ONE-DIMENSIONAL SCATTERING THEORY FOR QUANTUM SYSTEMS WITH NONTRIVIAL SPATIAL ASYMPTOTICS

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Abstract. We provide a general framework of stationary scattering theory for one-dimensional quantum systems with nontrivial spatial asymptotics. As a byproduct we characterize reflectionless potentials in terms of spectral multiplicities and properties of the diagonal Green's function of the underlying Schrödinger operator. Moreover, we prove that single (Crum-Darboux) and double commutation methods to insert eigenvalues into spectral gaps of a given background Schrödinger operator produce reflectionless potentials (i.e., solitons) if and only if the background potential is reflectionless.

Possible applications of our formalism include impurity (defect) scattering in (half)crystals and charge transport in mesoscopic quantum-interference devices.

1. Introduction

The purpose of this paper is to develop a general framework of stationary scattering theory for one-dimensional quantum systems which exhibit nontrivial spatial asymptotics as $x \to \pm\infty$ and to provide a unified treatment of a variety of physical phenomena including impurity (defect) scattering in (half-)crystals and charge transport in quasi-one-dimensional mesoscopic solid state structures. In addition, we give an explicit characterization of reflectionless potentials in terms of spectral multiplicities and properties of diagonal Green's functions of the underlying Schrödinger operator. The latter is of particular interest in connection with soliton solutions of the Korteweg-de Vries (KdV) equation with respect to general KdV background solutions.

Quantum systems with nontrivial spatial asymptotics (e.g., asymptotically periodic potentials with possibly different periods as $x \to \pm\infty$) have recently generated renewed interest

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due to their possible applications in mesoscopic solid state structures. A complete bibliography is impossible in this context but the interested reader may consult, e.g., [12], [37] and the references therein. From a mathematical perspective, scattering theory for one-dimensional systems with different spatial asymptotics has been pioneered by Ruijsenaars and Bongaarts [42] in connection with Dirac operators and by Davies and Simon [8] in connection with time-dependent aspects of scattering theory for Schrödinger operators on the line. Additional references to stationary scattering and inverse scattering problems in connection with nontrivial spatial asymptotics can be found, e.g., in [4]–[6], [14]–[16], [22], [29], [30], [34], [35], [37], [38], Example 4 in Sect. XI.4, [40], [41].

Our main tool in providing a unified treatment of (direct) stationary scattering theory for systems with different asymptotics as $x \to \pm\infty$ will be a systematic application of Weyl-Titchmarsh theory for second-order differential operators on $\mathbb{R}$ and explicit spectral representations in terms of (generalized) eigenfunction expansions for such operators. While the latter is a standard method in stationary scattering theory, the connections with the Weyl-Titchmarsh theory are our principal new contributions to the subject.

Section 2 reviews standard Weyl-Titchmarsh theory as needed in the remainder of this paper and Section 3 introduces spectral representations for one-dimensional Schrödinger operators H. Our principal Section 4 on scattering data then combines techniques from Sections 2 and 3 to arrive at explicit expressions of transmission and reflection coefficients in terms of Weyl m-functions and phases of asymptotic wave functions (cf. Theorem 4.2) and details the connection between scattering data and spectral representations of the underlying Schrödinger operator H. Moreover, we obtain a general criterion for reflectionless interactions in terms of spectral multiplicities and the diagonal Green's function of H. Section 5 finally provides the basis for a wide range of possible applications including impurity (defect) scattering in (half-)crystals and charge transport in quasi-one-dimensional solids.

Due to the broad range of possible applications, we made some efforts to keep our exposition accessible to theoretical and mathematical physicists alike and avoided technicalities at the expense of greater generality whenever possible. In particular, we included some motivations and partially formal arguments whenever they appeared to be helpful in bridging the usual gap between applied and pure science (though all our final results are formulated in a precise manner).

2. Background Material

In this section we provide some background material on the Weyl-Titchmarsh theory for one-dimensional Schrödinger operators on $\mathbb{R}$ needed in Sections 3 and 4. Details may be found, e.g., in [3], Ch. VI, [13], Sects. XIII.3–5, [31], Ch. 7, [32], Ch. 2, [33], Ch. VI, [36], Chs. 6, 7.

Given a real-valued potential $V \in L^1_{\text{loc}}(\mathbb{R})$ we introduce the differential expression

$$\tau = -\frac{d^2}{dx^2} + V(x), \quad x \in \mathbb{R} \tag{2.1}$$

and the associated operator H in $L^2(\mathbb{R})$,

$$Hf = \tau f,\ f \in \mathcal{D}(H) = \{g \in L^2(\mathbb{R}) \mid g, g' \in AC_{\text{loc}}(\mathbb{R}),\ \tau g \in L^2(\mathbb{R})\}. \tag{2.2}$$

(Here $AC_{\text{loc}}(\Omega)$ denotes the set of locally absolutely continuous functions on Ω.) Moreover, let $H^D_\pm$ be the corresponding Dirichlet operators in $L^2((0, \pm\infty))$ with a Dirichlet boundary condition at $x = 0$, i.e.,

$$\begin{aligned} &H^D_\pm f = \tau f,\ f \in \mathcal{D}(H^D_\pm) \\ &= \{g \in L^2((0, \pm\infty)) \mid g, g' \in AC_{\text{loc}}((0, \pm\infty)),\ \lim_{\epsilon \downarrow 0} g(\pm\epsilon) = 0,\ \tau g \in L^2((0, \pm\infty))\}. \end{aligned} \tag{2.3}$$

Our basic hypothesis in connection with τ then reads

(H.2.1) . *Define τ and H, $H^D_\pm$ as in* (2.1)–(2.3).
(i). Assume τ is in the limit point case at $\pm\infty$.
(ii). Suppose H has non-empty absolutely continuous spectrum and H, $H^D_\pm$ have no singularly continuous spectrum and no embedded eigenvalues, i.e.,

$$\sigma_{\text{ac}}(H) \neq \emptyset,\ \sigma_{\text{sc}}(H) = \sigma_{\text{sc}}(H^D_\pm) = \sigma_p(H) \cap \sigma_{\text{ac}}(H) = \sigma_p(H^D_\pm) \cap \sigma_{\text{ac}}(H^D_\pm) = \emptyset.$$

(Here $\sigma_{\text{ac}}(\cdot)$, $\sigma_{\text{sc}}(\cdot)$, and $\sigma_p(\cdot)$ denote the absolutely continuous, singularly continuous, and point spectrum (i.e., the set of eigenvalues), respectively.)

These conditions are not independent of each other since non-empty essential spectrum of τ implies self-adjointness of H, i.e., (H.2.1)(i), but this is of no concern to us in this context. Moreover, condition (ii) could be considerably relaxed but we decided to avoid unnecessary technicalities in this paper.

