline{z}}$ the orthogonal complement of $\mathrm{Ran}\,(H_+ - \overline{z}I)$, that is, the deficiency subspace of the operator H_+. Then,

$$0 = ((H_+ - \overline{z}I)u, v) = (u, (H_+^* - zI)v) \text{ for all } v \in N_{\overline{z}},\, u \in \mathrm{Dom}\,(H_+)\,.$$

Therefore, $N_{\overline{z}}$ coincides with the subspace of solutions of the equation $H_+^* v = zv$ or, because of the form of H_+^*, with the subspace of the solutions of the difference equation $(Lv)_j = zv_j$, $v_{-1} = 0$, which belong to $l^2(\mathbb{N}_0)$. By (3.1) each solution of this equation is represented in the form $v_j = v_0 P_{+,j}(z)$, and therefore the deficiency subspace is at most one-dimensional; moreover, it is nonzero if and only if $v = P_+(z) \in l^2(\mathbb{N}_0)$, that is, $\sum_{j=0}^{\infty} |P_{+,j}(z)|^2 < \infty$. □

Remark 3.3. *Because of the constancy of the deficiency indices in the open upper and lower complex half-planes, a sufficient condition for H_+ to be self-adjoint is that the series $\sum_{j=0}^{\infty} |P_{+,j}(z)|^2$ diverges for just one nonreal z.*

Definition 3.4. The difference expression L is said to be in the limit point case at ∞ if the deficiency indices of the operator H_+ are $(0,0)$, that is, the operator H_+ is self-adjoint, and L is said to be in the limit circle case at ∞ if the deficiency indices of H_+ are (1,1), that is, H_+ is symmetric but not self-adjoint.

Remark 3.5. *(i) $P_+(z)$ in (3.2) is called a generalized eigenvector of H_+ because*

$$(P_+(z), (H_+^* - \overline{z}I)u) = ((L - zI)P_+(z), u) = 0 \textit{ for all } u \in l_0^2(\mathbb{N}_0).$$

(ii) If the real-valued sequences $\{a_j\}_{j\in\mathbb{N}_0}$ and $\{b_j\}_{j\in\mathbb{N}_0}$ are bounded, then the operator H_+ is bounded and hence self-adjoint.

4 The eigenfunction expansion

The results in this section are taken from [2], p. 508-513.

In the following we will assume H_+ to be a self-adjoint operator.

By $\delta_k \in l^2(\mathbb{Z})$, $k \in \mathbb{Z}$ we will denote a vector, such that $(\delta_k)_j = \delta_{k,j}$, $j \in \mathbb{Z}$.

Theorem 4.1. *There is a family of projection operators $\{E_+(\lambda)\}_{\lambda\in\mathbb{R}}$ corresponding to the operator H_+ and the following representations are valid,*

$$I = \int_{\mathbb{R}} dE_+(\lambda) \quad \textit{and} \quad H_+ = \int_{\mathbb{R}} \lambda \, dE_+(\lambda).$$

Theorem 4.2. *The following formula is valid,*

$$\delta_{k,j} = \int_{\mathbb{R}} P_{+,k}(\lambda) P_{+,j}(\lambda) \, d(\delta_0, E_+(\lambda)\delta_0). \tag{4.1}$$

In particular, the polynomials $P_{+,j}(\lambda)$ are orthonormal with respect to the measure $d(\delta_0, E_+(\lambda)\delta_0)$ on $\mathbb{R}$.

Proof. First, note that because of

$$\begin{aligned}(H_+\delta_j, u) = (\delta_j, H_+u) &= (H_+u)_j \\ &= a_{j-1}u_{j-1} + a_j u_{j+1} + b_j u_j \\ &= (a_{j-1}\delta_{j-1} + a_j\delta_{j+1} + b_j\delta_j, u), \quad u \in l_0^2(\mathbb{N}_0),\end{aligned}$$

H_+ acts on each δ_j as

$$H_+\delta_j = a_{j-1}\delta_{j-1} + a_j\delta_{j+1} + b_j\delta_j, \quad j \in \mathbb{N}_0,$$

where we assume $\delta_{-1} = 0$. Therefore, δ_j belongs to the domain of any H_+^n, $n \in \mathbb{N}$, and analogously to (3.1) we find that

$$\delta_j = P_{+,j}(H_+)\delta_0.$$

Now it is easy to establish (4.1) using

$$\begin{aligned}\delta_{k,j} &= (\delta_k, \delta_j) \\ &= (P_{+,k}(H_+)\delta_0, P_{+,j}(H_+)\delta_0) \\ &= (\delta_0, P_{+,j}(H_+)P_{+,k}(H_+)\delta_0) \\ &= \int_{\mathbb{R}} P_{+,j}(\lambda)P_{+,k}(\lambda) \, d(\delta_0, E_+(\lambda)\delta_0).\end{aligned}$$

□

Definition 4.3. Let $\sigma_+(\lambda) = (\delta_0, E_+(\lambda)\delta_0)$, then $d\sigma_+(\lambda)$ is called the *spectral measure* associated with H_+.

Remark 4.4. *Following the usual conventions we also call $d\sigma_+(\lambda)$ the spectral measure of H_+ even though this terminology is usually reserved for the operator-valued spectral measure $dE_+(\lambda)$. (This slight abuse of notation should hardly cause any confusion.)*

Lemma 4.5. *The set of points of increase of the function $\sigma_+(\lambda)$ is infinite, that is, for all polynomials $P(\lambda) \in L^2(\mathbb{R}, d\sigma_+(\lambda))$,*

$$\int_{\mathbb{R}} |P(\lambda)|^2 \, d\sigma_+(\lambda) = 0 \quad \textit{if and only if} \quad P(\lambda) = 0.$$

5 Eigenfunction transforms

The results in this section are taken from [2], p. 513-518.

Definition 5.1. For any $u = (u_j)_{j \in \mathbb{N}_0} \in l^2(\mathbb{N}_0)$ the function

$$\widetilde{u}(\cdot) = \sum_{j=0}^{\infty} u_j P_{+,j}(\cdot) \in L^2(\mathbb{R}, d\sigma_+(\lambda)) \tag{5.1}$$

is called the *eigenfunction transform* of u.

Remark 5.2. *The sum in* (5.1) *converges in the $L^2(\mathbb{R}, d\sigma_+(\lambda))$ space for each $u \in l^2(\mathbb{N}_0)$ because $P_{+,j}(\lambda)$ form an orthonormal system of polynomials in $L^2(\mathbb{R}, d\sigma_+(\lambda))$.*

Lemma 5.3. *From* (4.1) *and* (5.1) *we have Parseval's relation*

$$(u, v) = \int_{\mathbb{R}} \widetilde{u}(\lambda) \widetilde{v}(\lambda) \, d\sigma_+(\lambda), \quad u, v \in l^2(\mathbb{N}_0). \tag{5.2}$$

Lemma 5.4. *From* (5.1) *it follows that the set of eigenfunction transforms of all sequences of finite support is the set of all polynomials in λ. And since $P_{+,j}(\lambda) \in L^2(\mathbb{R}, d\sigma_+(\lambda))$, any polynomial belongs to $L^2(\mathbb{R}, d\sigma_+(\lambda))$; in other words, the spectral measure $d\sigma_+(\lambda)$ satisfies*

$$\int_{\mathbb{R}} |\lambda|^m \, d\sigma_+(\lambda) < \infty, \quad m \in \mathbb{N}_0. \tag{5.3}$$

Lemma 5.5. *The operator H_+ on $l^2_0(\mathbb{N}_0)$ is transformed by the eigenfunction transform into the operator of multiplication by λ on the set of all polynomials in $L^2(\mathbb{R}, d\sigma_+(\lambda))$.*

Proof.

$$\begin{aligned}\widetilde{(H_+u)}(\lambda) &= \sum_{j=0}^{\infty}(H_+u)_j P_{+,j}(\lambda) = \sum_{j=0}^{\infty} u_j (H_+P_+(\lambda))_j \\ &= \lambda \sum_{j=0}^{\infty} u_j P_{+,j}(\lambda) = \lambda \widetilde{u}(\lambda).\end{aligned}$$

□

Theorem 5.6. *The operator H_+ is self-adjoint if and only if the set of eigenfunction transforms of all sequences of finite support $\widetilde{l^2_0(\mathbb{N}_0)}$ is dense in $L^2(\mathbb{R}, d\sigma_+(\lambda))$.*

Theorem 5.7. *Let $d\sigma_+(\lambda)$ be a nonnegative finite measure on $\mathbb{R}$ satisfying condition* (5.3)*. If Parseval's formula* (5.2) *holds for any finite sequences u, v and their eigenfunction transforms (or equivalently, if the orthogonality relations* (4.1) *hold), then $d\sigma_+(\lambda)$ is a spectral measure, that is, there exists a resolution of the identity $E_+(\lambda)$, such that $d\sigma_+(\lambda) = d(\delta_0, E_+(\lambda)\delta_0)$.*

Proof. Parseval's formula establishes an isometry between $l^2(\mathbb{N}_0)$ and $\widetilde{l^2(\mathbb{N}_0)} \subseteq L^2(\mathbb{R}, d\sigma_+(\lambda))$ by which the operator H_+ is transformed into the operator $\widetilde{H_+}$ of multiplication by λ, defined to be the closure of the operator of multiplication by λ on polynomials. Now we can consider an operator of multiplication by λ on $L^2(\mathbb{R}, d\sigma_+(\lambda))$, construct the resolution of identity for it, and then by isometry between the Hilbert spaces obtain the required resolution of identity for H_+. □

6 The inverse problem of spectral analysis on the semi-axis

The results in this section are taken from [2], p. 518-520.

So far we have considered the direct spectral problem: for a given difference operator H_+ we constructed a spectral decomposition. However, it is natural to consider the inverse problem, whether one can recover H_+ from appropriate spectral data. In this section we will show that such a recovery is possible when the spectral data consist of the spectral measure $d\sigma_+(\lambda)$.

Roughly speaking, this reconstruction procedure of $\{a_j, b_j\}_{j\in\mathbb{N}_0}$ starting from $d\sigma_+(\lambda)$ proceeds as follows: Given the spectral measure $d\sigma_+(\lambda)$, one first constructs the orthonormal set of polynomials $\{P_{+,j}(\lambda)\}_{j\in\mathbb{N}_0}$ with respect to $d\sigma_+(\lambda)$ using the Gram-Schmidt orthogonalization process as in the proof of Theorem 6.1 below. The fact that $P_{+,j}(\lambda)$ satisfies a second-order Jacobi difference equation and orthogonality properties of $P_{+,j}(\lambda)$ then yield explicit expressions for $\{a_j, b_j\}_{j\in\mathbb{N}_0}$.

To express the coefficients $\{a_j, b_j\}_{j\in\mathbb{N}_0}$ in terms of $P_{+,j}(\lambda)$ and $d\sigma_+(\lambda)$ one first notes that

$$\begin{aligned}&a_{j-1}P_{+,j-1}(\lambda) + a_j P_{+,j+1}(\lambda) + b_j P_{+,j}(\lambda) = \lambda P_{+,j}(\lambda), \quad j \in \mathbb{N}_0,\\ &P_{+,-1}(\lambda) = 0.\end{aligned}$$

Taking the scalar product in $L^2(\mathbb{R}, d\sigma_+(\lambda))$ of each side of this equation with $P_{+,k}(\lambda)$ and using the orthogonality relations (4.1), we obtain

$$a_j = \int_{\mathbb{R}} \lambda P_{+,j}(\lambda) P_{+,j+1}(\lambda)\, d\sigma_+(\lambda), \quad b_j = \int_{\mathbb{R}} \lambda P_{+,j}^2(\lambda)\, d\sigma_+(\lambda), \quad j \in \mathbb{N}_0. \tag{6.1}$$

Theorem 6.1. *Let $d\sigma_+(\lambda)$ be a nonnegative finite measure on $\mathbb{R}$, for which $\sigma_+(\lambda)$ has an infinite number of points of increase, such that*

$$\int_{\mathbb{R}} d\sigma_+(\lambda) = 1, \quad \int_{\mathbb{R}} |\lambda|^m\, d\sigma_+(\lambda) < \infty, \quad m \in \mathbb{N}_0.$$

Then $d\sigma_+(\lambda)$ is necessarily the spectral measure for some second order finite difference expression. The coefficients of this expression are uniquely determined by $d\sigma_+(\lambda)$ by formula (6.1), where $\{P_{+,j}(\lambda)\}_{j\in\mathbb{N}_0}$ is the orthonormal system of polynomials constructed by the orthogonalization process in the space $L^2(\mathbb{R}, d\sigma_+(\lambda))$ of the system of powers $1, \lambda, \lambda^2, \dots$.

Proof. Consider the space $L^2(\mathbb{R}, d\sigma_+(\lambda))$ and in it the system of functions $1, \lambda, \lambda^2, \dots$. Orthogonalize this sequence by applying the Gram-Schmidt orthogonalization process. If a polynomial is zero in the norm of $L^2(\mathbb{R}, d\sigma_+(\lambda))$, it is identically zero because of the infinite number of points of increase of $\sigma_+(\lambda)$. Thus, in the end we obtain an orthonormal sequence of real polynomials $P_{+,0}(\lambda) = 1, P_{+,1}(\lambda), \ldots$, where $P_{+,j}(\lambda)$ has degree j and its leading coefficient is positive.

Define a_j and b_j by means of the equation (6.1) for the polynomials $P_{+,j}(\lambda)$. It is easy to see that $a_j > 0$, $j \in \mathbb{N}_0$. In fact, $\lambda P_{+,j}(\lambda)$ is a polynomial of degree $j+1$ whose leading coefficient is positive, and therefore in the representation $\lambda P_{+,j}(\lambda) = c_{j+1}P_{+,j+1} + \cdots + c_0 P_{+,0}(\lambda)$, $c_{j+1} > 0$. But $c_{j+1} = a_j$, and thus the numbers a_j and b_j may be taken as the coefficients of some difference expression H_+.

Now we will show that the $P_{+,j}(\lambda)$ are polynomials of the first kind for the expression H_+ just constructed, that is, we will show that

$$\begin{aligned} &\lambda P_{+,j}(\lambda) = a_{j-1}P_{+,j-1}(\lambda) + a_j P_{+,j+1}(\lambda) + b_j P_{+,j}(\lambda), \quad j \in \mathbb{N}_0, \\ &P_{+,-1}(\lambda) = 0,\ P_{+,0}(\lambda) = 1. \end{aligned}$$

For the proof, it is sufficient to show that in the decomposition of the polynomial $\lambda P_{+,j}(\lambda)$ of degree $j+1$ with respect to $P_{+,0}(\lambda), \ldots, P_{+,j+1}(\lambda)$, the coefficients of $P_{+,0}(\lambda), \ldots, P_{+,j-2}$ are zero, that is,

$$\int_{\mathbb{R}} \lambda P_{+,j}(\lambda) P_{+,k}(\lambda)\, d\sigma_+(\lambda) = 0, \quad k = 0, \ldots, j-2.$$

But $\lambda P_{+,k}(\lambda)$ is a polynomial of degree at most $j-1$, so $P_{+,j}(\lambda)$ is orthogonal to it as required. □

7 Polynomials of the second kind

The results in this section are taken from [2], p. 520-523.

Consider the difference equation

$$\begin{aligned} &(Lu)_j = a_{j-1}u_{j-1} + b_j u_j + a_j u_{j+1} = z u_j, \quad j \in \mathbb{N}_0, \\ &u_0 = 0, \quad u_1 = 1/a_0, \end{aligned} \tag{7.1}$$

where z is some complex number. Let $Q_+(z) = (Q_{+,1}(z), Q_{+,2}(z), \ldots)$ be a solution of this equation. It is easy to see that $Q_{+,j}(z)$ is a polynomial of degree $j-1$ with real coefficients, and whose leading coefficient is positive. Therefore, $Q_{+,j}(z)$ is uniquely defined.

Definition 7.1. The polynomials $Q_{+,j}(z)$ are called *polynomials of the second kind*, generated by the difference expression L.

Remark 7.2. *Clearly $P_+(z)$ and $Q_+(z)$ form a linearly independent system of solutions of the second order difference equation $(Lu)_j = zu_j$, $j \in \mathbb{N}_0$.*

Lemma 7.3. *The polynomials $Q_{+,j}(z)$ and $P_{+,j}(z)$ are connected by the following relation*

$$Q_{+,j}(z) = \int_{\mathbb{R}} \frac{P_{+,j}(\lambda) - P_{+,j}(z)}{\lambda - z}\, d\sigma_+(\lambda), \quad j \in \mathbb{N}_0. \tag{7.2}$$

Proof. In fact, the sequence $u_j = \int_{\mathbb{R}} \frac{P_{+,j}(\lambda) - P_{+,j}(z)}{\lambda - z}\, d\sigma_+(\lambda)$ satisfies the equation

$$\begin{aligned}(Lu)_j &= \int_{\mathbb{R}} \frac{(LP_+(\lambda))_j - (LP_+(z))_j}{\lambda - z}\, d\sigma_+(\lambda) = z \int_{\mathbb{R}} \frac{P_{+,j}(\lambda) - P_{+,j}(z)}{\lambda - z}\, d\sigma_+(\lambda) \\ &\quad + \int_{\mathbb{R}} P_{+,j}(\lambda)\, d\sigma_+(\lambda) \\ &= z\, u_j, \quad j \in \mathbb{N}.\end{aligned}$$

Here we used $\int_{\mathbb{R}} P_{+,j}(\lambda)\, d\sigma_+(\lambda) = 0$, $j \in \mathbb{N}$, due to the orthogonality of $P_{+,j}$, $j \in \mathbb{N}$ with respect to $P_{+,0} = 1$. In addition, $u_0 = 0$ and

$$u_1 = \int_{\mathbb{R}} \frac{\frac{1}{a_0}(\lambda - b_0) - \frac{1}{a_0}(z - b_0)}{\lambda - z}\, d\sigma_+(\lambda) = \frac{1}{a_0}.$$

Thus, $u_j = Q_{+,j}(z)$, $j \in \mathbb{N}$, and relation (7.2) is established. □

Lemma 7.4. *Let $R_+(z) = (H_+ - zI)^{-1}$, $z \in \varrho(H_+)$ be the resolvent* [1] *of the difference operator H_+. Then*

$$R_+(z) = \int_{\mathbb{R}} (\lambda - z)^{-1} dE_+(\lambda)$$

and

$$(\delta_j, R_+(z)\delta_k) = \int_{\mathbb{R}} \frac{P_{+,j}(\lambda) P_{+,k}(\lambda)}{\lambda - z}\, d\sigma_+(\lambda), \quad j, k \in \mathbb{N}_0.$$

[1] $\varrho(H_+)$ denotes the resolvent set of H_+.

Definition 7.5. The function

$$m_+(z) = (\delta_0, R_+(z)\delta_0) = \int\limits_{\mathbb{R}} \frac{d\sigma_+(\lambda)}{\lambda - z}, \quad z \in \varrho\,(H_+)\,,$$

that is, the Stieltjes transform of the spectral measure, is called the *Weyl–Titchmarsh function* of the operator H_+.

Remark 7.6. *Let $\alpha, \beta \in \mathbb{R}$, $\alpha < \beta$. Then the spectral measure $d\sigma_+(\lambda)$ can be reconstructed from the Weyl–Titchmarsh function $m_+(z)$ as follows,*

$$\sigma_+((\alpha, \beta]) = \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int\limits_{\alpha+\delta}^{\beta+\delta} \operatorname{Im}\left(m_+(\lambda + i\varepsilon)\right)\, d\lambda. \tag{7.3}$$

This is a consequence of the fact that $m_+(z)$ is a Herglotz function, that is, $m_+(z) : \mathbb{C}_+ \to \mathbb{C}_+$ is analytic ($\mathbb{C}_+ = \{z \in \mathbb{C} \,|\, \operatorname{Im}(z) > 0\}$).

Theorem 7.7. *$R_+(z)\delta_0 = Q_+(z) + m_+(z)P_+(z)$, $z \in \varrho\,(H_+)$.*

Proof.

$$\begin{aligned}(R_+(z)\delta_0)_j &= \int\limits_{\mathbb{R}} \frac{P_{+,j}(\lambda)}{\lambda - z}\, d\sigma_+(\lambda) = \int\limits_{\mathbb{R}} \frac{P_{+,j}(\lambda) - P_{+,j}(z)}{\lambda - z}\, d\sigma_+(\lambda) \\ &\quad + P_{+,j}(z) \int\limits_{\mathbb{R}} \frac{d\sigma_+(\lambda)}{\lambda - z} = Q_{+,j}(z) + m_+(z)P_{+,j}(z), \quad j \in \mathbb{N}_0.\end{aligned}$$

□

Corollary 7.8. *For all $z \in \varrho\,(H_+)$*

$$Q_+(z) + m_+(z)P_+(z) \in l^2(\mathbb{N}_0). \tag{7.4}$$

Theorem 7.9. *If the operator H_+ is self-adjoint, then the Weyl–Titchmarsh function $m_+(z)$ is uniquely defined by the relation* (7.4)*.*

Proof. Suppose we have a function $f_+(z)$ which satisfies (7.4) for all $z \in \varrho\,(H_+)$, then

$$(f_+(z) - m_+(z))P_+(z) \in l^2(\mathbb{N}_0), \quad z \in \varrho\,(H_+)\,.$$

From the fact that $P_+(z) \notin l^2(\mathbb{N}_0)$ (since H_+ is assumed to be self-adjoint) for all $z \in \varrho\,(H_+)$ we get

$$f_+(z) - m_+(z) = 0, \quad z \in \varrho\,(H_+)\,.$$

Thus, the Weyl–Titchmarsh function $m_+(z)$ is uniquely defined by (7.4). □

8 Jacobi operators on $\mathbb{Z}$

The results in this section are taken from [2], p. 581-587, [3], and [4].

Definition 8.1. Let $l^2(\mathbb{Z})$ be the Hilbert space of all sequences

$$u = (\dots, u_{-1}, u_0, u_1, \dots), \text{ such that } \sum_{j=-\infty}^{\infty} |u_j|^2 < \infty$$

with the scalar product $(\cdot,\cdot)$ to be linear in the second argument. Moreover, let $l_0^2(\mathbb{Z}) \subset l^2(\mathbb{Z})$ be the dense subspace of all sequences of finite support

$$u = (\dots, 0, 0, u_K, \dots, u_{-1}, u_0, u_1, \dots, u_N, 0, 0, \dots),$$

where $N = N(u)$ and $K = K(u)$ depend on u.

Definition 8.2. Let $H' : l_0^2(\mathbb{Z}) \to l_0^2(\mathbb{Z})$ be the linear operator defined as $(H'u)_j = (Lu)_j,\ j \in \mathbb{Z}$ on the Hilbert space $l_0^2(\mathbb{Z})$.

Remark 8.3. *Using Green's formula* (1.2) *it is easy to see that the operator H' is symmetric.*

In the following we denote by $H = \overline{H'}$ the closure of the operator H'.

Lemma 8.4. *H is symmetric because H' defined on the dense subset of $l^2(\mathbb{Z})$ is symmetric and H is the closure of H'.*

The spectral theory of such operators is in many instances similar to the theory on the semi-axis; the difference is that now the spectrum may, in general, have multiplicity two on some subsets of $\mathbb{R}$. This multiplicity of the spectrum leads to a 2×2 matrix-valued spectral measure rather than a scalar spectral measure.

In the following we will assume H to be a self-adjoint operator, that is, we assume the difference expression L to be in the limit point case at $\pm\infty$.

Definition 8.5. Fix a site $n_0 \in \mathbb{Z}$ and define solutions $P_{+,j}(z, n_0+1)$ and $P_{-,j}(z, n_0)$ of the equation

$$(Hu)_j = a_{j-1}u_{j-1} + b_j u_j + a_j u_{j+1} = z u_j, \quad z \in \mathbb{C},\ j \in \mathbb{Z},$$

satisfying the initial conditions

$$P_{-,n_0}(z,n_0) = 1, \qquad P_{-,n_0+1}(z,n_0) = 0,$$
$$P_{+,n_0}(z,n_0+1) = 0, \qquad P_{+,n_0+1}(z,n_0+1) = 1.$$

Similarly to (3.1), $\{P_{-,j}(z,n_0)\}_{j\in\mathbb{Z}}$ and $\{P_{+,j}(z,n_0+1)\}_{j\in\mathbb{Z}}$ are two systems of polynomials.

Corollary 8.6. *Any solution of the equation*

$$(Hu)_j = a_{j-1}u_{j-1} + b_j u_j + a_j u_{j+1} = z u_j, \quad z \in \mathbb{C},\ j \in \mathbb{Z},$$

has the following form

$$u(z) = u_{n_0}(z)P_-(z,n_0) + u_{n_0+1}(z)P_+(z,n_0+1).$$

Remark 8.7. *Like the half-line difference operator H_+, the operator H has an associated family of spectral projection operators $\{E(\lambda)\}_{\lambda\in\mathbb{R}}$ and the following representations are valid,*

$$I = \int_{\mathbb{R}} dE(\lambda) \quad \textit{and} \quad H = \int_{\mathbb{R}} \lambda\, dE(\lambda).$$

Theorem 8.8. *The two-dimensional polynomials*

$$P_j(z) = \big(P_{-,j}(z,n_0), P_{+,j}(z,n_0+1)\big) : \mathbb{C} \to \mathbb{C}^2, \quad j \in \mathbb{Z},$$

are orthonormal with respect to the 2×2 matrix-valued spectral measure

$$d\Omega(\lambda,n_0) = d\begin{pmatrix} (\delta_{n_0}, E(\lambda)\delta_{n_0}) & (\delta_{n_0}, E(\lambda)\delta_{n_0+1}) \\ (\delta_{n_0+1}, E(\lambda)\delta_{n_0}) & (\delta_{n_0+1}, E(\lambda)\delta_{n_0+1}) \end{pmatrix},$$

that is,

$$\delta_{k,j} = \int_{\mathbb{R}} P_k(\lambda)\, d\Omega(\lambda,n_0)\, P_j(\lambda)^\top. \tag{8.1}$$

Proof. Like the half-line operator H_+, the operator H acts on each δ_j as

$$H\delta_j = a_{j-1}\delta_{j-1} + a_j\delta_{j+1} + b_j\delta_j, \quad j \in \mathbb{Z}.$$

Taking into account Corollary 8.6 and analogously to (3.1) we find that

$$\delta_j = P_{-,j}(L, n_0)\delta_{n_0} + P_{+,j}(L, n_0+1)\delta_{n_0+1}.$$

Now it is easy to establish (8.1) using

$$\begin{aligned}
\delta_{k,j} &= (\delta_k, \delta_j) \\
&= (P_{-,k}(L, n_0)\delta_{n_0},\ P_{-,j}(L, n_0)\delta_{n_0}) \\
&\quad + (P_{+,k}(L, n_0+1)\delta_{n_0+1},\ P_{-,j}(L, n_0)\delta_{n_0}) \\
&\quad + (P_{-,k}(L, n_0)\delta_{n_0},\ P_{+,j}(L, n_0+1)\delta_{n_0+1}) \\
&\quad + (P_{+,k}(L, n_0+1)\delta_{n_0+1},\ P_{+,j}(L, n_0+1)\delta_{n_0+1}) \\
&= \int_{\mathbb{R}} P_{-,j}(\lambda, n_0)P_{-,k}(\lambda, n_0)\, d(\delta_{n_0}, E(\lambda)\delta_{n_0}) \\
&\quad + \int_{\mathbb{R}} P_{-,j}(\lambda, n_0)P_{+,k}(\lambda, n_0+1)\, d(\delta_{n_0+1}, E(\lambda)\delta_{n_0}) \\
&\quad + \int_{\mathbb{R}} P_{+,j}(\lambda, n_0+1)P_{-,k}(\lambda, n_0)\, d(\delta_{n_0}, E(\lambda)\delta_{n_0+1}) \\
&\quad + \int_{\mathbb{R}} P_{+,j}(\lambda, n_0+1)P_{+,k}(\lambda, n_0+1)\, d(\delta_{n_0+1}, E(\lambda)\delta_{n_0+1}) \\
&= \int_{\mathbb{R}} P_k(\lambda)\, d\Omega(\lambda, n_0)\, P_j(\lambda)^\top.
\end{aligned}$$

□

Lemma 8.9. *The two-dimensional polynomials*

$$P_j(z) = \big(P_{+,j}(z, n_0+1), P_{-,j}(z, n_0)\big)$$

satisfy the following equation

$$a_{j-1}P_{j-1}(z) + a_j P_{j+1}(z) + b_j P_j(z) = zP_j(z), \quad z \in \mathbb{C},\ j \in \mathbb{Z},$$

and due to their orthonormality the following equalities hold,

$$a_j = \int_{\mathbb{R}} \lambda P_j(\lambda)\, d\Omega(\lambda, n_0)\, P_{j+1}(\lambda)^\top, \quad b_j = \int_{\mathbb{R}} \lambda P_j(\lambda)\, d\Omega(\lambda, n_0)\, P_j(\lambda)^\top,$$
$$j \in \mathbb{Z}. \qquad (8.2)$$

Definition 8.10. Let $\Psi_\pm(z,n_0) = (\Psi_{\pm,j}(z,n_0))_{j\in\mathbb{Z}}$ be two solutions of the following equation

$$\begin{aligned}&(Lu)_j = a_{j-1}u_{j-1} + b_j u_j + a_j u_{j+1} = z u_j, \quad z\in\mathbb{C},\ j\in\mathbb{Z},\\ &u_{n_0} = 1,\end{aligned} \tag{8.3}$$

such that for some (and hence for all) $m\in\mathbb{Z}$

$$\Psi_\pm(z,n_0)\in l^2([m,\pm\infty)\cap\mathbb{Z}), \quad z\in\mathbb{C}\backslash\mathbb{R}. \tag{8.4}$$

The fact that such solutions always exist will be shown in the next result.

Theorem 8.11. *If L is in the limit point case at $\pm\infty$, then the solutions $\Psi_\pm(z,n_0)$ in* (8.3) *and* (8.4) *exist and are unique.*

Proof. First of all note that $\Psi_{\pm,k}(z,n_0)\neq 0$ for all $z\in\mathbb{C}\backslash\mathbb{R}$ and $k\in\mathbb{Z}$, since otherwise they would be eigenfunctions corresponding to the nonreal eigenvalue z of the restrictions of the self-adjoint operator H to the half-lines $l^2((k,\pm\infty)\cap\mathbb{Z})$ with the Dirichlet boundary conditions at the point k.

Now suppose, for instance, we have two linearly independent functions $\Psi_+(z,n_0)$ and $\Phi_+(z,n_0)$ satisfying (8.3) and (8.4). Then the following function

$$f_+(z) = \Psi_+(z,n_0) - \Phi_+(z,n_0), \quad z\in\mathbb{C}\backslash\mathbb{R}.$$

also satisfies (8.3) and (8.4). Since $f_{+,n_0}(z)=0$, one obtains a contradiction by the previous consideration. Therefore, $\Psi_\pm(z,n_0)$ are unique.

Now consider the restriction H_+ of the operator H to $l^2(\mathbb{N}_0)$ with the Dirichlet boundary condition at -1 and apply the result (7.4) from the previous section,

$$u_j(z) = Q_{+,j}(z) + m_+(z)P_{+,j}(z), \quad j\in\mathbb{N}.$$

By definition of $Q_+(z)$ and $P_+(z)$

$$(Lu(z))_j = z u_j(z), \quad j\in\mathbb{N}.$$

The rest of the components of u_j, namely $\{u_j\}_{j=0}^{-\infty}$, can be determined recursively from (8.3). Now define $\Psi_+(z,n_0)$ as follows,

$$\Psi_{+,j}(z,n_0) = u_j(z)/u_{n_0}(z), \quad j\in\mathbb{Z}.$$

Therefore, there exists at least one function $\Psi_+(z,n_0)$. An analogous consideration is valid for $\Psi_-(z,n_0)$. □

Corollary 8.12. $\Psi_\pm(z,n) = \Psi_\pm(z,n_0)/\Psi_{\pm,n}(z,n_0)$, $n \in \mathbb{Z}$.

Definition 8.13. If the difference expression L is in the limit point case at $\pm\infty$, the (uniquely determined) solutions $\Psi_\pm(z,n_0)$ of (8.3) satisfying (8.4) are called the *Weyl–Titchmarsh solutions* of $Lu = zu$. Let $M_\pm(z,n_0)$ be functions, such that

$$\Psi_\pm(z,n_0) = P_-(z,n_0) - \frac{1}{a_{n_0}} M_\pm(z,n_0) P_+(z,n_0+1). \tag{8.5}$$

Such functions always exist due to Theorem 8.11 and Corollary 8.6.

In the following we denote by $H_{\pm,n_0}$ the restrictions of the operator H to the right and left half-line with the Dirichlet boundary condition at the point $n_0 \mp 1$, that is, $H_{\pm,n_0}$ acts on $l^2([n_0,\pm\infty)\cap\mathbb{Z})$ with the corresponding boundary condition $u_{n_0\mp 1} = 0$.

Next, let $m_\pm(z,n_0)$ be the Weyl–Titchmarsh functions for the half-line operators $H_{\pm,n_0}$ with $\sigma_\pm(\lambda,n_0)$ the associated spectral functions, that is,

$$m_\pm(z,n_0) = ((H_{\pm,n_0} - zI)^{-1}\delta_{n_0}, \delta_{n_0}) = \int\limits_{\mathbb{R}} \frac{d\sigma_\pm(\lambda,n_0)}{\lambda - z}, \quad z \in \varrho\left(H_{\pm,n_0}\right).$$

Then, analogously to (7.4),

$$Q_\pm(z,n_0) + m_\pm(z,n_0)P_\pm(z,n_0) \in l^2([n_0,\pm\infty)\cap\mathbb{Z}),$$

where $P_\pm(z,n_0)$ and $Q_\pm(z,n_0)$ are polynomials of the first and second kind for the half-line operators $H_{\pm,n_0}$, that is,

$$\begin{aligned}
(H_{\pm,n_0}P_\pm(z,n_0))_j &= zP_{\pm,j}(z,n_0), \quad j \in [n_0,\pm\infty)\cap\mathbb{Z},\\
(H_{\pm,n_0}Q_\pm(z,n_0))_j &= zQ_{\pm,j}(z,n_0), \quad j \in (n_0,\pm\infty)\cap\mathbb{Z},
\end{aligned}$$

and

$$\begin{aligned}
&P_{+,n_0-1}(z,n_0) = 0, && P_{+,n_0}(z,n_0) = 1,\\
&Q_{+,n_0}(z,n_0) = 0, && Q_{+,n_0+1}(z,n_0) = 1/a_{n_0},\\
&P_{-,n_0}(z,n_0) = 1, && P_{-,n_0+1}(z,n_0) = 0,\\
&Q_{-,n_0-1}(z,n_0) = 1/a_{n_0-1}, && Q_{-,n_0}(z,n_0) = 0.
\end{aligned}$$

Lemma 8.14. *The following relations hold*

$$\begin{aligned} M_+(z,n_0) &= -1/m_+(z,n_0) - z + b_{n_0}, \\ M_-(z,n_0) &= 1/m_-(z,n_0). \end{aligned} \tag{8.6}$$

Proof. From the uniqueness of the Weyl–Titchmarsh functions $\Psi_\pm(z,n_0)$ we get

$$\Psi_{\pm,j}(z,n_0) = c_\pm(z,n_0)\left(Q_{\pm,j}(z,n_0) + m_\pm(z,n_0)P_{\pm,j}(z,n_0)\right), \quad j \gtreqless n_0,$$
$$\Psi_{\pm,j}(z,n_0) = P_{-,j}(z,n_0) - \frac{1}{a_{n_0}} M_\pm(z,n_0)P_{+,j}(z,n_0+1), \quad j \in \mathbb{Z}.$$

Using the recursion formula (8.3) and

$$\begin{aligned} &P_{-,n_0}(z,n_0) = 1, && P_{-,n_0+1}(z,n_0) = 0, \\ &P_{+,n_0}(z,n_0+1) = 0, && P_{+,n_0+1}(z,n_0+1) = 1, \end{aligned}$$

one finds

$$1 = \Psi_{\pm,n_0}(z,n_0) = c_\pm(z,n_0)m_\pm(z,n_0),$$
$$-\frac{M_+(z,n_0)}{a_{n_0}} = \Psi_{+,n_0+1}(z,n_0) = c_+(z,n_0)\left(\frac{1}{a_{n_0}} + m_+(z,n_0)\frac{z-b_{n_0}}{a_{n_0}}\right), \tag{8.7}$$
$$-\frac{M_-(z,n_0)}{a_{n_0}} = \Psi_{-,n_0+1}(z,n_0) = c_-(z,n_0)\frac{-1}{a_{n_0}}. \tag{8.8}$$

Therefore,

$$c_\pm(z,n_0) = 1/m_\pm(z,n_0),$$

and

$$\begin{aligned} M_+(z,n_0) &= -1/m_+(z,n_0) - z + b_{n_0}, \\ M_-(z,n_0) &= 1/m_-(z,n_0). \end{aligned}$$

□

In particular, (8.7) and (8.8) yield

$$M_\pm(z,n_0) = -a_{n_0}\Psi_{\pm,n_0+1}(z,n_0). \tag{8.9}$$

Next, we introduce the Wronskian of two vectors u and v at the point m by

$$W(u,v)(m) = a_m(u_m v_{m+1} - u_{m+1}v_m).$$

Lemma 8.15. *The Wronskian of the Weyl–Titchmarsh functions* $\Psi_-(z, n_0)$ *and* $\Psi_+(z, n_0)$*,* $W(\Psi_-(z, n_0), \Psi_+(z, n_0))(m)$*, is independent of* m *and one obtains*

$$W(\Psi_-(z, n_0), \Psi_+(z, n_0)) = M_-(z, n_0) - M_+(z, n_0).$$

Proof.

$$\begin{aligned} W(\Psi_+, \Psi_-)(m) &= a_m[\Psi_{+,m}\Psi_{-,m+1} - \Psi_{+,m+1}\Psi_{-,m}] \\ &= -[a_{m+1}\Psi_{+,m+2} + (b_{m+1} - z)\Psi_{+,m+1}]\Psi_{-,m+1} \\ &\quad + [a_{m+1}\Psi_{-,m+2} + (b_{m+1} - z)\Psi_{-,m+1}]\Psi_{+,m+1} \\ &= a_{m+1}[\Psi_{+,m+1}\Psi_{-,m+2} - \Psi_{+,m+2}\Psi_{-,m+1}] \\ &= W(\Psi_+, \Psi_-)(m + 1). \end{aligned}$$

Therefore, to find the Wronskian of the Weyl–Titchmarsh functions $\Psi_\pm(z, n_0)$ it suffices to calculate it at any point, for instance, at n_0,

$$\begin{aligned} W(\Psi_+(z, n_0), \Psi_-(z, n_0))(n_0) =& a_{n_0}\left[-\frac{1}{a_{n_0}}M_-(z, n_0) + \frac{1}{a_{n_0}}M_+(z, n_0)\right] \\ =& M_+(z, n_0) - M_-(z, n_0). \end{aligned}$$

□

Next, let $R(z) = (H - zI)^{-1}$, $z \in \varrho(H)$, be the resolvent of the operator H. Then

$$R(z) = \int_{\mathbb{R}} (\lambda - z)^{-1} dE(\lambda), \quad z \in \varrho(H).$$

Lemma 8.16.

$$(\delta_j, R(z)\delta_k) = \frac{1}{W(\Psi_-(z, n_0), \Psi_+(z, n_0))} \begin{cases} \Psi_{-,j}(z, n_0)\Psi_{+,k}(z, n_0), & j \le k, \\ \Psi_{-,k}(z, n_0)\Psi_{+,j}(z, n_0), & j \ge k, \end{cases} \quad j, k \in \mathbb{Z}. \tag{8.10}$$

Moreover, (8.10) *does not depend on* n_0 *due to Corollary 8.12 and because it is homogeneous in* Ψ*.*

Proof. Denote the expression on the right-hand side of (8.10) as $T(z, j, k)$ and define a vector $\Psi(z, j) = (\Psi_k(z, j))_{k\in\mathbb{Z}} \in l^2(\mathbb{Z})$ as follows,

$$\Psi_k(z, j) = T(z, j, k), \quad k \in \mathbb{Z}.$$

Indeed, $\Psi(z,j) \in l^2(\mathbb{Z})$ because

$$\begin{aligned}\Psi =&\frac{1}{W}(\dots, \Psi_{+,j}\Psi_{-,j-1},\ \Psi_{+,j}\Psi_{-,j},\ \Psi_{-,j}\Psi_{+,j+1},\ \Psi_{-,j}\Psi_{+,j+2}, \dots)\\ =&\frac{1}{W}\big[\Psi_{+,j}(\dots, \Psi_{-,j-1}, \Psi_{-,j}, 0, 0\dots)\\ &\qquad + \Psi_{-,j}(\dots, 0, 0, \Psi_{+,j+1}, \Psi_{+,j+2}, \dots)\big]\end{aligned}$$

and

$$\begin{aligned}(\dots, \Psi_{-,j-1}, \Psi_{-,j}, 0, 0\dots) \in l^2(\mathbb{Z}),\\ (\dots, 0, 0, \Psi_{+,j+1}, \Psi_{+,j+2}, \dots) \in l^2(\mathbb{Z}).\end{aligned}$$

Define an operator $T(z)$ on $l_0^2(\mathbb{Z})$ as follows,

$$T(z)u = \left(\sum_{j\in\mathbb{Z}} T(z,j,k)u_j\right)_{k\in\mathbb{Z}} = \sum_{j\in\mathbb{Z}} \Psi(z,j)u_j, \quad u \in l_0^2(\mathbb{Z}).$$

To prove (8.10) it suffices to show that,

$$\begin{aligned}(H - zI)\, T(z)\, \delta_j = \delta_j, \quad j \in \mathbb{Z},\\ T(z)\, (H - zI)\, \delta_j = \delta_j, \quad j \in \mathbb{Z},\end{aligned}$$

because $\{\delta_j\}_{j\in\mathbb{Z}}$ is a basis in $l^2(\mathbb{Z})$.

$$\begin{aligned}(H - zI)\, T(z)\, \delta_j =&(H - zI)\Psi(z,j)\\ =&\frac{1}{W}(H - zI)\big[\Psi_{-,j}(\dots, 0, 0, a_j\Psi_{+,j+1}, -a_j\Psi_{+,j}, 0, 0, \dots)\\ &\qquad + \Psi_{+,j}(\dots, 0, 0, -a_j\Psi_{-,j+1}, a_j\Psi_{-,j}, 0, 0\dots)\big]\\ =&\frac{1}{W}\delta_j a_j\big[\Psi_{-,j}\Psi_{+,j+1} - \Psi_{+,j}\Psi_{-,j+1}\big]\\ =&\delta_j.\end{aligned}$$

$$
\begin{aligned}
T(z)\,(H-zI)\,\delta_j =& T(z)\big[a_{j-1}\delta_j + a_j\delta_{j+1} + (b_j - z)\delta_j\big] \\
=& a_{j-1}\Psi(z,j-1) + a_j\Psi(z,j+1) + (b_j-z)\Psi(z,j) \\
=& \delta_j \frac{1}{W}\big[a_{j-1}\Psi_{-,j-1}\Psi_{+,j} + a_j\Psi_{-,j}\Psi_{+,j+1} \\
&\qquad + (b_j - z)\Psi_{-,j}\Psi_{+,j}\big] \\
=& \delta_j \frac{1}{W}\big[a_{j-1}\Psi_{-,j-1}\Psi_{+,j} + a_j\Psi_{-,j+1}\Psi_{+,j} + W \\
&\qquad + (b_j - z)\Psi_{-,j}\Psi_{+,j}\big] \\
=& \delta_j.
\end{aligned}
$$

□

Corollary 8.17.

$$
\begin{aligned}
(\delta_j, R(z)\delta_k) =& \frac{1}{W(\Psi_-(z,n_0),\Psi_+(z,n_0))}\begin{cases}\Psi_{-,j}(z,n_0)\Psi_{+,k}(z,n_0), & j\le k\\ \Psi_{-,k}(z,n_0)\Psi_{+,j}(z,n_0), & j \ge k\end{cases} \\
=& \frac{1}{W(\Psi_-(z,n_0),\Psi_+(z,n_0))}\begin{cases}\Psi_{-,k}(z,n_0)\Psi_{+,j}(z,n_0), & j\ge k\\ \Psi_{-,j}(z,n_0)\Psi_{+,k}(z,n_0), & j \le k\end{cases} \\
=& (\delta_k, R(z)\delta_j), \quad j,k\in\mathbb{Z}.
\end{aligned}
$$

Corollary 8.18. *Using the definition of $M_\pm(z,n_0)$ one finds*

$$
\begin{aligned}
(\delta_{n_0+1}, R(z)\delta_{n_0+1}) &= \frac{\Psi_{-,n_0+1}(z,n_0)\Psi_{+,n_0+1}(z,n_0)}{W(\Psi_-(z,n_0),\Psi_+(z,n_0))} \\
&= \frac{1}{a_{n_0}^2}\frac{M_+(z,n_0)M_-(z,n_0)}{M_-(z,n_0)-M_+(z,n_0)}, \\
(\delta_{n_0}, R(z)\delta_{n_0}) &= \frac{\Psi_{-,n_0}(z,n_0)\Psi_{+,n_0}(z,n_0)}{W(\Psi_-(z,n_0),\Psi_+(z,n_0))} \\
&= \frac{1}{M_-(z,n_0)-M_+(z,n_0)}, \\
(\delta_{n_0}, R(z)\delta_{n_0+1}) &= (\delta_{n_0+1}, R(z)\delta_{n_0}) \\
&= \frac{\Psi_{-,n_0}(z,n_0)\Psi_{+,n_0+1}(z,n_0)}{W(\Psi_-(z,n_0),\Psi_+(z,n_0))} \\
&= -\frac{1}{a_{n_0}}\frac{M_+(z,n_0)}{M_-(z,n_0)-M_+(z,n_0)}.
\end{aligned}
$$

Definition 8.19. The following matrix $\mathcal{M}(z,n_0)$

$$\mathcal{M}(z,n_0) = \int\limits_{\mathbb{R}} \frac{1}{\lambda - z}\, d\Omega(\lambda,n_0) = \begin{pmatrix} (\delta_{n_0}, R(z)\delta_{n_0}) & (\delta_{n_0}, R(z)\delta_{n_0+1}) \\ (\delta_{n_0+1}, R(z)\delta_{n_0}) & (\delta_{n_0+1}, R(z)\delta_{n_0+1}) \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{M_-(z,n_0)-M_+(z,n_0)} & -\frac{1}{a_n}\frac{M_+(z,n_0)}{M_-(z,n_0)-M_+(z,n_0)} \\ -\frac{1}{a_n}\frac{M_+(z,n_0)}{M_-(z,n_0)-M_+(z,n_0)} & \frac{1}{a_n^2}\frac{M_+(z,n_0)M_-(z,n_0)}{M_-(z,n_0)-M_+(z,n_0)} \end{pmatrix}, \tag{8.11}$$

is called the *Weyl–Titchmarsh matrix* associated with the operator H.

Remark 8.20. *In connection with some applications (cf. [3]) it is sometimes more natural to use the following matrix $M(z,n_0)$ instead of the Weyl–Titchmarsh matrix $\mathcal{M}(z,n_0)$,*

$$M(z,n_0) = \begin{pmatrix} 1 & 0 \\ 0 & -a_{n_0} \end{pmatrix} \mathcal{M}(z,n_0) \begin{pmatrix} 1 & 0 \\ 0 & -a_{n_0} \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{M_-(z,n_0)-M_+(z,n_0)} & \frac{1}{2}\frac{M_+(z,n_0)+M_-(z,n_0)}{M_-(z,n_0)-M_+(z,n_0)} \\ \frac{1}{2}\frac{M_+(z,n_0)+M_-(z,n_0)}{M_-(z,n_0)-M_+(z,n_0)} & \frac{M_+(z,n_0)M_-(z,n_0)}{M_-(z,n_0)-M_+(z,n_0)} \end{pmatrix}.$$

Remark 8.21. *The spectral measure $d\Omega(\lambda,n_0)$ can be reconstructed from the Weyl–Titchmarsh matrix $\mathcal{M}(z,n_0)$ and hence from $M(z,n_0)$ as follows,*

$$\Omega((\alpha,\beta],n_0) = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int\limits_{\alpha+\delta}^{\beta+\delta} \mathrm{Im}\,(\mathcal{M}(\lambda+i\varepsilon,n_0))\, d\lambda. \tag{8.12}$$

Remark 8.22. *It is possible to treat a generalization of the previous sections by introducing the general linear homogeneous boundary condition in a neighborhood of the origin:*

$$\alpha u_{-1} + \beta u_0 = 0, \quad |\alpha| + |\beta| > 0.$$

From Green's formula (1.2) *it is easy to see that L is symmetric if and only if* $\mathrm{Im}\,(\alpha) = \mathrm{Im}\,(\beta) = 0$*. In this case all of the theory developed in the previous sections can be carried over to problems of the form*

$$(Lu)_j = a_{j-1}u_{j-1} + b_j u_j + a_j u_{j+1}, \quad j \in \mathbb{N}_0,$$
$$\alpha u_{-1} + \beta u_0 = 0, \quad |\alpha| + |\beta| > 0, \quad \mathrm{Im}\,(\alpha) = \mathrm{Im}\,(\beta) = 0.$$

9 Examples

The results in this section are taken from [2], p. 544-546 and p. 585-586.

Example 9.1. Consider the following difference expression on $\mathbb{N}_0$:

$$\begin{aligned} &(Lu)_j = \frac{1}{2}u_{j-1} + \frac{1}{2}u_{j+1}, \quad j \in \mathbb{N}_0, \\ &u_{-1} = 0, \end{aligned} \tag{9.1}$$

where $a_j = 1/2$, $b_j = 0$, $j \in \mathbb{N}_0$.

First, we determine $P_{+,j}(z)$. These polynomials are the solution of the following problem

$$\begin{aligned} &\frac{1}{2}u_{j-1} + \frac{1}{2}u_{j+1} = zu_j, \quad j \in \mathbb{N}_0, \\ &u_{-1} = 0, \quad u_0 = 1. \end{aligned}$$

The solution of the resulting recursion will again be unique; on the other hand, introducing $z = \cos(\theta)$, the sequence $u_j = \sin[(j+1)\theta]/\sin(\theta)$, $j \in \mathbb{N}_0$, obviously satisfies it. Thus,

$$P_{+,j}(z) = \frac{\sin[(j+1)\arccos(z)]}{\sin[\arccos(z)]}, \quad j \in \mathbb{N}_0$$

will be the solution of problem (9.1). These polynomials are known as Chebyshev polynomials of the second kind. The polynomials $Q_{+,j}(z)$ form the solution of the problem

$$\begin{aligned} &\frac{1}{2}u_{j-1} + \frac{1}{2}u_{j+1} = zu_j, \quad j \in \mathbb{N}_0, \\ &u_0 = 0, \quad u_1 = 1/a_0 = 2. \end{aligned}$$

Comparing this problem with the previous one, we obtain

$$Q_{+,j}(z) = 2P_{j-1}(z), \quad j \in \mathbb{N}_0.$$

Since the coefficients of L are bounded, the operator L is bounded. The unique spectral measure for L is given by[2]

$$d\sigma_+(\lambda) = \begin{cases} \frac{2}{\pi}\sqrt{1-\lambda^2}\, d\lambda, & |\lambda| \le 1, \\ 0, & |\lambda| \ge 1. \end{cases}$$

[2]We define $\sqrt{\cdot}$ to be the branch with $\sqrt{x} > 0$ for $x > 0$.

This follows from Theorem 5.7 and the well-known orthogonality relations for Chebyshev polynomials

$$\frac{2}{\pi}\int_{-1}^{1} P_{+,k}(\lambda)P_{+,j}(\lambda)\sqrt{1-\lambda^2}\,d\lambda = \frac{2}{\pi}\int_{0}^{\pi} \sin[(k+1)\theta]\sin[(j+1)\theta]\,d\theta = \delta_{kj},$$

$$j,k \in \mathbb{N}_0.$$

Thus,

$$\mathrm{Spec}\,(L) = [-1,1] \text{ and } \|L\| = 1.$$

The function $m_+(z)$ has the form

$$m_+(z) = \frac{2}{\pi}\int_{-1}^{1} \frac{\sqrt{1-\lambda^2}\,d\lambda}{\lambda - z} = 2(\sqrt{z^2-1} - z), \quad z \in \mathbb{C}\backslash[-1,1].$$

Example 9.2. Consider the following difference expression on $\mathbb{N}_0$:

$$\begin{aligned}&(Lu)_j = a_{j-1}u_{j-1} + a_j u_{j+1}, \quad j \in \mathbb{N}_0,\\ &u_{-1} = 0,\end{aligned}$$

where $a_0 = 1/\sqrt{2}$, $a_j = 1/2$, $j \in \mathbb{N}$, and $b_j = 0$, $j \in \mathbb{N}_0$.

First, we determine $P_{+,j}(z)$. These polynomials are the solution of the following problem

$$\begin{aligned}&\frac{1}{2}u_{j-1} + \frac{1}{2}u_{j+1} = zu_j, \quad j \geq 2,\\ &\frac{1}{\sqrt{2}}u_1 = zu_0, \quad \frac{1}{\sqrt{2}}u_0 + \frac{1}{2}u_2 = zu_1,\\ &u_{-1} = 0, \quad u_0 = 1.\end{aligned}$$

Set, as before, $z = \cos(\theta)$. It is not difficult to see that the solution of the resulting recursion relation is the sequence $u_j = \sqrt{2}\cos(j\theta)$, $j \in \mathbb{N}$. Thus,

$$\begin{aligned}&P_{+,0}(z) = 1,\\ &P_{+,j}(z) = \sqrt{2}\cos[j\arccos(z)], \quad j \in \mathbb{N}_0\end{aligned}$$

will be the solution of the problem. These polynomials are known as Chebyshev polynomials of the first kind. The polynomials $Q_{+,j}(z)$ satisfy the relation

$$\frac{1}{2}u_{j-1} + \frac{1}{2}u_{j+1} = zu_j, \quad j \in \mathbb{N},$$
$$u_0 = 0, \quad u_1 = 1/a_0 = \sqrt{2}.$$

Comparing this problem with the previous example, we obtain

$$Q_{+,j}(z) = \sqrt{2}\frac{\sin[j \arccos(z)]}{\sin[\arccos(z)]}, \quad j \in \mathbb{N}_0.$$

As in the previous example, it is easy to see that L is bounded, and

$$d\sigma_+(\lambda) = \begin{cases} \frac{d\lambda}{\pi\sqrt{1-\lambda^2}}, & |\lambda| < 1, \\ 0, & |\lambda| > 1, \end{cases}$$

$$\mathrm{Spec}\,(L) = [-1,1] \text{ and } \|L\| = 1,$$

$$m_+(z) = \frac{1}{\pi}\int_{-1}^{1} \frac{d\lambda}{(\lambda - z)\sqrt{1-\lambda^2}} = -\frac{1}{\sqrt{z^2-1}}, \quad z \in \mathbb{C}\backslash[-1,1].$$

Example 9.3. Consider the following difference expression on $\mathbb{Z}$:

$$(Lu)_j = \frac{1}{2}u_{j-1} + \frac{1}{2}u_{j+1}, \quad j \in \mathbb{Z},$$

where $a_j = 1/2$, $b_j = 0$, $j \in \mathbb{Z}$.

In this example it does not matter which point to choose as a reference point; therefore, without loss of generality, we will assume $n_0 = 0$.

The Weyl–Titchmarsh solutions $\Psi_{\pm,j}(z,0)$ are then seen to be of the form

$$\Psi_{\pm,j}(z,0) = \left(\mp\sqrt{z^2-1} + z\right)^j, \quad z \in \mathbb{C}\backslash[-1,1],\ j \in \mathbb{Z}.$$

By (8.7) and (8.8) one obtains

$$M_\pm(z,0) = \frac{1}{2}\left(\pm\sqrt{z^2-1} - z\right), \quad z \in \mathbb{C}\backslash[-1,1].$$

By (8.6) one infers

$$m_-(z,0) = m_+(z,0) = 2(\sqrt{z^2-1} - z), \quad z \in \mathbb{C}\backslash[-1,1].$$

Moreover, using (8.11), one finds for the Weyl–Titchmarsh matrix $\mathcal{M}(z,0)$,

$$\mathcal{M}(z,0) = \begin{pmatrix} \frac{-1}{\sqrt{z^2-1}} & \frac{-z}{\sqrt{z^2-1}} + 1 \\ \frac{-z}{\sqrt{z^2-1}} + 1 & \frac{-1}{\sqrt{z^2-1}} \end{pmatrix}, \quad z \in \mathbb{C}\backslash[-1,1].$$

By (8.12) this yields the corresponding spectral measure $d\Omega(\lambda,0)$,

$$d\Omega(\lambda,0) = \begin{cases} \frac{1}{\pi} \begin{pmatrix} \frac{1}{\sqrt{1-\lambda^2}} & \frac{\lambda}{\sqrt{1-\lambda^2}} \\ \frac{\lambda}{\sqrt{1-\lambda^2}} & \frac{1}{\sqrt{1-\lambda^2}} \end{pmatrix} d\lambda, & |\lambda| < 1, \\ 0, & |\lambda| > 1. \end{cases}$$

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Floquet and Spectral Theory for Periodic Schrödinger Operators

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- Floquet theory
- The Floquet discriminant in the real-valued case
- Some spectral theory
- Some connections between Floquet theory and the spectrum of periodic Schrödinger operators

1 Floquet theory

We consider the differential equation

$$L\psi(x) = \left[-\frac{d^2}{dx^2} + q(x)\right]\psi(x) = 0, \qquad x \in \mathbb{R}, \quad q \in C(\mathbb{R}), \tag{1.1}$$

where ψ, $\psi' \in AC_{loc}(\mathbb{R})$, and q is a periodic function (possibly complex-valued) with period $\Omega > 0$. That is,

$$q(x + \Omega) = q(x) \quad \text{for all} \quad x \in \mathbb{R}.$$

It is well-known that equation (1.1) has two linearly independent solutions and any solution of (1.1) can be written as a linear combination of these two linearly independent solutions. Also we can see that if $\psi(x)$ is a solution of (1.1), then so is $\psi(x + \Omega)$. Thus, one might ask whether or not these two solutions $\psi(x)$ and $\psi(x + \Omega)$ are linearly independent.

When $q(x) = 1$, in which case Ω can be any positive real number, say $\Omega = 1$, we know that $\psi_1(x) = e^x$ and $\psi_2(x) = e^{-x}$ are linearly independent solutions of (1.1). Then we see that $\psi_j(x)$ and $\psi_j(x+1)$ are linearly dependent for $j = 1, 2$, respectively. However, the solutions $(\psi_1 + \psi_2)(x)$ and $(\psi_1 + \psi_2)(x+1)$ are linearly independent. So for the special case $q(x) = 1$, whether solutions $\psi(x)$ and $\psi(x+\Omega)$ are linearly dependent depends upon the choice of the solution $\psi(x)$. In fact, this is true in general. (We will later see that in some exceptional cases, all solutions of (1.1) are periodic.)

Now we prove the following theorem on the existence of a non-trivial solution $\psi(x)$ of (1.1) such that $\psi(x)$ and $\psi(x + \Omega)$ are linearly dependent.

Theorem 1.1. *There exist a non-zero constant ρ and a non-trivial solution ψ of (1.1) such that*

$$\psi(x + \Omega) = \rho\psi(x), \quad x \in \mathbb{R}. \tag{1.2}$$

Proof. It is well-known that (1.1) has solutions ϕ_1 and ϕ_2 such that

$$\begin{aligned} \phi_1(0) &= 1, & \phi_2(0) &= 0, \\ \phi_1'(0) &= 0, & \phi_2'(0) &= 1. \end{aligned} \tag{1.3}$$

So in particular,

$$W(\phi_1, \phi_2)(x) = \phi_1(x)\phi_2'(x) - \phi_1'(x)\phi_2(x) = 1. \tag{1.4}$$

Then, since $\phi_1(x+\Omega)$ and $\phi_2(x+\Omega)$ are also solutions of (1.1), using (1.3) we get

$$\begin{aligned} \phi_1(x+\Omega) &= \phi_1(\Omega)\phi_1(x) + \phi_1'(\Omega)\phi_2(x), \\ \phi_2(x+\Omega) &= \phi_2(\Omega)\phi_1(x) + \phi_2'(\Omega)\phi_2(x). \end{aligned} \tag{1.5}$$

Since every solution $\psi(x)$ of (1.1) can be written as $\psi(x) = c_1\phi_1(x) + c_2\phi_2(x)$, it suffices to show that there exist a vector $(c_1, c_2) \in \mathbb{C}^2 \setminus \{0\}$ and a constant $\rho \in \mathbb{C}$ such that

$$\begin{pmatrix} \phi_1(\Omega) & \phi_2(\Omega) \\ \phi_1'(\Omega) & \phi_2'(\Omega) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \rho \begin{pmatrix} c_1 \\ c_2 \end{pmatrix},$$

which, by (1.5), is equivalent to

$$\psi(x+\Omega) = \rho\psi(x).$$

Now the question becomes whether the matrix

$$M = \begin{pmatrix} \phi_1(\Omega) & \phi_2(\Omega) \\ \phi_1'(\Omega) & \phi_2'(\Omega) \end{pmatrix} \tag{1.6}$$

has an eigenvector $(c_1, c_2)^T$ (the transpose of (c_1, c_2)) with the corresponding (non-zero) eigenvalue ρ. Since an eigenvalue is a solution of the quadratic equation

$$\rho^2 - [\phi_1(\Omega) + \phi_2'(\Omega)]\,\rho + 1 = 0, \tag{1.7}$$

where we used (1.4) to get the constant term 1, it is clear that every eigenvalue is non-zero. Therefore, matrix algebra completes the proof. □

We note that the matrix M in (1.6) is called the *monodromy matrix* of equation (1.1).

In addition to the previous theorem, one can show that equation (1.1) has two linearly independent solutions of a very special form:

Theorem 1.2. *The equation (1.1) has linearly independent solutions $\psi_1(x)$ and $\psi_2(x)$ such that either*
(i) $\psi_1(x) = e^{m_1 x}p_1(x)$, $\psi_2(x) = e^{m_2 x}p_2(x)$, where $m_1, m_2 \in \mathbb{C}$ and $p_1(x)$ and $p_2(x)$ are periodic functions with period Ω; or
(ii) $\psi_1(x) = e^{mx}p_1(x)$, $\psi_2(x) = e^{mx}\{xp_1(x) + p_2(x)\}$, where $m \in \mathbb{C}$ and $p_1(x)$ and $p_2(x)$ are periodic functions with period Ω.

Proof. We will divide the proof into two cases.
Case I: Suppose that the monodromy matrix M has two distinct eigenvalues ρ_1, ρ_2. Certainly, (1.1) has two linearly independent solutions $\psi_1(x)$ and $\psi_2(x)$ with $\psi_j(x+\Omega) = \rho_j\psi_j(x)$ for $j = 1, 2$. Next, we choose constants m_1 and m_2 so that

$$e^{m_j\Omega} = \rho_j, \quad j = 1, 2, \tag{1.8}$$

and define

$$p_j(x) = e^{-m_j x}\psi_j(x), \qquad j = 1, 2. \tag{1.9}$$

Then one can easily verify that $p_j(x)$ are periodic with period Ω as follows.

$$\begin{aligned} p_j(x+\Omega) &= e^{-m_j(x+\Omega)}\psi_j(x+\Omega) \\ &= e^{-m_j x}e^{-m_j\Omega}\,\rho_j\,\psi_j(x) \\ &= p_j(x), \quad j = 1,\ 2,\ x \in \mathbb{R}. \end{aligned}$$

Thus, $\psi_j(x) = e^{m_j x}p_j(x)$, where $p_j(x)$ has period Ω. So we have case (i) of the theorem.
Case II: Assume the matrix M has a repeated eigenvalue ρ. We then choose m so that $e^{m\Omega} = \rho$. By Theorem 1.1, there exists a non-trivial solution $\Psi_1(x)$ of (1.1) such that $\Psi_1(x+\Omega) = \rho\Psi_1(x)$. Since (1.1) has two linearly independent solutions, we can choose a second solution $\Psi_2(x)$ which is linearly independent of $\Psi_1(x)$. Then, since $\Psi_2(x+\Omega)$ is also a solution of (1.1), one can write

$$\Psi_2(x+\Omega) = d_1\Psi_1(x) + d_2\Psi_2(x) \text{ for some } d_1, d_2 \in \mathbb{C}.$$

Thus,

$$W(\Psi_1,\ \Psi_2)(x+\Omega) = W(\rho\Psi_1(x),\ \Psi_2(x+\Omega)) = \rho d_2 W(\Psi_1, \Psi_2)(x).$$

Since the Wronskian is a non-zero constant, we have

$$d_2 = \frac{1}{\rho} = \rho$$

and hence,

$$\Psi_2(x+\Omega) = d_1\Psi_1(x) + \rho\Psi_2(x) \quad \text{for some} \quad d_1 \in \mathbb{C}.$$

If $d_1 = 0$ this case reduces to case I with $\rho_1 = \rho_2 = \rho$. So we are again in case (i) of the theorem.

Now suppose that $d_1 \neq 0$. We define

$$P_1(x) = e^{-mx}\Psi_1(x)$$

and thus $P_1(x)$ is periodic with period Ω. Also, we define

$$P_2(x) = e^{-mx}\Psi_2(x) - \frac{d_1}{\rho\Omega} x P_1(x).$$

Then

$$\begin{aligned} P_2(x+\Omega) &= e^{-m(x+\Omega)}\Psi_2(x+\Omega) - \frac{d_1}{\rho\Omega}(x+\Omega)P_1(x+\Omega) \\ &= \frac{e^{-mx}}{\rho}\{d_1\Psi_1(x) + \rho\Psi_2(x)\} - \frac{d_1}{\rho\Omega}(x+\Omega)P_1(x) \\ &= \frac{d_1}{\rho}P_1(x) + e^{-mx}\Psi_2(x) - \frac{d_1}{\rho\Omega}xP_1(x) - \frac{d_1}{\rho}P_1(x) \\ &= P_2(x). \end{aligned}$$

So we have part (ii) of the theorem with $\psi_1(x) = \Psi_1(x)$ and $\psi_2(x) = \frac{\rho\Omega}{d_1}\Psi_2(x)$. □

The solutions ψ_1 and ψ_2 in Theorem 1.2 are called the *Floquet solutions* of (1.1).

Remark 1.3. These results form the basis of *Floquet Theory* of second-order scalar differential equations (see, e.g., Eastham [1, Ch. 1]).

Remark 1.4. Case (i) of Theorem 1.2 occurs when the matrix M has two linearly independent eigenvectors, while case (ii) occurs when M does not have two linearly independent eigenvectors.

Definition 1.5. One calls

$$\Delta = \frac{1}{2}\left(\phi_1(\Omega) + \phi_2'(\Omega)\right)$$

the *Floquet discriminant* of equation (1.1). The solutions ρ_1 and ρ_2 of

$$\rho^2 - 2\Delta\,\rho + 1 = 0 \tag{1.10}$$

are called the *Floquet multipliers* of equation (1.1).

Definition 1.6. The equation (1.1) is said to be (a) *unstable* if all non-trivial solutions are unbounded on $\mathbb{R}$, (b) *conditionally stable* if there is a non-trivial bounded solution, and (c) *stable* if all solutions are bounded.

Later we will see that the conditional stability is intimately related to the spectrum of the operator generated by L, defined in (1.1).

Remark 1.7. It is clear that ρ is a solution of the quadratic equation (1.10) if and only if $\frac{1}{\rho}$ is a solution of (1.10).

Remark 1.8. A non-trivial solution $\psi(x)$ of (1.1) with the property $\psi(x+\Omega) = \rho\psi(x)$ is bounded on $\mathbb{R}$ if and only if $|\rho| = 1$ since $\psi(x+n\Omega) = \rho^n\psi(x)$ for all $n \in \mathbb{Z}$.

We now prove the following theorem on stability of the equation (1.1).

Theorem 1.9. *Suppose that Δ is real.*
(i) If $|\Delta| < 1$, then all solutions of (1.1) are bounded on $\mathbb{R}$.
(ii) If $|\Delta| > 1$, then all non-trivial solutions of (1.1) are unbounded on $\mathbb{R}$.
(iii) If $\Delta = 1$, then there is at least one non-trivial solution of (1.1) that is periodic with period Ω. Moreover, if $\phi_1'(\Omega) = \phi_2(\Omega) = 0$, all solutions are periodic with period Ω. If either $\phi_1'(\Omega) \neq 0$ or $\phi_2(\Omega) \neq 0$, there do not exist two linearly independent periodic solutions.
(iv) If $\Delta = -1$, then there is at least one non-trivial solution ψ of (1.1) that is semi-periodic with semi-period Ω (i.e., $\psi(x+\Omega) = -\psi(x)$). Moreover, if $\phi_1'(\Omega) = \phi_2(\Omega) = 0$, all solutions are semi-periodic with semi-period Ω. If either $\phi_1'(\Omega) \neq 0$ or $\phi_2(\Omega) \neq 0$, there do not exist two linearly independent semi-periodic solutions.
If Δ is nonreal, then all non-trivial solutions of (1.1) are unbounded on $\mathbb{R}$.

Proof. Suppose Δ is real. Since the two solutions ρ_1 and ρ_2 of (1.10) are

$$\Delta \pm \sqrt{\Delta^2 - 1}, \tag{1.11}$$

we see that

$$|\rho_1| = 1, \quad \text{(and hence} \quad |\rho_2| = \frac{1}{|\rho_1|} = 1) \quad \text{if and only if} \quad |\Delta| \leq 1. \tag{1.12}$$

When $\rho_1 = e^{it}$ for some $t \in \mathbb{R}$, we have that

$$\Delta = \frac{1}{2}\left(\phi_1(\Omega) + \phi_2'(\Omega)\right) = \frac{1}{2}\left(\rho_1 + \frac{1}{\rho_1}\right) = \cos(t).$$

Proof of (i): Suppose $|\Delta| < 1$. By (1.12), we see that $|\rho_1| = |\rho_2| = 1$, and hence $\rho_1 = e^{it}$ and $\rho_2 = e^{-it}$ for some $t \in \mathbb{R}$. Then we have $\Delta = \cos(t)$. Since $|\Delta| < 1$, we get that t is not a multiple of π, and so $\rho_1 \neq \rho_2$. So we have case (i) of Theorem 1.2 with $m_1 = \frac{it}{\Omega}$ and $m_2 = -\frac{it}{\Omega}$ (see (1.8)), and every solution of (1.1) is bounded on $\mathbb{R}$.
Proof of (ii): Suppose $|\Delta| > 1$. By (1.11), we see that both ρ_1 and ρ_2 are real, and that either $|\rho_1| > 1$ and $|\rho_2| < 1$, or $|\rho_1| < 1$ and $|\rho_2| > 1$. In particular, they are different. So we have case (i) of Theorem 1.2 with $\operatorname{Re} m_j \neq 0$ for $j = 1, 2$, and every non-trivial solution of (1.1) is unbounded on $\mathbb{R}$ (see Remark 1.8).
Proof of (iii): Suppose $\Delta = 1$. Then $\rho_1 = \rho_2 = 1$ since they are solutions of (1.10). There is at least one eigenvector of the monodromy matrix M, and hence there exists at least one nontrivial periodic solution. When $\phi_1'(\Omega) = \phi_2(\Omega) = 0$, M is the identity matrix, and hence it has two linearly independent eigenvectors. So there are two linearly independent Floquet solutions that are periodic with period Ω. Thus every solution is periodic with period Ω.

If either $\phi_1'(\Omega) \neq 0$ or $\phi_2(\Omega) \neq 0$, then M has only one linearly independent eigenvector, and so we have case (ii) of Theorem 1.2. Thus, there exists a non-trivial solution that is not periodic.
Proof of (iv): Suppose $\Delta = -1$. Then $\rho_1 = \rho_2 = -1$ since they are solutions of (1.10). The proof is now similar to case (iii) above.

Finally, we suppose Δ is not real, and hence both ρ_1 and ρ_2 are not real. Also, $|\rho_1| \neq 1$ and $|\rho_2| \neq 1$, since otherwise Δ would be real. So from (1.8), $\operatorname{Re} m_j \neq 0$ for $j = 1, 2$, and every non-trivial solution is unbounded on $\mathbb{R}$ by Theorem 1.2. □

We note that if q is real-valued, then $\phi_1(\Omega)$ and $\phi_2'(\Omega)$ are real, and so is Δ.

2 The case where $q(x) \to q(x) - z$, $z \in \mathbb{C}$

In this section we introduce a complex parameter z into (1.1) and study the asymptotic behavior of $\Delta(z)$ as $|z| \to \infty$.

We consider

$$-\psi''(x) + [q(x) - z]\psi(x) = 0, \qquad x \in \mathbb{R}, \tag{2.1}$$

where ψ, $\psi' \in AC_{loc}(\mathbb{R})$, and $q \in C(\mathbb{R})$ is a periodic function (possibly complex-valued) with period $\Omega > 0$.

We know that for each $z \in \mathbb{C}$, (2.1) has the solutions $\phi_1(z,\cdot)$ and $\phi_2(z,\cdot)$ such that

$$\begin{aligned} \phi_1(z,0) &= 1, \qquad & \phi_2(z,0) &= 0, \\ \phi_1'(z,0) &= 0, \qquad & \phi_2'(z,0) &= 1, \end{aligned} \tag{2.2}$$

as in (1.3), where we denote $\frac{\partial}{\partial x} = {}'$.

Let

$$\Delta(z) = \frac{1}{2}\left(\phi_1(z,\Omega) + \phi_2'(z,\Omega)\right).$$

It is known that $\phi_j(z,x)$, $j = 1, 2$ for fixed $x \in \mathbb{R}$ as well as $\Delta(z)$ are entire functions of z. Next we will study the asymptotic behavior of $\Delta(z)$ using the following lemma.

Lemma 2.1. *For $x \geq 0$ and $z \neq 0$, we have the following bounds for $\phi_j(z,x)$, $j = 1, 2$,*

$$|\phi_1(z,x)| \leq \exp[|\mathrm{Im}\sqrt{z}|x] \exp\left[|z|^{-\frac{1}{2}} \int_0^x dx_1 |q(x_1)|\right], \tag{2.3}$$

$$|\phi_2(z,x)| \leq |z|^{-\frac{1}{2}} \exp[|\mathrm{Im}\sqrt{z}|x] \exp\left[|z|^{-\frac{1}{2}} \int_0^x dx_1 |q(x_1)|\right]. \tag{2.4}$$

Proof. One can see that $\phi_j(z,x)$ satisfy the following integral equations,

$$\phi_1(z,x) = \cos[\sqrt{z}x] + \int_0^x dx_1 \frac{\sin[\sqrt{z}(x-x_1)]}{\sqrt{z}} q(x_1)\phi_1(z,x_1), \tag{2.5}$$

$$\phi_2(z,x) = \frac{\sin[\sqrt{z}x]}{\sqrt{z}} + \int_0^x dx_1 \frac{\sin[\sqrt{z}(x-x_1)]}{\sqrt{z}} q(x_1)\phi_2(z,x_1). \tag{2.6}$$

We note that these integral equations are invariant under the change $\sqrt{z} \mapsto -\sqrt{z}$, so we can choose any branch for the square root.

Define a sequence $\{u_n(z,x)\}_{n\in\mathbb{N}_0}$ of functions recursively as follows:

$$\begin{aligned} u_0(z,x) &= 0, \\ u_n(z,x) &= \cos[\sqrt{z}x] + \int_0^x dx_1 \frac{\sin[\sqrt{z}(x-x_1)]}{\sqrt{z}} q(x_1) u_{n-1}(z,x_1), \quad n \geq 1. \end{aligned}$$

We will show that $\lim_{n\to\infty} u_n(z,x)$ exists, and that the limit is the solution of the integral equation (2.5).

Let $v_n(z,x) = u_n(z,x) - u_{n-1}(z,x)$ for $n \geq 1$. First, we claim that

$$|v_n(z,x)| \leq \exp[|\mathrm{Im}\sqrt{z}|x] \frac{\left(\int_0^x dx_1 |q(x_1)|\right)^{n-1}}{|z|^{\frac{n-1}{2}}(n-1)!}, \quad x \geq 0, \;\; n \geq 1, \tag{2.7}$$

which will be proven by induction.

The case $n = 1$ is clear since $v_1(z,x) = \cos[\sqrt{z}x]$. Suppose that (2.7) holds for some $n \geq 1$, that is, assume

$$|v_n(z,x)| \leq \exp[|\mathrm{Im}\sqrt{z}|x] \frac{\left(\int_0^x dx_1 |q(x_1)|\right)^{n-1}}{|z|^{\frac{n-1}{2}}(n-1)!}, \quad x \geq 0. \tag{2.8}$$

Then, since

$$v_{n+1}(z,x) = \int_0^x dx_1 \frac{\sin[\sqrt{z}(x-x_1)]}{\sqrt{z}} q(x_1) v_n(z,x_1),$$

we have

$$\begin{aligned}
|v_{n+1}(z,x)| &\leq \int_0^x dx_1 \frac{|\sin[\sqrt{z}(x-x_1)]|}{|\sqrt{z}|} |q(x_1)||v_n(z,x_1)| \\
&\leq \frac{|\exp[|\mathrm{Im}\sqrt{z}|x]}{|z|^{\frac{n}{2}}(n-1)!} \int_0^x dx_1 |q(x_1)| \left(\int_0^{x_1} dx_2 |q(x_2)|\right)^{n-1} \\
&= \exp[|\mathrm{Im}\sqrt{z}|x] \frac{\left(\int_0^x dx_1 |q(x_1)|\right)^{n}}{|z|^{\frac{n}{2}} n!}, \quad x \geq 0,
\end{aligned}$$

where we used (2.8) in the second step. Thus, by induction, (2.7) holds for all $n \geq 1$, and hence,

$$\begin{aligned}
\sum_{n=1}^{\infty} |v_n(z,x)| &\leq \exp[|\mathrm{Im}\sqrt{z}|x] \sum_{n=1}^{\infty} \frac{\left(\int_0^x dx_1 |q(x_1)|\right)^{n-1}}{|z|^{\frac{n-1}{2}}(n-1)!} \\
&= \exp[|\mathrm{Im}\sqrt{z}|x] \exp\left[\frac{\int_0^x dx_1 |q(x_1)|}{|\sqrt{z}|}\right].
\end{aligned} \tag{2.9}$$

Thus,

$$\lim_{n\to\infty} u_n(z,x) = \sum_{n=1}^{\infty} v_n(z,x)$$

exists and is the solution of the integral equation (2.5). Then by the uniqueness of the solution, we have $\lim_{n\to\infty} u_n(z,x) = \phi_1(z,x)$ and this proves (2.3).