Next we introduce the standard fundamental system $\theta(z,x)$, $\phi(z,x)$ of solutions of $\tau\psi = z\psi$, $z \in \mathbb{C}$ defined as

$$\theta(z,0) = \phi'(z,0) = 1, \ \theta'(z,0) = \phi(z,0) = 0, \ z \in \mathbb{C} \tag{2.4}$$

and introduce the Weyl solutions $f_\pm(z,x)$ uniquely determined by the requirements

$$\begin{aligned} &f_\pm(z,x) = \theta(z,x) + m_\pm(z)\phi(z,x), \\ &f_\pm(z,\cdot) \in L^2((R,\pm\infty)), \quad R \in \mathbb{R}, \ z \in \mathbb{C}\backslash\sigma(H) \end{aligned} \tag{2.5}$$

($\sigma(\cdot)$ abbreviating the spectrum). The coefficients $m_\pm(z)$ determined by (2.5) represent the Weyl-Titchmarsh m-functions associated with τ. In connection with the half-line m-functions $m_\pm(z)$ one also defines the Weyl-Titchmarsh M-matrix in $\mathbb{C}^2$ of H,

$$M(z) = (M_{p,q}(z))_{1\le p,q\le 2} = [m_-(z) - m_+(z)]^{-1} \begin{pmatrix} m_+(z)m_-(z) & [m_-(z)+m_+(z)]/2 \\ [m_-(z)+m_+(z)]/2 & 1 \end{pmatrix}, \quad z \in \mathbb{C}\backslash\sigma(H), \tag{2.6}$$

and the corresponding right-continuous self-adjoint spectral matrix $\rho(\lambda)$ of H,

$$\rho(\lambda) = (\rho_{p,q}(\lambda))_{1\le p,q\le 2}, \quad \lambda \in \mathbb{R}, \tag{2.7}$$

where

$$\rho_{p,q}(\lambda) - \rho_{p,q}(\mu) = \lim_{\delta\downarrow 0}\lim_{\epsilon\downarrow 0} \pi^{-1}\int_{\mu+\delta}^{\lambda+\delta} d\nu \, \mathrm{Im}[M_{p,q}(\nu + i\epsilon)], \quad \lambda,\mu \in \mathbb{R}, \ p,q = 1,2. \tag{2.8}$$

Next we introduce

$$\begin{aligned} \Sigma_1^\pm = \{\lambda \in \mathbb{R} \mid &\mathrm{Im}[m_-(\lambda+i0)] \text{ and } \mathrm{Im}[m_+(\lambda+i0)] \text{ exist}, \\ &\mathrm{Im}[m_\pm(\lambda+i0)] = 0 \text{ or } \infty, \ 0 < \mp\,\mathrm{Im}[m_\mp(\lambda+i0)] < \infty\}, \end{aligned} \tag{2.9}$$

$$\Sigma_2 = \{\lambda \in \mathbb{R} \mid \mathrm{Im}[m_\pm(\lambda+i0)] \text{ exist}, \ 0 < \pm\,\mathrm{Im}[m_\pm(\lambda+i0)] < \infty\}, \tag{2.10}$$

$$\Sigma_1 = \Sigma_1^+ \cup \Sigma_1^-, \ \Sigma = \Sigma_1 \cup \Sigma_2 \tag{2.11}$$

(abbreviating $m_\pm(\lambda + i0) = \lim_{\epsilon\downarrow 0} m_\pm(\lambda + i\epsilon)$ in obvious notation). By standard Weyl-Titchmarsh theory, Σ is a minimal support for $\sigma_{\mathrm{ac}}(H) = \sigma_{\mathrm{ac}}(H_+^D) \cup \sigma_{\mathrm{ac}}(H_-^D)$ (see, e.g., [1], [24], [25]) and due to Hypothesis (H.2.1), $\Sigma = \sigma_{\mathrm{ac}}(H)$ a.e. (with respect to Lebesgue measure). Moreover, H has uniform spectral multiplicity n on Σ_n, $n=1,2$ (see, e.g., [24], [26], [27]) assuming $|\Sigma_n|>0$ ($|\cdot|$ denoting Lebesgue measure) and

$$\dot\rho_{p,q}\in L^1_{\mathrm{loc}}(\sigma_{\mathrm{ac}}(H)),\ \dot\rho_{1,1}+\dot\rho_{2,2}>0 \text{ a.e. on } \sigma_{\mathrm{ac}}(H) \tag{2.12}$$

(abbreviating "$\dot{}$" $=d/d\lambda$). In order to avoid trivial situations in the following we assumed in (H.2.1)(ii) that at least one of $\Sigma_1^\pm$, Σ_2 has positive Lebesgue measure and we agree to identify Σ_1^- with the empty set $\emptyset$ whenever $|\Sigma_1^-|=0$ and similarly for Σ_1^+, Σ_2.

The (generalized) eigenfunction expansion associated with H then reads (cf., e.g., the references cited at the beginning of this section),

$$\begin{aligned}f(\cdot)=&\sum_{j\in J}\Psi(\lambda_j,\cdot)(\Psi(\lambda_j),f)+\operatorname*{s-lim}_{R\to\infty}\int_{\Sigma\cap[-R,R]}d\lambda\{\dot\rho_{1,1}(\lambda)\phi(\lambda,\cdot)(\phi(\lambda),f)\\&+\dot\rho_{2,2}(\lambda)\theta(\lambda,\cdot)(\theta(\lambda),f)+\dot\rho_{1,2}(\lambda)[\theta(\lambda,\cdot)(\phi(\lambda),f)+\phi(\lambda,\cdot)(\theta(\lambda),f)]\},\ f\in L^2(\mathbb{R}),\end{aligned} \tag{2.13}$$

where J denotes a (possibly empty) index set associated with the point spectrum $\sigma_p(H)=\{\lambda_j\}_{j\in J}$ of H, $\Psi(\lambda_j,x)$ are the corresponding normalized real-valued eigenfunctions

$$\Psi(\lambda_j)\in\mathcal{D}(H),\ H\Psi(\lambda_j)=\lambda_j\Psi(\lambda_j),\ \|\Psi(\lambda_j,\cdot)\|_2=1,\ j\in J, \tag{2.14}$$

and

$$\begin{aligned}(\phi(\cdot),f)&=\operatorname*{s-lim}_{R\to\infty}\int_{-R}^{R}dx\phi(\cdot,x)f(x)\text{ in }L^2(\Sigma),\\(\theta(\cdot),f)&=\operatorname*{s-lim}_{R\to\infty}\int_{-R}^{R}dx\theta(\cdot,x)f(x)\text{ in }L^2(\Sigma)\end{aligned} \tag{2.15}$$

are (generalized) Fourier coefficients. If J is infinite, $\sum_{j\in J}$ in (2.13) is to be interpreted as a strong limit in $L^2(\mathbb{R})$. (We agree to abbreviate $L^p(\Omega)=L^p(\Omega;d\mu)$ whenever $d\mu$ represents Lebesgue measure.)

It is customary to abbreviate (2.13)–(2.15) by the short-hand notation

$$\begin{aligned}\delta(x-x')=&\sum_{j\in J}\Psi(\lambda_j,x)\Psi(\lambda_j,x')+\int_\Sigma d\lambda\{\dot\rho_{1,1}(\lambda)\phi(\lambda,x)\phi(\lambda,x')\\&+\dot\rho_{2,2}(\lambda)\theta(\lambda,x)\theta(\lambda,x')+\dot\rho_{1,2}[\theta(\lambda,x)\phi(\lambda,x')+\phi(\lambda,x)\theta(\lambda,x')]\}.\end{aligned} \tag{2.16}$$

Next we are looking for an alternative but equivalent expression of (2.16) (respectively (2.13)) in terms of $f_\pm(\lambda,x)$, $\overline{f_\pm(\lambda,x)}$ ("$\overline{}$" denoting complex conjugation). We are searching for functions $\Psi_\pm(\lambda,x)$, $\lambda\in\Sigma$ satisfying

$$\text{for all } x\in\mathbb{R},\ \Psi_\pm(\lambda,x)=\Psi_\pm(\lambda,0)f_\pm(\lambda+i0,x)\text{ a.e. on }\Sigma \tag{2.17}$$

and

$$\delta(x-x') = \sum_{j\in J} \Psi(\lambda_j, x)\Psi(\lambda_j, x') + \int_\Sigma d\lambda[\Psi_-(\lambda, x)\overline{\Psi_-(\lambda, x')} + \Psi_+(\lambda, x)\overline{\Psi_+(\lambda, x')}]. \tag{2.18}$$