The proof of (2.4) is similar to the proof of (2.3), with (2.7) replaced by

$$|v_n(z,x)| \leq \exp[|\operatorname{Im}\sqrt{z}|x] \frac{\left(\int_0^x dx_1 |q(x_1)|\right)^{n-1}}{|z|^{\frac{n}{2}}(n-1)!}, \quad x \geq 0, \; n \geq 1.$$

□

Theorem 2.2.

$$2\Delta(z) \underset{|z|\to\infty}{=} 2\cos[\sqrt{z}\Omega] + \frac{\sin[\sqrt{z}\Omega]}{\sqrt{z}} \int_0^\Omega dx\, q(x) + O\left(\frac{\exp[|\operatorname{Im}\sqrt{z}|\Omega]}{|z|}\right). \tag{2.10}$$

In particular, $\Delta(z)$ is of order $\frac{1}{2}$ and type Ω. Also, for each $w \in \mathbb{C}$, there is an infinite set $\{z_n\}_{n\in\mathbb{N}_0} \subset \mathbb{C}$ such that $\Delta(z_n) = w$.

Proof. First we differentiate (2.6) with respect to x to get

$$\phi_2'(z,x) = \cos[\sqrt{z}x] + \int_0^x dx_1 \cos[\sqrt{z}(x-x_1)] q(x_1)\phi_2(z,x_1).$$

Then we have

$$\begin{aligned}
2\Delta(z) &= \phi_1(z,\Omega) + \phi_2'(z,\Omega) \\
&= \cos[\sqrt{z}\Omega] + \int_0^\Omega dx_1 \frac{\sin[\sqrt{z}(\Omega - x_1)]}{\sqrt{z}} q(x_1)\phi_1(z,x_1) \\
&\quad + \cos[\sqrt{z}\Omega] + \int_0^\Omega dx_1 \cos[\sqrt{z}(\Omega - x_1)] q(x_1)\phi_2(z,x_1) \\
&= 2\cos[\sqrt{z}\Omega] + \int_0^\Omega dx_1 \frac{\sin[\sqrt{z}(\Omega - x_1)]}{\sqrt{z}} q(x_1)\cos[\sqrt{z}x_1] \\
&\quad + \int_0^\Omega dx_1 \frac{\sin[\sqrt{z}(\Omega - x_1)]}{\sqrt{z}} q(x_1) \int_0^{x_1} dx_2 \frac{\sin[\sqrt{z}(x_1 - x_2)]}{\sqrt{z}} q(x_2)\phi_1(z,x_2) \\
&\quad + \int_0^\Omega dx_1 \cos[\sqrt{z}(\Omega - x_1)] q(x_1) \frac{\sin[\sqrt{z}x_1]}{\sqrt{z}}
\end{aligned}$$

$$
\begin{aligned}
&+\int_0^\Omega dx_1 \cos[\sqrt{z}(\Omega - x_1)]q(x_1)\int_0^{x_1} dx_2 \frac{\sin[\sqrt{z}(x_1-x_2)]}{\sqrt{z}} q(x_2)\phi_2(z,x_2)\\
&= 2\cos[\sqrt{z}\Omega] + \frac{\sin[\sqrt{z}\Omega]}{\sqrt{z}}\int_0^\Omega dx_1\, q(x_1)\\
&+\int_0^\Omega dx_1 \frac{\sin[\sqrt{z}(\Omega - x_1)]}{\sqrt{z}} q(x_1)\int_0^{x_1} dx_2 \frac{\sin[\sqrt{z}(x_1-x_2)]}{\sqrt{z}} q(x_2)\phi_1(z,x_2)\\
&+\int_0^\Omega dx_1 \cos[\sqrt{z}(\Omega - x_1)]q(x_1)\int_0^{x_1} dx_2 \frac{\sin[\sqrt{z}(x_1-x_2)]}{\sqrt{z}} q(x_2)\phi_2(z,x_2),
\end{aligned}
$$

where in the last step, we used $\sin(z_1+z_2) = \sin(z_1)\cos(z_2) + \cos(z_1)\sin(z_2)$.

Then, using (2.3) and (2.4) along with

$$
\begin{aligned}
& \left|\sin[\sqrt{z}(\Omega - x_1)]\sin[\sqrt{z}(x_1-x_2)]\right|\\
\le\ & \exp[|\mathrm{Im}\,\sqrt{z}|(\Omega - x_1)]\exp[|\mathrm{Im}\,\sqrt{z}|(x_1-x_2)]\\
=\ & \exp[|\mathrm{Im}\,\sqrt{z}|(\Omega - x_2)], \quad \text{where} \quad 0 \le x_2 \le x_1 \le \Omega,
\end{aligned}
$$

one can see that

$$
2\Delta(z) \underset{|z|\to\infty}{=} 2\cos[\sqrt{z}\Omega] + \frac{\sin[\sqrt{z}\Omega]}{\sqrt{z}}\int_0^\Omega dx\, q(x) + O\left(\frac{\exp[|\mathrm{Im}\,\sqrt{z}|\Omega]}{|z|}\right).
$$

Next, we recall the definitions of the order and type of entire functions. The *order* of an entire function f is defined as

$$
\mathit{order}\,(f) = \limsup_{r\to\infty} \frac{\log\left(\log\left(M(r,f)\right)\right)}{\log(r)},
$$

where $M(r,f) = \max\left\{|f(re^{i\theta})|\,|\,0 \le \theta \le 2\pi\right\}$ for $r > 0$. The *type* of f is defined by

$$
\mathit{type}\,(f) = \limsup_{r\to\infty} r^{-\mathit{order}\,(f)}\log\left(M(r,f)\right).
$$

If for some positive real numbers c_1, c_2, d, we have $M(r,f) \le c_1\exp[c_2 r^d]$ for all large r, then the order of f is less than or equal to d. Moreover,

$$
\mathit{type}\,(f) = \inf\{K > 0 \mid \text{for some } r_0 > 0, M(r,f) \le \exp[K r^{\mathit{order}\,(f)}] \text{ for all } r \ge r_0\}.
$$

Thus claims on the order and type of $\Delta(z)$ are clear from the asymptotic expression (2.10).

Finally, for each $w \in \mathbb{C}$ the existence of an infinite set $\{z_n\}_{n\in\mathbb{N}_0} \subset \mathbb{C}$ such that $\Delta(z_n) = w$ follows from Picard's little theorem that states that any entire function of non-integer order has such a set $\{z_n\}_{n\in\mathbb{N}_0}$. This completes the proof. $\square$

3 The Floquet discriminant $\Delta(\lambda)$ in the real-valued case

Assume $q \in C([0, \Omega])$ to be real-valued. In this section, we first investigate some periodic and semi-periodic eigenvalue problems. Then with the help of these eigenvalue problems, we study the behavior of the Floquet discriminant $\Delta(\lambda)$ as λ varies on the real line.

Consider the eigenvalue problem

$$-\psi''(x) + q(x)\psi(x) = \lambda\psi(x), \tag{3.1}$$

under the boundary conditions

$$\psi(\Omega) = \psi(0)e^{it}, \qquad \psi'(\Omega) = \psi'(0)e^{it}, \tag{3.2}$$

with $t \in (-\pi, \pi]$ fixed and $\psi, \psi' \in AC([0, \Omega])$. Then for every such t, the eigenvalue problem is self-adjoint. So the eigenvalues are all real if they exist. But the existence of countably infinitely many eigenvalues is clear by Theorem 2.2 since for each $t \in (-\pi, \pi]$,

$$\begin{aligned}&\lambda_n(t) \text{ is an eigenvalue (and hence real)}\\ &\text{if and only if } \Delta(\lambda_n(t)) = \cos(t),\ n \in \mathbb{N}_0.\end{aligned}$$

Thus for each $t \in (-\pi, \pi]$,

$$\{\lambda_n(t) \,|\, n \in \mathbb{N}_0\} = \{\lambda \in \mathbb{C} \,|\, \Delta(\lambda) = \cos(t)\} = \{\lambda_n(-t) \,|\, n \in \mathbb{N}_0\}.$$

Also, one can see that for each $t \in (-\pi, \pi]$, the eigenvalues are bounded from below since $\Delta(\lambda) \to \infty$ as $\lambda \to -\infty$.

(i) The *periodic eigenvalue problem* is the eigenvalue problem (3.1) under the boundary condition (3.2) with $t = 0$, that is,

$$\psi(\Omega) = \psi(0), \qquad \psi'(\Omega) = \psi'(0).$$

We denote the countably infinitely many eigenvalues by

$$\lambda_0 \le \lambda_1 \le \lambda_2 \le \lambda_3 \le \cdots, \quad \text{and} \quad \lambda_n \to \infty \quad \text{as} \quad n \to \infty.$$

(ii) The *semi-periodic eigenvalue problem* is the eigenvalue problem (3.1), under the boundary condition (3.2) with $t = \pi$, that is,

$$\psi(\Omega) = -\psi(0), \qquad \psi'(\Omega) = -\psi'(0).$$

We denote the countably infinitely many eigenvalues by

$$\mu_0 \le \mu_1 \le \mu_2 \le \mu_3 \le \cdots, \quad \text{and} \quad \mu_n \to \infty \quad \text{as} \quad n \to \infty.$$

Next, using these eigenvalue problems we examine the Floquet discriminant $\Delta(\lambda)$.

Theorem 3.1. *Suppose that $q \in C([0, \Omega])$ is real-valued and $\lambda \in \mathbb{R}$.*
(i) The numbers λ_n and μ_n occur in the order

$$\lambda_0 < \mu_0 \le \mu_1 < \lambda_1 \le \lambda_2 < \mu_2 \le \mu_3 < \lambda_3 \le \lambda_4 < \cdots.$$

(ii) In the intervals $[\lambda_{2m}, \mu_{2m}]$, $\Delta(\lambda)$ decreases from 1 to -1.
(iii) In the intervals $[\mu_{2m+1}, \lambda_{2m+1}]$, $\Delta(\lambda)$ increases from -1 to 1.
(iv) In the intervals $(-\infty, \lambda_0)$ and $(\lambda_{2m-1}, \lambda_{2m})$, $\Delta(\lambda) > 1$.
(v) In the intervals (μ_{2m}, μ_{2m+1}), $\Delta(\lambda) < -1$.

Proof. We give the proof in several stages.

(a) *There exists a $\Lambda \in \mathbb{R}$ such that $\Delta(\lambda) > 1$ if $\lambda \le \Lambda$. Moeover, $\Delta(\lambda)$ changes sign infinitely often near $+\infty$.*

From (2.10), we see that as $\lambda \to -\infty$,

$$\Delta(\lambda) = \exp[|\lambda|^{\frac{1}{2}}\Omega]\left(1 + O\left(\frac{1}{|\lambda|^{\frac{1}{2}}}\right)\right).$$

Since $\Delta(\lambda)$ is a continuous function of λ, there exists a $\Lambda \in \mathbb{R}$ such that if $\lambda \le \Lambda$, then $\Delta(\lambda) > 1$. Also from (2.10), we see that as $\lambda \to \infty$,

$$\Delta(\lambda) = \cos\left(|\lambda|^{\frac{1}{2}}\Omega\right) - \frac{\sin\left(|\lambda|^{\frac{1}{2}}\Omega\right)}{2|\lambda|^{\frac{1}{2}}}\int_0^\Omega dx\, q(x) + O\left(\frac{1}{|\lambda|}\right).$$

So $\Delta(\lambda)$ changes sign infinitely often near $+\infty$.

(b) $\overset{\bullet}{\Delta}(\lambda) \neq 0$ *if* $|\Delta(\lambda)| < 1$, *where* $\overset{\bullet}{\Delta}(\lambda) = \frac{d}{d\lambda}(\Delta(\lambda))$.

First we differentiate (3.1) with respect to λ. This gives

$$-\frac{d^2}{dx^2}\left(\frac{\partial \phi_1(\lambda,\, x)}{\partial \lambda}\right) + [q(x) - \lambda]\frac{\partial \phi_1(\lambda,\, x)}{\partial \lambda} = \phi_1(\lambda,\, x).$$

Also, from $\phi_1(\lambda, 0) = 1$, we have

$$\frac{\partial \phi_1(\lambda,\, 0)}{\partial \lambda} = \frac{d}{dx}\left(\frac{\partial \phi_1(\lambda,\, 0)}{\partial \lambda}\right) = 0.$$

Then one can check that

$$\frac{\partial \phi_1(\lambda,\, x)}{\partial \lambda} = \int_0^x dt\, [\phi_1(\lambda, x)\phi_2(\lambda, t) - \phi_2(\lambda, x)\phi_1(\lambda, t)]\, \phi_1(\lambda, t). \tag{3.3}$$

Similarly,

$$\frac{\partial \phi_2(\lambda,\, x)}{\partial \lambda} = \int_0^x dt\, [\phi_1(\lambda, x)\phi_2(\lambda, t) - \phi_2(\lambda, x)\phi_1(\lambda, t)]\, \phi_2(\lambda, t), \tag{3.4}$$

and we differentiate this with respect to x to obtain

$$\frac{\partial \phi_2'(\lambda,\, x)}{\partial \lambda} = \int_0^x dt\, [\phi_1'(\lambda, x)\phi_2(\lambda, t) - \phi_2'(\lambda, x)\phi_1(\lambda, t)]\, \phi_2(\lambda, t).$$

This, along with (3.3) yields

$$\begin{aligned} 2\overset{\bullet}{\Delta}(\lambda) = \int_0^\Omega dt \big[&\phi_1'(\lambda, \Omega)\phi_2^2(\lambda, t) + (\phi_1(\lambda, \Omega) - \phi_2'(\lambda, \Omega))\phi_1(\lambda, t)\phi_2(\lambda, t) \\ &- \phi_2(\lambda, \Omega)\phi_1^2(\lambda, t)\big], \end{aligned} \tag{3.5}$$

where $\phi_1 = \phi_1(\lambda, \Omega)$, $\phi_1' = \phi_1'(\lambda, \Omega)$, $\phi_2 = \phi_2(\lambda, \Omega)$, and $\phi_2' = \phi_2'(\lambda, \Omega)$.

Since $W(\phi_1, \phi_2)(\Omega) = \phi_1\phi_2' - \phi_1'\phi_2 = 1$,

$$\Delta^2 = \frac{1}{4}\left(\phi_1^2 + 2\phi_1\phi_2' + {\phi_2'}^2\right) = 1 + \frac{1}{4}(\phi_1 - \phi_2')^2 + \phi_2\phi_1'. \tag{3.6}$$

Multiplying (3.5) by ϕ_2 and rewriting the resulting equation one gets

$$\begin{aligned} 2\phi_2\overset{\bullet}{\Delta}(\lambda) \;&=\; -\int_0^\Omega dt\left[\phi_2\phi_1(\lambda, t) - \frac{\phi_1 - \phi_2'}{2}\phi_2(\lambda, t)\right]^2 \\ &\quad -(1 - \Delta^2(\lambda))\int_0^\Omega dt\, \phi_2^2(\lambda, t), \end{aligned} \tag{3.7}$$

where we used (3.6).

Next, we suppose that $|\Delta(\lambda)| < 1$. Then from (3.7), we have

$$\phi_2(\lambda,\,\Omega)\overset{\bullet}{\Delta}(\lambda) < 0, \text{ and in particular, } \overset{\bullet}{\Delta}(\lambda) \neq 0.$$

(c)*At a zero λ_n of $\Delta(\lambda) - 1$,*

$$\overset{\bullet}{\Delta}(\lambda_n) = 0 \quad \textit{if and only if} \quad \phi_2(\lambda_n, \Omega) = \phi_1'(\lambda_n, \Omega) = 0.$$

Also, if $\overset{\bullet}{\Delta}(\lambda_n) = 0$, then $\overset{\bullet\bullet}{\Delta}(\lambda_n) < 0$.

Suppose $\phi_2(\lambda_n, \Omega) = \phi_1'(\lambda_n, \Omega) = 0$. Then we have

$$\phi_2'(\lambda_n, \Omega) = \phi_1(\lambda_n, \Omega) = 1.$$

So by (3.5), we have $\overset{\bullet}{\Delta}(\lambda_n) = 0$. Conversely, if $\overset{\bullet}{\Delta}(\lambda_n) = 0$, by (3.7), we have $2\phi_2\phi_1(\lambda, t) + (\phi_1 - \phi_2')\phi_2(\lambda, t) = 0$. Since $\phi_1(\lambda, t)$ and $\phi_2(\lambda, t)$ are linearly independent, we get $\phi_2(\lambda_n, \Omega) = 0$ and $\phi_2'(\lambda_n, \Omega) = \phi_1(\lambda_n, \Omega)$. Finally, from (3.5) we infer $\phi_1'(\lambda_n, \Omega) = 0$.

Next, in order to prove that $\overset{\bullet\bullet}{\Delta}(\lambda_n) < 0$ if $\overset{\bullet}{\Delta}(\lambda_n) = 0$, we differentiate (3.5) with respect to λ, substitute $\lambda = \lambda_n$, and use $\phi_2(\lambda_n, \Omega) = \phi_1'(\lambda_n, \Omega) = 0$ and $\phi_2'(\lambda_n, \Omega) = \phi_1(\lambda_n, \Omega) = 1$ to arrive at

$$\begin{aligned} 2\overset{\bullet\bullet}{\Delta}(\lambda_n) = \int_0^\Omega dt \Bigg[& \frac{\partial \phi_1'(\lambda, \Omega)}{\partial \lambda}\bigg|_{\lambda_n} \phi_2^2(\lambda_n, t) \\ & + \left(\frac{\partial \phi_1(\lambda, \Omega)}{\partial \lambda}\bigg|_{\lambda_n} - \frac{\partial \phi_2'(\lambda, \Omega)}{\partial \lambda}\bigg|_{\lambda_n} \right) \phi_1(\lambda_n, t)\phi_2(\lambda_n, t) \\ & - \frac{\partial \phi_2(\lambda, \Omega)}{\partial \lambda}\bigg|_{\lambda_n} \phi_1^2(\lambda_n, t) \Bigg]. \end{aligned} \tag{3.8}$$

Now we use (3.3) and (3.4) to get

$$\begin{aligned} \frac{\partial \phi_1}{\partial \lambda}\bigg|_{\lambda_n} &= \int_0^\Omega dt\, \phi_2(\lambda_n, t)\phi_1(\lambda_n, t), \\ \frac{\partial \phi_1'}{\partial \lambda}\bigg|_{\lambda_n} &= -\int_0^\Omega dt\, \phi_1^2(\lambda_n, t), \\ \frac{\partial \phi_2}{\partial \lambda}\bigg|_{\lambda_n} &= \int_0^\Omega dt\, \phi_2^2(\lambda_n, t), \\ \frac{\partial \phi_2'}{\partial \lambda}\bigg|_{\lambda_n} &= -\int_0^\Omega dt\, \phi_1(\lambda_n, t)\phi_2(\lambda_n, t), \end{aligned}$$

where we used again $\phi_1(\lambda_n, \Omega) = \phi_2'(\lambda_n, \Omega) = 1$ and $\phi_1'(\lambda_n, \Omega) = \phi_2(\lambda_n, \Omega) = 0$.

Thus, (3.8) becomes

$$\ddot{\Delta}(\lambda_n) = \left[\int_0^\Omega dt\, \phi_1(\lambda_n, t)\phi_2(\lambda_n, t)\right]^2 - \int_0^\Omega dt\, \phi_1^2(\lambda_n, t) \int_0^\Omega ds\, \phi_2^2(\lambda_n, s) \le 0,$$

where the last step follows by the Schwarz inequality. Since $\phi_1(\lambda_n, t)$ and $\phi_2(\lambda_n, t)$ are linearly independent, we get $\ddot{\Delta}(\lambda_n) < 0$.

(d) *At a zero μ_n of $\Delta(\lambda) + 1$,*

$$\dot{\Delta}(\mu_n) = 0 \quad \textit{if and only if} \quad \phi_2(\mu_n, \Omega) = \phi_1'(\mu_n, \Omega) = 0.$$

Also, if $\dot{\Delta}(\mu_n) = 0$, then $\ddot{\Delta}(\mu_n) > 0$.

We omit the proof here because the proof is quite similar to case (c) above.

(e) Using the above (a)–(d), we now investigate the behavior of the continuous function $\Delta(\lambda)$ as λ increases from $-\infty$ to ∞.

Since $\Delta(\lambda) > 1$ near $-\infty$ and since it becomes negative for some λ near $+\infty$, we see that there exists a $\lambda_0 \in \mathbb{R}$ such that $\Delta(\lambda_0) = 1$, and $\Delta(\lambda) > 1$ if $\lambda < \lambda_0$. Since $\Delta(\lambda)$ does not have its local maximum at λ_0, we obtain that $\dot{\Delta}(\lambda_0) \ne 0$, by (c). Moreover, $\dot{\Delta}(\lambda_0) < 0$. So as λ increases from λ_0, $-1 < \Delta(\lambda) < 1$ until $\Delta(\lambda) = -1$ at μ_0, where $\Delta(\lambda)$ is decreasing by (b). So in the interval $(-\infty, \lambda_0)$, $\Delta(\lambda) > 1$, and in (λ_0, μ_0), $\Delta(\lambda)$ is decreasing from 1 to -1.

If $\dot{\Delta}(\mu_0) = 0$, then $\Delta(\lambda)$ has its local minimum at μ_0 by (d), and $\Delta(\lambda)+1$ has double zeros, and hence $\mu_1 = \mu_0$. Also, $\Delta(\lambda) > -1$ immediately to the right of μ_1, and it increases until it reaches 1 at λ_1. If $\dot{\Delta}(\mu_0) \ne 0$ (and so $\dot{\Delta}(\mu_0) < 0$), $\Delta(\lambda) < -1$ immediately to the right of μ_0. Since by (a), $\Delta(\lambda)$ changes sign infinitely often near $+\infty$, as λ increases, $\Delta(\lambda) = -1$ again at some μ_1 with $\Delta(\lambda) < -1$ for $\mu_0 < \lambda < \mu_1$. Since $\Delta(\lambda)$ does not have its local minimum at μ_1, we see by (d) that $\Delta(\lambda) > -1$ immediately to the right of μ_1 until it reaches 1 at λ_1.

A similar argument can be applied to the cases where $\dot{\Delta}(\lambda_1) = 0$ and $\dot{\Delta}(\lambda_1) \ne 0$. Continuing this argument completes the proof. □

Definition 3.2. The set

$$S = \bigcup_{m \in \mathbb{N}_0} \left([\lambda_{2m},\, \mu_{2m}] \cup [\mu_{2m+1},\, \lambda_{2m+1}] \right) \tag{3.9}$$

is called the *conditional stability set* of (3.1) in the case where q is real-valued.

One can show that

$$S = \bigcup_{t \in [0,\pi]} \{\lambda_m(t) | m \in \mathbb{N}_0\} .$$

4 Some spectral theory

In this section, we will study a differential operator associated with equation (3.1). But first we give various definitions of subsets of the spectrum of a densely defined closed linear operator in a complex separable Hilbert space $\mathcal{H}$.

Definition 4.1. Let $A : \mathcal{D}(A) \to \mathcal{H}$, $\overline{\mathcal{D}(A)} = \mathcal{H}$ be a densely defined closed linear operator in a complex separable Hilbert space $\mathcal{H}$. Let $B(\mathcal{H})$ be the set of all bounded linear operators in $\mathcal{H}$.
(i) The *resolvent set* $\varrho(A)$ of A is defined by

$$\varrho(A) = \{z \in \mathbb{C} \,|\, (A - zI)|_{\mathcal{D}(A)} \text{ is injective and } (A - zI)^{-1} \in \mathcal{B}(\mathcal{H})\}.$$

Moreover, $\sigma(A) = \mathbb{C} \setminus \varrho(A)$ is called the *spectrum* of A.
(ii) The set

$$\sigma_p(A) = \{\lambda \in \mathbb{C} \,|\, \text{there is a } 0 \neq \psi \in \mathcal{D}(A),\, A\psi = \lambda\psi\}$$

is called the *point spectrum* of A.
(iii) The set

$$\sigma_c(A) = \big\{\lambda \in \mathbb{C} \,\big|\, (A - \lambda I) : \mathcal{D}(A) \to \mathcal{H} \text{ is injective and } \overline{Ran(A - \lambda I)} = \mathcal{H},\, Ran(A - \lambda I) \subsetneq \mathcal{H}\big\}$$

is called the *continuous spectrum* of A. The set

$$\sigma_r(A) = \sigma(A) \setminus (\sigma_p(A) \cup \sigma_c(A))$$

is called the *residual spectrum* of A.
(iv) The set

$$\sigma_{ap}(A) = \big\{\lambda \in \mathbb{C} \,\big|\, \text{there is}\, \{f_n\}_{n\in\mathbb{N}} \subset \mathcal{D}(A)\, \text{s.t.}\, \|f_n\| = 1,\, n \in \mathbb{N}, \\ \|(A - \lambda I) f_n\| \xrightarrow{n\to\infty} 0\big\}. \tag{4.1}$$

is called the *approximate point spectrum* of A.

Theorem 4.2. *Let $A : \mathcal{D}(A) \to \mathcal{H}$, $\overline{\mathcal{D}(A)} = \mathcal{H}$ be a densely defined closed linear operator in a complex separable Hilbert space $\mathcal{H}$. Then*
(i) $\varrho(A)$ is open, and $\sigma = \mathbb{C} \setminus \varrho(A)$ is closed in $\mathbb{C}$.
(ii) The following relations are valid:

$$\sigma_r(A) = \big\{\lambda \in \mathbb{C} \,\big|\, (A - \lambda I) : \mathcal{D}(A) \to \mathcal{H} \textit{ is injective}, \overline{Ran(A - \lambda I)} \subsetneq \mathcal{H}\big\},$$
$$\sigma(A) = \sigma_p(A) \cup \sigma_c(A) \cup \sigma_r(A),$$
$$\sigma_p(A) \cap \sigma_c(A) = \sigma_p(A) \cap \sigma_r(A) = \sigma_c(A) \cap \sigma_r(A) = \emptyset.$$

(iii) If A is normal (i.e., $A^*A = AA^*$), then $\sigma_r(A) = \emptyset$.
(iv) $\sigma_p(A) \cup \sigma_c(A) \subseteq \sigma_{ap}(A) \subseteq \sigma(A)$.
(v) $\sigma_r(A) \subseteq [\sigma_p(A^*)]^{cc} \subseteq \sigma_r(A) \cup \sigma_p(A)$.
(Here $E^{cc} = \{\overline{z} \in \mathbb{C} \,|\, z \in E\}$.)

Proof of (i). Write $R(z) = (A - zI)^{-1}$ for $z \in \varrho(A)$. Suppose that $z_0 \in \varrho(A)$ and $|z - z_0| < \frac{1}{\|R(z_0)\|}$. Then

$$\sum_{n=0}^{\infty} (z - z_0)^n R(z_0)^{n+1}$$

converges to a bounded operator. Moreover, one obtains

$$\begin{aligned}(A - zI)R(z_0)^{n+1} &= [A - z_0 I + (z_0 - z)I](A - z_0 I)^{-1} R(z_0)^n \\ &= R(z_0)^n - (z - z_0) R(z_0)^{n+1}.\end{aligned}$$

Thus,

$$
\begin{aligned}
&(A - zI) \sum_{n=0}^{\infty} (z - z_0)^n R(z_0)^{n+1} \\
&= \sum_{n=0}^{\infty} (z - z_0)^n (A - zI) R(z_0)^{n+1} \\
&= \sum_{n=0}^{\infty} (z - z_0)^n \left[R(z_0)^n - (z - z_0) R(z_0)^{n+1} \right] \\
&= \sum_{n=0}^{\infty} (z - z_0)^n R(z_0)^n - \sum_{n=0}^{\infty} (z - z_0)^{n+1} R(z_0)^{n+1} \\
&= I.
\end{aligned}
$$

Similarly, one can show that $\sum_{n=0}^{\infty}(z - z_0)^n R(z_0)^{n+1}(A - zI) = I$. Thus,

$$(A - zI)^{-1} = \sum_{n=0}^{\infty} (z - z_0)^n R(z_0)^{n+1},$$

and in particular, $z \in \varrho(A)$. Thus $\varrho(A) \subset \mathbb{C}$ is open, and hence $\sigma(A) = \mathbb{C} \setminus \varrho(A)$ is closed.

Proof of (iii). Suppose that A is normal. Then $Ker(A - zI) = Ker(A^* - \overline{z}I)$ since $((A - zI)f, (A - zI)f) = ((A^* - \overline{z}I)(A - zI)f, f) = ((A - zI)(A^* - \overline{z}I)f, f) = ((A^* - \overline{z}I)f, (A^* - \overline{z}I)f)$. Here we want to show that if $A - zI$ is injective, then $\overline{(A - zI)\mathcal{D}(A)} = \mathcal{H}$. But $\overline{(A - zI)\mathcal{D}(A)}^{\perp} = Ker(A^* - \overline{z}I) = Ker(A - zI) = \{0\}$. This proves (iii).

Proof of (iv). This is a consequence of the fact that $(A - zI)$ has a continuous inverse if and only if it is injective and its image is closed. So $(A - zI)$ does not have a continuous inverse if and only if either it is not injective or its image is not closed.

Proof of (v). Suppose that $z \in \sigma_r(A)$. Then $\overline{(A - zI)\mathcal{D}(A)} \subsetneqq \mathcal{H}$, and hence there exists $g_0(\neq 0) \in [(A - zI)\mathcal{D}(A)]^{\perp}$. So $((A - zI)f, g_0) = 0$ for all $f \in \mathcal{D}(A)$. Since $|(Af, g_0)| \leq |z|\|g_0\|\|f\|$ for all $f \in \mathcal{D}(A)$, we see that $g_0 \in \mathcal{D}(A^*)$, and $(f, (A^* - \overline{z}I)g_0) = 0$ for all $f \in \mathcal{D}(A)$. Since $\overline{\mathcal{D}(A)} = \mathcal{H}$, we have $(A^* - \overline{z}I)g_0 = 0$, and hence $\overline{z} \in \sigma_p(A^*)$.

Next suppose that $\overline{z} \in \sigma_p(A^*)$. Then there exists $g_0(\neq 0) \in \mathcal{D}(A^*)$ such that $A^* g_0 = \overline{z} g_0$. So for all $f \in \mathcal{D}(A)$,

$$0 = (f, (A^* - \overline{z}I)g_0) = ((A - zI)f, g_0).$$

So $g_0 \notin \overline{(A-zI)\mathcal{D}(A)}$, and $z \in \sigma(A) \setminus \sigma_c(A) = \sigma_p(A) \cup \sigma_r(A)$. ☐

5 The conditional stability set and the spectrum of periodic Schrödinger operators

In this section, we prove the main theorem regarding the connection between the Floquet theory and the spectrum of the associated Schrödinger differential operator L on $H^{2,2}(\mathbb{R})$ defined by

$$(Lf)(x) = \left[-\frac{d^2}{dx^2} + q(x)\right] f(x), \quad x \in \mathbb{R}, \quad f \in dom(L) = H^{2,2}(\mathbb{R}), \quad (5.1)$$

where $q \in C(\mathbb{R})$ is periodic with period Ω (and possibly complex-valued).

Theorem 5.1. *The spectrum of L is purely continuous. That is, $\sigma(L) = \sigma_c(L)$ and $\sigma_p(L) = \sigma_r(L) = \emptyset$.*

Proof. We first show that $\sigma_p(L) = \emptyset$. Suppose that L has an eigenvalue λ with the corresponding eigenfunction $\psi \in L^2(\mathbb{R})$. Then by Theorem 1.9, ψ is unbounded (and then one can easily show that it is not in $L^2(\mathbb{R})$), unless ψ is a multiple of a Floquet solution with $|\rho| = 1$. But even in the case that ψ is a Floquet solution with $|\rho| = 1$, $\psi \notin L^2(\mathbb{R})$. So L does not have any eigenvalues.

Next we show $\sigma_r(L) = \emptyset$. In doing so, we will use Theorem 4.2 (iv) (i. e., $\sigma_r(L) \subseteq \sigma_p(L^*)^{cc}$), where

$$(L^*f)(x) = -f''(x) + \overline{q(x)}f(x), \; f \in dom(L^*) = H^{2,2}(\mathbb{R}).$$

The above argument showing $\sigma_p(L) = \emptyset$ can be applied to show $\sigma_p(L^*) = \emptyset$. Thus, $\sigma_r(L) = \emptyset$. ☐

In the general case where q is complex-valued, the conditional stability set S is defined as follows,

$$S = \{z \in \mathbb{C} \,|\, \text{there exists a non-trivial distributional}\, \psi \in L^\infty(\mathbb{R}) \; \text{of}\, L\psi = z\psi\}.$$

It is not difficult to see that

$$S = \{z \in \mathbb{C} \,|\, \Delta(z) \in [-1, 1]\}.$$

The following is the main theorem of this section.

Theorem 5.2. $\sigma(L) = S$.

Proof. We first show that $S \subseteq \sigma_{ap}(L) = \sigma(L)$. Suppose $\gamma \in S$. Then there exists a non-trivial solution $\psi(\gamma, \cdot)$ of (3.1) such that

$$\psi(\gamma, x+\Omega) = \rho\psi(\gamma, x), \quad \text{where} \quad |\rho| = 1. \tag{5.2}$$

In order to define a sequence $\{f_n\}_{n\in\mathbb{N}}$ as in the definition (4.1) of $\sigma_{ap}(L)$, we choose $g \in C^2([0,\Omega])$ such that

$$\begin{aligned} &g(0) = 0,\ g(\Omega) = 1, \\ &g'(0) = g''(0) = g'(\Omega) = g''(\Omega) = 0, \\ &0 \le g(x) \le 1,\ x \in [0,\Omega]. \end{aligned}$$

Define

$$f_n(\gamma, x) = c_n(\gamma)\psi(\gamma, x)h_n(x), \quad x \in \mathbb{R},$$

where

$$h_n(x) = \begin{cases} 1 & \text{if } |x| \le (n-1)\Omega, \\ g(n\Omega - |x|) & \text{if } (n-1)\Omega < |x| \le n\Omega, \\ 0 & \text{if } |x| > n\Omega, \end{cases}$$

and the normalization constant $c_n(\gamma)$ is chosen to guarantee $\|f_n\|_{L^2(\mathbb{R})} = 1$. From (5.2) and the definition of $h_n(x)$, we see that

$$c_n(\gamma) = \left(2n\int_0^\Omega dx\,|\psi(\gamma,x)|^2 + O(1)\right)^{-\frac{1}{2}} \to 0 \quad \text{as} \quad n \to \infty.$$

Next, using $L\psi = \gamma\psi$,

$$\begin{aligned} &(L-\gamma I)f_n(x) \\ &\quad = -c_n(\gamma)\left[\psi''(\gamma,x)h_n(x) + 2\psi'(\gamma,x)h_n'(x) + \psi(\gamma,x)h_n''(x)\right] \\ &\qquad + c_n(\gamma)[q(x)-\gamma]\psi(\gamma,x)h_n(x) \\ &\quad = c_n h_n(x)(L-\gamma I)\psi(\gamma,x) - c_n(\gamma)\left[2\psi'(\gamma,x)h_n'(x) + \psi(\gamma,x)h_n''(x)\right] \\ &\quad = -c_n(\gamma)\left[2\psi'(\gamma,x)h_n'(x) + \psi(\gamma,x)h_n''(x)\right]. \end{aligned}$$

So we have

$$\|(L-\gamma I)f_n\| \le c_n(\gamma)\left[2\|\psi'(\gamma,\cdot)h_n'(\cdot)\| + \|\psi(\gamma,\cdot)h_n''(\cdot)\|\right].$$

From (5.2) and the definition of h_n one infers that

$$\begin{aligned}
\|\psi'(\gamma,\cdot)h_n'(\cdot)\|^2 &= \int_{(n-1)\Omega\le|x|\le n\Omega} dx\ |\psi'(\gamma,x)h_n'(x)|^2 \\
&= \int_0^\Omega dx\ \left[|\psi'(\gamma,-x)|^2+|\psi'(\gamma,x)|^2\right]|g'(x)|^2 \\
&\underset{n\to\infty}{=} O(1).
\end{aligned}$$

Similarly, one can show that

$$\|\psi(\gamma,\cdot)h_n''(\cdot)\| \underset{n\to\infty}{=} O(1).$$

Thus, since $c_n(\gamma)\to 0$ as $n\to\infty$, we have

$$\|(L-\gamma I)f_n\|\to 0 \quad \text{as} \quad n\to\infty.$$

Since $\|f_n\|=1$ for all $n\in\mathbb{N}$, we see that $\gamma\in\sigma_{ap}(L)$. So $S\subseteq\sigma_{ap}(L)=\sigma(L)$.

Next, in order to show $\sigma(L)\subseteq S$, we suppose that $z\in\mathbb{C}\setminus S$. Then $\Delta(z)\in\mathbb{C}\setminus[-1,\,1]$.

First, we note that since $\rho_+(z)\neq\rho_-(z)$ we have by Theorem 1.2 (i) that

$$\psi_+(z,x)=e^{-m(z)x}p_+(z,x),\quad \psi_-(z,x)=e^{m(z)x}p_-(z,x),$$

where $\operatorname{Re}(m(z))>0$, and $p_\pm(z,\cdot)$ are periodic with period Ω. Hence

$$\begin{aligned}
\psi_\pm(z,\cdot) &\in L^2((R,\pm\infty)),\quad R\in\mathbb{R}, \\
\psi_\pm(z,x+\Omega) &= e^{\mp m(z)\Omega}\psi_\pm(z,x),\quad |e^{\mp m(z)\Omega}|=|\rho_\pm(z)|\neq 1.
\end{aligned}$$

Define the Green's function $G(z,x,x')$ by

$$G(z,x,x')=W(\psi_+,\,\psi_-)^{-1}\begin{cases}\psi_+(z,x)\psi_-(z,x') & \text{if } x'\le x,\\ \psi_+(z,x')\psi_-(z,x) & \text{if } x'\ge x.\end{cases}$$

Then we will prove below that

$$\left(R(z)f\right)(x)=\int_{\mathbb{R}}dx'\,G(z,x,x')f(x'),\quad f\in L^2(\mathbb{R})$$

is a bounded operator in $L^2(\mathbb{R})$.

We note that

$$|(R(z)f)(x)| \leq \frac{K^2}{|W(\psi_+, \psi_-)|}\left(G_1(x) + G_2(x)\right),$$

where K is an upper bound of $|p_\pm(z,\, x)|$, $x \in \mathbb{R}$, and

$$\begin{aligned} G_1(x) &= e^{-m_0 x}\int_{-\infty}^{x} dx'\, e^{m_0 x'}|f(x')|, \\ G_2(x) &= e^{m_0 x}\int_{x}^{\infty} dx'\, e^{-m_0 x'}|f(x')|, \quad f \in L^2(\mathbb{R}), \end{aligned}$$

where $m_0 = \mathrm{Re}\,(m(z)) > 0$.

See [1, page 84] for the proof of

$$\|G_1\| \leq \frac{1}{m_0}\|f\|. \tag{5.3}$$

Here we will prove that

$$\|G_2\| \leq \frac{1}{m_0}\|f\|.$$

We will closely follow the proof of (5.3) in [1, page 84]. For any $X < Y$, an integration by parts yields

$$\begin{aligned} \int_X^Y dx\, G_2^2(x) &= \int_X^Y dx\, e^{2m_0 x}\left(\int_x^\infty dx'\, e^{-m_0 x'}|f(x')|\right)^2 \\ &= \left[\frac{e^{2m_0 x}}{2m_0}\left(\int_x^\infty dx'\, e^{-m_0 x'}|f(x')|\right)^2\right]_X^Y \\ &\quad + \frac{1}{m_0}\int_X^Y dx\, e^{m_0 x}|f(x)|\left(\int_x^\infty dx'\, e^{-m_0 x'}|f(x')|\right) \\ &= \frac{1}{2m_0}\left[G_2^2(Y) - G_2^2(X)\right] + \frac{1}{m_0}\int_X^Y dx\, G_2(x)|f(x)| \\ &\leq \frac{1}{2m_0}G_2^2(Y) + \frac{1}{m_0}\left[\int_X^Y dx\, G_2^2(x)\int_X^Y dx\, |f(x)|^2\right]^{\frac{1}{2}} \\ &\leq \frac{1}{2m_0}G_2^2(Y) + \frac{1}{m_0}\left[\int_X^Y dx\, G_2^2(x)\right]^{\frac{1}{2}}\|f\|. \end{aligned} \tag{5.4}$$

Also,

$$\begin{aligned} G_2(Y) &= e^{m_0 Y} \int_Y^\infty dx'\, e^{-m_0 x'} |f(x')| \\ &\leq e^{m_0 Y} \left[\int_Y^\infty dx\, e^{-2m_0 x} \int_Y^\infty dx\, |f(x)|^2 \right]^{\frac{1}{2}} \\ &\leq e^{m_0 Y} \left[\frac{1}{2m_0} e^{-2m_0 Y} \int_Y^\infty dx\, |f(x)|^2 \right]^{\frac{1}{2}}. \end{aligned}$$

Thus, as $Y \to \infty$, $G_2(Y) \to 0$, and hence by letting $X \to -\infty$ and $Y \to \infty$ in (5.4), we see that $0 < \|G_2\| < \infty$ and so

$$\|G_2\| \leq \frac{1}{m_0} \|f\|.$$

Next, we show that

$$(L - zI)R(z)f = f \text{ for all } f \in L^2(\mathbb{R}), \tag{5.5}$$
$$R(z)(L - zI)f = f \text{ for all } f \in L^2(\mathbb{R}) \cap H^{2,2}(\mathbb{R}). \tag{5.6}$$

First, let $f \in L^2(\mathbb{R})$. Then,

$$\begin{aligned} & - W(\psi_+, \psi_-) \frac{d^2}{dx^2} [R(z)f](x) \\ & = -\frac{d^2}{dx^2} \left[\int_{-\infty}^x dx'\, \psi_+(z,x)\psi_-(z,x')f(x') + \int_x^\infty dx'\, \psi_+(z,x')\psi_-(z,x) \right] \\ & = -\frac{d}{dx} \left[\int_{-\infty}^x dx'\, \psi_+'(z,x)\psi_-(z,x')f(x') + \int_x^\infty dx'\, \psi_+(z,x')\psi_-'(z,x)f(x') \right] \\ & = W(\psi_+, \psi_-)f(x) \\ & - \left[\int_{-\infty}^x dx'\, \psi_+''(z,x)\psi_-(z,x')f(x') + \int_x^\infty dx'\, \psi_+(z,x')\psi_-''(z,x)f(x') \right] \\ & = W(\psi_+, \psi_-)f(x) + (z - q(x)) \left[\int_{-\infty}^x dx'\, \psi_+(z,x)\psi_-(z,x')f(x') \right. \\ & \left. + \int_x^\infty dx'\, \psi_+(z,x')\psi_-(z,x)f(x') \right] \\ & = W(\psi_+, \psi_-)f(x) + W(\psi_+, \psi_-)(z - q(x)) \int_{\mathbb{R}} dx'\, G(z,x,x')f(x'). \end{aligned}$$

This proves (5.5). Similarly, one can show (5.6). Thus, $(L - zI)^{-1}$ exists and is bounded on $L^2(\mathbb{R})$. Hence, $z \in \varrho(L) = \mathbb{C} \setminus \sigma(L)$ and this proves $\sigma(L) \subseteq S$. □

Before we introduce our next theorem, we give some definitions first.

Definition 5.3. A set $\sigma \subset \mathbb{C}$ is an *arc* if there exists $\gamma \in C([a, b])$, $a, b \in \mathbb{R}$, $a \leq b$ such that $\sigma = \{\gamma(t) \mid t \in [a, b]\}$. Then we call γ a *parameterization* of the arc σ. The arc σ is called *simple* if it has a one-to-one parameterization. And the arc σ is called an *analytic arc* if it has a parameterization $\gamma \in C^\infty([a, b])$ such that $t \mapsto \gamma(t)$ is analytic on $[a, b]$.

Theorem 5.4. *The conditional stability set S consists of countably infinitely many simple analytic arcs in $\mathbb{C}$.*

Moreover,

$$S = \sigma(L) \subset \{z \in \mathbb{C} \mid M_1 \leq \mathrm{Im}\,(z) \leq M_2,\, \mathrm{Re}\,(z) \geq M_3\},$$

where

$$M_1 = \inf_{x \in [0,\, \Omega]} [\mathrm{Im}\,(q(x))], \quad M_2 = \sup_{x \in [0,\, \Omega]} [\mathrm{Im}\,(q(x))], \quad M_3 = \inf_{x \in [0,\, \Omega]} [\mathrm{Re}\,(q(x))].$$

Next, we provide, without proofs, some additional results of Tkachenko [9, 10].

Theorem 5.5 ([9, Theorem 1]). *For a function Δ to be a Floquet discriminant of the operator L in (5.1) with $q \in L^2([0, \Omega])$, it is necessary and sufficient that it be an entire function of exponential type Ω of the form*

$$\Delta(z) = \cos(\Omega\sqrt{z}) + \frac{Q}{\sqrt{z}}\sin(\Omega\sqrt{z}) - \frac{Q^2}{2z}\cos(\Omega\sqrt{z}) + \frac{f(\sqrt{z})}{z} \quad \textit{for some} \quad Q \in \mathbb{C},$$

where f is an even entire function of exponential type not exceeding Ω satisfying the conditions

$$\int_{-\infty}^{+\infty} d\lambda\, |f(\lambda)|^2 < +\infty, \quad \sum_{n=-\infty}^{+\infty} |f(n)| < +\infty.$$

Theorem 5.6 ([9, Theorem 2]). *For any operator L in (5.1) with a potential $q \in L^2_{loc}(\mathbb{R})$ periodic of period Ω and for any $\epsilon > 0$ there exists a potential $q_\epsilon \in L^2_{loc}(\mathbb{R})$ periodic of period Ω such that $\|q - q_\epsilon\|_{L^2([0,\Omega])} \leq \epsilon$ and the spectrum of the corresponding periodic Schrödinger operator L_ϵ in $L^2(\mathbb{R})$ with potential q_ϵ is the union of nonintersecting analytic arcs. Each spectral arc is one-to-one mapped on the interval $[-1, 1]$ by the Floquet discriminant Δ_ϵ of L_ϵ.*

Also, see [10] for some results regarding one-to-one correspondence between classes of operators L with $q \in L^2([0, \Omega])$ and certain Riemann surfaces.

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ON HALF-LINE SPECTRA FOR A CLASS OF NON-SELF-ADJOINT HILL OPERATORS

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ABSTRACT. In 1980, Gasymov showed that non-self-adjoint Hill operators with complex-valued periodic potentials of the type

$$V(x) = \sum_{k=1}^{\infty} a_k e^{ikx}, \text{ with } \sum_{k=1}^{\infty} |a_k| < \infty,$$

have spectra $[0, \infty)$. In this note, we provide an alternative and elementary proof of this result.

1. INTRODUCTION

We study the Schrödinger equation

$$-\psi''(z,x) + V(x)\psi(z,x) = z\psi(z,x), \quad x \in \mathbb{R}, \tag{1}$$

where $z \in \mathbb{C}$ and $V \in L^\infty(\mathbb{R})$ is a continuous complex-valued periodic function of period 2π, that is, $V(x+2\pi) = V(x)$ for all $x \in \mathbb{R}$. The *Hill operator* H in $L^2(\mathbb{R})$ associated with (1) is defined by

$$(Hf)(x) = -f''(x) + V(x)f(x), \quad f \in W^{2,2}(\mathbb{R}),$$

where $W^{2,2}(\mathbb{R})$ denotes the usual Sobolev space. Then H is a densely defined closed operator in $L^2(\mathbb{R})$ (see, e.g., [2, Chap. 5]).

The spectrum of H is purely continuous and a union of countablely many analytic arcs in the complex plane [9]. In general it is not easy to explicitly determine the spectrum of H with specific potentials. However, in 1980, Gasymov [3] proved the following remarkable result:

Theorem 1 ([3])**.** *Let* $V(x) = \sum_{k=1}^{\infty} a_k e^{ikx}$ *with* $\{a_k\}_{k\in\mathbb{N}} \in \ell^1(\mathbb{N})$. *Then the spectrum of the associated Hill operator* H *is purely continuous and equals* $[0, \infty)$.

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In this note we provide an alternative and elementary proof of this result. Gasymov [3] proved the existence of a solution ψ of (1) of the form

$$\psi(z,x) = e^{i\sqrt{z}x}\left(1 + \sum_{j=1}^{\infty} \frac{1}{j+2\sqrt{z}} \sum_{k=j}^{\infty} \nu_{j,k} e^{ikx}\right),$$

where the series

$$\sum_{j=1}^{\infty} \frac{1}{j} \sum_{k=j+1}^{\infty} k(k-j)|\nu_{j,k}| \quad \text{and} \quad \sum_{j=1}^{\infty} j|\nu_{j,k}|$$

converge, and used this fact to show that the spectrum of H equals $[0,\infty)$. He also discussed the corresponding inverse spectral problem. This inverse spectral problem was subsequently considered by Pastur and Tkachenko [8] for 2π-periodic potentials in $L^2_{\rm loc}(\mathbb{R})$ of the form $\sum_{k=1}^{\infty} a_k e^{ikx}$.

In this paper, we will provide an elementary proof of the following result.

Theorem 2. *Let* $V(x) = \sum_{k=1}^{\infty} a_k e^{ikx}$ *with* $\{a_k\}_{k\in\mathbb{N}} \in \ell^1(\mathbb{N})$. *Then*

$$\Delta(V;z) = \cos(2\pi\sqrt{z}),$$

where $\Delta(V;z)$ *denotes the Floquet discriminant associated with* (1) *(cf. equation* (2)*).*

Corollary 3. *Theorem 2 implies that the spectrum of* H *equals* $[0,\infty)$*; it also implies Theorem 1.*

Proof. In general, one-dimensional Schrödinger operators with periodic potentials have purely continuous spectra (cf. [9]). Since $-1 \le \cos(2\pi\sqrt{z}) \le 1$ if and only if $z \in [0,\infty)$, one concludes that the spectrum of H equals $[0,\infty)$ and that Theorem 1 holds (see Lemma 5 below). □

Remark. We note that the potentials V in Theorem 1 are nonreal and hence H is non-self-adjoint in $L^2(\mathbb{R})$ except when $V=0$. It is known that $V=0$ is the only *real* periodic potential for which the spectrum of H equals $[0,\infty)$ (see [1]). However, if we allow the potential V to be complex-valued, Theorem 1 provides a family of complex-valued potentials such that spectra of the associated Hill operators equal $[0, \infty)$. From the point of view of inverse spectral theory this yields an interesting and significant nonuniqueness property of non-self-adjoint Hill operators in stark contrast to self-adjoint ones. For an explanation of this nonuniqueness property of non-self-adjoint Hill operators in terms of associated Dirichlet eigenvalues, we refer to [4, p. 113].

As a final remark we mention some related work of Guillemin and Uribe [5]. Consider the differential equation (1) on the interval $[0, 2\pi]$ with the periodic boundary conditions. It is shown in [5] that all potentials in Theorem 1 generate the same spectrum $\{n^2 : n = 0, 1, 2, \dots\}$, that is, $\Delta(V; n^2) = 1$ for all $n = 0, 1, 2, \dots$.

2. Some known facts

In this section we recall some definitions and known results regarding (1).

For each $z \in \mathbb{C}$, there exists a fundamental system of solutions $c(V; z, x)$, $s(V; z, x)$ of (1) such that

$$c(V; z, 0) = 1, \qquad c'(V; z, 0) = 0,$$
$$s(V; z, 0) = 0, \qquad s'(V; z, 0) = 1,$$

where we use $'$ for $\frac{\partial}{\partial x}$ throughout this note. The *Floquet discriminant* $\Delta(V; z)$ of (1) is then defined by

$$\Delta(V; z) = \frac{1}{2}\left(c(V; z, 2\pi) + s'(V; z, 2\pi)\right). \tag{2}$$

The Floquet discriminant $\Delta(V; z)$ is an entire function of order $\frac{1}{2}$ with respect to z (see [10, Chap. 21]).

Lemma 4. *For every $z \in \mathbb{C}$ there exists a solution $\psi(z, \cdot) \neq 0$ of (1) and a number $\rho(z) \in \mathbb{C} \setminus \{0\}$ such that $\psi(z, x + 2\pi) = \rho(z)\psi(z, x)$ for all $x \in \mathbb{R}$. Moreover,*

$$\Delta(V; z) = \frac{1}{2}\left(\rho(z) + \frac{1}{\rho(z)}\right). \tag{3}$$

In particular, if $V = 0$, then $\Delta(0; z) = \cos(2\pi\sqrt{z})$.

For obvious reasons one calls $\rho(z)$ the *Floquet multiplier* of equation (1).

Lemma 5. *Let H be the Hill operator associated with (1) and $z \in \mathbb{C}$. Then the following four assertions are equivalent:*

(i) *z lies in the spectrum of H.*
(ii) *$\Delta(V; z)$ is real and $|\Delta(V; z)| \leq 1$.*
(iii) *$\rho(z) = e^{i\alpha}$ for some $\alpha \in \mathbb{R}$.*
(iv) *Equation (1) has a non-trivial bounded solution $\psi(z, \cdot)$ on $\mathbb{R}$.*

For proofs of Lemmas 4 and 5, see, for instance, [2, Chs. 1, 2, 5], [7], [9] (we note that V is permitted to be locally integrable on $\mathbb{R}$).

3. Proof of Theorem 2

In this section we prove Theorem 2. In doing so, we will use the standard identity theorem in complex analysis which asserts that two analytic functions coinciding on an infinite set with an accumulation point in their common domain of analyticity, in fact coincide throughout that domain. Since both $\Delta(V; z)$ and $\cos(2\pi\sqrt{z})$ are entire functions, to prove that $\Delta(V; z) = \cos(2\pi\sqrt{z})$, it thus suffices to show that $\Delta(V; 1/n^2) = \cos(2\pi/n)$ for all integers $n \geq 3$.

Let $n \in \mathbb{N}$, $n \geq 3$ be fixed and let $\psi \neq 0$ be the solution of (1) such that $\psi(z, x+2\pi) = \rho(z)\psi(z, x)$, $x \in \mathbb{R}$ for some $\rho(z) \in \mathbb{C}$. The existence of such ψ and ρ is guaranteed by Lemma 4. We set $\phi(z, x) = \psi(z, nx)$. Then

$$\phi(z, x + 2\pi) = \rho^n(z)\phi(z, x), \tag{4}$$

and

$$-\phi''(z, x) + q_n(x)\phi(z, x) = n^2 z\phi(z, x), \tag{5}$$

where

$$q_n(x) = n^2 V(nx) = n^2 \sum_{k=1}^{\infty} a_k e^{iknx}, \tag{6}$$

with period 2π. Moreover, by (3) and (4),

$$\Delta(q_n; w) = \frac{1}{2}\left(\rho^n(z) + \frac{1}{\rho^n(z)}\right), \quad \text{where } w = n^2 z. \tag{7}$$

We will show below that

$$\Delta(q_n; 1) = 1 \text{ for every positive integer } n \geq 3. \tag{8}$$

First, if $w = 1$ (i.e., if $z = \frac{1}{n^2}$), then the fundamental system of solutions $c(q_n; 1, x)$ and $s(q_n; 1, x)$ of (5) satisfies

$$\begin{aligned} c(q_n; 1, x) &= \cos(x) + \int_0^x \sin(x-t) q_n(t) c(q_n; 1, t)\, dt, \\ s(q_n; 1, x) &= \sin(x) + \int_0^x \sin(x-t) q_n(t) s(q_n; 1, t)\, dt. \end{aligned} \tag{9}$$

Moreover, we have

$$s'(q_n; 1, x) = \cos(x) + \int_0^x \cos(x-t) q_n(t) s(q_n; 1, t)\, dt. \tag{10}$$

We use the Picard iterative method of solving the above integral equations. Define sequences $\{u_j(x)\}_{j\geq 0}$ and $\{v_j(x)\}_{j\geq 0}$ of functions as follows.

$$u_0(x) = \cos(x), \quad u_j(x) = \int_0^x \sin(x-t) q_n(t) u_{j-1}(t)\, dt, \tag{11}$$

$$v_0(x) = \sin(x), \quad v_j(x) = \int_0^x \sin(x-t) q_n(t) v_{j-1}(t)\, dt, \quad j \geq 1. \tag{12}$$

Then one verifies in a standard manner that

$$c(q_n; 1, x) = \sum_{j=0}^{\infty} u_j(x), \quad s(q_n; 1, x) = \sum_{j=0}^{\infty} v_j(x), \tag{13}$$

where the sums converge uniformly over $[0, 2\pi]$. Since

$$\Delta(q_n; 1) = \frac{1}{2}\left(c(q_n; 1, 2\pi) + s'(q_n; 1, 2\pi)\right),$$

to prove that $\Delta(q_n; 1) = 1$, it suffices to show that the integrals in (9) and (10) vanish at $x = 2\pi$.

Next, we will rewrite (11) as

$$u_0(x) = \frac{1}{2}(e^{ix} + e^{-ix}),$$
$$u_j(x) = \frac{e^{ix}}{2i}\int_0^x e^{-it} q_n(t)u_{j-1}(t)\,dt - \frac{e^{-ix}}{2i}\int_0^x e^{it} q_n(t)u_{j-1}(t)\,dt, \quad j \ge 1. \tag{14}$$

Using this and (6), one shows by induction on j that u_j, $j \ge 0$, is of the form

$$u_j(x) = \sum_{\ell=-1}^{\infty} b_{j,\ell}\, e^{i\ell x} \text{ for some } b_{j,\ell} \in \mathbb{C}, \tag{15}$$

the sum converging uniformly for $x \in \mathbb{R}$. This follows from $n \ge 3$ because the smallest exponent of e^{it} that $q_n u_{j-1}$ can have in (14) equals 2. (The first three terms in (15) are due to the antiderivatives of $e^{\pm it} q_n(t)u_{j-1}(t)$, evaluated at $t = 0$.) Next we will use (13) and (15) to show that

$$\int_0^{2\pi} \sin(2\pi - t) q_n(t) c(q_n; 1, t)\,dt = 0. \tag{16}$$

We begin with

$$\begin{aligned}
&\int_0^{2\pi} \sin(2\pi - t) q_n(t) c(q_n; 1, t)\,dt \\
= &-\frac{1}{2i}\int_0^{2\pi} (e^{it} - e^{-it}) q_n(t) c(q_n; 1, t)\,dt \\
= &-\frac{1}{2i}\int_0^{2\pi} (e^{it} - e^{-it}) \left(\sum_{k=1}^{\infty} a_k e^{iknt}\right)\left(\sum_{j=0}^{\infty} u_j(t)\right) dt \\
= &-\frac{1}{2i}\sum_{k=1}^{\infty}\sum_{j=0}^{\infty} a_k \int_0^{2\pi} (e^{i(kn+1)t} - e^{i(kn-1)t}) u_j(t)\,dt,
\end{aligned} \tag{17}$$

where the change of the order of integration and summations is permitted due to the uniform convergence of the sums involved. The function $(e^{i(kn+1)t} - e^{i(kn-1)t})u_j(t)$ is a power series in e^{it} with no constant term (cf. (15)), and hence its antiderivative is a periodic function of period 2π. Thus, every integral in (17) vanishes, and hence (16) holds. So from (9) we conclude that $c(q_n; 1, 2\pi) = 1$.

Similarly, one can show by induction that v_j for each $j \geq 0$ is of the form (15). Hence, from (10), one concludes that $s'(q_n; 1, 2\pi) = 1$ in close analogy to the proof of $c(q_n; 1, 2\pi) = 1$. Thus, (8) holds for each $n \geq 3$.

So by (7),

$$\Delta(q_n; 1) = \frac{1}{2}\left(\rho^n(1/n^2) + \frac{1}{\rho^n(1/n^2)}\right) = 1 \text{ for every } n \geq 3.$$

This implies that $\rho^n(1/n^2) = 1$. So $\rho(1/n^2) \in \{\xi \in \mathbb{C} : \xi^n = 1\}$. Thus, $\Delta(V; 1/n^2) \in \{\cos(2k\pi/n) : k \in \mathbb{Z}\}$. Next, we will show that $\Delta(V; 1/n^2) = \cos(2\pi/n)$.

We consider a family of potentials $q_\varepsilon(x) = \varepsilon V(x)$ for $0 \leq \varepsilon \leq 1$. For each $0 \leq \varepsilon \leq 1$, we apply the above argument to get that $\rho(\varepsilon, 1/n^2) \in \{\xi \in \mathbb{C} : \xi^n = 1\}$, where we use the notation $\rho(\varepsilon, 1/n^2)$ to indicate the possible ε-dependence of $\rho(1/n^2)$. Next, by the integral equations (9)–(12) with $q_\varepsilon = \varepsilon V$ instead of q_n, one sees that $\Delta(\varepsilon V; 1/n^2)$ can be written as a power series in ε that converges uniformly for $0 \leq \varepsilon \leq 1$. Thus, the function $\varepsilon \mapsto \Delta(\varepsilon V; 1/n^2) \in \{\cos(2k\pi/n) : k \in \mathbb{Z}\}$ is continuous for $0 \leq \varepsilon \leq 1$ (in fact, it is entire w.r.t. ε). Since $\{\cos(2k\pi/n) : k \in \mathbb{Z}\}$ is discrete, and since $\Delta(\varepsilon V; 1/n^2) = \cos(2\pi/n)$ for $\varepsilon = 0$, we conclude that

$$\Delta(\varepsilon V; 1/n^2) = \Delta(0; 1/n^2) = \cos(2\pi/n) \text{ for all } 0 \leq \varepsilon \leq 1.$$

In particular, $\Delta(V; 1/n^2) = \cos(2\pi/n)$ for every positive integer $n \geq 3$. Since $\Delta(V; z)$ and $\cos(2\pi\sqrt{z})$ are both entire and since they coincide at $z = 1/n^2$, $n \geq 3$, we conclude that

$$\Delta(V; z) = \cos(2\pi\sqrt{z}) \text{ for all } z \in \mathbb{C}$$

by the identity theorem for analytic functions alluded to at the beginning of this section. This completes proof of Theorem 2 and hence that of Theorem 1 by Corollary 3.

Remarks. (i) Adding a constant term to the potential V yields a translation of the spectrum. (ii) If the potential V is a power series in e^{-ix} with no constant term, then the spectrum of H is still $[0, \infty)$, by complex conjugation. (iii) If V lies in the $L^2([0,\, 2\pi])$-span of $\{e^{ikx}\}_{k\in\mathbb{N}}$, then by continuity of $V \mapsto \Delta(V;z)$ one concludes $\Delta(V;z) = \cos(2\pi\sqrt{z})$ and hence the spectrum of H equals $[0,\, \infty)$ (see [8]).

(iv) Potentials V that include negative and positive integer powers of e^{ix} are not included in our note. Consider, for example, equation (1) with $V(x) = 2\cos(x)$, the so-called Mathieu equation. The spectrum of H in this case is known to be a disjoint union of infinitely many closed intervals on the real line [6] (also, see [2], [7]). In particular, the spectrum of H is not $[0,\, \infty)$. In such a case the antiderivatives of $(e^{i(kn+1)t} - e^{i(kn-1)t})u_j(t)$ in (17) need not be periodic and our proof breaks down.

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ON THE SPECTRUM OF QUASI-PERIODIC ALGEBRO-GEOMETRIC KDV POTENTIALS

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Dedicated with great pleasure to Vladimir A. Marchenko on the occasion of his 80th birthday.

Abstract. We characterize the spectrum of one-dimensional Schrödinger operators $H = -d^2/dx^2 + V$ in $L^2(\mathbb{R}; dx)$ with quasi-periodic complex-valued algebro-geometric potentials V (i.e., potentials V which satisfy one (and hence infinitely many) equation(s) of the stationary Korteweg–deVries (KdV) hierarchy). The spectrum of H coincides with the conditional stability set of H and can explicitly be described in terms of the mean value of the inverse of the diagonal Green's function of H.

As a result, the spectrum of H consists of finitely many simple analytic arcs and one semi-infinite simple analytic arc in the complex plane. Crossings as well as confluences of spectral arcs are possible and discussed as well. Our results extend to the $L^p(\mathbb{R}; dx)$-setting for $p \in [1, \infty)$.

1. Introduction

It is well-known since the work of Novikov [44], Its and Matveev [31], Dubrovin, Matveev, and Novikov [16] (see also [7, Sects. 3.4, 3.5], [24, p. 111–112, App. J], [45, Sects. II.6–II.10] and the references therein) that the self-adjoint Schrödinger operator

$$H = -\frac{d^2}{dx^2} + V, \quad \operatorname{dom}(H) = H^{2,2}(\mathbb{R}) \tag{1.1}$$

in $L^2(\mathbb{R}; dx)$ with a real-valued periodic, or more generally, *quasi-periodic* and *real-valued* potential V, that satisfies one (and hence infinitely many) equation(s) of the stationary Korteweg–deVries (KdV) equations, leads to a finite-gap, or perhaps more appropriately, to a

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finite-band spectrum $\sigma(H)$ of the form

$$\sigma(H) = \bigcup_{m=0}^{n-1} [E_{2m}, E_{2m+1}] \cup [E_{2n}, \infty). \tag{1.2}$$

It is also well-known, due to work of Serov [50] and Rofe-Beketov [48] in 1960 and 1963, respectively (see also [53]), that if V is *periodic* and *complex-valued* then the spectrum of the non-self-adjoint Schrödinger operator H defined as in (1.1) consists either of infinitely many simple analytic arcs, or else, of a finite number of simple analytic arcs and one semi-infinite simple analytic arc tending to infinity. It seems plausible that the latter case is again connected with (complex-valued) stationary solutions of equations of the KdV hierarchy, but to the best of our knowledge, this has not been studied in the literature. In particular, the next scenario in line, the determination of the spectrum of H in the case of *quasi-periodic* and *complex-valued* solutions of the stationary KdV equation apparently has never been clarified. The latter problem is open since the mid-seventies and it is the purpose of this paper to provide a comprehensive solution of it.

To describe our results, a bit of preparation is needed. Let

$$G(z,x,x') = (H-z)^{-1}(x,x'), \quad z \in \mathbb{C}\backslash\sigma(H), \ x,x' \in \mathbb{R}, \tag{1.3}$$

be the Green's function of H (here $\sigma(H)$ denotes the spectrum of H) and denote by $g(z,x)$ the corresponding diagonal Green's function of H defined by

$$g(z,x) = G(z,x,x) = \frac{i\prod_{j=1}^n [z-\mu_j(x)]}{2R_{2n+1}(z)^{1/2}}, \tag{1.4}$$

$$R_{2n+1}(z) = \prod_{m=0}^{2n} (z-E_m), \quad \{E_m\}_{m=0}^{2n} \subset \mathbb{C}, \tag{1.5}$$

$$E_m \neq E_{m'} \text{ for } m \neq m', \quad m,m' = 0,1,\dots,2n. \tag{1.6}$$

For any quasi-periodic (in fact, Bohr (uniformly) almost periodic) function f the mean value $\langle f \rangle$ of f is defined by

$$\langle f \rangle = \lim_{R\to\infty} \frac{1}{2R} \int_{-R}^{R} dx\, f(x). \tag{1.7}$$

Moreover, we introduce the set Σ by

$$\Sigma = \big\{\lambda \in \mathbb{C} \,\big|\, \mathrm{Re}\big(\langle g(\lambda,\cdot)^{-1}\rangle\big) = 0\big\} \tag{1.8}$$

and note that

$$\langle g(z,\cdot)\rangle = \frac{i\prod_{j=1}^n \big(z-\widetilde{\lambda}_j\big)}{2R_{2n+1}(z)^{1/2}} \tag{1.9}$$

for some constants $\{\widetilde{\lambda}_j\}_{j=1}^n \subset \mathbb{C}$.

Finally, we denote by $\sigma_{\rm p}(T)$, $\sigma_{\rm d}(T)$, $\sigma_{\rm c}(T)$, $\sigma_{\rm e}(T)$, and $\sigma_{\rm ap}(T)$, the point spectrum (i.e., the set of eigenvalues), the discrete spectrum, the continuous spectrum, the essential spectrum (cf. (4.15)), and the approximate point spectrum of a densely defined closed operator T in a complex Hilbert space, respectively.

Our principal new results, to be proved in Section 4, then read as follows:

Theorem 1.1. *Assume that V is a quasi-periodic (complex-valued) solution of the nth stationary KdV equation. Then the following assertions hold:*
(i) The point spectrum and residual spectrum of H are empty and hence the spectrum of H is purely continuous,

$$\sigma_{\rm p}(H) = \sigma_{\rm r}(H) = \emptyset, \tag{1.10}$$

$$\sigma(H) = \sigma_{\rm c}(H) = \sigma_{\rm e}(H) = \sigma_{\rm ap}(H). \tag{1.11}$$

(ii) The spectrum of H coincides with Σ and equals the conditional stability set of H,

$$\sigma(H) = \big\{\lambda \in \mathbb{C} \,\big|\, \mathrm{Re}\big(\langle g(\lambda,\cdot)^{-1}\rangle\big) = 0\big\} \tag{1.12}$$

$$= \{\lambda \in \mathbb{C} \,|\, \textit{there exists at least one bounded distributional solution } 0 \neq \psi \in L^\infty(\mathbb{R}; dx) \textit{ of } H\psi = \lambda\psi\}. \tag{1.13}$$

(iii) $\sigma(H)$ is contained in the semi-strip

$$\sigma(H) \subset \{z \in \mathbb{C} \,|\, \mathrm{Im}(z) \in [M_1, M_2],\, \mathrm{Re}(z) \geq M_3\}, \tag{1.14}$$

where

$$M_1 = \inf_{x\in\mathbb{R}}[\mathrm{Im}(V(x))], \quad M_2 = \sup_{x\in\mathbb{R}}[\mathrm{Im}(V(x))], \quad M_3 = \inf_{x\in\mathbb{R}}[\mathrm{Re}(V(x))]. \tag{1.15}$$

(iv) $\sigma(H)$ consists of finitely many simple analytic arcs and one simple semi-infinite arc. These analytic arcs may only end at the points $\widetilde{\lambda}_1, \dots, \widetilde{\lambda}_n$, $E_0, \dots, E_{2n}$, and at infinity. The semi-infinite arc, σ_∞, asymptotically approaches the half-line $L_{\langle V\rangle} = \{z \in \mathbb{C} \,|\, z = \langle V\rangle + x,\, x \geq 0\}$ in the following sense: asymptotically, σ_∞ can be parameterized by

$$\sigma_\infty = \big\{z \in \mathbb{C} \,\big|\, z = R + i\,\mathrm{Im}(\langle V\rangle) + O\big(R^{-1/2}\big) \text{ as } R \uparrow \infty\big\}. \tag{1.16}$$

(v) Each E_m, $m = 0, \dots, 2n$, is met by at least one of these arcs. More precisely, a particular E_{m_0} is hit by precisely $2N_0 + 1$ analytic arcs, where $N_0 \in \{0, \dots, n\}$ denotes the number of $\widetilde{\lambda}_j$ that coincide with E_{m_0}. Adjacent arcs meet at an angle $2\pi/(2N_0 + 1)$ at E_{m_0}. (Thus,

generically, $N_0 = 0$ and precisely one arc hits E_{m_0}.)
(vi) Crossings of spectral arcs are permitted and take place precisely when

$$\operatorname{Re}\big(\langle g(\widetilde\lambda_{j_0},\cdot)^{-1}\rangle\big) = 0 \ \text{ for some } j_0 \in \{1,\dots,n\} \text{ with } \widetilde\lambda_{j_0} \notin \{E_m\}_{m=0}^{2n}. \tag{1.17}$$

In this case $2M_0+2$ analytic arcs are converging toward $\widetilde\lambda_{j_0}$, where $M_0 \in \{1,\dots,n\}$ denotes the number of $\widetilde\lambda_j$ that coincide with $\widetilde\lambda_{j_0}$. Adjacent arcs meet at an angle $\pi/(M_0+1)$ at $\widetilde\lambda_{j_0}$.
(vii) The resolvent set $\mathbb{C}\backslash\sigma(H)$ of H is path-connected.

Naturally, Theorem 1.1 applies to the special case where V is a periodic (complex-valued) solution of the nth stationary KdV equation. Even in this special case, items (v) and (vi) of Theorem 1.1 provide additional new details on the nature of the spectrum of H.

As described in Remark 4.10, these results extend to the $L^p(\mathbb{R};dx)$-setting for $p \in [1,\infty)$.

Theorem 1.1 focuses on stationary quasi-periodic solutions of the KdV hierarchy for the following reasons. First of all, the class of algebro-geometric solutions of the (time-dependent) KdV hierarchy is defined as the class of all solutions of some (and hence infinitely many) equations of the stationary KdV hierarchy. Secondly, time-dependent algebro-geometric solutions of a particular equation of the (time-dependent) KdV hierarchy just represent isospectral deformations (the deformation parameter being the time variable) of a fixed stationary algebro-geometric KdV solution (the latter can be viewed as the initial condition at a fixed time t_0). In the present case of quasi-periodic algebro-geometric solutions of the nth KdV equation, the isospectral manifold of such a given solution is an n-dimensional real torus, and time-dependent solutions trace out a path in that isospectral torus (cf. the discussion in [24, p. 12]).

Finally, we give a brief discussion of the contents of each section. In Section 2 we provide the necessary background material including a quick construction of the KdV hierarchy of nonlinear evolution equations and its Lax pairs using a polynomial recursion formalism. We also discuss the hyperelliptic Riemann surface underlying the stationary KdV hierarchy, the corresponding Baker–Akhiezer function, and the necessary ingredients to describe the Its–Matveev formula for stationary KdV solutions. Section 3 focuses on the diagonal Green's function of the Schrödinger operator H, a key ingredient in our characterization of the spectrum $\sigma(H)$ of H in Section 4 (cf. (1.12)). Our principal Section 4 is then devoted to a proof of Theorem 1.1. Appendix A provides the necessary summary of tools needed from elementary algebraic geometry (most notably the theory of compact (hyperelliptic) Riemann surfaces) and sets the stage for some of the notation used in Sections 2–4. Appendix B provides additional insight into one ingredient of the Its–Matveev formula; Appendix C illustrates our results in the special periodic non-self-adjoint case and provides a simple yet nontrivial example in the elliptic genus one case.

Our methods extend to the case of algebro-geometric non-self-adjoint second order finite difference (Jacobi) operators associated with the Toda lattice hierarchy. Moreover, they extend to the infinite genus limit $n \to \infty$ (cf. (1.2)–(1.5)) using the approach in [23]. This will be studied elsewhere.

Dedication. It is with great pleasure that we dedicate this paper to Vladimir A. Marchenko on the occasion of his 80th birthday. His strong influence on the subject at hand is universally admired.

2. The KdV hierarchy, hyperelliptic curves, and the Its–Matveev formula

In this section we briefly review the recursive construction of the KdV hierarchy and associated Lax pairs following [25] and especially, [24, Ch. 1]. Moreover, we discuss the class of algebro-geometric solutions of the KdV hierarchy corresponding to the underlying hyperelliptic curve and recall the Its–Matveev formula for such solutions. The material in this preparatory section is known and detailed accounts with proofs can be found, for instance, in [24, Ch. 1]. For the notation employed in connection with elementary concepts in algebraic geometry (more precisely, the theory of compact Riemann surfaces), we refer to Appendix A.

Throughout this section we suppose the hypothesis

$$V \in C^\infty(\mathbb{R}) \tag{2.1}$$

and consider the one-dimensional Schrödinger differential expression

$$L = -\frac{d^2}{dx^2} + V. \tag{2.2}$$

To construct the KdV hierarchy we need a second differential expression P_{2n+1} of order $2n+1$, $n \in \mathbb{N}_0$, defined recursively in the following. We take the quickest route to the construction of P_{2n+1}, and hence to that of the KdV hierarchy, by starting from the recursion relation (2.3) below.

Define $\{f_\ell\}_{\ell\in\mathbb{N}_0}$ recursively by

$$f_0 = 1, \quad f_{\ell,x} = -(1/4)f_{\ell-1,xxx} + Vf_{\ell-1,x} + (1/2)V_x f_{\ell-1}, \quad \ell\in\mathbb{N}. \tag{2.3}$$

Explicitly, one finds

$$\begin{aligned} f_0 &= 1,\\ f_1 &= \tfrac{1}{2}V + c_1,\\ f_2 &= -\tfrac{1}{8}V_{xx} + \tfrac{3}{8}V^2 + c_1\tfrac{1}{2}V + c_2,\\ f_3 &= \tfrac{1}{32}V_{xxxx} - \tfrac{5}{16}VV_{xx} - \tfrac{5}{32}V_x^2 + \tfrac{5}{16}V^3\\ &\quad + c_1\big(-\tfrac{1}{8}V_{xx} + \tfrac{3}{8}V^2\big) + c_2\tfrac{1}{2}V + c_3, \quad \text{etc.} \end{aligned} \tag{2.4}$$

Here $\{c_k\}_{k\in\mathbb{N}}\subset\mathbb{C}$ denote integration constants which naturally arise when solving (2.3).

Subsequently, it will be convenient to also introduce the corresponding homogeneous coefficients $\hat f_\ell$, defined by the vanishing of the integration constants c_k for $k=1,\dots,\ell$,

$$\hat f_0 = f_0 = 1, \quad \hat f_\ell = f_\ell\big|_{c_k=0,\,k=1,\dots,\ell}, \quad \ell\in\mathbb{N}. \tag{2.5}$$

Hence,

$$f_\ell = \sum_{k=0}^{\ell} c_{\ell-k}\hat f_k, \quad \ell\in\mathbb{N}_0, \tag{2.6}$$

introducing

$$c_0 = 1. \tag{2.7}$$

One can prove inductively that all homogeneous elements $\hat f_\ell$ (and hence all f_ℓ) are differential polynomials in V, that is, polynomials with respect to V and its x-derivatives up to order $2\ell-2$, $\ell\in\mathbb{N}$.

Next we define differential expressions P_{2n+1} of order $2n+1$ by

$$P_{2n+1} = \sum_{\ell=0}^{n}\Big(f_{n-\ell}\frac{d}{dx} - \frac{1}{2}f_{n-\ell,x}\Big)L^\ell, \quad n\in\mathbb{N}_0. \tag{2.8}$$

Using the recursion (2.3), the commutator of P_{2n+1} and L can be explicitly computed and one obtains

$$[P_{2n+1}, L] = 2f_{n+1,x}, \quad n\in\mathbb{N}_0. \tag{2.9}$$

In particular, (L, P_{2n+1}) represents the celebrated *Lax pair* of the KdV hierarchy. Varying $n\in\mathbb{N}_0$, the stationary KdV hierarchy is then defined in terms of the vanishing of the commutator of P_{2n+1} and L in

(2.9) by[1],

$$-[P_{2n+1}, L] = -2f_{n+1,x}(V) = \text{s-KdV}_n(V) = 0, \quad n \in \mathbb{N}_0. \tag{2.10}$$

Explicitly,

$$\begin{aligned} &\text{s-KdV}_0(V) = -V_x = 0, \\ &\text{s-KdV}_1(V) = \tfrac{1}{4}V_{xxx} - \tfrac{3}{2}VV_x + c_1(-V_x) = 0, \\ &\text{s-KdV}_2(V) = -\tfrac{1}{16}V_{xxxxx} + \tfrac{5}{8}V_{xxx} + \tfrac{5}{4}V_xV_{xx} - \tfrac{15}{8}V^2V_x \\ &\qquad + c_1\big(\tfrac{1}{4}V_{xxx} - \tfrac{3}{2}VV_x\big) + c_2(-V_x) = 0, \quad \text{etc.,} \end{aligned} \tag{2.11}$$

represent the first few equations of the stationary KdV hierarchy. By definition, the set of solutions of (2.10), with n ranging in $\mathbb{N}_0$ and c_k in $\mathbb{C}$, $k \in \mathbb{N}$, represents the class of algebro-geometric KdV solutions. At times it will be convenient to abbreviate algebro-geometric stationary KdV solutions V simply as KdV *potentials*.