At this point (2.17), (2.18) determine $\Psi_\pm(\lambda, x)$ only up to the phase of $\Psi_\pm(\lambda, 0)$. We shall fix that phase later on in a natural manner (see (4.9)). In order to determine $|\Psi_\pm(\lambda, 0)|$ we first recall the Wronskian relations,

$$\begin{aligned} W(\Psi_\pm(\lambda),\ \overline{\Psi_\pm(\lambda)}) &= -2i|\Psi_\pm(\lambda, 0)|^2 \operatorname{Im}[m_\pm(\lambda+i0)], \\ W(\Psi_-(\lambda), \Psi_+(\lambda)) &= \Psi_-(\lambda, 0)\Psi_+(\lambda, 0)[m_+(\lambda+i0) - m_-(\lambda+i0)] \\ &\qquad \text{a.e. on } \Sigma \end{aligned} \tag{2.19}$$

using (2.4), (2.5), and (2.17). Here $W(f,g)(x) = f(x)g'(x) - f'(x)g(x)$ denotes the Wronskian of f and g. Next, a comparison of (2.16) and (2.18) yields

$$\begin{aligned} \dot\rho_{1,1}(\lambda) &= |\Psi_-(\lambda, 0)|^2 |m_-(\lambda+i0)|^2 + |\Psi_+(\lambda, 0)|^2 |m_+(\lambda+i0)|^2 \\ &= |\Psi'_-(\lambda, 0)|^2 + |\Psi'_+(\lambda, 0)|^2, \end{aligned} \tag{2.20}$$

$$\dot\rho_{2,2}(\lambda) = |\Psi_-(\lambda, 0)|^2 + |\Psi_+(\lambda, 0)|^2, \tag{2.21}$$

$$\begin{aligned} \dot\rho_{1,2}(\lambda) = \dot\rho_{2,1}(\lambda) &= |\Psi_-(\lambda, 0)|^2 m_-(\lambda+i0) + |\Psi_+(\lambda, 0)|^2 m_+(\lambda+i0) \\ &= |\Psi_-(\lambda, 0)|^2\, \overline{m_-(\lambda+i0)} + |\Psi_+(\lambda, 0)|^2\, \overline{m_+(\lambda+i0)} \\ &\qquad \text{a.e. on } \Sigma. \end{aligned} \tag{2.22}$$

On the other hand, (2.6), (2.8), and (2.13) imply

$$\dot\rho_{1,1}(\lambda) = \frac{1}{\pi}\frac{|m_-(\lambda+i0)|^2 \operatorname{Im}[m_+(\lambda+i0)] - |m_+(\lambda+i0)|^2 \operatorname{Im}[m_-(\lambda+i0)]}{|m_-(\lambda+i0) - m_+(\lambda+i0)|^2}, \tag{2.23}$$

$$\dot\rho_{2,2}(\lambda) = \frac{1}{\pi}\frac{\operatorname{Im}[m_+(\lambda+i0)] - \operatorname{Im}[m_-(\lambda+i0)]}{|m_-(\lambda+i0) - m_+(\lambda+i0)|^2}, \tag{2.24}$$

$$\begin{aligned} \dot\rho_{1,2}(\lambda) = \dot\rho_{2,1}(\lambda) &= \frac{1}{2i\pi}\frac{m_+(\lambda+i0)\,\overline{m_-(\lambda+i0)} - \overline{m_+(\lambda+i0)}m_-(\lambda+i0)}{|m_-(\lambda+i0) - m_+(\lambda+i0)|^2}, \\ &\qquad \text{a.e. on } \Sigma. \end{aligned} \tag{2.25}$$

Thus we obtain

Lemma 2.1. *Assume hypothesis (H.2.1), then*

$$|\Psi_\pm(\lambda,0)|^2 = \mp\pi^{-1}|m_-(\lambda+i0) - m_+(\lambda+i0)|^{-2}\operatorname{Im}[m_\mp(\lambda+i0)] \tag{2.26}$$

for a.e. $\lambda\in\Sigma$.

Proof. It suffices to combine (2.21), (2.22), and (2.24).

One observes that (2.26) is consistent with the well-known Herglotz property of $\pm m_\pm(z)$ (i.e., $\pm m_\pm : \mathbb{C}_+ \to \mathbb{C}_+$ are holomorphic, where $\mathbb{C}_+ = \{z\in\mathbb{C} \mid \operatorname{Im}(z) > 0\}$). Moreover, a comparison of (2.19) and (2.26) also yields

$$\begin{aligned} W(\Psi_\pm(\lambda), \overline{\Psi_\pm(\lambda)}) &= \mp 2\pi i |W(\Psi_-(\lambda),\Psi_+(\lambda))|^2 \\ &= \mp 2i\pi^{-1}|m_-(\lambda+i0)-m_+(\lambda+i0)|^{-2}\{-\operatorname{Im}[m_-(\lambda+i0)]\operatorname{Im}[m_+(\lambda+i0)]\} \\ &\qquad\qquad \text{a.e. on } \Sigma. \end{aligned} \tag{2.27}$$

3. Spectral Representations

With the preliminaries on Weyl-Titchmarsh theory out of the way, we now turn to spectral representations for $HP_{\rm ac}(H)$, where $P_{\rm ac}(H) = \chi_{\sigma_{ac}(H)}(H)$ denotes the projection onto the absolutely continuous subspace $\mathcal{H}_{\rm ac}(H) = P_{\rm ac}(H)L^2(\mathbb{R})$ of H ($\chi_\Omega(\cdot)$ the characteristic function of $\Omega\subseteq\mathbb{R}$). Due to Hypothesis (H.2.1), $\mathcal{H}_{\rm ac}(H) = \mathcal{H}_p(H)^\perp$, with $\mathcal{H}_p(H)$ the pure point subspace of H.

We introduce the isometric bijections

$$T : \begin{cases} \mathcal{H}_{\rm ac}(H) & \to L^2(\Sigma_1^-)\oplus L^2(\Sigma_1^+)\oplus[L^2(\Sigma_2)\otimes\mathbb{C}^2] \\ f & \mapsto \Big((\Psi_-(\cdot),f),(\Psi_+(\cdot),f),\Big(\begin{smallmatrix}(\Psi_+(\cdot),f)\\(\Psi_-(\cdot),f)\end{smallmatrix}\Big)\Big) \end{cases}, \tag{3.1}$$

$$\tilde T : \begin{cases} \mathcal{H}_{\rm ac}(H) & \to L^2(\Sigma_1^-)\oplus L^2(\Sigma_1^+)\oplus[L^2(\Sigma_2)\otimes\mathbb{C}^2] \\ f & \mapsto \Big((\overline{\Psi_-(\cdot)},f),(\overline{\Psi_+(\cdot)},f),\Big(\begin{smallmatrix}(\overline{\Psi_-(\cdot)},f)\\(\overline{\Psi_+(\cdot)},f)\end{smallmatrix}\Big)\Big) \end{cases}, \tag{3.2}$$

where

$$\begin{aligned} (\Psi_\pm(\cdot),f) &= \operatorname*{s-lim}_{R\to\infty}\int_{-R}^R dx\overline{\Psi_\pm(\cdot,x)}f(x) \text{ in } L^2(\Sigma_1^\pm \text{ or } \Sigma_2), \\ (\overline{\Psi_\pm(\cdot)},f) &= \operatorname*{s-lim}_{R\to\infty}\int_{-R}^R dx\Psi_\pm(\cdot,x)f(x) \text{ in } L^2(\Sigma_1^\pm \text{ or } \Sigma_2). \end{aligned} \tag{3.3}$$