In the following we will frequently assume that V satisfies the nth stationary KdV equation. By this we mean it satisfies one of the nth stationary KdV equations after a particular choice of integration constants $c_k \in \mathbb{C}$, $k = 1, \dots, n$, $n \in \mathbb{N}$, has been made.

Next, we introduce a polynomial F_n of degree n with respect to the spectral parameter $z \in \mathbb{C}$ by

$$F_n(z,x) = \sum_{\ell=0}^{n} f_{n-\ell}(x) z^\ell. \tag{2.12}$$

Explicitly, one obtains

$$\begin{aligned} &F_0 = 1, \\ &F_1 = z + \tfrac{1}{2}V + c_1, \\ &F_2 = z^2 + \tfrac{1}{2}Vz - \tfrac{1}{8}V_{xx} + \tfrac{3}{8}V^2 + c_1\big(\tfrac{1}{2}V + z\big) + c_2, \\ &F_3 = z^3 + \tfrac{1}{2}Vz^2 + \big(-\tfrac{1}{8}V_{xx} + \tfrac{3}{8}V^2\big)z + \tfrac{1}{32}V_{xxxx} - \tfrac{5}{16}VV_{xx} - \tfrac{5}{32}V_x^2 \\ &\qquad + \tfrac{5}{16}V^3 + c_1\big(z^2 + \tfrac{1}{2}Vz - \tfrac{1}{8}V_{xx} + \tfrac{3}{8}V^2\big) + c_2\big(z + \tfrac{1}{2}V\big) + c_3, \quad \text{etc.} \end{aligned} \tag{2.13}$$

The recursion relation (2.3) and equation (2.10) imply that

$$F_{n,xxx} - 4(V-z)F_{n,x} - 2V_xF_n = 0. \tag{2.14}$$

Multiplying (2.14) by F_n, a subsequent integration with respect to x results in

$$(1/2)F_{n,xx}F_n - (1/4)F_{n,x}^2 - (V-z)F_n^2 = R_{2n+1}, \tag{2.15}$$

[1]In a slight abuse of notation we will occasionally stress the functional dependence of f_ℓ on V, writing $f_\ell(V)$.

where R_{2n+1} is a monic polynomial of degree $2n+1$. We denote its roots by $\{E_m\}_{m=0}^{2n}$, and hence write

$$R_{2n+1}(z) = \prod_{m=0}^{2n}(z - E_m), \quad \{E_m\}_{m=0}^{2n} \subset \mathbb{C}. \tag{2.16}$$

One can show that equation (2.15) leads to an explicit determination of the integration constants $c_1, \dots, c_n$ in

$$\text{s-KdV}_n(V) = -2f_{n+1,x}(V) = 0 \tag{2.17}$$

in terms of the zeros $E_0, \dots, E_{2n}$ of the associated polynomial R_{2n+1} in (2.16). In fact, one can prove

$$c_k = c_k(\underline{E}), \quad k = 1, \dots, n, \tag{2.18}$$

where

$$c_k(\underline{E}) = -\sum_{\substack{j_0,\dots,j_{2n}=0 \\ j_0+\cdots+j_{2n}=k}}^{k} \frac{(2j_0)!\cdots(2j_{2n})!}{2^{2k}(j_0!)^2\cdots(j_{2n}!)^2(2j_0-1)\cdots(2j_{2n}-1)} \times E_0^{j_0}\cdots E_{2n}^{j_{2n}}, \quad k = 1, \dots, n. \tag{2.19}$$

Remark 2.1. Suppose $V \in C^{2n+1}(\mathbb{R})$ satisfies the nth stationary KdV equation $\text{s-KdV}_n(V) = -2f_{n+1,x}(V) = 0$ for a given set of integration constants c_k, $k = 1, \dots, n$. Introducing F_n as in (2.12) with $f_0, \dots, f_n$ given by (2.6) then yields equation (2.14) and hence (2.15). The latter equation in turn, as shown inductively in [27, Prop. 2.1], yields

$$V \in C^\infty(\mathbb{R}) \text{ and } f_\ell \in C^\infty(\mathbb{R}), \ \ell = 0, \dots, n. \tag{2.20}$$

Thus, without loss of generality, we may assume in the following that solutions of $\text{s-KdV}_n(V) = 0$ satisfy $V \in C^\infty(\mathbb{R})$.

Next, we study the restriction of the differential expression P_{2n+1} to the two-dimensional kernel (i.e., the formal null space in an algebraic sense as opposed to the functional analytic one) of $(L - z)$. More precisely, let

$$\ker(L - z) = \{\psi\colon \mathbb{R} \to \mathbb{C}_\infty \text{ meromorphic} \mid (L - z)\psi = 0\}, \quad z \in \mathbb{C}. \tag{2.21}$$

Then (2.8) implies

$$P_{2n+1}\big|_{\ker(L-z)} = \Big(F_n(z)\frac{d}{dx} - \frac{1}{2}F_{n,x}(z)\Big)\Big|_{\ker(L-z)}. \tag{2.22}$$

We emphasize that the result (2.22) is valid independently of whether or not P_{2n+1} and L commute. However, if one makes the additional assumption that P_{2n+1} and L commute, one can prove that this implies an algebraic relationship between P_{2n+1} and L.

Theorem 2.2. *Fix $n \in \mathbb{N}_0$ and assume that P_{2n+1} and L commute, $[P_{2n+1}, L] = 0$, or equivalently, suppose* s-KdV$_n(V) = -2f_{n+1,x}(V) = 0$. *Then L and P_{2n+1} satisfy an algebraic relationship of the type* (*cf.* (2.16))

$$\begin{aligned} &\mathcal{F}_n(L, -iP_{2n+1}) = -P_{2n+1}^2 - R_{2n+1}(L) = 0, \\ &R_{2n+1}(z) = \prod_{m=0}^{2n} (z - E_m), \quad z \in \mathbb{C}. \end{aligned} \tag{2.23}$$

The expression $\mathcal{F}_n(L, -iP_{2n+1})$ is called the Burchnall–Chaundy polynomial of the pair (L, P_{2n+1}). Equation (2.23) naturally leads to the hyperelliptic curve $\mathcal{K}_n$ of (arithmetic) genus $n \in \mathbb{N}_0$ (possibly with a singular affine part), where

$$\begin{aligned} &\mathcal{K}_n \colon \mathcal{F}_n(z, y) = y^2 - R_{2n+1}(z) = 0, \\ &R_{2n+1}(z) = \prod_{m=0}^{2n} (z - E_m), \quad \{E_m\}_{m=0}^{2n} \subset \mathbb{C}. \end{aligned} \tag{2.24}$$

The curve $\mathcal{K}_n$ is compactified by joining the point P_∞ but for notational simplicity the compactification is also denoted by $\mathcal{K}_n$. Points P on $\mathcal{K}_n \backslash \{P_\infty\}$ are represented as pairs $P = (z, y)$, where $y(\cdot)$ is the meromorphic function on $\mathcal{K}_n$ satisfying $\mathcal{F}_n(z, y) = 0$. The complex structure on $\mathcal{K}_n$ is then defined in the usual way, see Appendix A. Hence, $\mathcal{K}_n$ becomes a two-sheeted hyperelliptic Riemann surface of (arithmetic) genus $n \in \mathbb{N}_0$ (possibly with a singular affine part) in a standard manner.

We also emphasize that by fixing the curve $\mathcal{K}_n$ (i.e., by fixing the constants $E_0, \dots, E_{2n}$), the integration constants $c_1, \dots, c_n$ in $f_{n+1,x}$ (and hence in the corresponding stationary KdV$_n$ equation) are uniquely determined as is clear from (2.18) and (2.19), which establish the integration constants c_k as symmetric functions of $E_0, \dots, E_{2n}$.

For notational simplicity we will usually tacitly assume that $n \in \mathbb{N}$. The trivial case $n = 0$ which leads to $V(x) = E_0$ is of no interest to us in this paper.

In the following, the zeros[2] of the polynomial $F_n(\cdot,x)$ (cf. (2.12)) will play a special role. We denote them by $\{\mu_j(x)\}_{j=1}^n$ and hence write

$$F_n(z,x)=\prod_{j=1}^n[z-\mu_j(x)]. \tag{2.25}$$

From (2.15) we see that

$$R_{2n+1}+(1/4)F_{n,x}^2=F_nH_{n+1}, \tag{2.26}$$

where

$$H_{n+1}(z,x)=(1/2)F_{n,xx}(z,x)+(z-V(x))F_n(z,x) \tag{2.27}$$

is a monic polynomial of degree $n+1$. We introduce the corresponding roots[3] $\{\nu_\ell(x)\}_{\ell=0}^n$ of $H_{n+1}(\cdot,x)$ by

$$H_{n+1}(z,x)=\prod_{\ell=0}^n[z-\nu_\ell(x)]. \tag{2.28}$$

Explicitly, one computes from (2.4) and (2.12),

$$\begin{aligned}
H_1&=z-V,\\
H_2&=z^2-\tfrac12 Vz+\tfrac14 V_{xx}-\tfrac12 V^2+c_1(z-V),\\
H_3&=z^3-\tfrac12 Vz^2+\tfrac18\big(V_{xx}-V^2\big)z-\tfrac1{16}V_{xxxx}+\tfrac38 V_x^2+\tfrac12 VV_{xx}\\
&\quad-\tfrac38 V^3+c_1\big(z^2-\tfrac12 Vz+\tfrac14 V_{xx}-\tfrac12 V^2\big)+c_2(z-V), \quad \text{etc.}
\end{aligned} \tag{2.29}$$

The next step is crucial; it permits us to "lift" the zeros μ_j and ν_ℓ of F_n and H_{n+1} from $\mathbb{C}$ to the curve $\mathcal{K}_n$. From (2.26) one infers

$$R_{2n+1}(z)+(1/4)F_{n,x}(z)^2=0, \quad z\in\{\mu_j,\nu_\ell\}_{j=1,\dots,n,\ell=0,\dots,n}. \tag{2.30}$$

We now introduce $\{\hat\mu_j(x)\}_{j=1,\dots,n}\subset\mathcal{K}_n$ and $\{\hat\nu_\ell(x)\}_{\ell=0,\dots,n}\subset\mathcal{K}_n$ by

$$\hat\mu_j(x)=(\mu_j(x),-(i/2)F_{n,x}(\mu_j(x),x)), \quad j=1,\dots,n,\ x\in\mathbb{R} \tag{2.31}$$

and

$$\hat\nu_\ell(x)=(\nu_\ell(x),(i/2)F_{n,x}(\nu_\ell(x),x)), \quad \ell=0,\dots,n,\ x\in\mathbb{R}. \tag{2.32}$$

Due to the $C^\infty(\mathbb{R})$ assumption (2.1) on V, $F_n(z,\cdot)\in C^\infty(\mathbb{R})$ by (2.3) and (2.12), and hence also $H_{n+1}(z,\cdot)\in C^\infty(\mathbb{R})$ by (2.27). Thus, one concludes

$$\mu_j,\nu_\ell\in C(\mathbb{R}),\ \ j=1,\dots,n,\ \ell=0,\dots,n, \tag{2.33}$$

[2]If $V\in L^\infty(\mathbb{R};dx)$, these zeros are the Dirichlet eigenvalues of a closed operator in $L^2(\mathbb{R})$ associated with the differential expression L and a Dirichlet boundary condition at $x\in\mathbb{R}$.

[3]If $V\in L^\infty(\mathbb{R};dx)$, these roots are the Neumann eigenvalues of a closed operator in $L^2(\mathbb{R})$ associated with L and a Neumann boundary condition at $x\in\mathbb{R}$.

taking multiplicities (and appropriate renumbering) of the zeros of F_n and H_{n+1} into account. (Away from collisions of zeros, μ_j and ν_ℓ are of course C^∞.)

Next, we define the fundamental meromorphic function $\phi(\cdot, x)$ on $\mathcal{K}_n$,

$$\phi(P,x) = \frac{iy + (1/2)F_{n,x}(z,x)}{F_n(z,x)} \tag{2.34}$$

$$= \frac{-H_{n+1}(z,x)}{iy - (1/2)F_{n,x}(z,x)}, \tag{2.35}$$

$$P = (z,y) \in \mathcal{K}_n, \ x \in \mathbb{R}$$

with divisor $(\phi(\cdot,x))$ of $\phi(\cdot,x)$ given by

$$(\phi(\cdot,x)) = \mathcal{D}_{\hat{\nu}_0(x)\underline{\hat{\nu}}(x)} - \mathcal{D}_{P_\infty \underline{\hat{\mu}}(x)}, \tag{2.36}$$

using (2.25), (2.28), and (2.33). Here we abbreviated

$$\underline{\hat{\mu}} = \{\hat{\mu}_1, \dots, \hat{\mu}_n\}, \, \underline{\hat{\nu}} = \{\hat{\nu}_1, \dots, \hat{\nu}_n\} \in \operatorname{Sym}^n(\mathcal{K}_n) \tag{2.37}$$

(cf. the notation introduced in Appendix A). The stationary Baker–Akhiezer function $\psi(\cdot, x, x_0)$ on $\mathcal{K}_n \backslash \{P_\infty\}$ is then defined in terms of $\phi(\cdot, x)$ by

$$\psi(P,x,x_0) = \exp\left(\int_{x_0}^x dx'\, \phi(P,x')\right), \quad P \in \mathcal{K}_n\backslash\{P_\infty\}, \, (x,x_0) \in \mathbb{R}^2. \tag{2.38}$$

Basic properties of ϕ and ψ are summarized in the following result (where $W(f,g) = fg' - f'g$ denotes the Wronskian of f and g, and P^* abbreviates $P^* = (z,-y)$ for $P = (z,y)$).

Lemma 2.3. *Assume $V \in C^\infty(\mathbb{R})$ satisfies the nth stationary KdV equation* (2.10). *Moreover, let $P = (z,y) \in \mathcal{K}_n\backslash\{P_\infty\}$ and $(x,x_0) \in \mathbb{R}^2$. Then ϕ satisfies the Riccati-type equation*

$$\phi_x(P) + \phi(P)^2 = V - z, \tag{2.39}$$

as well as

$$\phi(P)\phi(P^*) = \frac{H_{n+1}(z)}{F_n(z)}, \tag{2.40}$$

$$\phi(P) + \phi(P^*) = \frac{F_{n,x}(z)}{F_n(z)}, \tag{2.41}$$

$$\phi(P) - \phi(P^*) = \frac{2iy}{F_n(z)}. \tag{2.42}$$

Moreover, ψ satisfies

$$(L - z(P))\psi(P) = 0, \quad (P_{2n+1} - iy(P))\psi(P) = 0, \tag{2.43}$$

$$\psi(P, x, x_0) = \left(\frac{F_n(z,x)}{F_n(z,x_0)}\right)^{1/2} \exp\left(iy \int_{x_0}^{x} dx'\, F_n(z,x')^{-1}\right), \tag{2.44}$$

$$\psi(P, x, x_0)\psi(P^*, x, x_0) = \frac{F_n(z,x)}{F_n(z,x_0)}, \tag{2.45}$$

$$\psi_x(P, x, x_0)\psi_x(P^*, x, x_0) = \frac{H_{n+1}(z,x)}{F_n(z,x_0)}, \tag{2.46}$$

$$\psi(P, x, x_0)\psi_x(P^*, x, x_0) + \psi(P^*, x, x_0)\psi_x(P, x, x_0) = \frac{F_{n,x}(z,x)}{F_n(z,x_0)}, \tag{2.47}$$

$$W(\psi(P, \cdot, x_0), \psi(P^*, \cdot, x_0)) = -\frac{2iy}{F_n(z,x_0)}. \tag{2.48}$$

In addition, as long as the zeros of $F_n(\cdot, x)$ are all simple for $x \in \Omega$, $\Omega \subseteq \mathbb{R}$ an open interval, $\psi(\cdot, x, x_0)$ is meromorphic on $\mathcal{K}_n \backslash \{P_\infty\}$ for $x, x_0 \in \Omega$.

Next, we recall that the affine part of $\mathcal{K}_n$ is nonsingular if

$$E_m \neq E_{m'} \text{ for } m \neq m', \quad m, m' = 0, 1, \dots, 2n. \tag{2.49}$$

Combining the polynomial recursion approach with (2.25) readily yields trace formulas for the KdV invariants, that is, expressions of f_ℓ in terms of symmetric functions of the zeros μ_j of F_n.

Lemma 2.4. *Assume $V \in C^\infty(\mathbb{R})$ satisfies the nth stationary KdV equation* (2.10)*. Then,*

$$V = \sum_{m=0}^{2n} E_m - 2\sum_{j=1}^{n} \mu_j, \tag{2.50}$$

$$V^2 - (1/2)V_{xx} = \sum_{m=0}^{2n} E_m^2 - 2\sum_{j=1}^{n} \mu_j^2, \ \textit{etc.} \tag{2.51}$$

Equation (2.50) represents the trace formula for the algebro-geometric potential V. In addition, (2.51) indicates that higher-order trace formulas associated with the KdV hierarchy can be obtained from (2.25) comparing powers of z. We omit further details and refer to [24, Ch. 1] and [25].

Since nonspecial divisors play a fundamental role in this context we also recall the following fact.

Lemma 2.5. *Assume that* $V \in C^\infty(\mathbb{R}) \cap L^\infty(\mathbb{R}; dx)$ *satisfies the* n*th stationary KdV equation* (2.10)*. Let* $\mathcal{D}_{\underline{\hat{\mu}}}$*,* $\underline{\hat{\mu}} = (\hat{\mu}_1, \dots, \hat{\mu}_n)$ *be the Dirichlet divisor of degree* n *associated with* V *defined according to* (2.31)*, that is,*

$$\hat{\mu}_j(x) = (\mu_j(x), -(i/2)F_{n,x}(\mu_j(x), x)), \quad j = 1, \dots, n, \ x \in \mathbb{R}. \quad (2.52)$$

Then $\mathcal{D}_{\underline{\hat{\mu}}(x)}$ *is nonspecial for all* $x \in \mathbb{R}$*. Moreover, there exists a constant* $C > 0$ *such that*

$$|\mu_j(x)| \le C, \quad j = 1, \dots, n, \ x \in \mathbb{R}. \quad (2.53)$$

Remark 2.6. Assume that $V \in C^\infty(\mathbb{R}) \cap L^\infty(\mathbb{R}; dx)$ satisfies the nth stationary KdV equation (2.10). We recall that $f_\ell \in C^\infty(\mathbb{R})$, $\ell \in \mathbb{N}_0$, by (2.20) since f_ℓ are differential polynomials in V. Moreover, we note that (2.53) implies that $f_\ell \in L^\infty(\mathbb{R}; dx)$, $\ell = 0, \dots, n$, employing the fact that f_ℓ, $\ell = 0, \dots, n$, are elementary symmetric functions of $\mu_1, \dots, \mu_n$ (cf. (2.12) and (2.25)). Since $f_{n+1,x} = 0$, one can use the recursion relation (2.3) to reduce f_k for $k \ge n+2$ to a linear combination of $f_1, \dots, f_n$. Thus,

$$f_\ell \in C^\infty(\mathbb{R}) \cap L^\infty(\mathbb{R}; dx), \quad \ell \in \mathbb{N}_0. \quad (2.54)$$

Using the fact that for fixed $1 \le p \le \infty$,

$$h, h^{(k)} \in L^p(\mathbb{R}; dx) \ \text{ imply } \ h^{(\ell)} \in L^p(\mathbb{R}; dx), \ \ \ell = 1, \dots, k-1 \quad (2.55)$$

(cf., e.g., [6, p. 168–170]), one then infers

$$V^{(\ell)} \in L^\infty(\mathbb{R}; dx), \quad \ell \in \mathbb{N}_0, \quad (2.56)$$

applying (2.55) with $p = \infty$.

We continue with the theta function representation for ψ and V. For general background information and the notation employed we refer to Appendix A.

Let θ denote the Riemann theta function associated with $\mathcal{K}_n$ (whose affine part is assumed to be nonsingular) and let $\{a_j, b_j\}_{j=1}^n$ be a fixed homology basis on $\mathcal{K}_n$. Next, choosing a base point $Q_0 \in \mathcal{K}_n \backslash P_\infty$, the Abel maps $\underline{A}_{Q_0}$ and $\underline{\alpha}_{Q_0}$ are defined by (A.41) and (A.42), and the Riemann vector $\underline{\Xi}_{Q_0}$ is given by (A.54).

Next, let $\omega^{(2)}_{P_\infty,0}$ denote the normalized differential of the second kind defined by

$$\omega^{(2)}_{P_\infty,0} = -\frac{1}{2y}\prod_{j=1}^n (z - \lambda_j)dz \underset{\zeta \to 0}{=} \big(\zeta^{-2} + O(1)\big)d\zeta \text{ as } P \to P_\infty, \quad (2.57)$$

$$\zeta = \sigma/z^{1/2}, \ \sigma \in \{1. -1\},$$

where the constants $\lambda_j \in \mathbb{C}$, $j = 1, \dots, n$, are determined by employing the normalization

$$\int_{a_j} \omega^{(2)}_{P_\infty,0} = 0, \quad j = 1, \dots, n. \tag{2.58}$$

One then infers

$$\int_{Q_0}^{P} \omega^{(2)}_{P_\infty,0} \underset{\zeta\to 0}{=} -\zeta^{-1} + e^{(2)}_0(Q_0) + O(\zeta) \text{ as } P \to P_\infty \tag{2.59}$$

for some constant $e^{(2)}_0(Q_0) \in \mathbb{C}$. The vector of b-periods of $\omega^{(2)}_{P_\infty,0}/(2\pi i)$ is denoted by

$$\underline{U}^{(2)}_0 = (U^{(2)}_{0,1}, \dots, U^{(2)}_{0,n}), \quad U^{(2)}_{0,j} = \frac{1}{2\pi i}\int_{b_j} \omega^{(2)}_{P_\infty,0}, \ j = 1, \dots, n. \tag{2.60}$$

By (A.26) one concludes

$$U^{(2)}_{0,j} = -2c_j(n), \quad j = 1, \dots, n. \tag{2.61}$$

In the following it will be convenient to introduce the abbreviation

$$\begin{aligned} &\underline{z}(P, \underline{Q}) = \underline{\Xi}_{Q_0} - \underline{A}_{Q_0}(P) + \underline{\alpha}_{Q_0}(\mathcal{D}_{\underline{Q}}), \\ &P \in \mathcal{K}_n, \ \underline{Q} = \{Q_1, \dots, Q_n\} \in \operatorname{Sym}^n(\mathcal{K}_n). \end{aligned} \tag{2.62}$$

We note that $\underline{z}(\cdot, \underline{Q})$ is independent of the choice of base point Q_0.

Theorem 2.7. *Suppose that $V \in C^\infty(\mathbb{R}) \cap L^\infty(\mathbb{R}; dx)$ satisfies the nth stationary KdV equation* (2.10) *on $\mathbb{R}$. In addition, assume the affine part of $\mathcal{K}_n$ to be nonsingular and let $P \in \mathcal{K}_n\backslash\{P_\infty\}$ and $x, x_0 \in \mathbb{R}$. Then $\mathcal{D}_{\hat{\underline{\mu}}(x)}$ and $\mathcal{D}_{\hat{\underline{\nu}}(x)}$ are nonspecial for $x \in \mathbb{R}$. Moreover,*[4]

$$\begin{aligned} \psi(P, x, x_0) = &\frac{\theta(\underline{z}(P_\infty, \hat{\underline{\mu}}(x_0)))\theta(\underline{z}(P, \hat{\underline{\mu}}(x)))}{\theta(\underline{z}(P_\infty, \hat{\underline{\mu}}(x)))\theta(\underline{z}(P, \hat{\underline{\mu}}(x_0)))} \\ &\times \exp\bigg[-i(x - x_0)\bigg(\int_{Q_0}^{P} \omega^{(2)}_{P_\infty,0} - e^{(2)}_0(Q_0)\bigg)\bigg], \end{aligned} \tag{2.63}$$

with the linearizing property of the Abel map,

$$\underline{\alpha}_{Q_0}(\mathcal{D}_{\hat{\underline{\mu}}(x)}) = \Big(\underline{\alpha}_{Q_0}(\mathcal{D}_{\hat{\underline{\mu}}(x_0)}) + i\underline{U}^{(2)}_0(x - x_0)\Big) \pmod{L_n}. \tag{2.64}$$

The Its–Matveev formula for V reads

$$V(x) = E_0 + \sum_{j=1}^{n}(E_{2j-1} + E_{2j} - 2\lambda_j)$$

[4]To avoid multi-valued expressions in formulas such as (2.63), etc., we agree to always choose the same path of integration connecting Q_0 and P and refer to Remark A.4 for additional tacitly assumed conventions.

$$- 2\partial_x^2 \ln\big(\theta(\underline{\Xi}_{Q_0} - \underline{A}_{Q_0}(P_\infty) + \underline{\alpha}_{Q_0}(\mathcal{D}_{\underline{\hat{\mu}}(x)}))\big). \tag{2.65}$$

Combining (2.64) and (2.65) shows the remarkable linearity of the theta function with respect to x in the Its–Matveev formula for V. In fact, one can rewrite (2.65) as

$$V(x) = \Lambda_0 - 2\partial_x^2 \ln(\theta(\underline{A} + \underline{B}x)), \tag{2.66}$$

where

$$\underline{A} = \underline{\Xi}_{Q_0} - \underline{A}_{Q_0}(P_\infty) - i\underline{U}_0^{(2)}x_0 + \underline{\alpha}_{Q_0}(\mathcal{D}_{\underline{\hat{\mu}}(x_0)}), \tag{2.67}$$

$$\underline{B} = i\underline{U}_0^{(2)}, \tag{2.68}$$

$$\Lambda_0 = E_0 + \sum_{j=1}^n (E_{2j-1} + E_{2j} - 2\lambda_j). \tag{2.69}$$

Hence the constants $\Lambda_0 \in \mathbb{C}$ and $\underline{B} \in \mathbb{C}^n$ are uniquely determined by $\mathcal{K}_n$ (and its homology basis), and the constant $\underline{A} \in \mathbb{C}^n$ is in one-to-one correspondence with the Dirichlet data $\underline{\hat{\mu}}(x_0) = (\hat{\mu}_1(x_0), \dots, \hat{\mu}_n(x_0)) \in \mathrm{Sym}^n(\mathcal{K}_n)$ at the point x_0.

Remark 2.8. If one assumes V in (2.65) (or (2.66)) to be quasi-periodic (cf. (3.16) and (3.17)), then there exists a homology basis $\{\tilde{a}_j, \tilde{b}_j\}_{j=1}^n$ on $\mathcal{K}_n$ such that $\underline{\widetilde{B}} = i\underline{\widetilde{U}}_0^{(2)}$ satisfies the constraint

$$\underline{\widetilde{B}} = i\underline{\widetilde{U}}_0^{(2)} \in \mathbb{R}^n. \tag{2.70}$$

This is studied in detail in Appendix B.

An example illustrating some of the general results of this section is provided in Appendix C.

3. The diagonal Green's function of H

In this section we focus on the diagonal Green's function of H and derive a variety of results to be used in our principal Section 4.

We start with some preparations. We denote by

$$W(f,g)(x) = f(x)g_x(x) - f_x(x)g(x) \text{ for a.e. } x \in \mathbb{R} \tag{3.1}$$

the Wronskian of $f, g \in AC_{\mathrm{loc}}(\mathbb{R})$ (with $AC_{\mathrm{loc}}(\mathbb{R})$ the set of locally absolutely continuous functions on $\mathbb{R}$).

Lemma 3.1. *Assume*[5] $q \in L^1_{\mathrm{loc}}(\mathbb{R})$, *define* $\tau = -d^2/dx^2 + q$, *and let* $u_j(z)$, $j = 1, 2$ *be two* (*not necessarily distinct*) *distributional solutions*[6]

[5]One could admit more severe local singularities; in particular, one could assume q to be meromorphic, but we will not need this in this paper.

[6]That is, $u, u_x \in AC_{\mathrm{loc}}(\mathbb{R})$.

of $\tau u = zu$ *for some* $z \in \mathbb{C}$. *Define* $U(z,x) = u_1(z,x)u_2(z,x)$, $(z,x) \in \mathbb{C} \times \mathbb{R}$. *Then,*

$$2U_{xx}U - U_x^2 - 4(q-z)U^2 = -W(u_1,u_2)^2. \tag{3.2}$$

If in addition $q_x \in L^1_{\text{loc}}(\mathbb{R})$, *then*

$$U_{xxx} - 4(q-z)U_x - 2q_xU = 0. \tag{3.3}$$

Proof. Equation (3.3) is a well-known fact going back to at least Appell [2]. Equation (3.2) either follows upon integration using the integrating factor U, or alternatively, can be verified directly from the definition of U. We omit the straightforward computations. □

Introducing

$$\mathfrak{g}(z,x) = u_1(z,x)u_2(z,x)/W(u_1(z),u_2(z)), \quad z \in \mathbb{C},\ x \in \mathbb{R}, \tag{3.4}$$

Lemma 3.1 implies the following result.

Lemma 3.2. *Assume that* $q \in L^1_{\text{loc}}(\mathbb{R})$ *and* $(z,x) \in \mathbb{C} \times \mathbb{R}$. *Then,*

$$2\mathfrak{g}_{xx}\mathfrak{g} - \mathfrak{g}_x^2 - 4(q-z)\mathfrak{g}^2 = -1, \tag{3.5}$$

$$-\big(\mathfrak{g}^{-1}\big)_z = 2\mathfrak{g} + \big\{\mathfrak{g}\big[u_1^{-2}W(u_1,u_{1,z}) + u_2^{-2}W(u_2,u_{2,z})\big]\big\}_x, \tag{3.6}$$

$$-\big(\mathfrak{g}^{-1}\big)_z = 2\mathfrak{g} - \mathfrak{g}_{xxz} + \big[\mathfrak{g}^{-1}\mathfrak{g}_x\mathfrak{g}_z\big]_x \tag{3.7}$$

$$= 2\mathfrak{g} - \Big\{\Big[\big(\mathfrak{g}^{-1}\big)\big(\mathfrak{g}^{-1}\big)_{zx} - \big(\mathfrak{g}^{-1}\big)_x\big(\mathfrak{g}^{-1}\big)_z\Big]\Big/\big(\mathfrak{g}^{-3}\big)\Big\}_x. \tag{3.8}$$

If in addition $q_x \in L^1_{\text{loc}}(\mathbb{R})$, *then*

$$\mathfrak{g}_{xxx} - 4(q-z)\mathfrak{g}_x - 2q_x\mathfrak{g} = 0. \tag{3.9}$$

Proof. Equations (3.9) and (3.5) are clear from (3.3) and (3.2). Equation (3.6) follows from

$$\big(\mathfrak{g}^{-1}\big)_z = u_2^{-2}W(u_2,u_{2,z}) - u_1^{-2}W(u_1,u_{1,z}) \tag{3.10}$$

and

$$W(u_j,u_{j,z})_x = -u_j^2, \quad j = 1,2. \tag{3.11}$$

Finally, (3.8) (and hence (3.7)) follows from (3.4), (3.5), and (3.6) by a straightforward, though tedious, computation. □

Equation (3.7) is known and can be found, for instance, in [22]. Similarly, (3.6) can be inferred, for example, from the results in [12, p. 369].

Next, we turn to the analog of $\mathfrak{g}$ in connection with the algebro-geometric potential V in (2.65). Introducing

$$g(P,x) = \frac{\psi(P,x,x_0)\psi(P^*,x,x_0)}{W(\psi(P,\cdot,x_0),\psi(P^*,\cdot,x_0))}, \quad P \in \mathcal{K}_n \backslash \{P_\infty\},\ x,x_0 \in \mathbb{R}, \tag{3.12}$$

equations (2.45) and (2.48) imply

$$g(P,x) = \frac{iF_n(z,x)}{2y}, \quad P=(z,y) \in \mathcal{K}_n \backslash \{P_\infty\},\ x \in \mathbb{R}. \tag{3.13}$$

Together with $g(P,x)$ we also introduce its two branches $g_\pm(z,x)$ defined on the upper and lower sheets $\Pi_\pm$ of $\mathcal{K}_n$ (cf. (A.3), (A.4), and (A.14))

$$g_\pm(z,x) = \pm\frac{iF_n(z,x)}{2R_{2n+1}(z)^{1/2}}, \quad z \in \Pi,\ x \in \mathbb{R} \tag{3.14}$$

with $\Pi = \mathbb{C}\backslash\mathcal{C}$ the cut plane introduced in (A.4). A comparison of (3.4), (3.12)–(3.14), then shows that $g_\pm(z,\cdot)$ satisfy (3.5)–(3.9).

For convenience we will subsequently focus on g_+ whenever possible and then use the simplified notation

$$g(z,x) = g_+(z,x), \quad z \in \Pi,\ x \in \mathbb{R}. \tag{3.15}$$

Next, we assume that V is quasi-periodic and compute the mean value of $g(z,\cdot)^{-1}$ using (3.7). Before embarking on this task we briefly review a few properties of quasi-periodic functions.

We denote by $CP(\mathbb{R})$ and $QP(\mathbb{R})$, the sets of continuous periodic and quasi-periodic functions on $\mathbb{R}$, respectively. In particular, f is called quasi-periodic with fundamental periods $(\Omega_1,\dots,\Omega_N) \in (0,\infty)^N$ if the frequencies $2\pi/\Omega_1,\dots,2\pi/\Omega_N$ are linearly independent over $\mathbb{Q}$ and if there exists a continuous function $F \in C(\mathbb{R}^N)$, periodic of period 1 in each of its arguments

$$F(x_1,\dots,x_j+1,\dots,x_N) = F(x_1,\dots,x_N), \quad x_j \in \mathbb{R},\ j=1,\dots,N, \tag{3.16}$$

such that

$$f(x) = F(\Omega_1^{-1}x,\dots,\Omega_N^{-1}x), \quad x \in \mathbb{R}. \tag{3.17}$$

The frequency module $\mathrm{Mod}\,(f)$ of f is then of the type

$$\mathrm{Mod}\,(f) = \{2\pi m_1/\Omega_1 + \dots + 2\pi m_N/\Omega_N \,|\, m_j \in \mathbb{Z},\ j=1,\dots,N\}. \tag{3.18}$$

We note that $f \in CP(\mathbb{R})$ if and only if there are $r_j \in \mathbb{Q}\backslash\{0\}$ such that $\Omega_j = r_j\widehat{\Omega}$ for some $\widehat{\Omega} > 0$, or equivalently, if and only if $\Omega_j = m_j\widetilde{\Omega}$,

$m_j \in \mathbb{Z}\backslash\{0\}$ for some $\widetilde{\Omega} > 0$. f has the fundamental period $\Omega > 0$ if every period of f is an integer multiple of Ω.

For any quasi-periodic (in fact, Bohr (uniformly) almost periodic) function f, the mean value $\langle f \rangle$ of f, defined by

$$\langle f \rangle = \lim_{R\to\infty} \frac{1}{2R} \int_{x_0-R}^{x_0+R} dx\, f(x), \tag{3.19}$$

exists and is independent of $x_0 \in \mathbb{R}$. Moreover, we recall the following facts (also valid for Bohr (uniformly) almost periodic functions on $\mathbb{R}$), see, for instance, [8, Ch. I], [11, Sects. 39–92], [15, Ch. I], [21, Chs. 1,3,6], [32], [40, Chs. 1,2,6], and [49].

Theorem 3.3. *Assume $f, g \in QP(\mathbb{R})$ and $x_0, x \in \mathbb{R}$. Then the following assertions hold:*
(i) f is uniformly continuous on $\mathbb{R}$ and $f \in L^\infty(\mathbb{R}; dx)$.
(ii) $\overline{f}$, $d\,f$, $d \in \mathbb{C}$, $f(\cdot + c)$, $f(c\cdot)$, $c \in \mathbb{R}$, $|f|^\alpha$, $\alpha \geq 0$ are all in $QP(\mathbb{R})$.
(iii) $f + g, fg \in QP(\mathbb{R})$.
(iv) $f/g \in QP(\mathbb{R})$ if and only if $\inf_{s\in\mathbb{R}}[|g(s)|] > 0$.
(v) Let G be uniformly continuous on $\mathcal{M} \subseteq \mathbb{R}$ and $f(s) \in \mathcal{M}$ for all $s \in \mathbb{R}$. Then $G(f) \in QP(\mathbb{R})$.
(vi) $f' \in QP(\mathbb{R})$ if and only if f' is uniformly continuous on $\mathbb{R}$.
(vii) Let $F(x) = \int_{x_0}^x dx'\, f(x')$ with $\langle f \rangle = 0$. Then $\int_{x_0}^x dx'\, f(x') \underset{|x|\to\infty}{=} o(|x|)$.
(viii) Let $F(x) = \int_{x_0}^x dx'\, f(x')$. Then $F \in QP(\mathbb{R})$ if and only if $F \in L^\infty(\mathbb{R}; dx)$.
(ix) If $0 \leq f \in QP(\mathbb{R})$, $f \not\equiv 0$, then $\langle f \rangle > 0$.
(x) If $f = |f| \exp(i\varphi)$, then $|f| \in QP(\mathbb{R})$ and φ is of the type $\varphi(x) = cx + \psi(x)$, where $c \in \mathbb{R}$ and $\psi \in QP(\mathbb{R})$ (and real-valued).
(xi) If $F(x) = \exp\Big(\int_{x_0}^x dx'\, f(x')\Big)$, then $F \in QP(\mathbb{R})$ if and only if $f(x) = i\beta + \psi(x)$, where $\beta \in \mathbb{R}$, $\psi \in QP(\mathbb{R})$, and $\Psi \in L^\infty(\mathbb{R}; dx)$, where $\Psi(x) = \int_{x_0}^x dx'\, \psi(x')$.

For the rest of this section and the next it will be convenient to introduce the following hypothesis:

Hypothesis 3.4. Assume the affine part of $\mathcal{K}_n$ to be nonsingular. Moreover, suppose that $V \in C^\infty(\mathbb{R}) \cap QP(\mathbb{R})$ satisfies the nth stationary KdV equation (2.10) on $\mathbb{R}$.

Next, we note the following result.