One verifies

$$T^{-1}:\begin{cases} L^2(\Sigma_1^-)\oplus L^2(\Sigma_1^+)\oplus[L^2(\Sigma_2)\otimes\mathbb{C}^2]\to\mathcal{H}_{\mathrm{ac}}(H) \\ \left(g_-,g_+,\binom{h_+}{h_-}\right)\mapsto \underset{R\to\infty}{\text{s-lim}}\Big\{\int_{\Sigma_1^-\cap[-R,R]} d\lambda g_-(\lambda)\Psi_-(\lambda,\cdot) \\ \qquad\qquad + \int_{\Sigma_1^+\cap[-R,R]} d\lambda g_+(\lambda)\Psi_+(\lambda,\cdot) \\ \qquad\qquad + \int_{\Sigma_2\cap[-R,R]} d\lambda [h_-(\lambda)\Psi_-(\lambda,\cdot)+h_+(\lambda)\Psi_+(\lambda,\cdot)]\Big\} \end{cases}, \tag{3.4}$$

$$\bar{T}^{-1}:\begin{cases} L^2(\Sigma_1^-)\oplus L^2(\Sigma_1^+)\oplus[L^2(\Sigma_2)\otimes\mathbb{C}^2]\to\mathcal{H}_{\mathrm{ac}}(H) \\ \left(g_-,g_+,\binom{h_+}{h_-}\right)\mapsto \underset{R\to\infty}{\text{s-lim}}\Big\{\int_{\Sigma_1^-\cap[-R,R]} d\lambda g_-(\lambda)\overline{\Psi_-(\lambda,\cdot)} \\ \qquad\qquad + \int_{\Sigma_1^+\cap[-R,R]} d\lambda g_+(\lambda)\overline{\Psi_+(\lambda,\cdot)} \\ \qquad\qquad + \int_{\Sigma_2\cap[-R,R]} d\lambda [h_-(\lambda)\overline{\Psi_+(\lambda,\cdot)}+h_+(\lambda)\overline{\Psi_-(\lambda,\cdot)}]\Big\} \end{cases}. \tag{3.5}$$

At first sight it might be somewhat surprising that even though $\mathrm{Im}[m_\pm(\lambda+i0)]|_{\Sigma_1^\pm}=0$, one is using $f_\pm(\lambda+i0,x)$ in (3.1), (3.2), (3.4), and (3.5) in connection with $\Sigma_1^\pm$. The point is that, in general, $f_\pm(\lambda,x)$, $\lambda\in\Sigma_1^\pm$ will be decreasing as $x\to\pm\infty$ and oscillatory as $x\to\mp\infty$ whereas $f_\mp(\lambda+i0,x)$, $\lambda\in\Sigma_1^\pm$ will be oscillatory as $x\to\mp\infty$ and contain an increasing (unbounded) component as $x\to\pm\infty$ (cf., e.g., Example 5.3).

Standard spectral theory for the self-adjoint operator H then yields (see, e.g., [2], Chs. 3, 4, [43], Ch. 5 and the references cited at the beginning of Section 2),

$$T^{-1}T=\bar{T}^{-1}\bar{T}=P_{\mathrm{ac}}(H),\ \|\overset{(-)}{T}f\|_{\hat{\mathcal{H}}}=\|f\|_{\mathcal{H}_{\mathrm{ac}}(H)} \tag{3.6}$$

and

$$TT^{-1}=\bar{T}\bar{T}^{-1}=1_{\hat{\mathcal{H}}}, \tag{3.7}$$

where we abbreviated

$$\hat{\mathcal{H}}=L^2(\Sigma_1^-)\oplus L^2(\Sigma_1^+)\oplus[L^2(\Sigma_2)\otimes\mathbb{C}^2]. \tag{3.8}$$

While (3.6) is formally summed up in (2.18) restricted to $\mathcal{H}_{\mathrm{ac}}(H)=\mathcal{H}_p(H)^\perp$, (3.7) formally reads

$$\int_{\mathbb{R}} dx\overline{\Psi_\mp(\mu,x)}\Psi_\pm(\lambda,x)=0,\qquad \int_{\mathbb{R}} dx\overline{\Psi_\mp(\mu,x)}\Psi_\mp(\lambda,x)=\delta(\lambda-\mu),\quad \lambda,\mu\in\Sigma. \tag{3.9}$$

In particular, (3.1)–(3.7) yield the following form of the spectral theorem for $HP_{\text{ac}}(H)$,

$$TH P_{\text{ac}}(H) T^{-1} = \bar{T} H P_{\text{ac}}(H) \bar{T}^{-1} = \{\lambda, \lambda, \lambda 1_2\} \tag{3.10}$$

(with $1_2 = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$ in $\mathbb{C}^2$), where we used the usual short-hand notation for direct integrals,

$$\{\lambda, \lambda, \lambda 1_2\} = \int_{\Sigma_1^-}^{\oplus} d\lambda\, \lambda \oplus \int_{\Sigma_1^+}^{\oplus} d\lambda\, \lambda \oplus \int_{\Sigma_2}^{\oplus} d\lambda\, \lambda 1_2 \tag{3.11}$$

with respect to the decomposition $\hat{\mathcal{H}} = \int_{\Sigma_1^-} d\lambda\, \mathbb{C} \oplus \int_{\Sigma_1^+} d\lambda\, \mathbb{C} \oplus \int_{\Sigma_2}^{\oplus} d\lambda\, \mathbb{C}^2$ (see, e.g., [2], Ch. 4, [39], Sect. XIII. 16, and [43], Chs. 1, 5 for direct integral representations).

Finally, we introduce appropriate scattering data associated with $\Sigma_1^{\pm}$, Σ_2. We start with the regions $\Sigma_1^{\pm}$ of uniform spectral multiplicity one (assuming $|\Sigma_1^{\pm}| > 0$ or $\Sigma_1^{\pm} = \emptyset$ according to our conventions).

$\boldsymbol{\Sigma_1^{\pm}}$: By (2.9) and (2.26), $\text{Im}[m_{\pm}(\lambda + i0)] = 0$ implies $\Psi_{\mp}(\lambda, x) = 0$ for all $x \in \mathbb{R}$ and a.e. $\lambda \in \Sigma_1^{\pm}$.

Moreover, (2.26) and (2.27) also yield $W(\Psi_{\pm}(\lambda), \overline{\Psi_{\pm}(\lambda)}) = 0$ a.e. on $\Sigma_1^{\pm}$ and hence

$$\Psi_{\pm}(\lambda, x) = \overset{\ell}{R}{}^{r}(\lambda) \overline{\Psi_{\pm}(\lambda, x)} \text{ for all } x \in \mathbb{R} \text{ and a.e. } \lambda \in \Sigma_1^{\pm} \tag{3.12}$$

for some (reflection) coefficients $\overset{\ell}{R}{}^{r}(.)$ since $\Psi_{\pm}(\lambda, 0) \neq 0$ a.e. on $\Sigma_1^{\pm}$ by (2.9) and (2.26). In particular,

$$\overset{\ell}{R}{}^{r}(\lambda) = \Psi_{\pm}(\lambda, 0) / \overline{\Psi_{\pm}(\lambda, 0)}, \ |\overset{\ell}{R}{}^{r}(\lambda)| = 1 \text{ a.e. on } \Sigma_1^{\pm}. \tag{3.13}$$

Next we turn to the regime Σ_2 of uniform spectral multiplicity two (assuming $|\Sigma_2| > 0$).