Lemma 3.5. *Assume Hypothesis* 3.4*. Then $V^{(k)}$, $k \in \mathbb{N}$, and f_ℓ, $\ell \in \mathbb{N}$, and hence all x and z-derivatives of $F_n(z, \cdot)$, $z \in \mathbb{C}$, and $g(z, \cdot)$,*

$z \in \Pi$, are quasi-periodic. Moreover, taking limits to points on $\mathcal{C}$, the last result extends to either side of the cuts in the set $\mathcal{C}\backslash\{E_m\}_{m=0}^{2n}$ (cf. (A.3)) *by continuity with respect to z.*

Proof. Since by hypothesis $V \in C^\infty(\mathbb{R}) \cap L^\infty(\mathbb{R}; dx)$, s-KdV$_n(V) = 0$ implies $V^{(k)} \in L^\infty(\mathbb{R}; dx)$, $k \in \mathbb{N}$ and $f_\ell \in C^\infty(\mathbb{R}) \cap L^\infty(\mathbb{R}; dx)$, $\ell \in \mathbb{N}_0$, applying Remark 2.6. In particular $V^{(k)}$ is uniformly continuous on $\mathbb{R}$ and hence quasi-periodic for all $k \in \mathbb{N}$. Since the f_ℓ are differential polynomials with respect to V, also f_ℓ, $\ell \in \mathbb{N}$ are quasi-periodic. The corresponding assertion for $F_n(z, \cdot)$ then follows from (2.12) and that for $g(z, \cdot)$ follows from (3.14). □

For future purposes we introduce the set

$$\begin{aligned}\Pi_C = \Pi \Big\backslash \Big\{ &\{z \in \mathbb{C} \,|\, |z| \leq C+1\} \\ &\cup \{z \in \mathbb{C} \,|\, \mathrm{Re}(z) \geq \min_{m=0,\dots,2n} [\mathrm{Re}(E_m)] - 1, \\ &\qquad \min_{m=0,\dots,2n} [\mathrm{Im}(E_m)] - 1 \leq \mathrm{Im}(z) \leq \max_{m=0,\dots,2n} [\mathrm{Im}(E_m)] + 1\} \Big\},\end{aligned} \tag{3.20}$$

where $C > 0$ is the constant in (2.53). Moreover, without loss of generality, we may assume Π_C contains no cuts, that is,

$$\Pi_C \cap \mathcal{C} = \emptyset. \tag{3.21}$$

Lemma 3.6. *Assume Hypothesis* 3.4 *and let $z, z_0 \in \Pi$. Then*

$$\big\langle g(z, \cdot)^{-1} \big\rangle = -2 \int_{z_0}^{z} dz' \, \langle g(z', \cdot) \rangle + \big\langle g(z_0, \cdot)^{-1} \big\rangle, \tag{3.22}$$

where the path connecting z_0 and z is assumed to lie in the cut plane Π. Moreover, by taking limits to points on $\mathcal{C}$ in (3.22)*, the result* (3.22) *extends to either side of the cuts in the set $\mathcal{C}$ by continuity with respect to z.*

Proof. Let $z, z_0 \in \Pi_C$. Integrating equation (3.7) from z_0 to z along a smooth path in Π_C yields

$$\begin{aligned} g(z,x)^{-1} - g(z_0,x)^{-1} &= -2 \int_{z_0}^{z} dz' \, g(z',x) + [g_{xx}(z,x) - g_{xx}(z_0,x)] \\ &\quad - \int_{z_0}^{z} dz' \, \big[g(z',x)^{-1} g_x(z',x) g_z(z',x) \big]_x \\ &= -2 \int_{z_0}^{z} dz' \, g(z',x) + g_{xx}(z,x) - g_{xx}(z_0,x) \\ &\quad - \bigg[\int_{z_0}^{z} dz' \, g(z',x)^{-1} g_x(z',x) g_z(z',x) \bigg]_x. \end{aligned} \tag{3.23}$$

By Lemma 3.5 $g(z,\cdot)$ and all its x-derivatives are quasi-periodic,

$$\langle g_{xx}(z,\cdot)\rangle = 0, \quad z \in \Pi. \tag{3.24}$$

Since we actually assumed $z \in \Pi_C$, also $g(z,\cdot)^{-1}$ is quasi-periodic. Consequently, also

$$\int_{z_0}^{z} dz'\, g(z',\cdot)^{-1} g_x(z',\cdot) g_z(z',\cdot), \quad z \in \Pi_C, \tag{3.25}$$

is a family of uniformly almost periodic functions for z varying in compact subsets of Π_C as discussed in [21, Sect. 2.7] and one obtains

$$\bigg\langle \bigg[\int_{z_0}^{z} dz'\, g(z',\cdot)^{-1} g_x(z',\cdot) g_z(z',\cdot) \bigg]_x \bigg\rangle = 0. \tag{3.26}$$

Hence, taking mean values in (3.23) (taking into account (3.24) and (3.26)), proves (3.22) for $z \in \Pi_C$. Since f_ℓ, $\ell \in \mathbb{N}_0$, are quasi-periodic by Lemma 3.5 (we recall that $f_0 = 1$), (2.12) and (3.13) yield

$$\int_{z_0}^{z} dz'\, \langle g(z',\cdot)\rangle = \frac{i}{2} \sum_{\ell=0}^{n} \langle f_{n-\ell}\rangle \int_{z_0}^{z} dz' \, \frac{(z')^\ell}{R_{2n+1}(z')^{1/2}}. \tag{3.27}$$

Thus, $\int_{z_0}^{z} dz'\, \langle g(z',\cdot)\rangle$ has an analytic continuation with respect to z to all of Π and consequently, (3.22) for $z \in \Pi_C$ extends by analytic continuation to $z \in \Pi$. By continuity this extends to either side of the cuts in $\mathcal{C}$. Interchanging the role of z and z_0, analytic continuation with respect to z_0 then yields (3.22) for $z, z_0 \in \Pi$. □

Remark 3.7. For $z \in \Pi_C$, $g(z,\cdot)^{-1}$ is quasi-periodic and hence the mean value $\langle g(z,\cdot)^{-1}\rangle$ is well-defined. If one analytically continues $g(z,x)$ with respect to z, $g(z,x)$ will acquire zeros for some $x \in \mathbb{R}$ and hence $g(z,\cdot)^{-1} \notin QP(\mathbb{R})$. Nevertheless, as shown by the right-hand side of (3.22), $\langle g(z,\cdot)^{-1}\rangle$ admits an analytic continuation in z from Π_C to all of Π, and from now on, $\langle g(z,\cdot)^{-1}\rangle$, $z \in \Pi$, always denotes that analytic continuation (cf. also (3.29)).

Next, we will invoke the Baker–Akhiezer function $\psi(P,x,x_0)$ and analyze the expression $\langle g(z,\cdot)^{-1}\rangle$ in more detail.

Theorem 3.8. *Assume Hypothesis* 3.4*, let* $P = (z,y) \in \Pi_\pm$*, and* $x, x_0 \in \mathbb{R}$*. Moreover, select a homology basis* $\{\tilde a_j, \tilde b_j\}_{j=1}^n$ *on* $\mathcal{K}_n$ *such that* $\underline{\widetilde B} = i\underline{\widetilde U}_0^{(2)}$*, with* $\underline{\widetilde U}_0^{(2)}$ *the vector of* $\tilde b$*-periods of the normalized differential of the second kind,* $\widetilde\omega_{P_\infty,0}^{(2)}$*, satisfies the constraint*

$$\underline{\widetilde B} = i\underline{\widetilde U}_0^{(2)} \in \mathbb{R}^n \tag{3.28}$$

(*cf. Appendix* B). *Then,*

$$\mathrm{Re}\big(\big\langle g(P,\cdot)^{-1}\big\rangle\big) = -2\mathrm{Im}\big(y\big\langle F_n(z,\cdot)^{-1}\big\rangle\big) = 2\mathrm{Im}\bigg(\int_{Q_0}^{P} \widetilde{\omega}^{(2)}_{P_\infty,0} - \tilde{e}^{(2)}_0(Q_0)\bigg). \tag{3.29}$$

Proof. Using (2.44), one obtains for $z \in \Pi_C$,

$$\begin{aligned}\psi(P,x,x_0) &= \bigg(\frac{F_n(z,x)}{F_n(z,x_0)}\bigg)^{1/2} \exp\bigg(iy\int_{x_0}^{x} dx'\, F_n(z,x')^{-1}\bigg)\\ &= \bigg(\frac{F_n(z,x)}{F_n(z,x_0)}\bigg)^{1/2} \exp\bigg(iy\int_{x_0}^{x} dx'\, \big[F_n(z,x')^{-1} - \big\langle F_n(z,\cdot)^{-1}\big\rangle\big]\bigg)\\ &\quad\times \exp\big(i(x-x_0)y\big\langle F_n(z,\cdot)^{-1}\big\rangle\big), \\ &\quad P=(z,y)\in\Pi_\pm,\ z\in\Pi_C,\ x,x_0\in\mathbb{R}.\end{aligned} \tag{3.30}$$

Since $\big[F_n(z,x')^{-1} - \big\langle F_n(z,\cdot)^{-1}\big\rangle\big]$ has mean zero,

$$\bigg|\int_{x_0}^{x} dx'\, \big[F_n(z,x')^{-1} - \langle F_n(z,\cdot)^{-1}\rangle\big]\bigg| \underset{|x|\to\infty}{=} o(|x|), \quad z\in\Pi_C \tag{3.31}$$

by Theorem 3.3 (vii). In addition, the factor $F_n(z,x)/F_n(z,x_0)$ in (3.30) is quasi-periodic and hence bounded on $\mathbb{R}$.

On the other hand, (2.63) yields

$$\begin{aligned}\psi(P,x,x_0) &= \frac{\theta(\underline{z}(P_\infty,\underline{\hat{\mu}}(x_0)))\theta(\underline{z}(P,\underline{\hat{\mu}}(x)))}{\theta(\underline{z}(P_\infty,\underline{\hat{\mu}}(x)))\theta(\underline{z}(P,\underline{\hat{\mu}}(x_0)))}\\ &\qquad\times \exp\bigg[-i(x-x_0)\bigg(\int_{Q_0}^{P}\widetilde{\omega}^{(2)}_{P_\infty,0} - \tilde{e}^{(0)}_0(Q_0)\bigg)\bigg]\\ &= \Theta(P,x,x_0)\exp\bigg[-i(x-x_0)\bigg(\int_{Q_0}^{P}\widetilde{\omega}^{(2)}_{P_\infty,0} - \tilde{e}^{(2)}_0(Q_0)\bigg)\bigg],\\ &\qquad P\in\mathcal{K}_n\backslash\big\{\{P_\infty\}\cup\{\hat{\mu}_j(x_0)\}_{j=1}^n\big\}.\end{aligned} \tag{3.32}$$

Taking into account (2.62), (2.64), (2.70), (A.30), and the fact that by (2.53) no $\hat{\mu}_j(x)$ can reach P_∞ as x varies in $\mathbb{R}$, one concludes that

$$\Theta(P,\cdot,x_0)\in L^\infty(\mathbb{R};dx), \quad P\in\mathcal{K}_n\backslash\{\hat{\mu}_j(x_0)\}_{j=1}^n. \tag{3.33}$$

A comparison of (3.30) and (3.32) then shows that the $o(|x|)$-term in (3.31) must actually be bounded on $\mathbb{R}$ and hence the left-hand side of (3.31) is quasi-periodic. In addition, the term

$$\exp\bigg(iR_{2n+1}(z)^{1/2}\int_{x_0}^{x} dx'\,\big[F_n(z,x')^{-1} - \big\langle F_n(z,\cdot)^{-1}\big\rangle\big]\bigg), \quad z\in\Pi_C, \tag{3.34}$$

is then quasi-periodic by Theorem 3.3 (xi). A further comparison of (3.30) and (3.32) then yields (3.29) for $z \in \Pi_C$. Analytic continuation with respect to z then yields (3.29) for $z \in \Pi$. By continuity with respect to z, taking boundary values to either side of the cuts in the set $\mathcal{C}$, this then extends to $z \in \mathcal{C}$ (cf. (A.3), (A.4)) and hence proves (3.29) for $P = (z, y) \in \mathcal{K}_n \backslash \{P_\infty\}$. □

4. Spectra of Schrödinger operators with quasi-periodic algebro-geometric KdV potentials

In this section we establish the connection between the algebro-geometric formalism of Section 2 and the spectral theoretic description of Schrödinger operators H in $L^2(\mathbb{R}; dx)$ with quasi-periodic algebro-geometric KdV potentials. In particular, we introduce the conditional stability set of H and prove our principal result, the characterization of the spectrum of H. Finally, we provide a qualitative description of the spectrum of H in terms of analytic spectral arcs.

Suppose that $V \in C^\infty(\mathbb{R}) \cap QP(\mathbb{R})$ satisfies the nth stationary KdV equation (2.10) on $\mathbb{R}$. The corresponding Schrödinger operator H in $L^2(\mathbb{R}; dx)$ is then introduced by

$$H = -\frac{d^2}{dx^2} + V, \quad \mathrm{dom}(H) = H^{2,2}(\mathbb{R}). \tag{4.1}$$

Thus, H is a densely defined closed operator in $L^2(\mathbb{R}; dx)$ (it is self-adjoint if and only if V is real-valued).

Before we turn to the spectrum of H in the general non-self-adjoint case, we briefly mention the following result on the spectrum of H in the self-adjoint case with a quasi-periodic (or almost periodic) real-valued potential q. We denote by $\sigma(A)$, $\sigma_{\mathrm{e}}(A)$, and $\sigma_{\mathrm{d}}(A)$ the spectrum, essential spectrum, and discrete spectrum of a self-adjoint operator A in a complex Hilbert space, respectively.

Theorem 4.1 (See, e.g., [51]). *Let $V \in QP(\mathbb{R})$ and q be real-valued. Define the self-adjoint Schrödinger operator H in $L^2(\mathbb{R}; dx)$ as in* (4.1). *Then,*

$$\sigma(H) = \sigma_{\mathrm{e}}(H) \subseteq \big[\min_{x\in\mathbb{R}}(V(x)), \infty\big), \quad \sigma_{\mathrm{d}}(H) = \emptyset. \tag{4.2}$$

Moreover, $\sigma(H)$ contains no isolated points, that is, $\sigma(H)$ is a perfect set.

In the special periodic case where $V \in CP(\mathbb{R})$ is real-valued, the spectrum of H is purely absolutely continuous and either a finite union of some compact intervals and a half-line or an infinite union of compact intervals (see, e.g., [18, Sect. 5.3], [47, Sect. XIII.16]). If $V \in CP(\mathbb{R})$

and V is complex-valued, then the spectrum of H is purely continuous and it consists of either a finite union of simple analytic arcs and one simple semi-infinite analytic arc tending to infinity or an infinite union of simple analytic arcs (cf. [48], [50], and [53])[7].

Remark 4.2. Here $\sigma \subset \mathbb{C}$ is called an *arc* if there exists a parameterization $\gamma \in C([0,1])$ such that $\sigma = \{\gamma(t) \,|\, t \in [0,1]\}$. The arc σ is called *simple* if there exists a parameterization γ such that $\gamma\colon [0,1] \to \mathbb{C}$ is injective. The arc σ is called *analytic* if there is a parameterization γ that is analytic at each $t \in [0,1]$. Finally, σ_∞ is called a *semi-infinite* arc if there exists a parameterization $\gamma \in C([0,\infty))$ such that $\sigma_\infty = \{\gamma(t) \,|\, t \in [0,\infty)\}$ and σ_∞ is an unbounded subset of $\mathbb{C}$. Analytic semi-infinite arcs are defined analogously and by a simple semi-infinite arc we mean one that is without self-intersection (i.e., corresponds to a injective parameterization) with the additional restriction that the unbounded part of σ_∞ consists of precisely one branch tending to infinity.

Now we turn to the analyis of the generally non-self-adjoint operator H in (4.1). Assuming Hypothesis 3.4 we now introduce the set $\Sigma \subset \mathbb{C}$ by

$$\Sigma = \big\{\lambda \in \mathbb{C} \,\big|\, \mathrm{Re}\big(\big\langle g(\lambda,\cdot)^{-1}\big\rangle\big) = 0\big\}. \tag{4.3}$$

Below we will show that Σ plays the role of the conditional stability set of H, familiar from the spectral theory of one-dimensional periodic Schrödinger operators (cf. [18, Sect. 5.3], [48], [57], [58]).

Lemma 4.3. *Assume Hypothesis* 3.4*. Then Σ coincides with the conditional stability set of H, that is,*

$$\begin{aligned}\Sigma = \{\lambda \in \mathbb{C} \,|\, &\textit{there exists at least one bounded distributional solution} \\ &0 \neq \psi \in L^\infty(\mathbb{R};dx) \ \textit{of } H\psi = \lambda\psi.\}\end{aligned} \tag{4.4}$$

Proof. By (3.32) and (3.33),

$$\psi(P,x) = \frac{\theta(\underline{z}(P,\underline{\hat\mu}(x)))}{\theta(\underline{z}(P_\infty,\underline{\hat\mu}(x)))} \exp\bigg[-ix\bigg(\int_{Q_0}^{P} \widetilde\omega^{(2)}_{P_\infty,0} - \tilde e^{(0)}_0(Q_0)\bigg)\bigg], \quad P = (z,y) \in \Pi_\pm, \tag{4.5}$$

is a distributional solution of $H\psi = z\psi$ which is bounded on $\mathbb{R}$ if and only if the exponential function in (4.5) is bounded on $\mathbb{R}$. By (3.29), the latter holds if and only if

$$\mathrm{Re}\big(\big\langle g(z,\cdot)^{-1}\big\rangle\big) = 0. \tag{4.6}$$

□

[7] in either case the resolvent set is connected.

Remark 4.4. At first sight our *a priori* choice of cuts $\mathcal{C}$ for $R_{2n+1}(\cdot)^{1/2}$, as described in Appendix A, might seem unnatural as they completely ignore the actual spectrum of H. However, the spectrum of H is not known from the outset, and in the case of complex-valued periodic potentials, spectral arcs of H may actually cross each other (cf. [26], [46], and Theorem 4.9 (iv)) which renders them unsuitable for cuts of $R_{2n+1}(\cdot)^{1/2}$.

Before we state our first principal result on the spectrum of H, we find it convenient to recall a number of basic definitions and well-known facts in connection with the spectral theory of non-self-adjoint operators (we refer to [19, Chs. I, III, IX], [29, Sects. 1, 21–23], [33, Sects. IV.5.6, V.3.2], and [47, p. 178–179] for more details). Let S be a densely defined closed operator in a complex separable Hilbert space $\mathcal{H}$. Denote by $\mathcal{B}(\mathcal{H})$ the Banach space of all bounded linear operators on $\mathcal{H}$ and by $\ker(T)$ and $\operatorname{ran}(T)$ the kernel (null space) and range of a linear operator T in $\mathcal{H}$. The resolvent set, $\rho(S)$, spectrum, $\sigma(S)$, point spectrum (the set of eigenvalues), $\sigma_{\rm p}(S)$, continuous spectrum, $\sigma_{\rm c}(S)$, residual spectrum, $\sigma_{\rm r}(S)$, field of regularity, $\pi(S)$, approximate point spectrum, $\sigma_{\rm ap}(S)$, two kinds of essential spectra, $\sigma_{\rm e}(S)$, and $\widetilde{\sigma}_{\rm e}(S)$, the numerical range of S, $\Theta(S)$, and the sets $\Delta(S)$ and $\widetilde{\Delta}(S)$ are defined as follows:

$$\rho(S) = \{z \in \mathbb{C} \,|\, (S - zI)^{-1} \in \mathcal{B}(\mathcal{H})\}, \tag{4.7}$$

$$\sigma(S) = \mathbb{C} \backslash \rho(S), \tag{4.8}$$

$$\sigma_{\rm p}(S) = \{\lambda \in \mathbb{C} \,|\, \ker(S - \lambda I) \neq \{0\}\}, \tag{4.9}$$

$$\sigma_{\rm c}(S) = \{\lambda \in \mathbb{C} \,|\, \ker(S - \lambda I) = \{0\} \text{ and } \operatorname{ran}(S - \lambda I) \text{ is dense in } \mathcal{H} \text{ but not equal to } \mathcal{H}\}, \tag{4.10}$$

$$\sigma_{\rm r}(S) = \{\lambda \in \mathbb{C} \,|\, \ker(S - \lambda I) = \{0\} \text{ and } \operatorname{ran}(S - \lambda I) \text{ is not dense in } \mathcal{H}\}, \tag{4.11}$$

$$\pi(S) = \{z \in \mathbb{C} \,|\, \text{there exists } k_z > 0 \text{ s.t. } \|(S - zI)u\|_{\mathcal{H}} \geq k_z \|u\|_{\mathcal{H}} \text{ for all } u \in \operatorname{dom}(S)\}, \tag{4.12}$$

$$\sigma_{\rm ap}(S) = \mathbb{C} \backslash \pi(S), \tag{4.13}$$

$$\Delta(S) = \{z \in \mathbb{C} \,|\, \dim(\ker(S - zI)) < \infty \text{ and } \operatorname{ran}(S - zI) \text{ is closed}\}, \tag{4.14}$$

$$\sigma_{\rm e}(S) = \mathbb{C} \backslash \Delta(S), \tag{4.15}$$

$$\widetilde{\Delta}(S) = \{z \in \mathbb{C} \,|\, \dim(\ker(S - zI)) < \infty \text{ or } \dim(\ker(S^* - \overline{z}I)) < \infty\}, \tag{4.16}$$

$$\widetilde{\sigma}_{\rm e}(S) = \mathbb{C} \backslash \widetilde{\Delta}(S), \tag{4.17}$$

$$\Theta(S) = \{(f, Sf) \in \mathbb{C} \,|\, f \in \mathrm{dom}(S),\ \|f\|_{\mathcal{H}} = 1\}, \tag{4.18}$$

respectively. One then has

$$\begin{aligned}
\sigma(S) &= \sigma_{\mathrm{p}}(S) \cup \sigma_{\mathrm{c}}(S) \cup \sigma_{\mathrm{r}}(S) \quad \text{(disjoint union)} && (4.19)\\
&= \sigma_{\mathrm{p}}(S) \cup \sigma_{\mathrm{e}}(S) \cup \sigma_{\mathrm{r}}(S), && (4.20)\\
\sigma_{\mathrm{c}}(S) &\subseteq \sigma_{\mathrm{e}}(S)\backslash(\sigma_{\mathrm{p}}(S) \cup \sigma_{\mathrm{r}}(S)), && (4.21)\\
\sigma_{\mathrm{r}}(S) &= \sigma_{\mathrm{p}}(S^*)^*\backslash\sigma_{\mathrm{p}}(S), && (4.22)\\
\sigma_{\mathrm{ap}}(S) &= \{\lambda \in \mathbb{C} \,|\, \text{there exists a sequence } \{f_n\}_{n\in\mathbb{N}} \subset \mathrm{dom}(S)\\
&\qquad \text{with } \|f_n\|_{\mathcal{H}} = 1,\ n \in \mathbb{N}, \text{ and } \lim_{n\to\infty} \|(S - \lambda I)f_n\|_{\mathcal{H}} = 0\}, && (4.23)\\
\widetilde{\sigma}_{\mathrm{e}}(S) &\subseteq \sigma_{\mathrm{e}}(S) \subseteq \sigma_{\mathrm{ap}}(S) \subseteq \sigma(S) \ \text{ (all four sets are closed)}, && (4.24)\\
\rho(S) &\subseteq \pi(S) \subseteq \Delta(S) \subseteq \widetilde{\Delta}(S) \quad \text{(all four sets are open)}, && (4.25)\\
\widetilde{\sigma}_{\mathrm{e}}(S) &\subseteq \overline{\Theta(S)}, \quad \Theta(S) \ \text{ is convex}, && (4.26)\\
\widetilde{\sigma}_{\mathrm{e}}(S) &= \sigma_{\mathrm{e}}(S) \ \text{ if } S = S^*. && (4.27)
\end{aligned}$$

Here σ^* in the context of (4.22) denotes the complex conjugate of the set $\sigma \subseteq \mathbb{C}$, that is,

$$\sigma^* = \{\overline{\lambda} \in \mathbb{C} \,|\, \lambda \in \sigma\}. \tag{4.28}$$

We note that there are several other versions of the concept of the essential spectrum in the non-self-adjoint context (cf. [19, Ch. IX]) but we will only use the two in (4.15) and in (4.17) in this paper.

Finally, we recall the following result due to Talenti [52] and Tomaselli [56] (see also Chisholm and Everitt [13], Chisholm, Everitt, and Littlejohn [14], and Muckenhoupt [42]).

Lemma 4.5. *Let $f \in L^2(\mathbb{R}; dx)$, $U \in L^2((-\infty, R]; dx)$, and $V \in L^2([R, \infty); dx)$ for all $R \in \mathbb{R}$. Then the following assertions (i)–(iii) are equivalent:*
(i) *There exists a finite constant $C > 0$ such that*

$$\int_{\mathbb{R}} dx \left| U(x) \int_x^\infty dx'\, V(x')f(x') \right|^2 \leq C \int_{\mathbb{R}} dx\, |f(x)|^2. \tag{4.29}$$

(ii) *There exists a finite constant $D > 0$ such that*

$$\int_{\mathbb{R}} dx \left| V(x) \int_{-\infty}^x dx'\, U(x')f(x') \right|^2 \leq D \int_{\mathbb{R}} dx\, |f(x)|^2. \tag{4.30}$$

(iii)

$$\sup_{r\in\mathbb{R}} \left[\left(\int_{-\infty}^r dx\, |U(x)|^2 \right) \left(\int_r^\infty dx\, |V(x)|^2 \right) \right] < \infty. \tag{4.31}$$

We start with the following elementary result.

Lemma 4.6. *Let* H *be defined as in* (4.1). *Then,*

$$\sigma_{\mathrm{e}}(H) = \widetilde{\sigma}_{\mathrm{e}}(H) \subseteq \overline{\Theta(H)}. \tag{4.32}$$

Proof. Since H and H^* are second-order ordinary differential operators on $\mathbb{R}$,

$$\dim(\ker(H - zI)) \le 2, \quad \dim(\ker(H^* - \overline{z}I)) \le 2. \tag{4.33}$$

Equations (4.14)–(4.17) and (4.26) then prove (4.32). □

Theorem 4.7. *Assume Hypothesis* 3.4. *Then the point spectrum and residual spectrum of* H *are empty and hence the spectrum of* H *is purely continuous,*

$$\sigma_{\mathrm{p}}(H) = \sigma_{\mathrm{r}}(H) = \emptyset, \tag{4.34}$$

$$\sigma(H) = \sigma_{\mathrm{c}}(H) = \sigma_{\mathrm{e}}(H) = \sigma_{\mathrm{ap}}(H). \tag{4.35}$$

Proof. First we prove the absence of the point spectrum of H. Suppose $z \in \Pi\backslash\{\Sigma \cup \{\mu_j(x_0)\}_{j=1}^n\}$. Then $\psi(P,\cdot,x_0)$ and $\psi(P^*,\cdot,x_0)$ are linearly independent distributional solutions of $H\psi = z\psi$ which are unbounded at $+\infty$ or $-\infty$. This argument extends to all $z \in \Pi\backslash\Sigma$ by multiplying $\psi(P,\cdot,x_0)$ and $\psi(P^*,\cdot,x_0)$ with an appropriate function of z and x_0 (independent of x). It also extends to either side of the cut $\mathcal{C}\backslash\Sigma$ by continuity with respect to z. On the other hand, since $V^{(k)} \in L^\infty(\mathbb{R};dx)$ for all $k \in \mathbb{N}_0$, any distributional solution $\psi(z,\cdot) \in L^2(\mathbb{R};dx)$ of $H\psi = z\psi$, $z \in \mathbb{C}$, is necessarily bounded. In fact,

$$\psi^{(k)}(z,\cdot) \in L^\infty(\mathbb{R};dx) \cap L^2(\mathbb{R};dx), \quad k \in \mathbb{N}_0, \tag{4.36}$$

applying $\psi''(z,x) = (V(x)-z)\psi(z,x)$ and (2.55) with $p = 2$ and $p = \infty$ repeatedly. (Indeed, $\psi(z,\cdot) \in L^2(\mathbb{R};dx)$ implies $\psi''(z,\cdot) \in L^2(\mathbb{R};dx)$ which in turn implies $\psi'(z,\cdot) \in L^2(\mathbb{R};dx)$. Integrating $(\psi^2)' = 2\psi\psi'$ then yields $\psi(z,\cdot) \in L^\infty(\mathbb{R};dx)$. The latter yields $\psi''(z,\cdot) \in L^\infty(\mathbb{R};dx)$, etc.) Thus,

$$\{\mathbb{C}\backslash\Sigma\} \cap \sigma_{\mathrm{p}}(H) = \emptyset. \tag{4.37}$$

Hence, it remains to rule out eigenvalues located in Σ. We consider a fixed $\lambda \in \Sigma$ and note that by (2.45), there exists at least one distributional solution $\psi_1(\lambda,\cdot) \in L^\infty(\mathbb{R};dx)$ of $H\psi = \lambda\psi$. Actually, a comparison of (2.44) and (4.3) shows that we may choose $\psi_1(\lambda,\cdot)$ such that $|\psi_1(\lambda,\cdot)| \in QP(\mathbb{R})$ and hence $\psi_1(\lambda,\cdot) \notin L^2(\mathbb{R};dx)$. As in (4.36) one then infers from repeated use of $\psi''(\lambda) = (V-\lambda)\psi(\lambda)$ and (2.55) with $p = \infty$ that

$$\psi_1^{(k)}(\lambda,\cdot) \in L^\infty(\mathbb{R};dx), \quad k \in \mathbb{N}_0. \tag{4.38}$$

Next, suppose there exists a second distributional solution $\psi_2(\lambda,\cdot)$ of $H\psi = \lambda\psi$ which is linearly independent of $\psi_1(\lambda,\cdot)$ and which satisfies $\psi_2(\lambda,\cdot) \in L^2(\mathbb{R}; dx)$. Applying (4.36) then yields

$$\psi_2^{(k)}(\lambda,\cdot) \in L^2(\mathbb{R}; dx), \quad k \in \mathbb{N}_0. \tag{4.39}$$

Combining (4.38) and (4.39), one concludes that the Wronskian of $\psi_1(\lambda,\cdot)$ and $\psi_2(\lambda,\cdot)$ lies in $L^2(\mathbb{R}; dx)$,

$$W(\psi_1(\lambda,\cdot), \psi_2(\lambda,\cdot)) \in L^2(\mathbb{R}; dx). \tag{4.40}$$

However, by hypothesis, $W(\psi_1(\lambda,\cdot), \psi_2(\lambda,\cdot)) = c(\lambda) \neq 0$ is a nonzero constant. This contradiction proves that

$$\Sigma \cap \sigma_{\mathrm{p}}(H) = \emptyset \tag{4.41}$$

and hence $\sigma_{\mathrm{p}}(H) = \emptyset$.

Next, we note that the same argument yields that H^* also has no point spectrum,

$$\sigma_{\mathrm{p}}(H^*) = \emptyset. \tag{4.42}$$

Indeed, if $V \in C^\infty(\mathbb{R}) \cap QP(\mathbb{R})$ satisfies the nth stationary KdV equation (2.10) on $\mathbb{R}$, then $\overline{V}$ also satisfies one of the nth stationary KdV equations (2.10) associated with a hyperelliptic curve of genus n with $\{E_m\}_{m=0}^{2n}$ replaced by $\{\overline{E}_m\}_{m=0}^{2n}$, etc. Since by general principles (cf. (4.28)),

$$\sigma_{\mathrm{r}}(B) \subseteq \sigma_{\mathrm{p}}(B^*)^* \tag{4.43}$$

for any densely defined closed linear operator B in some complex separable Hilbert space (see, e.g., [30, p. 71]), one obtains $\sigma_{\mathrm{r}}(H) = \emptyset$ and hence (4.34). This proves that the spectrum of H is purely continuous, $\sigma(H) = \sigma_{\mathrm{c}}(H)$. The remaining equalities in (4.35) then follow from (4.21) and (4.24). □

The following result is a fundamental one:

Theorem 4.8. *Assume Hypothesis* 3.4. *Then the spectrum of H coincides with Σ and hence equals the conditional stability set of H,*

$$\sigma(H) = \big\{\lambda \in \mathbb{C} \,\big|\, \mathrm{Re}\big(\big\langle g(\lambda,\cdot)^{-1}\big\rangle\big) = 0\big\} \tag{4.44}$$

$$= \{\lambda \in \mathbb{C} \,|\, \textit{there exists at least one bounded distributional solution } 0 \neq \psi \in L^\infty(\mathbb{R}; dx) \textit{ of } H\psi = \lambda\psi\}. \tag{4.45}$$

In particular,

$$\{E_m\}_{m=0}^{2n} \subset \sigma(H), \tag{4.46}$$

and $\sigma(H)$ contains no isolated points.

Proof. First we will prove that

$$\sigma(H) \subseteq \Sigma \tag{4.47}$$

by adapting a method due to Chisholm and Everitt [13]. For this purpose we temporarily choose $z \in \Pi\backslash\{\Sigma \cup \{\mu_j(x_0)\}_{j=1}^n\}$ and construct the resolvent of H as follows. Introducing the two branches $\psi_\pm(P,x,x_0)$ of the Baker–Akhiezer function $\psi(P,x,x_0)$ by

$$\psi_\pm(P,x,x_0) = \psi(P,x,x_0), \quad P = (z,y) \in \Pi_\pm, \ x, x_0 \in \mathbb{R}, \tag{4.48}$$

we define

$$\hat\psi_+(z,x,x_0) = \begin{cases} \psi_+(z,x,x_0) & \text{if } \psi_+(z,\cdot,x_0) \in L^2((x_0,\infty);dx), \\ \psi_-(z,x,x_0) & \text{if } \psi_-(z,\cdot,x_0) \in L^2((x_0,\infty);dx), \end{cases} \tag{4.49}$$

$$\hat\psi_-(z,x,x_0) = \begin{cases} \psi_-(z,x,x_0) & \text{if } \psi_-(z,\cdot,x_0) \in L^2((-\infty,x_0);dx), \\ \psi_+(z,x,x_0) & \text{if } \psi_+(z,\cdot,x_0) \in L^2((-\infty,x_0);dx), \end{cases}$$
$$z \in \Pi\backslash\Sigma, \ x, x_0 \in \mathbb{R}, \tag{4.50}$$

and

$$\begin{aligned} G(z,x,x') = {} & \frac{1}{W(\hat\psi_+(z,x,x_0), \hat\psi_-(z,x,x_0))} \\ & \times \begin{cases} \hat\psi_-(z,x',x_0)\hat\psi_+(z,x,x_0), & x \geq x', \\ \hat\psi_-(z,x,x_0)\hat\psi_+(z,x',x_0), & x \leq x', \end{cases} \\ & z \in \Pi\backslash\Sigma, \ x, x_0 \in \mathbb{R}. \end{aligned} \tag{4.51}$$

Due to the homogeneous nature of G, (4.51) extends to all $z \in \Pi$. Moreover, we extend (4.49)–(4.51) to either side of the cut $\mathcal{C}$ except at possible points in Σ (i.e., to $\mathcal{C}\backslash\Sigma$) by continuity with respect to z, taking limits to $\mathcal{C}\backslash\Sigma$. Next, we introduce the operator $R(z)$ in $L^2(\mathbb{R};dx)$ defined by

$$(R(z)f)(x) = \int_{\mathbb{R}} dx'\, G(z,x,x')f(x'), \quad f \in C_0^\infty(\mathbb{R}), \ z \in \Pi, \tag{4.52}$$

and extend it to $z \in \mathcal{C}\backslash\Sigma$, as discussed in connection with $G(\cdot,x,x')$. The explicit form of $\hat\psi_\pm(z,x,x_0)$, inferred from (3.32) by restricting P to $\Pi_\pm$, then yields the estimates

$$|\hat\psi_\pm(z,x,x_0)| \leq C_\pm(z,x_0)e^{\mp\kappa(z)x}, \quad z \in \Pi\backslash\Sigma, \ x \in \mathbb{R} \tag{4.53}$$

for some constants $C_\pm(z,x_0) > 0$, $\kappa(z) > 0$, $z \in \Pi\backslash\Sigma$. An application of Lemma 4.5 identifying $U(x) = \exp(-\kappa(z)x)$ and $V(x) = \exp(\kappa(z)x)$ then proves that $R(z)$, $z \in \mathbb{C}\backslash\Sigma$, extends from $C_0^\infty(\mathbb{R})$ to a bounded linear operator defined on all of $L^2(\mathbb{R};dx)$. (Alternatively, one can follow the second part of the proof of Theorem 5.3.2 in [18] line by line.) A straightforward differentiation then proves

$$(H - zI)R(z)f = f, \quad f \in L^2(\mathbb{R}; dx),\ z \in \mathbb{C}\backslash\Sigma \tag{4.54}$$

and hence also

$$R(z)(H - zI)g = g, \quad g \in \mathrm{dom}(H),\ z \in \mathbb{C}\backslash\Sigma. \tag{4.55}$$

Thus, $R(z) = (H - zI)^{-1}$, $z \in \mathbb{C}\backslash\Sigma$, and hence (4.47) holds.

Next we will prove that

$$\sigma(H) \supseteq \Sigma. \tag{4.56}$$

We will adapt a strategy of proof applied by Eastham in the case of (real-valued) periodic potentials [17] (reproduced in the proof of Theorem 5.3.2 of [18]) to the (complex-valued) quasi-periodic case at hand. Suppose $\lambda \in \Sigma$. By the characterization (4.4) of Σ, there exists a bounded distributional solution $\psi(\lambda, \cdot)$ of $H\psi = \lambda\psi$. A comparison with the Baker-Akhiezer function (2.44) then shows that we can assume, without loss of generality, that

$$|\psi(\lambda, \cdot)| \in QP(\mathbb{R}). \tag{4.57}$$

Moreover, by the same argument as in the proof of Theorem 4.7 (cf. (4.38)), one obtains

$$\psi^{(k)}(\lambda, \cdot) \in L^\infty(\mathbb{R}; dx), \quad k \in \mathbb{N}_0. \tag{4.58}$$

Next, we pick $\Omega > 0$ and consider $g \in C^\infty([0, \Omega])$ satisfying

$$\begin{aligned} &g(0) = 0, \quad g(\Omega) = 1, \\ &g'(0) = g''(0) = g'(\Omega) = g''(\Omega) = 0, \\ &0 \le g(x) \le 1, \quad x \in [0, \Omega]. \end{aligned} \tag{4.59}$$

Moreover, we introduce the sequence $\{h_n\}_{n\in\mathbb{N}} \in L^2(\mathbb{R}; dx)$ by

$$h_n(x) = \begin{cases} 1, & |x| \le (n-1)\Omega, \\ g(n\Omega - |x|), & (n-1)\Omega \le |x| \le n\Omega, \\ 0, & |x| \ge n\Omega \end{cases} \tag{4.60}$$

and the sequence $\{f_n(\lambda)\}_{n\in\mathbb{N}} \in L^2(\mathbb{R}; dx)$ by

$$f_n(\lambda, x) = d_n(\lambda)\psi(\lambda, x)h_n(x), \quad x \in \mathbb{R},\ d_n(\lambda) > 0,\ n \in \mathbb{N}. \tag{4.61}$$

Here $d_n(\lambda)$ is determined by the requirement

$$\|f_n(\lambda)\|_2 = 1, \quad n \in \mathbb{N}. \tag{4.62}$$

One readily verifies that

$$f_n(\lambda, \cdot) \in \mathrm{dom}(H) = H^{2,2}(\mathbb{R}), \quad n \in \mathbb{N}. \tag{4.63}$$

Next, we note that as a consequence of Theorem 3.3 (ix),

$$\int_{-T}^{T} dx\, |\psi(\lambda,x)|^2 \underset{T\to\infty}{=} 2\big\langle |\psi(\lambda,\cdot)|^2\big\rangle T + o(T) \tag{4.64}$$

with

$$\big\langle |\psi(\lambda,\cdot)|^2\big\rangle > 0. \tag{4.65}$$

Thus, one computes

$$\begin{aligned} 1 &= \|f_n(\lambda)\|_2^2 = d_n(\lambda)^2 \int_{\mathbb{R}} dx\, |\psi(\lambda,x)|^2 h_n(x)^2 \\ &= d_n(\lambda)^2 \int_{|x|\le n\Omega} dx\, |\psi(\lambda,x)|^2 h_n(x)^2 \ge d_n(\lambda)^2 \int_{|x|\le (n-1)\Omega} dx\, |\psi(\lambda,x)|^2 \\ &\ge d_n(\lambda)^2 \big[\big\langle |\psi(\lambda,\cdot)|^2\big\rangle (n-1)\Omega + o(n)\big]. \end{aligned} \tag{4.66}$$

Consequently,

$$d_n(\lambda) \underset{n\to\infty}{=} O\big(n^{-1/2}\big). \tag{4.67}$$

Next, one computes

$$(H-\lambda I) f_n(\lambda,x) = -d_n(\lambda)[2\psi'(\lambda,x)h_n'(x) + \psi(\lambda,x)h_n''(x)] \tag{4.68}$$

and hence

$$\|(H-\lambda I)f_n\|_2 \le d_n(\lambda)[2\|\psi'(\lambda)h_n'\|_2 + \|\psi(\lambda)h_n''\|_2], \quad n\in\mathbb{N}. \tag{4.69}$$

Using (4.58) and (4.60) one estimates

$$\begin{aligned} \|\psi'(\lambda)h_n'\|_2^2 &= \int_{(n-1)\Omega\le |x|\le n\Omega} dx\, |\psi'(\lambda,x)|^2 |h_n'(x)|^2 \\ &\le 2\|\psi'(\lambda)\|_\infty^2 \int_0^\Omega dx\, |g'(x)|^2 \\ &\le 2\Omega \|\psi'(\lambda)\|_\infty^2 \|g'\|_{L^\infty([0,\Omega];dx)}^2, \end{aligned} \tag{4.70}$$

and similarly,

$$\begin{aligned} \|\psi(\lambda)h_n''\|_2^2 &= \int_{(n-1)\Omega\le |x|\le n\Omega} dx\, |\psi(\lambda,x)|^2 |h_n''(x)|^2 \\ &\le 2\|\psi(\lambda)\|_\infty^2 \int_0^\Omega dx\, |g''(x)|^2 \\ &\le 2\Omega \|\psi(\lambda)\|_\infty^2 \|g''\|_{L^\infty([0,\Omega];dx)}^2. \end{aligned} \tag{4.71}$$

Thus, combining (4.67) and (4.69)–(4.71) one infers

$$\lim_{n\to\infty} \|(H-\lambda I)f_n\|_2 = 0, \tag{4.72}$$

and hence $\lambda \in \sigma_{\rm ap}(H) = \sigma(H)$ by (4.23) and (4.35).