$\boldsymbol{\Sigma_2}$: Since by (2.10) and (2.26), $\Psi_{\pm}(\lambda, 0) \neq 0$ a.e. on Σ_2, the pairs $(\Psi_-(\lambda, x), \Psi_+(\lambda, x))$ and $(\overline{\Psi_-(\lambda, x)}, \overline{\Psi_+(\lambda, x)})$ are both fundamental systems for $\tau\psi = \lambda\psi$ and hence we may write

$$\begin{aligned} \Psi_-(\lambda, x) &= T^r(\lambda) \overline{\Psi_+(\lambda, x)} + R^r(\lambda) \overline{\Psi_-(\lambda, x)}, \\ \Psi_+(\lambda, x) &= T^\ell(\lambda) \overline{\Psi_-(\lambda, x)} + R^\ell(\lambda) \overline{\Psi_+(\lambda, x)} \end{aligned} \tag{3.14}$$

$$\text{for all } x \in \mathbb{R} \text{ and a.e. } \lambda \in \Sigma_2$$

for appropriate (transmission and reflection) coefficients $T^{\ell,r}(.)$, $R^{\ell,r}(.)$. One verifies

$$\begin{aligned} T^{\ell}(\lambda) &= \frac{W(\Psi_+(\lambda), \overline{\Psi_+(\lambda)})}{W(\overline{\Psi_-(\lambda)}, \overline{\Psi_+(\lambda)})}, \quad T^{r}(\lambda) = -\frac{W(\Psi_-(\lambda), \overline{\Psi_-(\lambda)})}{W(\overline{\Psi_-(\lambda)}, \overline{\Psi_+(\lambda)})}, \\ R^{\ell}(\lambda) &= \frac{W(\overline{\Psi_-(\lambda)}, \Psi_+(\lambda))}{W(\overline{\Psi_-(\lambda)}, \overline{\Psi_+(\lambda)})}, \quad R^{r}(\lambda) = \frac{W(\Psi_-(\lambda), \overline{\Psi_+(\lambda)})}{W(\overline{\Psi_-(\lambda)}, \overline{\Psi_+(\lambda)})} \\ & \qquad\qquad\qquad\qquad\qquad \text{a.e. on } \Sigma_2. \end{aligned} \tag{3.15}$$

In particular, taking into account (2.27), one infers

$$T^{\ell}(\lambda) = T^{r}(\lambda) := T(\lambda) \text{ a.e. on } \Sigma_2 \tag{3.16}$$

and introducing the matrix

$$S(\lambda) = \begin{pmatrix} T(\lambda) & R^{r}(\lambda) \\ R^{\ell}(\lambda) & T(\lambda) \end{pmatrix} \text{ for a.e. } \lambda \in \Sigma_2 \tag{3.17}$$

in $\mathbb{C}^2$, $S(.)$ is easily seen to be unitary by appealing to the standard Wronskian identity,

$$\begin{aligned} W(f_1, g_1)(x) W(f_2, g_2)(x) = W(f_1, g_2)(x) W(f_2, g_1)(x) \\ - W(f_1, f_2)(x) W(g_2, g_1)(x). \end{aligned} \tag{3.18}$$

Moreover, one verifies

$$|R^{\ell}(\lambda)| = |R^{r}(\lambda)| \text{ for a.e. } \lambda \in \Sigma_2. \tag{3.19}$$

We repeat at this point that $T(\cdot)$, $R^{\ell,r}(\cdot)$ are only defined up to phase factors thus far since we have not yet fixed the open phases in $\Psi_\pm(\lambda, 0)$, $\lambda \in \Sigma$. This will be taken up in the following Section 4 (cf. (4.9)).

4. Scattering Data

In this section we shall establish the connection between spectral representations (such as (3.1), (3.2)) of $HP_{\mathrm{ac}}(H)$ and the scattering data (3.13), (3.15)–(3.17). Moreover, we derive expressions for the transmission and reflection coefficients in terms of Weyl m-functions and phases of suitably chosen asymptotic wave functions.

In order to motivate our approach we envisage a suitably chosen set of self-adjoint comparison Hamiltonians H^{ϵ} in $L^2(\mathbb{R})$ and their generalized eigenfunctions $\Psi^{\epsilon}_{\pm}(\lambda, x)$ near $\epsilon\infty$,

$\epsilon \in \{+,-\}$. Specifically, we have in mind the following (partly heuristic) scenario: Suppose

$$
\begin{aligned}
&H^\epsilon \Psi_\epsilon^\epsilon(\lambda,x) = \lambda \Psi_\epsilon^\epsilon(\lambda,x), \quad \lambda \in \Sigma_1^{-\epsilon}, \\
&H^\epsilon \Psi_\epsilon^\epsilon(\lambda,x) = \lambda \Psi_\epsilon^\epsilon(\lambda,x), \quad \lambda \in \Sigma_2,\ \epsilon \in \{+,-\},
\end{aligned}
\tag{4.1}
$$

where $H^\epsilon P_{\Sigma_1^{-\epsilon}}(H^\epsilon)$, $H^\epsilon P_{\Sigma_2}(H^\epsilon)$ have purely absolutely continuous spectra such that (in the spirit of (2.18), (3.9))

$$
P_\Omega(H^\epsilon,x,x') = \int_\Omega d\lambda \Psi_\epsilon^\epsilon(\lambda,x)\overline{\Psi_\epsilon^\epsilon(\lambda,x')},\ \Omega = \Sigma_1^{-\epsilon}, \Sigma_2,\ \epsilon \in \{+,-\} \tag{4.2}
$$

and

$$
\int_{\mathbb{R}} dx \overline{\Psi_\epsilon^\epsilon(\mu,x)}\Psi_\epsilon^\epsilon(\lambda,x) = \delta(\lambda-\mu), \quad \epsilon \in \{+,-\}. \tag{4.3}
$$

Here $P_\Omega(\cdot) = \chi_\Omega(\cdot)$ denotes the corresponding spectral projection associated with the measurable set $\Omega \subseteq \mathbb{R}$, and $P_\Omega(\cdot,x,x')$ the corresponding (formal) integral kernel. In contrast to Sections 2 and 3 we assume that the phase of $\Psi_\epsilon^\epsilon(\lambda,0)$ has been prescribed a priori. Since $H^\pm$ are asymptotic Hamiltonians for H relevant near $\pm\infty$, we are only concerned with $\Psi_\pm^\pm(\lambda,x)$, $\overline{\Psi_\pm^\pm(\lambda,x)}$ (as opposed to $\overset{(\text{—})}{\Psi_\pm^\mp(\lambda,x)}$) which becomes especially clear when we make the explicit connection between $\Psi_\pm(\lambda,x)$ (respectively $f_\pm(\lambda,x)$) and $\Psi_\pm^\pm(\lambda,x)$. $H^\pm$, or more precisely, $\Psi_\pm^\pm(\lambda,x)$ are selected as follows. Consider multiples $\psi_\pm(\lambda,x)$ of $f_\pm(\lambda,x)$ such that

$$
\begin{aligned}
&\left|\frac{d^n}{dx^n}\psi_\pm(\lambda,x) - \frac{d^n}{dx^n}\Psi_\pm^\pm(\lambda,x)\right| \underset{x\to\pm\infty}{\longrightarrow} 0 \text{ a.e. on } \Sigma_1^\mp, \\
&\left|\frac{d^n}{dx^n}\psi_\pm(\lambda,x) - \frac{d^n}{dx^n}\Psi_\pm^\pm(\lambda,x)\right| \underset{x\to\pm\infty}{\longrightarrow} 0 \text{ a.e. on } \Sigma_2, \\
&\qquad n = 0,1,
\end{aligned}
\tag{4.4}
$$

$$
W(\psi_\pm(\lambda), \overline{\psi_\pm(\lambda)}) = W(\Psi_\pm^\pm(\lambda), \overline{\Psi_\pm^\pm(\lambda)}) \text{ a.e. on } \Sigma, \tag{4.5}
$$

where, in analogy to (2.17),

$$
\psi_\pm(\lambda,x) = \psi_\pm(\lambda,0) f_\pm(\lambda,x) \text{ for all } x \in \mathbb{R} \text{ and a.e. } \lambda \in \Sigma. \tag{4.6}
$$

The actual form of the asymptotic Hamiltonians H^ϵ, although convenient to shape ones intuition in this context, is no longer of crucial importance from this point on and the emphasis is shifted to the asymptotic wave functions $\Psi_\epsilon^\epsilon(\lambda,x)$ instead. Our basic hypothesis concerning the asymptotic relation (4.4) can now be formulated as follows.