Relation (4.46) is clear from (4.4) and the fact that by (2.45) there exists a distributional solution $\psi((E_m,0),\cdot,x_0)\in L^\infty(\mathbb{R};dx)$ of $H\psi = E_m\psi$ for all $m=0,\dots,2n$.

Finally, $\sigma(H)$ contains no isolated points since those would necessarily be essential singularities of the resolvent of H, as H has no eigenvalues by (4.34) (cf. [33, Sect. III.6.5]). An explicit investigation of the Green's function of H reveals at most a square root singularity at the points $\{E_m\}_{m=0}^{2n}$ and hence excludes the possibility of an essential singularity of $(H-zI)^{-1}$. □

In the special self-adjoint case where V is real-valued, the result (4.44) is equivalent to the vanishing of the Lyapunov exponent of H which characterizes the (purely absolutely continous) spectrum of H as discussed by Kotani [34], [35], [36], [37] (see also [12, p. 372]). In the case where V is periodic and complex-valued, this has also been studied by Kotani [37].

The explicit formula for Σ in (4.3) permits a qualitative description of the spectrum of H as follows. We recall (3.22) and write

$$\frac{d}{dz}\big\langle g(z,\cdot)^{-1}\big\rangle = -2\langle g(z,\cdot)\rangle = -i\frac{\prod_{j=1}^{n}\big(z-\widetilde{\lambda}_j\big)}{\big(\prod_{m=0}^{2n}(z-E_m)\big)^{1/2}}, \quad z\in\Pi, \tag{4.73}$$

for some constants

$$\{\widetilde{\lambda}_j\}_{j=1}^{n}\subset\mathbb{C}. \tag{4.74}$$

As in similar situations before, (4.73) extends to either side of the cuts in $\mathcal{C}$ by continuity with respect to z.

Theorem 4.9. *Assume Hypothesis* 3.4. *Then the spectrum $\sigma(H)$ of H has the following properties:*
(i) $\sigma(H)$ is contained in the semi-strip

$$\sigma(H)\subset\{z\in\mathbb{C}\,|\,\mathrm{Im}(z)\in[M_1,M_2],\ \mathrm{Re}(z)\geq M_3\}, \tag{4.75}$$

where

$$M_1=\inf_{x\in\mathbb{R}}[\mathrm{Im}(V(x))],\quad M_2=\sup_{x\in\mathbb{R}}[\mathrm{Im}(V(x))],\quad M_3=\inf_{x\in\mathbb{R}}[\mathrm{Re}(V(x))]. \tag{4.76}$$

(ii) $\sigma(H)$ consists of finitely many simple analytic arcs and one simple semi-infinite arc. These analytic arcs may only end at the points $\widetilde{\lambda}_1,\dots,\widetilde{\lambda}_n$, $E_0,\dots,E_{2n}$, and at infinity. The semi-infinite arc, σ_∞, asymptotically approaches the half-line $L_{\langle V\rangle}=\{z\in\mathbb{C}\,|\,z=\langle V\rangle+$

$x,\, x \geq 0\}$ *in the following sense: asymptotically, σ_∞ can be parameterized by*

$$\sigma_\infty = \big\{ z \in \mathbb{C} \,\big|\, z = R + i \operatorname{Im}(\langle V \rangle) + O\big(R^{-1/2}\big) \text{ as } R \uparrow \infty \big\}. \tag{4.77}$$

(iii) Each E_m, $m = 0, \dots, 2n$, is met by at least one of these arcs. More precisely, a particular E_{m_0} is hit by precisely $2N_0 + 1$ analytic arcs, where $N_0 \in \{0, \dots, n\}$ denotes the number of $\widetilde{\lambda}_j$ that coincide with E_{m_0}. Adjacent arcs meet at an angle $2\pi/(2N_0+1)$ at E_{m_0}. (Thus, generically, $N_0 = 0$ and precisely one arc hits E_{m_0}.)
(iv) Crossings of spectral arcs are permitted. This phenomenon and takes place precisely when for a particular $j_0 \in \{1, \dots, n\}$, $\widetilde{\lambda}_{j_0} \in \sigma(H)$ such that

$$\operatorname{Re}\big(\big\langle g(\widetilde{\lambda}_{j_0}, \cdot)^{-1} \big\rangle\big) = 0 \text{ for some } j_0 \in \{1, \dots, n\} \text{ with } \widetilde{\lambda}_{j_0} \notin \{E_m\}_{m=0}^{2n}. \tag{4.78}$$

In this case $2M_0+2$ analytic arcs are converging toward $\widetilde{\lambda}_{j_0}$, where $M_0 \in \{1, \dots, n\}$ denotes the number of $\widetilde{\lambda}_j$ that coincide with $\widetilde{\lambda}_{j_0}$. Adjacent arcs meet at an angle $\pi/(M_0 + 1)$ at $\widetilde{\lambda}_{j_0}$.
(v) The resolvent set $\mathbb{C}\backslash\sigma(H)$ of H is path-connected.

Proof. Item (i) follows from (4.32) and (4.35) by noting that

$$(f, Hf) = \|f'\|^2 + (f, \operatorname{Re}(V)f) + i(f, \operatorname{Im}(V)f), \quad f \in H^{2,2}(\mathbb{R}). \tag{4.79}$$

To prove (ii) we first introduce the meromorphic differential of the second kind

$$\Omega^{(2)} = \langle g(P, \cdot) \rangle dz = \frac{i \langle F_n(z, \cdot) \rangle dz}{2y} = \frac{i}{2} \frac{\prod_{j=1}^n \big(z - \widetilde{\lambda}_j\big) dz}{R_{2n+1}(z)^{1/2}}, \quad P = (z, y) \in \mathcal{K}_n \backslash \{P_\infty\} \tag{4.80}$$

(cf. (4.74)). Then, by Lemma 3.6,

$$\big\langle g(P, \cdot)^{-1} \big\rangle = -2 \int_{Q_0}^P \Omega^{(2)} + \big\langle g(Q_0, \cdot)^{-1} \big\rangle, \quad P \in \mathcal{K}_n \backslash \{P_\infty\} \tag{4.81}$$

for some fixed $Q_0 \in \mathcal{K}_n \backslash \{P_\infty\}$, is holomorphic on $\mathcal{K}_n \backslash \{P_\infty\}$. By (4.73), (4.74), the characterization (4.44) of the spectrum,

$$\sigma(H) = \big\{ \lambda \in \mathbb{C} \,\big|\, \operatorname{Re}\big(\big\langle g(\lambda, \cdot)^{-1} \big\rangle\big) = 0 \big\}, \tag{4.82}$$

and the fact that $\operatorname{Re}\big(\big\langle g(z, \cdot)^{-1} \big\rangle\big)$ is a harmonic function on the cut plane Π, the spectrum $\sigma(H)$ of H consists of analytic arcs which may only end at the points $\widetilde{\lambda}_1, \dots, \widetilde{\lambda}_n$, $E_0, \dots, E_{2n}$, and possibly tend to infinity. (Since $\sigma(H)$ is independent of the chosen set of cuts, if a spectral arc crosses or runs along a part of one of the cuts in $\mathcal{C}$, one can slightly deform the original set of cuts to extend an analytic arc along or across such an original cut.) To study the behavior of spectral arcs near infinity we first note that

$$g(z,x) \underset{|z|\to\infty}{=} \frac{i}{2z^{1/2}} + \frac{i}{4z^{3/2}}V(x) + O\big(|z|^{-3/2}\big), \tag{4.83}$$

combining (2.4), (2.12), (2.16), and (3.14). Thus, one computes

$$g(z,x)^{-1} \underset{|z|\to\infty}{=} -2iz^{1/2} + \frac{i}{z^{1/2}}V(x) + O\big(|z|^{-3/2}\big) \tag{4.84}$$

and hence

$$\big\langle g(z,\cdot)^{-1}\big\rangle \underset{|z|\to\infty}{=} -2iz^{1/2} + \frac{i}{z^{1/2}}\langle V\rangle + O\big(|z|^{-3/2}\big). \tag{4.85}$$

Writing $z = Re^{i\varphi}$ this yields

$$\begin{aligned} 0 = \mathrm{Re}\big(\big\langle g(z,\cdot)^{-1}\big\rangle\big) \underset{R\to\infty}{=} 2\mathrm{Im}\big\{&R^{1/2}e^{i\varphi/2} - 2^{-1}R^{-1/2}e^{-i\varphi/2}\langle V\rangle \\ &+ O\big(R^{-3/2}\big)\big\} \end{aligned} \tag{4.86}$$

implying

$$\varphi \underset{R\to\infty}{=} \mathrm{Im}(\langle V\rangle)R^{-1} + O\big(R^{-3/2}\big) \tag{4.87}$$

and hence (4.77). In particular, there is precisely one analytic semi-infinite arc σ_∞ that tends to infinity and asymptotically approaches the half-line $L_{\langle V\rangle}$. This proves item (ii).

To prove (iii) one first recalls that by Theorem 4.8 the spectrum of H contains no isolated points. On the other hand, since $\{E_m\}_{m=0}^{2n} \subset \sigma(H)$ by (4.46), one concludes that at least one spectral arc meets each E_m, $m = 0, \dots, 2n$. Choosing $Q_0 = (E_{m_0}, 0)$ in (4.81) one obtains

$$\begin{aligned} \big\langle g(z,\cdot)^{-1}\big\rangle &= -2\int_{E_{m_0}}^{z} dz'\,\langle g(z',\cdot)\rangle + \big\langle g(E_{m_0},\cdot)^{-1}\big\rangle \\ &= -i\int_{E_{m_0}}^{z} dz' \frac{\prod_{j=1}^{n}\big(z'-\widetilde{\lambda}_j\big)}{\big(\prod_{m=0}^{2n}(z'-E_m)\big)^{1/2}} + \big\langle g(E_{m_0},\cdot)^{-1}\big\rangle \\ &\underset{z\to E_{m_0}}{=} -i\int_{E_{m_0}}^{z} dz'\,(z'-E_{m_0})^{N_0-(1/2)}[C + O(z'-E_{m_0})] \\ &\qquad + \big\langle g(E_{m_0},\cdot)^{-1}\big\rangle \\ &\underset{z\to E_{m_0}}{=} -i[N_0+(1/2)]^{-1}(z-E_{m_0})^{N_0+(1/2)}[C + O(z-E_{m_0})] \\ &\qquad + \big\langle g(E_{m_0},\cdot)^{-1}\big\rangle, \quad z\in\Pi \end{aligned} \tag{4.88}$$

for some $C = |C|e^{i\varphi_0} \in \mathbb{C}\backslash\{0\}$. Using

$$\operatorname{Re}\big(\big\langle g(E_m, \cdot)^{-1}\big\rangle\big) = 0, \quad m = 0, \dots, 2n, \tag{4.89}$$

as a consequence of (4.46), $\operatorname{Re}\big(\big\langle g(z, \cdot)^{-1}\big\rangle\big) = 0$ and $z = E_{m_0} + \rho e^{i\varphi}$ imply

$$0 \underset{\rho\downarrow 0}{=} \sin[(N_0 + (1/2))\varphi + \varphi_0]\rho^{N_0+(1/2)}[|C| + O(\rho)]. \tag{4.90}$$

This proves the assertions made in item *(iii)*.

To prove *(iv)* it suffices to refer to (4.73) and to note that locally, $d\big\langle g(z, \cdot)^{-1}\big\rangle/dz$ behaves like $C_0(z - \widetilde{\lambda}_{j_0})^{M_0}$ for some $C_0 \in \mathbb{C}\backslash\{0\}$ in a sufficiently small neighborhood of $\widetilde{\lambda}_{j_0}$.

Finally we will show that all arcs are simple (i.e., do not self-intersect each other). Assume that the spectrum of H contains a simple closed loop γ, $\gamma \subset \sigma(H)$. Then

$$\operatorname{Re}\big(\big\langle g(P, \cdot)^{-1}\big\rangle\big) = 0, \quad P \in \Gamma, \tag{4.91}$$

where the closed simple curve $\Gamma \subset \mathcal{K}_n$ denotes the lift of γ to $\mathcal{K}_n$, yields the contradiction

$$\operatorname{Re}\big(\big\langle g(P, \cdot)^{-1}\big\rangle\big) = 0 \text{ for all } P \text{ in the interior of } \Gamma \tag{4.92}$$

by Corollary 8.2.5 in [5]. Therefore, since there are no closed loops in $\sigma(H)$ and precisely one semi-infinite arc tends to infinity, the resolvent set of H is connected and hence path-connected, proving *(v)*. □

Remark 4.10. For simplicity we focused on $L^2(\mathbb{R}; dx)$-spectra thus far. However, since $V \in L^\infty(\mathbb{R}; dx)$, H in $L^2(\mathbb{R}; dx)$ is the generator of a C_0-semigroup $T(t)$ in $L^2(\mathbb{R}; dx)$, $t > 0$, whose integral kernel $T(t, x, x')$ satisfies the Gaussian upper bound (cf., e.g., [4])

$$\big|T(t, x, x')\big| \leq C_1 t^{-1/2} e^{C_2 t} e^{-C_3|x-x'|^2/t}, \quad t > 0, \ x, x' \in \mathbb{R} \tag{4.93}$$

for some $C_1 > 0$, $C_2 \geq 0$, $C_3 > 0$. Thus, $T(t)$ in $L^2(\mathbb{R}; dx)$ defines, for $p \in [1, \infty)$, consistent C_0-semigroups $T_p(t)$ in $L^p(\mathbb{R}; dx)$ with generators denoted by H_p (i.e., $H = H_2$, $T(t) = T_2(t)$, etc.). Applying Theorem 1.1 of Kunstman [38] one then infers the p-independence of the spectrum,

$$\sigma(H_p) = \sigma(H), \quad p \in [1, \infty). \tag{4.94}$$

Actually, since $\mathbb{C}\backslash\sigma(H)$ is connected by Theorem 4.9 (v), (4.94) also follows from Theorem 4.2 of Arendt [3].

Of course, these results apply to the special case of algebro-geometric complex-valued periodic potentials (see [9], [10], [57], [58]) and we briefly point out the corresponding connections between the algebro-geometric approach and standard Floquet theory in Appendix C. But even in this special case, items (iii) and (iv) of Theorem 1.1 provide additional new details on the nature of the spectrum of H. We briefly illustrate the results of this section in Example C.1 of Appendix C.

The methods of this paper extend to the case of algebro-geometric non-self-adjoint second order finite difference (Jacobi) operators associated with the Toda lattice hierarchy. Moreover, they extend to the infinite genus limit $n \to \infty$ using the approach in [23]. This will be studied elsewhere.

Appendix A. Hyperelliptic curves and their theta functions

We provide a brief summary of some of the fundamental notations needed from the theory of hyperelliptic Riemann surfaces. More details can be found in some of the standard textbooks [20] and [43], as well as in monographs dedicated to integrable systems such as [7, Ch. 2], [24, App. A, B]. In particular, the following material is taken from [24, App. A, B].

Fix $n \in \mathbb{N}$. We intend to describe the hyperelliptic Riemann surface $\mathcal{K}_n$ of genus n of the KdV-type curve (2.24), associated with the polynomial

$$\begin{aligned} &\mathcal{F}_n(z,y) = y^2 - R_{2n+1}(z) = 0, \\ &R_{2n+1}(z) = \prod_{m=0}^{2n} (z - E_m), \quad \{E_m\}_{m=0}^{2n} \subset \mathbb{C}. \end{aligned} \tag{A.1}$$

To simplify the discussion we will assume that the affine part of $\mathcal{K}_n$ is nonsingular, that is, we suppose that

$$E_m \neq E_{m'} \text{ for } m \neq m',\ m, m' = 0, \dots, 2n \tag{A.2}$$

throughout this appendix. Introducing an appropriate set of (nonintersecting) cuts $\mathcal{C}_j$ joining $E_{m(j)}$ and $E_{m'(j)}$, $j = 1, \dots, n$, and $\mathcal{C}_{n+1}$, joining E_{2n} and ∞, we denote

$$\mathcal{C} = \bigcup_{j=1}^{n+1} \mathcal{C}_j, \quad \mathcal{C}_j \cap \mathcal{C}_k = \emptyset, \quad j \neq k. \tag{A.3}$$

Define the cut plane Π by

$$\Pi = \mathbb{C} \backslash \mathcal{C}, \tag{A.4}$$

and introduce the holomorphic function

$$R_{2n+1}(\cdot)^{1/2} \colon \Pi \to \mathbb{C}, \quad z \mapsto \bigg(\prod_{m=0}^{2n}(z-E_m)\bigg)^{1/2} \tag{A.5}$$

on Π with an appropriate choice of the square root branch in (A.5). Define

$$\mathcal{M}_n = \{(z, \sigma R_{2n+1}(z)^{1/2}) \mid z \in \mathbb{C},\ \sigma \in \{1,-1\}\} \cup \{P_\infty\} \tag{A.6}$$

by extending $R_{2n+1}(\cdot)^{1/2}$ to $\mathcal{C}$. The hyperelliptic curve $\mathcal{K}_n$ is then the set $\mathcal{M}_n$ with its natural complex structure obtained upon gluing the two sheets of $\mathcal{M}_n$ crosswise along the cuts. The set of branch points $\mathcal{B}(\mathcal{K}_n)$ of $\mathcal{K}_n$ is given by

$$\mathcal{B}(\mathcal{K}_n) = \{(E_m, 0)\}_{m=0}^{2n}. \tag{A.7}$$

Points $P \in \mathcal{K}_n \backslash \{P_\infty\}$ are denoted by

$$P = (z, \sigma R_{2n+1}(z)^{1/2}) = (z, y), \tag{A.8}$$

where $y(P)$ denotes the meromorphic function on $\mathcal{K}_n$ satisfying $\mathcal{F}_n(z,y) = y^2 - R_{2n+1}(z) = 0$ and

$$y(P) \underset{\zeta\to 0}{=} \bigg(1 - \frac{1}{2}\bigg(\sum_{m=0}^{2n} E_m\bigg)\zeta^2 + O(\zeta^4)\bigg)\zeta^{-2n-1} \text{ as } P \to P_\infty, \quad \zeta = \sigma'/z^{1/2},\ \sigma' \in \{1,-1\} \tag{A.9}$$

(i.e., we abbreviate $y(P) = \sigma R_{2n+1}(z)^{1/2}$). Local coordinates near $P_0 = (z_0, y_0) \in \mathcal{K}_n \backslash \{\mathcal{B}(\mathcal{K}_n) \cup \{P_\infty\}\}$ are given by $\zeta_{P_0} = z - z_0$, near P_∞ by $\zeta_{P_{\infty_\pm}} = 1/z^{1/2}$, and near branch points $(E_{m_0}, 0) \in \mathcal{B}(\mathcal{K}_n)$ by $\zeta_{(E_{m_0},0)} = (z - E_{m_0})^{1/2}$. The compact hyperelliptic Riemann surface $\mathcal{K}_n$ resulting in this manner has topological genus n.

Moreover, we introduce the holomorphic sheet exchange map (involution)

$$* \colon \mathcal{K}_n \to \mathcal{K}_n, \quad P = (z,y) \mapsto P^* = (z,-y),\ P_\infty \mapsto P_\infty^* = P_\infty \tag{A.10}$$

and the two meromorphic projection maps

$$\tilde\pi \colon \mathcal{K}_n \to \mathbb{C} \cup \{\infty\}, \quad P = (z,y) \mapsto z,\ P_\infty \mapsto \infty \tag{A.11}$$

and

$$y \colon \mathcal{K}_n \to \mathbb{C} \cup \{\infty\}, \quad P = (z,y) \mapsto y,\ P_\infty \mapsto \infty. \tag{A.12}$$

The map $\tilde\pi$ has a pole of order 2 at P_∞, and y has a pole of order $2n+1$ at P_∞. Moreover,

$$\tilde\pi(P^*) = \tilde\pi(P), \quad y(P^*) = -y(P), \quad P \in \mathcal{K}_n. \tag{A.13}$$

Thus $\mathcal{K}_n$ is a two-sheeted branched covering of the Riemann sphere $\mathbb{CP}^1$ ($\cong \mathbb{C} \cup \{\infty\}$) branched at the $2n+2$ points $\{(E_m, 0)\}_{m=0}^{2n}, P_\infty$.

We introduce the upper and lower sheets $\Pi_\pm$ by

$$\Pi_\pm = \{(z, \pm R_{2n+1}(z)^{1/2}) \in \mathcal{M}_n \mid z \in \Pi\} \tag{A.14}$$

and the associated charts

$$\zeta_\pm \colon \Pi_\pm \to \Pi, \quad P \mapsto z. \tag{A.15}$$

Next, let $\{a_j, b_j\}_{j=1}^n$ be a homology basis for $\mathcal{K}_n$ with intersection matrix of the cycles satisfying

$$a_j \circ b_k = \delta_{j,k}, \quad a_j \circ a_k = 0, \quad b_j \circ b_k = 0, \quad j, k = 1, \dots, n. \tag{A.16}$$

Associated with the homology basis $\{a_j, b_j\}_{j=1}^n$ we also recall the canonical dissection of $\mathcal{K}_n$ along its cycles yielding the simply connected interior $\widehat{\mathcal{K}}_n$ of the fundamental polygon $\partial\widehat{\mathcal{K}}_n$ given by

$$\partial\widehat{\mathcal{K}}_n = a_1 b_1 a_1^{-1} b_1^{-1} a_2 b_2 a_2^{-1} b_2^{-1} \cdots a_n^{-1} b_n^{-1}. \tag{A.17}$$

Let $\mathcal{M}(\mathcal{K}_n)$ and $\mathcal{M}^1(\mathcal{K}_n)$ denote the set of meromorphic functions (0-forms) and meromorphic differentials (1-forms) on $\mathcal{K}_n$, respectively. The residue of a meromorphic differential $\nu \in \mathcal{M}^1(\mathcal{K}_n)$ at a point $Q \in \mathcal{K}_n$ is defined by

$$\operatorname{res}_Q(\nu) = \frac{1}{2\pi i} \int_{\gamma_Q} \nu, \tag{A.18}$$

where γ_Q is a counterclockwise oriented smooth simple closed contour encircling Q but no other pole of ν. Holomorphic differentials are also called Abelian differentials of the first kind. Abelian differentials of the second kind $\omega^{(2)} \in \mathcal{M}^1(\mathcal{K}_n)$ are characterized by the property that all their residues vanish. They will usually be normalized by demanding that all their a-periods vanish, that is,

$$\int_{a_j} \omega^{(2)} = 0, \quad j = 1, \dots, n. \tag{A.19}$$

If $\omega_{P_1,n}^{(2)}$ is a differential of the second kind on $\mathcal{K}_n$ whose only pole is $P_1 \in \widehat{\mathcal{K}}_n$ with principal part $\zeta^{-n-2}\, d\zeta$, $n \in \mathbb{N}_0$ near P_1 and $\omega_j = (\sum_{m=0}^\infty d_{j,m}(P_1)\zeta^m)\, d\zeta$ near P_1, then

$$\frac{1}{2\pi i} \int_{b_j} \omega_{P_1,m}^{(2)} = \frac{d_{j,m}(P_1)}{m+1}, \quad m = 0, 1, \dots . \tag{A.20}$$

Using the local chart near P_∞, one verifies that dz/y is a holomorphic differential on $\mathcal{K}_n$ with zeros of order $2(n-1)$ at P_∞ and hence

$$\eta_j = \frac{z^{j-1}dz}{y}, \quad j = 1, \dots, n, \tag{A.21}$$

form a basis for the space of holomorphic differentials on $\mathcal{K}_n$. Upon introduction of the invertible matrix C in $\mathbb{C}^n$,

$$C = \big(C_{j,k}\big)_{j,k=1,\dots,n}, \quad C_{j,k} = \int_{a_k} \eta_j, \tag{A.22}$$

$$\underline{c}(k) = (c_1(k), \dots, c_n(k)), \quad c_j(k) = \big(C^{-1}\big)_{j,k}, \quad j,k = 1, \dots, n, \tag{A.23}$$

the normalized differentials ω_j for $j = 1, \dots, n$,

$$\omega_j = \sum_{\ell=1}^{n} c_j(\ell)\eta_\ell, \quad \int_{a_k} \omega_j = \delta_{j,k}, \quad j,k = 1, \dots, n, \tag{A.24}$$

form a canonical basis for the space of holomorphic differentials on $\mathcal{K}_n$.

In the chart $(U_{P_\infty}, \zeta_{P_\infty})$ induced by $1/\tilde{\pi}^{1/2}$ near P_∞ one infers,

$$\begin{aligned}
\underline{\omega} = (\omega_1, \dots, \omega_n) &= -2\bigg(\sum_{j=1}^{n} \frac{\underline{c}(j)\zeta^{2(n-j)}}{\big(\prod_{m=0}^{2n}(1-\zeta^2 E_m)\big)^{1/2}} \bigg) d\zeta \qquad \text{(A.25)} \\
&= -2\bigg(\underline{c}(n) + \bigg(\frac{1}{2}\underline{c}(n) \sum_{m=0}^{2n} E_m + \underline{c}(n-1) \bigg)\zeta^2 + O(\zeta^4) \bigg) d\zeta \\
&\qquad \text{as } P \to P_\infty, \quad \zeta = \sigma/z^{1/2},\ \sigma \in \{1,-1\},
\end{aligned}$$

where $\underline{E} = (E_0, \dots, E_{2n})$ and we used (A.9). Given (A.25), one computes for the vector $\underline{U}_0^{(2)}$ of b-periods of $\omega^{(2)}_{P_\infty,0}/(2\pi i)$, the normalized differential of the second kind, holomorphic on $\mathcal{K}_n \backslash \{P_\infty\}$, with principal part $\zeta^{-2}d\zeta/(2\pi i)$,

$$\underline{U}_0^{(2)} = \big(U_{0,1}^{(2)}, \dots, U_{0,n}^{(2)}\big), \quad U_{0,j}^{(2)} = \frac{1}{2\pi i} \int_{b_j} \omega^{(2)}_{P_\infty,0} = -2c_j(n), \quad j = 1, \dots, n. \tag{A.26}$$

Next, define the matrix $\tau = \big(\tau_{j,\ell}\big)_{j,\ell=1}^{n}$ by

$$\tau_{j,\ell} = \int_{b_j} \omega_\ell, \quad j,\ell = 1, \dots, n. \tag{A.27}$$

Then

$$\mathrm{Im}(\tau) > 0, \quad \text{and} \quad \tau_{j,\ell} = \tau_{\ell,j}, \quad j,\ell = 1, \dots, n. \tag{A.28}$$

Associated with τ one introduces the period lattice

$$L_n = \{\underline{z} \in \mathbb{C}^n \mid \underline{z} = \underline{m} + \underline{n}\tau,\ \underline{m}, \underline{n} \in \mathbb{Z}^n\} \tag{A.29}$$

and the Riemann theta function associated with $\mathcal{K}_n$ and the given homology basis $\{a_j, b_j\}_{j=1,\dots,n}$,

$$\theta(\underline{z}) = \sum_{\underline{n}\in\mathbb{Z}^n} \exp\big(2\pi i(\underline{n}, \underline{z}) + \pi i(\underline{n}, \underline{n}\tau)\big), \quad \underline{z} \in \mathbb{C}^n, \tag{A.30}$$

where $(\underline{u}, \underline{v}) = \overline{\underline{u}}\,\underline{v}^\top = \sum_{j=1}^n \overline{u}_j v_j$ denotes the scalar product in $\mathbb{C}^n$. It has the fundamental properties

$$\theta(z_1, \dots, z_{j-1}, -z_j, z_{j+1}, \dots, z_n) = \theta(\underline{z}), \tag{A.31}$$

$$\theta(\underline{z} + \underline{m} + \underline{n}\tau) = \exp\big(-2\pi i(\underline{n}, \underline{z}) - \pi i(\underline{n}, \underline{n}\tau)\big)\theta(\underline{z}), \quad \underline{m}, \underline{n} \in \mathbb{Z}^n. \tag{A.32}$$

Next we briefly study some consequences of a change of homology basis. Let

$$\{a_1, \dots, a_n, b_1, \dots, b_n\} \tag{A.33}$$

be a canonical homology basis on $\mathcal{K}_n$ with intersection matrix satisfying (A.16) and let

$$\{a_1', \dots, a_n', b_1', \dots, b_n'\} \tag{A.34}$$

be a homology basis on $\mathcal{K}_n$ related to each other by

$$\begin{pmatrix} \underline{a'}^\top \\ \underline{b'}^\top \end{pmatrix} = X \begin{pmatrix} \underline{a}^\top \\ \underline{b}^\top \end{pmatrix}, \tag{A.35}$$

where

$$\begin{aligned} \underline{a}^\top &= (a_1, \dots, a_n)^\top, \quad \underline{b}^\top = (b_1, \dots, b_n)^\top, \\ \underline{a'}^\top &= (a_1', \dots, a_n')^\top, \quad \underline{b'}^\top = (b_1', \dots, b_n')^\top, \end{aligned} \tag{A.36}$$

$$X = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \tag{A.37}$$

with A, B, C, and D being $n \times n$ matrices with integer entries. Then (A.34) is also a canonical homology basis on $\mathcal{K}_n$ with intersection matrix satisfying (A.16) if and only if

$$X \in \mathrm{Sp}(n, \mathbb{Z}), \tag{A.38}$$

where

$$\mathrm{Sp}(n, \mathbb{Z}) = \left\{ X = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \,\middle|\, X \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix} X^\top = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}, \det(X) = 1 \right\} \tag{A.39}$$

denotes the symplectic modular group (here A, B, C, D in X are again $n \times n$ matrices with integer entries). If $\{\omega_j\}_{j=1}^n$ and $\{\omega'_j\}_{j=1}^n$ are the normalized bases of holomorphic differentials corresponding to the canonical homology bases (A.33) and (A.34), with τ and τ' the associated b and b'-periods of $\omega_1, \dots, \omega_n$ and $\omega'_1, \dots, \omega'_n$, respectively, one computes

$$\underline{\omega}' = \underline{\omega}(A + B\tau)^{-1}, \quad \tau' = (C + D\tau)(A + B\tau)^{-1}, \tag{A.40}$$

where $\underline{\omega} = (\omega_1, \dots, \omega_n)$ and $\underline{\omega}' = (\omega'_1, \dots, \omega'_n)$.

Fixing a base point $Q_0 \in \mathcal{K}_n \backslash \{P_\infty\}$, one denotes by $J(\mathcal{K}_n) = \mathbb{C}^n / L_n$ the Jacobi variety of $\mathcal{K}_n$, and defines the Abel map $\underline{A}_{Q_0}$ by

$$\underline{A}_{Q_0} \colon \mathcal{K}_n \to J(\mathcal{K}_n), \quad \underline{A}_{Q_0}(P) = \left(\int_{Q_0}^P \omega_1, \dots, \int_{Q_0}^P \omega_n \right) \pmod{L_n}, \quad P \in \mathcal{K}_n. \tag{A.41}$$

Similarly, we introduce

$$\underline{\alpha}_{Q_0} \colon \operatorname{Div}(\mathcal{K}_n) \to J(\mathcal{K}_n), \quad \mathcal{D} \mapsto \underline{\alpha}_{Q_0}(\mathcal{D}) = \sum_{P \in \mathcal{K}_n} \mathcal{D}(P) \underline{A}_{Q_0}(P), \tag{A.42}$$

where $\operatorname{Div}(\mathcal{K}_n)$ denotes the set of divisors on $\mathcal{K}_n$. Here $\mathcal{D} \colon \mathcal{K}_n \to \mathbb{Z}$ is called a divisor on $\mathcal{K}_n$ if $\mathcal{D}(P) \neq 0$ for only finitely many $P \in \mathcal{K}_n$. (In the main body of this paper we will choose Q_0 to be one of the branch points, i.e., $Q_0 \in \mathcal{B}(\mathcal{K}_n)$, and for simplicity we will always choose the same path of integration from Q_0 to P in all Abelian integrals.) For subsequent use in Remark A.4 we also introduce

$$\begin{aligned} &\widehat{\underline{A}}_{Q_0} \colon \widehat{\mathcal{K}}_n \to \mathbb{C}^n, \\ &\quad P \mapsto \widehat{\underline{A}}_{Q_0}(P) = \big(\widehat{A}_{Q_0,1}(P), \dots, \widehat{A}_{Q_0,n}(P)\big) = \left(\int_{Q_0}^P \omega_1, \dots, \int_{Q_0}^P \omega_n \right) \end{aligned} \tag{A.43}$$

and

$$\widehat{\underline{\alpha}}_{Q_0} \colon \operatorname{Div}(\widehat{\mathcal{K}}_n) \to \mathbb{C}^n, \quad \mathcal{D} \mapsto \widehat{\underline{\alpha}}_{Q_0}(\mathcal{D}) = \sum_{P \in \widehat{\mathcal{K}}_n} \mathcal{D}(P) \widehat{\underline{A}}_{Q_0}(P). \tag{A.44}$$

In connection with divisors on $\mathcal{K}_n$ we shall employ the following (additive) notation,

$$\begin{aligned} &\mathcal{D}_{Q_0 \underline{Q}} = \mathcal{D}_{Q_0} + \mathcal{D}_{\underline{Q}}, \quad \mathcal{D}_{\underline{Q}} = \mathcal{D}_{Q_1} + \cdots + \mathcal{D}_{Q_m}, \\ &\underline{Q} = \{Q_1, \dots, Q_m\} \in \operatorname{Sym}^m \mathcal{K}_n, \quad Q_0 \in \mathcal{K}_n, \ m \in \mathbb{N}, \end{aligned} \tag{A.45}$$

where for any $Q \in \mathcal{K}_n$,

$$\mathcal{D}_Q \colon \mathcal{K}_n \to \mathbb{N}_0, \quad P \mapsto \mathcal{D}_Q(P) = \begin{cases} 1 & \text{for } P = Q, \\ 0 & \text{for } P \in \mathcal{K}_n \backslash \{Q\}, \end{cases} \tag{A.46}$$

and $\operatorname{Sym}^m \mathcal{K}_n$ denotes the mth symmetric product of $\mathcal{K}_n$. In particular, $\operatorname{Sym}^m \mathcal{K}_n$ can be identified with the set of nonnegative divisors $0 \leq \mathcal{D} \in \operatorname{Div}(\mathcal{K}_n)$ of degree $m \in \mathbb{N}$.

For $f \in \mathcal{M}(\mathcal{K}_n)\backslash\{0\}$ and $\omega \in \mathcal{M}^1(\mathcal{K}_n)\backslash\{0\}$ the divisors of f and ω are denoted by (f) and (ω), respectively. Two divisors $\mathcal{D}, \mathcal{E} \in \operatorname{Div}(\mathcal{K}_n)$ are called equivalent, denoted by $\mathcal{D} \sim \mathcal{E}$, if and only if $\mathcal{D} - \mathcal{E} = (f)$ for some $f \in \mathcal{M}(\mathcal{K}_n)\backslash\{0\}$. The divisor class $[\mathcal{D}]$ of $\mathcal{D}$ is then given by $[\mathcal{D}] = \{\mathcal{E} \in \operatorname{Div}(\mathcal{K}_n) \mid \mathcal{E} \sim \mathcal{D}\}$. We recall that

$$\deg((f)) = 0,\ \deg((\omega)) = 2(n-1),\ f \in \mathcal{M}(\mathcal{K}_n)\backslash\{0\},\ \omega \in \mathcal{M}^1(\mathcal{K}_n)\backslash\{0\}, \tag{A.47}$$

where the degree $\deg(\mathcal{D})$ of $\mathcal{D}$ is given by $\deg(\mathcal{D}) = \sum_{P \in \mathcal{K}_n} \mathcal{D}(P)$. It is customary to call (f) (respectively, (ω)) a principal (respectively, canonical) divisor.

Introducing the complex linear spaces

$$\mathcal{L}(\mathcal{D}) = \{f \in \mathcal{M}(\mathcal{K}_n) \mid f = 0 \text{ or } (f) \geq \mathcal{D}\},\ r(\mathcal{D}) = \dim_{\mathbb{C}} \mathcal{L}(\mathcal{D}), \tag{A.48}$$

$$\mathcal{L}^1(\mathcal{D}) = \{\omega \in \mathcal{M}^1(\mathcal{K}_n) \mid \omega = 0 \text{ or } (\omega) \geq \mathcal{D}\},\ i(\mathcal{D}) = \dim_{\mathbb{C}} \mathcal{L}^1(\mathcal{D}) \tag{A.49}$$

(with $i(\mathcal{D})$ the index of specialty of $\mathcal{D}$), one infers that $\deg(\mathcal{D})$, $r(\mathcal{D})$, and $i(\mathcal{D})$ only depend on the divisor class $[\mathcal{D}]$ of $\mathcal{D}$. Moreover, we recall the following fundamental facts.