(H.4.1) . *Assume the existence of* $\Psi^{\pm}_{\pm}(\cdot,\cdot)$ *on* $\Sigma\times\mathbb{R}$ *with* $\Psi^{\pm}_{\pm}(\lambda,\cdot)\in C^1(\mathbb{R})$, $\lambda\in\Sigma$, $\frac{d^n}{dx^n}\Psi^{\pm}_{\pm}(\cdot,x)\in L^{\infty}_{\mathrm{loc}}(\Sigma)$, $n=0,1$, $x\in\mathbb{R}$ *such that* (4.4) *and* (4.6) *are satisfied for some multiples* $\psi_{\pm}(\lambda,x)$ *of* $f_{\pm}(\lambda,x)$.

In concrete applications, Hypothesis (H.4.1) can frequently be verified by setting up Volterra integral equations for $\psi_{\pm}(\lambda,x)$ and $\Psi^{\pm}_{\pm}(\lambda,x)$ involving $V(x)$ and its appropriate asymptotic forms $V^{\pm}(x)$ as $x\to\pm\infty$ (see Section 5). In these cases $\Psi^{\pm}_{\pm}(\lambda,x)$ are generalized eigenfunctions of $H^{\pm}=-\frac{d^2}{dx^2}+V^{\pm}$ which are conveniently normalized as in (2.17), (3.9) (with their phases prescribed a priori) and our heuristic introductory treatment in (4.1)–(4.3) can be put on a sound mathematical basis.

Equations (4.5) and (4.6) yield (cf. (2.19)),

$$\begin{aligned} W(\psi_{\pm}(\lambda),\overline{\psi_{\pm}(\lambda)}) &= W(\Psi^{\pm}_{\pm}(\lambda),\overline{\Psi^{\pm}_{\pm}(\lambda)}) \\ &= -2i|\psi_{\pm}(\lambda,0)|^2\,\mathrm{Im}[m_{\pm}(\lambda+i0)], \\ W(\psi_{-}(\lambda),\psi_{+}(\lambda)) &= \psi_{-}(\lambda,0)\psi_{+}(\lambda,0)[m_{+}(\lambda+i0)-m_{-}(\lambda+i0)] \\ &\qquad \text{a.e. on } \Sigma. \end{aligned} \tag{4.7}$$

Combining (2.26) and (4.7) one derives

$$\begin{aligned} |\Psi_{\pm}(\lambda,0)|^2 &= \mp\pi^{-1}|m_{-}(\lambda+i0)-m_{+}(\lambda+i0)|^{-2}\,\mathrm{Im}[m_{\mp}(\lambda+i0)] \\ &= (2\pi)^{-1}|\psi_{\mp}(\lambda,0)|^{-2}|m_{-}(\lambda+i0)-m_{+}(\lambda+i0)|^{-2}[\mp iW(\Psi^{\mp}_{\mp}(\lambda),\overline{\Psi^{\mp}_{\mp}(\lambda)})] \\ &\qquad \text{a.e. on } \Sigma, \end{aligned} \tag{4.8}$$

which enables one to define the phase of $\Psi_{\pm}(\lambda,0)$ (and hence of $\Psi_{\pm}(\lambda,x)$, $x\in\mathbb{R}$) in a natural manner (motivated by comparision with the short-range case) by

$$\Psi_{\pm}(\lambda,0):=-i(2\pi)^{-1/2}\psi_{\mp}(\lambda,0)^{-1}[m_{-}(\lambda+i0)-m_{+}(\lambda+i0)]^{-1}[\mp iW(\Psi^{\mp}_{\mp}(\lambda),\overline{\Psi^{\mp}_{\mp}(\lambda)})]^{1/2} \quad \text{a.e. on } \Sigma. \tag{4.9}$$

Having fixed $\Psi_{\pm}(\lambda,0)$, the scattering data $R^{\ell,r}(\lambda)$, $T(\lambda)$ in (3.13), (3.15)–(3.17) get their following final form.

Theorem 4.2. *Assume Hypotheses (H.2.1) and (H.4.1). Then*

$$R^{\ell}_{r}(\lambda)=-\frac{\overline{\psi_{\mp}(\lambda,0)[m_{-}(\lambda+i0)-m_{+}(\lambda+i0)]}}{\psi_{\mp}(\lambda,0)[m_{-}(\lambda+i0)-m_{+}(\lambda+i0)]} \text{ a.e. on } \Sigma_1^{\pm} \tag{4.10}$$

(if $|\Sigma_1^{\pm}| > 0$),

$$
\begin{aligned}
T(\lambda) &= \frac{i[W(\Psi_-^-(\lambda), \overline{\Psi_-^-(\lambda)})W(\Psi_+^+(\lambda), \overline{\Psi_+^+(\lambda)})]^{1/2}}{W(\psi_-(\lambda), \psi_+(\lambda))} \\
&= -2i\frac{|\psi_-(\lambda,0)\psi_+(\lambda,0)|}{\psi_-(\lambda,0)\psi_+(\lambda,0)}\frac{\{-\operatorname{Im}[m_-(\lambda+i0)]\operatorname{Im}[m_+(\lambda+i0)]\}^{1/2}}{m_-(\lambda+i0)-m_+(\lambda+i0)}, \\
R^{\ell}_{R}(\lambda) &= \pm\frac{W(\psi_\pm(\lambda), \overline{\psi_\mp(\lambda)})}{W(\psi_-(\lambda), \psi_+(\lambda))} = \pm\frac{\overline{\psi_\mp(\lambda,0)}[m_\pm(\lambda+i0)-\overline{m_\mp(\lambda+i0)}]}{\psi_\mp(\lambda,0)[m_-(\lambda+i0)-m_+(\lambda+i0)]} \\
&\qquad\qquad\qquad\qquad\qquad\qquad a.e. \ on \ \Sigma_2
\end{aligned}
\tag{4.11}
$$

(if $|\Sigma_2| > 0$).

Proof. It suffices to insert (4.9) into (3.13) and (3.15), taking into account (3.16).

Remark 4.3. (i). The fact that

$$|R^{\ell,r}(\lambda)| = 1 \text{ a.e. on } \Sigma_1, \tag{4.12}$$

in physical terms, indicates that total reflection is associated with the energy regime Σ_1 of spectral multiplicity one as opposed to the regime Σ_2 of spectral multiplicity two which supports nonvanishing transmission. This phenomenon has first been rigorously established by Davies and Simon [8] (see also [39], Example 4 of Sect. XI.4 and [16]).
(ii). As is evident from (4.4), (4.10), and (4.11), the choice of normalization of $|\Psi_\pm^\pm(\lambda,0)|$ does not influence the reflection and transmission coefficients $R^{\ell,r}$, T. However, the choice of phase of $\Psi_\pm^\pm(\lambda,0)$ (and hence that of $\psi_\pm(\lambda,0)$) enters crucially in (4.10) and (4.11).