Theorem A.1. *Let $\mathcal{D} \in \operatorname{Div}(\mathcal{K}_n)$, $\omega \in \mathcal{M}^1(\mathcal{K}_n)\backslash\{0\}$. Then*

$$i(\mathcal{D}) = r(\mathcal{D} - (\omega)), \quad n \in \mathbb{N}_0. \tag{A.50}$$

The Riemann-Roch theorem reads

$$r(-\mathcal{D}) = \deg(\mathcal{D}) + i(\mathcal{D}) - n + 1, \quad n \in \mathbb{N}_0. \tag{A.51}$$

By Abel's theorem, $\mathcal{D} \in \operatorname{Div}(\mathcal{K}_n)$, $n \in \mathbb{N}$, is principal if and only if

$$\deg(\mathcal{D}) = 0 \text{ and } \underline{\alpha}_{Q_0}(\mathcal{D}) = \underline{0}. \tag{A.52}$$

Finally, assume $n \in \mathbb{N}$. Then $\underline{\alpha}_{Q_0} : \operatorname{Div}(\mathcal{K}_n) \to J(\mathcal{K}_n)$ is surjective (Jacobi's inversion theorem).

Theorem A.2. *Let $\mathcal{D}_{\underline{Q}} \in \operatorname{Sym}^n \mathcal{K}_n$, $\underline{Q} = \{Q_1, \dots, Q_n\}$. Then*

$$1 \leq i(\mathcal{D}_{\underline{Q}}) = s \tag{A.53}$$

if and only if there are s pairs of the type $\{P, P^*\} \subseteq \{Q_1, \dots, Q_n\}$ (this includes, of course, branch points for which $P = P^*$). Obviously, one has $s \leq n/2$.

Next, denote by $\underline{\Xi}_{Q_0} = (\Xi_{Q_{0,1}}, \dots, \Xi_{Q_{0,n}})$ the vector of Riemann constants,

$$\Xi_{Q_{0,j}} = \frac{1}{2}(1+\tau_{j,j}) - \sum_{\substack{\ell=1\\ \ell\neq j}}^{n} \int_{a_\ell} \omega_\ell(P) \int_{Q_0}^{P} \omega_j, \quad j=1,\dots,n. \tag{A.54}$$

Theorem A.3. *Let $\underline{Q} = \{Q_1, \dots, Q_n\} \in \operatorname{Sym}^n \mathcal{K}_n$ and assume $\mathcal{D}_{\underline{Q}}$ to be nonspecial, that is, $i(\mathcal{D}_{\underline{Q}}) = 0$. Then*

$$\theta(\underline{\Xi}_{Q_0} - \underline{A}_{Q_0}(P) + \alpha_{Q_0}(\mathcal{D}_{\underline{Q}})) = 0 \text{ if and only if } P \in \{Q_1, \dots, Q_n\}. \tag{A.55}$$

Remark A.4. In Section 2 we dealt with theta function expressions of the type

$$\psi(P) = \frac{\theta(\underline{\Xi}_{Q_0} - \underline{A}_{Q_0}(P) + \underline{\alpha}_{Q_0}(\mathcal{D}_1))}{\theta(\underline{\Xi}_{Q_0} - \underline{A}_{Q_0}(P) + \underline{\alpha}_{Q_0}(\mathcal{D}_2))} \exp\bigg(-c\int_{Q_0}^{P} \Omega^{(2)}\bigg), \quad P \in \mathcal{K}_n, \tag{A.56}$$

where $\mathcal{D}_j \in \operatorname{Sym}^n \mathcal{K}_n$, $j=1,2$, are nonspecial positive divisors of degree n, $c \in \mathbb{C}$ is a constant, and $\Omega^{(2)}$ is a normalized differential of the second kind with a prescribed singularity at P_∞. Even though we agree to always choose identical paths of integration from P_0 to P in all Abelian integrals (A.56), this is not sufficient to render ψ single-valued on $\mathcal{K}_n$. To achieve single-valuedness one needs to replace $\mathcal{K}_n$ by its simply connected canonical dissection $\widehat{\mathcal{K}}_n$ and then replace $\underline{A}_{Q_0}$ and $\underline{\alpha}_{Q_0}$ in (A.56) with $\underline{\widehat{A}}_{Q_0}$ and $\underline{\widehat{\alpha}}_{Q_0}$ as introduced in (A.43) and (A.44). In particular, one regards a_j, b_j, $j=1,\dots,n$, as curves (being a part of $\partial\widehat{\mathcal{K}}_n$, cf. (A.17)) and not as homology classes. Similarly, one then replaces $\underline{\Xi}_{Q_0}$ by $\underline{\widehat{\Xi}}_{Q_0}$ (replacing $\underline{A}_{Q_0}$ by $\underline{\widehat{A}}_{Q_0}$ in (A.54), etc.). Moreover, in connection with ψ, one introduces the vector of b-periods $\underline{U}^{(2)}$ of $\Omega^{(2)}$ by

$$\underline{U}^{(2)} = (U_1^{(2)}, \dots, U_g^{(2)}), \quad U_j^{(2)} = \frac{1}{2\pi i}\int_{b_j} \Omega^{(2)}, \quad j=1,\dots,n, \tag{A.57}$$

and then renders ψ single-valued on $\widehat{\mathcal{K}}_n$ by requiring

$$\underline{\widehat{\alpha}}_{Q_0}(\mathcal{D}_1) - \underline{\widehat{\alpha}}_{Q_0}(\mathcal{D}_2) = c\,\underline{U}^{(2)} \tag{A.58}$$

(as opposed to merely $\underline{\alpha}_{Q_0}(\mathcal{D}_1) - \underline{\alpha}_{Q_0}(\mathcal{D}_2) = c\,\underline{U}^{(2)} \pmod{L_n}$). Actually, by (A.32),

$$\underline{\widehat{\alpha}}_{Q_0}(\mathcal{D}_1) - \underline{\widehat{\alpha}}_{Q_0}(\mathcal{D}_2) - c\,\underline{U}^{(2)} \in \mathbb{Z}^n, \tag{A.59}$$

suffices to guarantee single-valuedness of ψ on $\widehat{\mathcal{K}}_n$. Without the replacement of $\underline{A}_{Q_0}$ and $\underline{\alpha}_{Q_0}$ by $\widehat{\underline{A}}_{Q_0}$ and $\widehat{\underline{\alpha}}_{Q_0}$ in (A.56) and without the assumption (A.58) (or (A.59)), ψ is a multiplicative (multi-valued) function on $\mathcal{K}_n$, and then most effectively discussed by introducing the notion of characters on $\mathcal{K}_n$ (cf. [20, Sect. III.9]). For simplicity, we decided to avoid the latter possibility and throughout this paper will always tacitly assume (A.58) or (A.59).

Appendix B. Restrictions on $\underline{B} = i\underline{U}_0^{(2)}$

The purpose of this appendix is to prove the result (2.70), $\underline{B} = i\underline{U}_0^{(2)} \in \mathbb{R}^n$, for some choice of homology basis $\{a_j, b_j\}_{j=1}^n$ on $\mathcal{K}_n$ as recorded in Remark 2.8.

To this end we first recall a few notions in connection with periodic meromorphic functions of p complex variables.

Definition B.1. Let $p \in \mathbb{N}$ and $F\colon \mathbb{C}^p \to \mathbb{C} \cup \{\infty\}$ be meromorphic (i.e., a ratio of two entire functions of p complex variables). Then,
(i) $\underline{\omega} = (\omega_1, \dots, \omega_p) \in \mathbb{C}^p \backslash \{0\}$ is called a *period* of F if

$$F(\underline{z} + \underline{\omega}) = F(\underline{z}) \tag{B.1}$$

for all $\underline{z} \in \mathbb{C}^p$ for which F is analytic. The set of all periods of F is denoted by $\mathcal{P}_F$.
(ii) F is called *degenerate* if it depends on less than p complex variables; otherwise, F is called *nondegenerate*.

Theorem B.2. *Let $p \in \mathbb{N}$, $F\colon \mathbb{C}^p \to \mathbb{C} \cup \{\infty\}$ be meromorphic, and $\mathcal{P}_F$ be the set of all periods of F. Then either*
(i) $\mathcal{P}_F$ has a finite limit point,
or
(ii) $\mathcal{P}_F$ has no finite limit point.
In case (i), $\mathcal{P}_F$ contains infinitesimal periods (i.e., sequences of nonzero periods converging to zero). In addition, in case (i) each period is a limit point of periods and hence $\mathcal{P}_F$ is a perfect set.
Moreover, F is degenerate if and only if F admits infinitesimal periods. In particular, for nondegenerate functions F only alternative (ii) applies.

Next, let $\underline{\omega}_q \in \mathbb{C}^p \backslash \{0\}$, $q = 1, \dots, r$ for some $r \in \mathbb{N}$. Then $\underline{\omega}_1, \dots, \underline{\omega}_r$ are called *linearly independent over* $\mathbb{Z}$ (*resp.* $\mathbb{R}$) if

$$\begin{aligned}&\nu_1\underline{\omega}_1 + \cdots + \nu_r\underline{\omega}_r = 0, \quad \nu_q \in \mathbb{Z} \text{ (resp., } \nu_q \in \mathbb{R}),\ q = 1, \dots, r,\\ &\text{implies } \nu_1 = \cdots = \nu_r = 0.\end{aligned} \tag{B.2}$$

Clearly, the maximal number of vectors in $\mathbb{C}^p$ linearly independent over $\mathbb{R}$ equals $2p$.

Theorem B.3. *Let $p \in \mathbb{N}$.*
(i) If $F\colon \mathbb{C}^p \to \mathbb{C} \cup \{\infty\}$ is a nondegenerate meromorphic function with periods $\underline{\omega}_q \in \mathbb{C}^p\backslash\{0\}$, $q = 1, \dots, r$, $r \in \mathbb{N}$, linearly independent over $\mathbb{Z}$, then $\underline{\omega}_1, \dots, \underline{\omega}_r$ are also linearly independent over $\mathbb{R}$. In particular, $r \leq 2p$.
(ii) A nondegenerate entire function $F\colon \mathbb{C}^p \to \mathbb{C}$ cannot have more than p periods linearly independent over $\mathbb{Z}$ (or $\mathbb{R}$).

For $p = 1$, $\exp(z)$, $\sin(z)$ are examples of entire functions with precisely one period. Any non-constant doubly periodic meromorphic function of one complex variable is elliptic (and hence has indeed poles).

Definition B.4. Let $p, r \in \mathbb{N}$. A system of periods $\underline{\omega}_q \in \mathbb{C}^p\backslash\{0\}$, $q = 1, \dots, r$ of a nondegenerate meromorphic function $F\colon \mathbb{C}^p \to \mathbb{C} \cup \{\infty\}$, linearly independent over $\mathbb{Z}$, is called *fundamental* or a *basis* of periods for F if every period $\underline{\omega}$ of F is of the form

$$\underline{\omega} = m_1\underline{\omega}_1 + \cdots + m_r\underline{\omega}_r \text{ for some } m_q \in \mathbb{Z},\ q = 1, \dots, r. \tag{B.3}$$

The representation of $\underline{\omega}$ in (B.3) is unique since by hypothesis $\underline{\omega}_1, \dots, \underline{\omega}_r$ are linearly independent over $\mathbb{Z}$. In addition, $\mathcal{P}_F$ is countable in this case. (This rules out case (i) in Theorem B.2 since a perfect set is uncountable. Hence, one does not have to assume that F is nondegenerate in Definition B.4.)

This material is standard and can be found, for instance, in [41, Ch. 2].

Next, returning to the Riemann theta function $\theta(\underline{\cdot})$ in (A.30), we introduce the vectors $\{\underline{e}_j\}_{j=1}^n, \{\underline{\tau}_j\}_{j=1}^n \subset \mathbb{C}^n\backslash\{0\}$ by

$$\underline{e}_j = (0, \dots, 0, \underbrace{1}_{j}, 0, \dots, 0), \quad \underline{\tau}_j = \underline{e}_j\tau, \quad j = 1, \dots, n. \tag{B.4}$$

Then

$$\{\underline{e}_j\}_{j=1}^n \tag{B.5}$$

is a basis of periods for the entire (nondegenerate) function $\theta(\underline{\cdot})\colon \mathbb{C}^n \to \mathbb{C}$. Moreover, fixing $k, k' \in \{1, \dots, n\}$, then

$$\{\underline{e}_j, \underline{\tau}_j\}_{j=1}^n \tag{B.6}$$

is a basis of periods for the meromorphic function $\partial^2_{z_k z_{k'}} \ln\big(\theta(\underline{\cdot})\big)\colon \mathbb{C}^n \to \mathbb{C} \cup \{\infty\}$ (cf. (A.32) and [20, p. 91]).

Next, let $\underline{A} \in \mathbb{C}^n$, $\underline{D} = (D_1, \dots, D_n) \in \mathbb{R}^n$, $D_j \in \mathbb{R}\backslash\{0\}$, $j = 1, \dots, n$ and consider

$$\begin{aligned} f_{k,k'}\colon \mathbb{R} \to \mathbb{C}, \quad f_{k,k'}(x) &= \partial^2_{z_k z_{k'}} \ln\big(\theta(\underline{A} + \underline{z})\big)\big|_{\underline{z}=\underline{D}x} \\ &= \partial^2_{z_k z_{k'}} \ln\big(\theta(\underline{A} + \underline{z}\,\mathrm{diag}(\underline{D}))\big)\big|_{\underline{z}=(x,\dots,x)}. \end{aligned} \tag{B.7}$$

Here $\mathrm{diag}(\underline{D})$ denotes the diagonal matrix

$$\mathrm{diag}(\underline{D}) = \big(D_j \delta_{j,j'}\big)_{j,j'=1}^n. \tag{B.8}$$

Then the quasi-periods D_j^{-1}, $j = 1, \dots, n$, of $f_{k,k'}$ are in a one-one correspondence with the periods of

$$F_{k,k'}\colon \mathbb{C}^n \to \mathbb{C} \cup \{\infty\}, \quad F_{k,k'}(\underline{z}) = \partial^2_{z_k z_{k'}} \ln\big(\theta(\underline{A} + \underline{z}\,\mathrm{diag}(\underline{D})\big) \tag{B.9}$$

of the special type

$$\underline{e}_j\big(\,\mathrm{diag}(\underline{D})\big)^{-1} = \big(0, \dots, 0, \underbrace{D_j^{-1}}_{j}, 0, \dots, 0\big). \tag{B.10}$$

Moreover,

$$f_{k,k'}(x) = F_{k,k'}(\underline{z})|_{\underline{z}=(x,\dots,x)}, \quad x \in \mathbb{R}. \tag{B.11}$$

Theorem B.5. *Suppose V in (2.65) (or (2.66)) to be quasi-periodic. Then there exists a homology basis $\{\tilde a_j, \tilde b_j\}_{j=1}^n$ on $\mathcal{K}_n$ such that the vector $\underline{\widetilde{B}} = i\underline{\widetilde{U}}_0^{(2)}$ with $\underline{\widetilde{U}}_0^{(2)}$ the vector of $\tilde b$-periods of the corresponding normalized differential of the second kind, $\widetilde{\omega}^{(2)}_{P_\infty,0}$, satisfies the constraint*

$$\underline{\widetilde{B}} = i\underline{\widetilde{U}}_0^{(2)} \in \mathbb{R}^n. \tag{B.12}$$

Proof. By (A.26), the vector of b-periods $\underline{U}_0^{(2)}$ associated with a given homology basis $\{a_j, b_j\}_{j=1}^n$ on $\mathcal{K}_n$ and the normalized differential of the 2nd kind, $\omega^{(2)}_{P_\infty,0}$, is continuous with respect to $E_0, \dots, E_{2n}$. Hence, we may assume in the following that

$$B_j \neq 0,\ j = 1, \dots, n, \quad \underline{B} = (B_1, \dots, B_n) \tag{B.13}$$

by slightly altering $E_0, \dots, E_{2n}$, if necessary. By comparison with the Its–Matveev formula (2.66), we may write

$$\begin{aligned} V(x) &= \Lambda_0 - 2\partial_x^2 \ln(\theta(\underline{A} + \underline{B}x)) \\ &= \Lambda_0 + 2\sum_{j,k=1}^n U^{(2)}_{0,j} U^{(2)}_{0,k} \partial^2_{z_k z_j} \ln\big(\theta(\underline{A} + \underline{z})\big)\big|_{\underline{z}=\underline{B}x}. \end{aligned} \tag{B.14}$$

Introducing the meromorphic (nondegenerate) function $\mathcal{V}\colon \mathbb{C}^n \to \mathbb{C} \cup \{\infty\}$ by

$$\mathcal{V}(\underline{z}) = \Lambda_0 + 2 \sum_{j,k=1}^{n} U_{0,j}^{(2)} U_{0,k}^{(2)} \partial_{z_k z_j}^2 \ln\big(\theta(\underline{A} + \underline{z}\,\mathrm{diag}(\underline{B}))\big), \tag{B.15}$$

one observes that

$$V(x) = \mathcal{V}(\underline{z})|_{\underline{z}=(x,\dots,x)}. \tag{B.16}$$

In addition, $\mathcal{V}$ has a basis of periods

$$\Big\{\underline{e}_j\big(\,\mathrm{diag}(\underline{B})\big)^{-1}, \underline{\tau}_j\big(\,\mathrm{diag}(\underline{B})\big)^{-1}\Big\}_{j=1}^{n} \tag{B.17}$$

by (B.6), where

$$\underline{e}_j\big(\,\mathrm{diag}(\underline{B})\big)^{-1} = \big(0,\dots,0,\underbrace{B_j^{-1}}_{j},0,\dots,0\big), \quad j = 1,\dots,n, \tag{B.18}$$

$$\underline{\tau}_j\big(\,\mathrm{diag}(\underline{B})\big)^{-1} = \big(\tau_{j,1}B_1^{-1},\dots,\tau_{j,n}B_n^{-1}\big), \quad j = 1,\dots,n. \tag{B.19}$$

By hypothesis, V in (B.14) is quasi-periodic and hence has n real (scalar) quasi-periods. The latter are not necessarily linearly independent over $\mathbb{Q}$ from the outset, but by slightly changing the locations of branchpoints $\{E_m\}_{m=0}^{2n}$ into, say, $\{\widetilde{E}_m\}_{m=0}^{2n}$, one can assume they are. In particular, since the period vectors in (B.17) are linearly independent and the (scalar) quasi-periods of V are in a one-one correspondence with vector periods of $\mathcal{V}$ of the special form (B.18) (cf. (B.9), (B.10)), there exists a homology basis $\{\tilde{a}_j, \tilde{b}_j\}_{j=1}^n$ on $\mathcal{K}_n$ such that the vector $\underline{\widetilde{B}} = i\underline{\widetilde{U}}_0^{(2)}$ corresponding to the normalized differential of the second kind, $\widetilde{\omega}_{P_\infty,0}^{(2)}$ and this particular homology basis, is real-valued. By continuity of $\underline{\widetilde{U}}_0^2$ with respect to $\widetilde{E}_0,\dots,\widetilde{E}_{2m}$, this proves (B.12). ☐

Remark B.6. Given the existence of a homology basis with associated real vector $\underline{\widetilde{B}} = i\underline{\widetilde{U}}_0^{(2)}$, one can follow the proof of Theorem 10.3.1 in [39] and show that each μ_j, $j = 1,\dots,n$, is quasi-periodic with the same quasi-periods as V.

Appendix C. Floquet theory and an explicit example

In this appendix we discuss the special case of algebro-geometric complex-valued periodic potentials and we briefly point out the connections between the algebro-geometric approach and standard Floquet theory. We then conclude with the explicit genus $n = 1$ example which illustrates both, the algebro-geometric as well as the periodic case.

We start with the periodic case. Suppose V satisfies

$$V \in CP(\mathbb{R}) \text{ and for all } x \in \mathbb{R},\ V(x+\Omega) = V(x) \tag{C.1}$$

for some period $\Omega > 0$. In addition, we suppose that V satisfies Hypothesis 3.4.

Under these assumptions the Riemann surface associated with V, which by Floquet theoretic arguments, in general, would be a two-sheeted Riemann surface of infinite genus, can be reduced to the compact hyperelliptic Riemann surface corresponding to $\mathcal{K}_n$ induced by $y^2 = R_{2n+1}(z)$. Moreover, the corresponding Schrödinger operator H is then defined as in (4.1) and one introduces the fundamental system of distributional solutions $c(z,\cdot,x_0)$ and $s(z,\cdot,x_0)$ of $H\psi = z\psi$ satisfying

$$c(z,x_0,x_0) = s_x(z,x_0,x_0) = 1, \tag{C.2}$$

$$c_x(z,x_0,x_0) = s(z,x_0,x_0) = 0, \quad z \in \mathbb{C} \tag{C.3}$$

with $x_0 \in \mathbb{R}$ a fixed reference point. For each $x, x_0 \in \mathbb{R}$, $c(z,x,x_0)$ and $s(z,x,x_0)$ are entire with respect to z. The monodromy matrix $\mathcal{M}(z,x_0)$ is then given by

$$\mathcal{M}(z,x_0) = \begin{pmatrix} c(z,x_0+\Omega,x_0) & s(z,x_0+\Omega,x_0) \\ c_x(z,x_0+\Omega,x_0) & s_x(z,x_0+\Omega,x_0) \end{pmatrix}, \quad z \in \mathbb{C} \tag{C.4}$$

and its eigenvalues $\rho_\pm(z)$, the (x_0-independent) Floquet multipliers, satisfy

$$\rho_+(z)\rho_-(z) = 1 \tag{C.5}$$

since $\det(\mathcal{M}(z,x_0)) = 1$. The Floquet discriminant $\Delta(\cdot)$ is then defined by

$$\Delta(z) = \operatorname{tr}(\mathcal{M}(z,x_0))/2 = [c(z,x_0+\Omega,x_0) + s_x(z,x_0+\Omega,x_0)]/2 \tag{C.6}$$

and one obtains

$$\rho_\pm(z) = \Delta(z) \pm [\Delta(z)^2 - 1]^{1/2}. \tag{C.7}$$

We also note that

$$|\rho_\pm(z)| = 1 \text{ if and only if } \Delta(z) \in [-1,1]. \tag{C.8}$$

The Floquet solutions $\psi_\pm(z,x,x_0)$, the analog of the functions in (4.48), are then given by

$$\begin{aligned} \psi_\pm(z,x,x_0) = c(z,x,x_0) + s(z,x,x_0)[\rho_\pm(z) - c(z,x_0+\Omega,x_0)] \\ \times s(z,x_0+\Omega,x_0)^{-1}, \quad z \in \Pi\backslash\{\mu_j(x_0)\}_{j=1,\dots,n} \end{aligned} \tag{C.9}$$

and one verifies (for $x, x_0 \in \mathbb{R}$),

$$\psi_\pm(z, x+\Omega, x_0) = \rho_\pm(z)\psi_\pm(z, x, x_0), \quad z \in \Pi\backslash\{\mu_j(x_0)\}_{j=1,\dots,n}, \tag{C.10}$$

$$\psi_+(z, x, x_0)\psi_-(z, x, x_0) = \frac{s(z, x+\Omega, x)}{s(z, x_0+\Omega, x_0)}, \quad z \in \mathbb{C}\backslash\{\mu_j(x_0)\}_{j=1,\dots,n}, \tag{C.11}$$

$$W(\psi_+(z, \cdot, x_0), \psi_-(z, \cdot, x_0)) = -\frac{2[\Delta(z)^2 - 1]^{1/2}}{s(z, x_0+\Omega, x_0)}, \quad z \in \Pi\backslash\{\mu_j(x_0)\}_{j=1,\dots,n}, \tag{C.12}$$

$$g(z, x) = -\frac{s(z, x+\Omega, x)}{2[\Delta(z)^2 - 1]^{1/2}} = \frac{iF_n(z, x)}{2R_{2n+1}(z)^{1/2}}, \quad z \in \Pi. \tag{C.13}$$

Moreover, one computes

$$\begin{aligned} \frac{d\Delta(z)}{dz} &= -s(z, x_0+\Omega, x_0)\frac{1}{2}\int_{x_0}^{x_0+\Omega} dx\, \psi_+(z, x, x_0)\psi_-(z, x, x_0) \\ &= \Omega[\Delta(z)^2 - 1]^{1/2}\langle g(z, \cdot)\rangle, \quad z \in \mathbb{C} \end{aligned} \tag{C.14}$$

and hence

$$\frac{d\Delta(z)/dz}{[\Delta(z)^2 - 1]^{1/2}} = \frac{d}{dz}\big\{\ln\big[\Delta(z) + [\Delta(z)^2 - 1]^{1/2}\big]\big\} = \Omega\langle g(z, \cdot)\rangle, \quad z \in \Pi. \tag{C.15}$$

∎

Here the mean value $\langle f\rangle$ of a periodic function $f \in CP(\mathbb{R})$ of period $\Omega > 0$ is simply given by

$$\langle f\rangle = \frac{1}{\Omega}\int_{x_0}^{x_0+\Omega} dx\, f(x), \tag{C.16}$$

independent of the choice of $x_0 \in \mathbb{R}$. Thus, applying (3.22) one obtains

$$\begin{aligned} &\int_{z_0}^{z} \frac{dz'\,[d\Delta(z')/dz']}{[\Delta(z')^2 - 1]^{1/2}} = \ln\left(\frac{\Delta(z) + [\Delta(z)^2 - 1]^{1/2}}{\Delta(z_0) + [\Delta(z_0)^2 - 1]^{1/2}}\right) \\ &\quad = \Omega\int_{z_0}^{z} dz'\,\langle g(z', \cdot)\rangle = -(\Omega/2)\big[\big\langle g(z, \cdot)^{-1}\big\rangle - \big\langle g(z_0, \cdot)^{-1}\big\rangle\big], \\ &\qquad z, z_0 \in \Pi \end{aligned} \tag{C.17}$$

and hence

$$\ln\big[\Delta(z) + [\Delta(z)^2 - 1]^{1/2}\big] = -(\Omega/2)\big\langle g(z, \cdot)^{-1}\big\rangle + C. \tag{C.18}$$

Letting $|z| \to \infty$ one verifies that $C = 0$ and thus

$$\ln\big[\Delta(z) + [\Delta(z)^2 - 1]^{1/2}\big] = -(\Omega/2)\big\langle g(z, \cdot)^{-1}\big\rangle, \quad z \in \Pi. \tag{C.19}$$

We note that by continuity with respect to z, equations (C.12), (C.13), (C.15), (C.17), and (C.19) all extend to either side of the set of cuts in $\mathcal{C}$. Consequently,

$$\Delta(z) \in [-1,1] \text{ if and only if } \operatorname{Re}\big(\langle g(z,\cdot)^{-1}\rangle\big) = 0. \tag{C.20}$$

In particular, our characterization of the spectrum of H in (4.44) is thus equivalent to the standard Floquet theoretic characterization of H in terms of the Floquet discriminant,

$$\sigma(H) = \{\lambda \in \mathbb{C} \,|\, \Delta(\lambda) \in [-1,1]\}. \tag{C.21}$$

The result (C.21) was originally proven in [48] and [50] for complex-valued periodic (not necessarily algebro-geometric) potentials (cf. also [53], and more recently, [54], [55]).

We will end this appendix by providing an explicit example of the simple yet nontrivial genus $n = 1$ case which illustrates the periodic case as well as some of the general results of Sections 2–4 and Appendix B. For more general elliptic examples we refer to [27], [28] and the references therein.

By $\wp(\cdot) = \wp(\cdot\,|\,\Omega_1,\Omega_3)$ we denote the Weierstrass $\wp$-function with fundamental half-periods Ω_j, $j = 1,3$, $\Omega_1 > 0$, $\Omega_3 \in \mathbb{C}\backslash\{0\}$, $\operatorname{Im}(\Omega_3) > 0$, $\Omega_2 = \Omega_1 + \Omega_3$, and invariants g_2 and g_3 (cf. [1, Ch. 18]). By $\zeta(\cdot) = \zeta(\cdot\,|\Omega_1,\Omega_3)$ and $\sigma(\cdot) = \sigma(\cdot\,|\Omega_1,\Omega_3)$ we denote the Weierstrass zeta and sigma functions, respectively. We also denote $\tau = \Omega_3/\Omega_1$ and hence stress that $\operatorname{Im}(\tau) > 0$.

Example C.1. Consider the genus one ($n = 1$) Lamé potential

$$\begin{aligned} V(x) &= 2\wp(x+\Omega_3) && \text{(C.22)}\\ &= -2\bigg\{\ln\bigg[\theta\bigg(\frac{1}{2}+\frac{x}{2\Omega_1}\bigg)\bigg]\bigg\}'' - 2\frac{\zeta(\Omega_1)}{\Omega_1}, \quad x \in \mathbb{R}, && \text{(C.23)}\end{aligned}$$

where

$$\theta(z) = \sum_{n\in\mathbb{Z}} \exp\big(2\pi i n z + \pi i n^2 \tau\big), \quad z \in \mathbb{C},\ \tau = \Omega_3/\Omega_1, \tag{C.24}$$

and introduce

$$L = -\frac{d^2}{dx^2} + 2\wp(x+\Omega_3), \quad P_3 = -\frac{d^3}{dx^3} + 3\wp(x+\Omega_3)\frac{d}{dx} + \frac{3}{2}\wp'(x+\Omega_3). \tag{C.25}$$

Then one obtains

$$[L, P_3] = 0 \tag{C.26}$$

which yields the elliptic curve

$$\mathcal{K}_1\colon \mathcal{F}_1(z,y) = y^2 - R_3(z) = y^2 - \big(z^3 - (g_2/4)z + (g_3/4)\big) = 0,$$

$$R_3(z) = \prod_{m=0}^{2}(z - E_m) = z^3 - (g_2/4)z + (g_3/4), \tag{C.27}$$
$$E_0 = -\wp(\Omega_1),\ E_1 = -\wp(\Omega_2),\ E_2 = -\wp(\Omega_3).$$

Moreover, one has

$$F_1(z,x) = z + \wp(x+\Omega_3), \quad \mu_1(x) = -\wp(x+\Omega_3), \tag{C.28}$$
$$H_2(z,x) = z^2 - \wp(x+\Omega_3)z + \wp(x+\Omega_3)^2 - (g_2/4), \tag{C.29}$$
$$\nu_\ell(x) = \big[\wp(x+\Omega_3) - (-1)^\ell[g_2 - 3\wp(x+\Omega_3)^2]^{1/2}\big]/2, \quad \ell = 0,1$$

and

$$\text{s-}\widehat{\text{KdV}}_1(V) = 0, \tag{C.30}$$
$$\text{s-}\widehat{\text{KdV}}_2(V) - (g_2/8)\,\text{s-}\widehat{\text{KdV}}_0(V) = 0, \text{ etc.} \tag{C.31}$$

In addition, we record

$$\psi_\pm(z,x,x_0) = \frac{\sigma(x+\Omega_3 \pm b)\sigma(x_0+\Omega_3)}{\sigma(x+\Omega_3)\sigma(x_0+\Omega_3 \pm b)} e^{\mp\zeta(b)(x-x_0)}, \tag{C.32}$$
$$\psi_\pm(z,x+2\Omega_1,x_0) = \rho_\pm(z)\psi_\pm(z,x,x_0), \quad \rho_\pm(z) = e^{\pm[(b/\Omega_1)\zeta(\Omega_1)-\zeta(b)]2\Omega_1} \tag{C.33}$$

with Floquet parameter corresponding to Ω_1-direction given by

$$k_1(b) = i[\zeta(b)\Omega_1 - \zeta(\Omega_1)b]/\Omega_1. \tag{C.34}$$

Here

$$\begin{aligned} P &= (z,y) = (-\wp(b), -(i/2)\wp'(b)) \in \Pi_+, \\ P^* &= (z,-y) = (-\wp(b), (i/2)\wp'(b)) \in \Pi_-, \end{aligned} \tag{C.35}$$

where b varies in the fundamental period parallelogram spanned by the vertices 0, $2\Omega_1$, $2\Omega_2$, and $2\Omega_3$. One then computes

$$\Delta(z) = \cosh[2(\Omega_1\zeta(b) - b\zeta(\Omega_1))], \tag{C.36}$$
$$\langle\mu_1\rangle = \zeta(\Omega_1)/\Omega_1, \quad \langle V\rangle = -2\zeta(\Omega_1)/\Omega_1, \tag{C.37}$$
$$g(z,x) = -\frac{z+\wp(x+\Omega_3)}{\wp'(b)}, \tag{C.38}$$
$$\frac{d}{dz}\big\langle g(z,\cdot)^{-1}\big\rangle = 2\frac{z - [\zeta(\Omega_1)/\Omega_1]}{\wp'(b)} = -2\langle g(z,\cdot)\rangle, \tag{C.39}$$
$$\big\langle g(z,\cdot)^{-1}\big\rangle = -2[\zeta(b) - (b/\Omega_1)\zeta(\Omega_1)], \tag{C.40}$$

where $(z,y) = (-\wp(b), -(i/2)\wp'(b)) \in \Pi_+$. The spectrum of the operator H with potential $V(x) = 2\wp(x+\Omega_3)$ is then determined as follows

$$\sigma(H) = \{\lambda \in \mathbb{C} \,|\, \Delta(\lambda) \in [-1,1]\} \tag{C.41}$$

$$= \big\{\lambda \in \mathbb{C} \,\big|\, \mathrm{Re}\big(\langle g(\lambda,\cdot)^{-1}\rangle\big) = 0\big\} \tag{C.42}$$
$$= \{\lambda \in \mathbb{C} \,|\, \mathrm{Re}[\Omega_1\zeta(b) - b\zeta(\Omega_1)] = 0,\, \lambda = -\wp(b)\}. \tag{C.43}$$

Generically (cf. [54]), $\sigma(H)$ consists of one simple analytic arc (connecting two of the three branch points E_m, $m = 0, 1, 2$) and one simple semi-infinite analytic arc (connecting the remaining of the branch points and infinity). The semi-infinite arc σ_∞ asymptotically approaches the half-line $L_{\langle V\rangle} = \{z \in \mathbb{C} \,|\, z = -2\zeta(\Omega_1)/\Omega_1 + x,\, x \geq 0\}$ in the following sense: asymptotically, σ_∞ can be parameterized by

$$\sigma_\infty = \big\{z \in \mathbb{C} \,\big|\, z = R - 2i\,[\mathrm{Im}(\zeta(\Omega_1))/\Omega_1] + O\big(R^{-1/2}\big) \text{ as } R \uparrow \infty\big\}. \tag{C.44}$$

We note that a slight change in the setup of Example C.1 permits one to construct crossing spectral arcs as shown in [26]. One only needs to choose complex conjugate fundamental half-periods $\widehat{\Omega}_1 \notin \mathbb{R}$, $\widehat{\Omega}_3 = \overline{\widehat{\Omega}_1}$ with real period $\Omega = 2\big(\widehat{\Omega}_1 + \widehat{\Omega}_3\big) > 0$ and consider the potential $V(x) = 2\wp\big(x + a\,\big|\widehat{\Omega}_1, \widehat{\Omega}_3\big)$, $0 < \mathrm{Im}(a) < 2\big|\mathrm{Im}\big(\widehat{\Omega}_1\big)\big|$.

Finally, we briefly consider a change of homology basis and illustrate Theorem B.5. Let $\Omega_1 > 0$ and $\Omega_3 \in \mathbb{C}$, $\mathrm{Im}(\Omega_3) > 0$. We choose the homology basis $\{\tilde a_1, \tilde b_1\}$ such that $\tilde b_1$ encircles E_0 and E_1 counterclockwise on Π_+ and $\tilde a_1$ starts near E_1, intersects $\tilde b_1$ on Π_+, surrounds E_2 clockwise and then continues on Π_- back to its initial point surrounding E_1 such that (A.16) holds. Then,

$$\omega_1 = c_1(1)\, dz/y, \quad c_1(1) = (4i\Omega_1)^{-1}, \tag{C.45}$$
$$\int_{\tilde a_1} \omega_1 = 1, \quad \int_{\tilde b_1} \omega_1 = \tau, \quad \tau = \Omega_3/\Omega_1, \tag{C.46}$$
$$\widetilde{\omega}^{(2)}_{P_\infty,0} = -\frac{(z-\lambda_1)dz}{2y}, \quad \lambda_1 = \zeta(\Omega_1)/\Omega_1, \tag{C.47}$$
$$\int_{\tilde a_1} \widetilde{\omega}^{(2)}_{P_\infty,0} = 0, \quad \frac{1}{2\pi i}\int_{\tilde b_1} \widetilde{\omega}^{(2)}_{P_\infty,0} = -2c_1(1) = \widetilde{U}_{0,1}, \tag{C.48}$$
$$\widetilde{U}_{0,1} = \frac{i}{2\Omega_1} \in i\mathbb{R}, \tag{C.49}$$
$$\int_{Q_0}^{P} \widetilde{\omega}^{(2)}_{P_\infty,0} - \tilde e^{(2)}_0(Q_0) \underset{b\to 0}{=} \frac{i}{b} + O(b)$$
$$\underset{\zeta\to 0}{=} -\zeta^{-1} + O(\zeta), \quad \zeta = \sigma/z^{1/2},\, \sigma \in \{1,-1\}, \tag{C.50}$$
$$\tilde e^{(2)}_0(Q_0) = -i[\zeta(b_0)\Omega_1 - \zeta(\Omega_1)b_0]/\Omega_1, \tag{C.51}$$
$$i\bigg[\int_{Q_0}^{P} \widetilde{\omega}^{(2)}_{P_\infty,0} - \tilde e^{(2)}_0(Q_0)\bigg] = [\zeta(\Omega_1)b - \zeta(b)\Omega_1]/\Omega_1, \tag{C.52}$$

$$P = (-\wp(b), -(i/2)\wp'(b)),\ Q_0 = (-\wp(b_0), -(i/2)\wp'(b_0)).$$

The change of homology basis (cf. (A.33)–(A.39))

$$\begin{pmatrix} \tilde a_1 \\ \tilde b_1 \end{pmatrix} \mapsto \begin{pmatrix} a_1' \\ b_1' \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} \tilde a_1 \\ \tilde b_1 \end{pmatrix} = \begin{pmatrix} A\tilde a_1 + B\tilde b_1 \\ Ca_1 + Db_1 \end{pmatrix}, \tag{C.53}$$

$$A, B, C, D \in \mathbb{Z}, \quad AD - BC = 1, \tag{C.54}$$

then implies

$$\omega_1' = \frac{\omega_1}{A + B\tau}, \tag{C.55}$$

$$\tau' = \frac{\Omega_3'}{\Omega_1'} = \frac{C + D\tau}{A + B\tau}, \tag{C.56}$$

$$\Omega_1' = A\Omega_1 + B\Omega_3, \quad \Omega_3' = C\Omega_1 + D\Omega_3, \tag{C.57}$$

$$\omega_{P_\infty,0}^{(2)\,\prime} = -\frac{(z - \lambda_1')dz}{2y}, \quad \lambda_1' = \lambda_1 - \frac{\pi i B}{2\Omega_1\Omega_1'}, \tag{C.58}$$

$$\int_{a_1'} \omega_{P_\infty,0}^{(2)\,\prime} = 0, \quad \frac{1}{2\pi i}\int_{b_1'} \omega_{P_\infty,0}^{(2)\,\prime} = -\frac{2c_1(1)}{A + B\tau} = U_{0,1}', \tag{C.59}$$

$$U_{0,1}' = \frac{\widetilde U_{0,1}}{A + B\tau} = \frac{i}{2\Omega_1'}. \tag{C.60}$$

Moreover, one infers

$$\begin{aligned} &\psi_\pm(z, x + 2\Omega_1', x_0) = \rho_\pm(z)'\psi_\pm(z, x, x_0), \\ &\rho_\pm(z)' = e^{\pm[(b/\Omega_1')(A\zeta(\Omega_1) + B\zeta(\Omega_3)) - \zeta(b)]2\Omega_1'} \end{aligned} \tag{C.61}$$

with Floquet parameter $k_1(b)'$ corresponding to Ω_1'-direction given by

$$k_1(b)' = i\left[\zeta(b)\Omega_1 - \zeta(\Omega_1)b + \frac{\pi i B}{2\Omega_1'}b\right]\Big/\Omega_1. \tag{C.62}$$

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