Asymptotically, one verifies

$$\Psi_+(\lambda,x) \underset{x\to-\infty}{=} [-2\pi i W(\Psi_-^-(\lambda), \overline{\Psi_-^-(\lambda)})]^{-1/2}[\overline{\Psi_-^-(\lambda,x)} + R^\ell(\lambda)\Psi_-^-(\lambda,x)], \quad \lambda \in \Sigma_1^+, \tag{4.13}$$

$$\Psi_-(\lambda,x) \underset{x\to+\infty}{=} [2\pi i W(\Psi_+^+(\lambda), \overline{\Psi_+^+(\lambda)})]^{-1/2}[\overline{\Psi_+^+(\lambda,x)} + R^r(\lambda)\Psi_+^+(\lambda,x)], \quad \lambda \in \Sigma_1^-, \tag{4.14}$$

$$\Psi_+(\lambda,x) = \begin{cases} [2\pi i W(\Psi_+^+(\lambda), \overline{\Psi_+^+(\lambda)})]^{-1/2}T(\lambda)\Psi_+^+(\lambda,x), & x\to+\infty \\ [-2\pi i W(\Psi_-^-(\lambda), \overline{\Psi_-^-(\lambda)})]^{-1/2}[\overline{\Psi_-^-(\lambda,x)} + R^\ell(\lambda)\Psi_-^-(\lambda,x)], & x\to-\infty \end{cases}, \quad \lambda \in \Sigma_2, \tag{4.15}$$

$$\Psi_-(\lambda,x)=\begin{cases}[-2\pi i W(\Psi_-^-(\lambda),\overline{\Psi_-^-(\lambda)})]^{-1/2}T(\lambda)\Psi_-^-(\lambda,x), & x\to-\infty\\ [2\pi i W(\Psi_+^+(\lambda),\overline{\Psi_+^+(\lambda)})]^{-1/2}[\overline{\Psi_+^+(\lambda,x)}+R^r(\lambda)\Psi_+^+(\lambda,x)], & x\to+\infty\end{cases},\quad \lambda\in\Sigma_2. \tag{4.16}$$

Next we state the precise connection between the spectral representations of $HP_{\mathrm{ac}}(H)$ in Section 3 and the stationary scattering data. (We recall our convention to identify Σ_1^- and $\emptyset$ if $|\Sigma_1^-|=0$ and similarly for Σ_1^+, Σ_2.)

Theorem 4.4. *Assume Hypotheses (H.2.1) and (H.4.1) and abbreviate*

$$s(\cdot)=\begin{cases}R^r(\cdot) & a.e.\ on\ \Sigma_1^-\\ R^\ell(\cdot) & a.e.\ on\ \Sigma_1^+\\ S(\cdot) & a.e.\ on\ \Sigma_2\end{cases}, \tag{4.17}$$

with $R^{\ell,r}(\cdot)$, $S(\cdot)$ defined in (3.13), (3.15)–(3.17) *and* (4.10), (4.11), *respectively. Then*

$$\bar{T}T^{-1}=\int_\Sigma^\oplus d\lambda\, s(\lambda)=\{R^r(\cdot),R^\ell(\cdot),S(\cdot)\} \tag{4.18}$$

with respect to the direct integral decomposition $\hat{\mathcal{H}}=\int_{\Sigma_1^-}^\oplus d\lambda\,\mathbb{C}\oplus\int_{\Sigma_1^+}^\oplus d\lambda\,\mathbb{C}\oplus\int_{\Sigma_2}^\oplus d\lambda\,\mathbb{C}^2$. In addition, $s(\cdot)$ is unimodular on Σ_1 and unitary on Σ_2.

Proof. Let $(g_-,g_+,\binom{h_+}{h_-})\in\hat{\mathcal{H}}$. Then (3.2), (3.4), (3.12), (3.14), and (3.7) imply

$$\bar{T}T^{-1}\left(g_-,g_+,\begin{pmatrix}h_+\\h_-\end{pmatrix}\right)=\left(R^rg_-,R^\ell g_+,S\begin{pmatrix}g_+\\g_-\end{pmatrix}\right) \tag{4.19}$$

proving (4.18). The remaining assertion has been discussed at the end of Section 3.

We continue with a few remarks on reflectionless scattering, i.e., $R^{\ell,r}(\lambda)=0$ for a.e. $\lambda\in\Sigma$. Since $R^{\overset{\ell}{r}}(\cdot)$ would be unimodular on $\Sigma_1^\pm$, we necessarily need the absence of the spectral multiplicity one part $\Sigma_1=\Sigma_1^-\cup\Sigma_1^+$, i.e.,

$$\Sigma_1=\emptyset. \tag{4.20}$$

Moreover, by (4.11),

$$R^{\ell,r}(\lambda)=0 \text{ a.e. on } \Sigma_2 \tag{4.21}$$

is equivalent to

$$m_+(\lambda+i0)=\overline{m_-(\lambda+i0)} \text{ a.e. on } \Sigma_2, \tag{4.22}$$

i.e., to

$$f_+(\lambda + i0, x) = \overline{f_-(\lambda + i0, x)} \text{ for all } x \in \mathbb{R} \text{ and a.e. } \lambda \in \Sigma_2. \tag{4.23}$$

The latter equation is easily seen to be equivalent to the fact that the diagonal Green's function $G(\lambda + i0, x, x)$ of H is purely imaginary for all $x \in \mathbb{R}$ and a.e. $\lambda \in \Sigma_2$. In fact, $G(z, x, x')$, the integral kernel of the resolvent $(H - z)^{-1}$ of H,

$$\begin{aligned} G(z, x, x') &= W(f_+(z), f_-(z))^{-1} f_+(z, x) f_-(z, x'), \quad x' \le x, \\ G(z, 0, 0) &= [m_-(z) - m_+(z)]^{-1}, \end{aligned} \tag{4.24}$$

satisfies

$$\arg[G(\lambda + i0, x, x)] = \pi/2 \text{ for all } x \in \mathbb{R} \text{ and a.e. } \lambda \in \Sigma_2 \tag{4.25}$$

if (4.23) (or (4.22)) holds. (This is in accordance with the Herglotz property of $G(\cdot, x, x) : \mathbb{C}_+ \to \mathbb{C}_+$ for all $x \in \mathbb{R}$.) Thus we arrive at

Theorem 4.5. *Assume Hypotheses (H.2.1) and (H.4.1). Then H is reflectionless, i.e., $R^{\ell,r}(\cdot) = 0$ a.e. on Σ, if and only if the following two conditions hold:*
(i). $\Sigma_1 = \emptyset$.
(ii). For all $x \in \mathbb{R} : \arg[G(\lambda + i0, x, x)] = \pi/2$ a.e. on Σ_2.
Condition (ii) is equivalent to
(ii'). $m_+(\lambda + i0) = \overline{m_-(\lambda + i0)}$ a.e. on Σ_2.

Proof. It remains to prove the equivalence of (ii) and (ii'). Since (ii') clearly implies (ii) we focus on the converse statement. Assuming (ii), the special case $x = 0$ leads to $\mathrm{Re}[m_+(\lambda + i0)] = \mathrm{Re}[m_-(\lambda + i0)]$ a.e. on Σ_2. In general, $\overline{G(\lambda + i0, x, x)} = -G(\lambda + i0, x, x)$ and (2.5) (taking into account the real-valuedness of $\theta(\lambda, x)$, $\phi(\lambda, x)$, $\lambda \in \mathbb{R}$) yield

$$\begin{aligned} &\phi(\lambda, x)^2 [\overline{m_+(\lambda + i0)}\,\overline{m_-(\lambda + i0)} - m_+(\lambda + i0) m_-(\lambda + i0)] \\ &+ \theta(\lambda, x)\phi(\lambda, x)[\overline{m_-(\lambda + i0)} - m_-(\lambda + i0) + \overline{m_+(\lambda + i0)} - m_+(\lambda + i0)] = 0 \\ &\qquad \text{for all } x \in \mathbb{R} \text{ and a.e. } \lambda \in \Sigma_2. \end{aligned} \tag{4.26}$$

Linear independence of $\phi(z, x)^2$ and $\theta(z, x)\phi(z, x)$ then yields (ii').

If H is reflectionless, (4.11) reduces to

$$T(\lambda) = \frac{|\psi_-(\lambda,0)\psi_+(\lambda,0)|}{\psi_-(\lambda,0)\psi_+(\lambda,0)}, \qquad R^{\ell,r}(\lambda) = 0 \qquad \text{a.e. on } \Sigma = \Sigma_2. \tag{4.27}$$

A closer look at Theorem 4.5 reveals that the asymptotic condition in Hypothesis (H.4.1) is not essential in our notion of reflectionless Schrödinger operators and we adopt the following general definition used previously in [7], [10], [28] in the context of almost periodic potentials.

Definition 4.6. Assume Hypothesis (H.2.1). Then H (respectively V) is called reflectionless if and only if conditions (i) and (ii) (or (i) and (ii')) of Theorem 4.5 hold.

The following well-known (stationary) one-soliton solution of the KdV equation illustrates Theorem 4.5.

Example 4.7 (One-soliton potential). Consider

$$V(x) = -2\kappa^2\cosh^2(\kappa x), \quad \kappa > 0, \tag{4.28}$$

$$H = -\frac{d^2}{dx^2} + V, \ \mathcal{D}(H) = H^{2,2}(\mathbb{R}) \tag{4.29}$$

($H^{m,n}(\mathbb{R})$, m, $n \in \mathbb{N}$ the usual Sobolev spaces). Then one computes

$$f_\pm(z,x) = \mp iz^{-1/2}\{(\pm iz^{1/2}+\kappa) - 2\kappa[1+e^{-2\kappa_1 x}]^{-1}\}e^{\pm iz^{1/2}x}, \tag{4.30}$$

$$m_\pm(z) = f'_\pm(z,0) = \pm i(z^{1/2} + \kappa_1^2 z^{-1/2}) \tag{4.31}$$

(we use the branch $\mathrm{Im}(z^{1/2}) \geq 0$). Moreover, using $V(x) = 0$, $x \in \mathbb{R}$ as the asymptotic comparison potential and hence making the natural choice (see Example 5.1 with $V_0 = 0$)

$$\Psi^\pm_\pm(\lambda,x) = 2^{-1}\pi^{-1/2}\lambda^{-1/4}e^{\pm i\lambda^{1/2}x}, \quad \lambda > 0, \tag{4.32}$$

one obtains

$$\psi_\pm(\lambda,0) = 2^{-1}\pi^{-1/2}\lambda^{1/4}(\lambda^{1/2}+i\kappa)^{-1}, \quad \lambda > 0, \tag{4.33}$$

$$\Psi_\pm(\lambda,0) = 2^{-1}\pi^{-1/2}\lambda^{1/4}(\lambda^{1/2}-i\kappa)^{-1}, \quad \lambda > 0, \tag{4.34}$$

$$\Sigma_1 = \Sigma_1^+ = \emptyset, \quad \Sigma_2 = (0,\infty), \tag{4.35}$$

$$\sigma(H) = \{-\kappa^2\} \cup [0,\infty), \ \sigma_{\mathrm{sc}}(H) = \sigma_p(H) \cap [0,\infty) = \emptyset. \tag{4.36}$$

By (4.22) and (4.30), $m_+(\lambda+i0)=\overline{m_-(\lambda+i0)}$, $\lambda>0$ shows that H is reflectionless and (4.11) then yields

$$T(\lambda)=(\lambda^{1/2}+i\kappa)(\lambda^{1/2}-i\kappa)^{-1},\ R^{\ell,r}(\lambda)=0,\quad \lambda>0. \tag{4.37}$$

The scattering data (4.10), (4.11) contain spectral information about H and the asymptotic wave functions $\Psi^{\pm}_{\pm}(\lambda,x)$ (respectively the asymptotic operators $H^{\pm}$) in a subtle way. While the Weyl m-functions $m_\pm(\lambda+i0)$ of H enter explicitly, the phase factors $\psi_\pm(\lambda,0)/|\psi_\pm(\lambda,0)|$ encode information about H and $\Psi^{\pm}_{\pm}(\lambda,x)(H^{\pm})$ in a rather intricate manner.

Another point that deserves attention is the following. Even if one would choose the generalized eigenfunctions $\Psi_\pm(\lambda,x)$ of H as its asymptotic wave functions, i.e., $\Psi^{\pm}_{\pm}(\lambda,x)=\Psi_\pm(\lambda,x)$, the corresponding scattering matrix $S(\lambda)$, $\lambda\in\Sigma_2$ will not be diagonal (in particular, $S(\lambda)\neq 1_2$) unless H is reflectionless. (This follows from the fact that the pairs $(f_+(\lambda,x),\overline{f_+(\lambda,x)})$ as $x\to-\infty$ and $(\overline{f_-(\lambda,x)},f_-(\lambda,x))$ as $x\to+\infty$ only coincide in the reflectionless case.) For such reasons we prefer to call (4.10), (4.11) scattering data as opposed to scattering matrices.

5. Some Applications

We illustrate the preceding formalism in a variety of different situations which have a broad range of applications from standard short-range scattering to impurity (defect) scattering in (half-)crystals and related phenomena of charge transport in quasi-one-dimensional mesoscopic solid state structures. At the end we discuss reflectionless scattering off certain background potentials using commutation methods. The latter subject is relevant in generalized soliton-type solutions for the KdV hierarchy of nonlinear evolution equations.

We start with the simplest possible case of constant potentials.

Example 5.1 (Constant potentials). Let

$$V^{(0)}(x)=V_0,\quad V_0\in\mathbb{R}, \tag{5.1}$$

$$H^{(0)}=-\frac{d^2}{dx^2}+V_0,\ \mathcal{D}(H^{(0)})=H^{2,2}(\mathbb{R}), \tag{5.2}$$

$$m^{(0)}_\pm(z)=\pm i(z-V_0)^{1/2} \tag{5.3}$$

(we choose $\mathrm{Im}[(z-V_0)^{1/2}] \geq 0$ in (5.3) and in analogous situations below),

$$\Psi_{\pm}^{(0)}(\lambda,x) = 2^{-1}\pi^{-1/2}(\lambda-V_0)^{-1/4}e^{\pm i(\lambda-V_0)^{1/2}x}, \quad \lambda > V_0, \tag{5.4}$$

$$W(\Psi_{\mp}^{(0)}(\lambda), \overline{\Psi_{\mp}^{(0)}(\lambda)}) = \mp(2\pi i)^{-1}, \quad \lambda > V_0, \tag{5.5}$$

$$\Sigma_1 = \Sigma_1^{\pm} = \emptyset,\ \Sigma_2 = (V_0,\infty), \tag{5.6}$$

$$\sigma(H^{(0)}) = \sigma_{\mathrm{ac}}(H^{(0)}) = [V_0,\infty),\ \sigma_{\mathrm{sc}}(H^{(0)}) = \sigma_p(H^{(0)}) = \emptyset. \tag{5.7}$$

$H^{(0)}$ is reflectionless since $\Sigma_1 = \emptyset$ and $m_+(\lambda+i0) = \overline{m_-(\lambda+i0)}$, $\lambda \in \Sigma_2$.

Next we briefly discuss standard short-range scattering.

Example 5.2 (Short-range potentials). Let

$$V \in L^1(\mathbb{R};(1+|x|)dx) \text{ be real-valued,} \tag{5.8}$$

define H as in (2.2), and $\Psi_{\pm}^{\pm}(\lambda,x) = \Psi_{\pm}^{(0)}(\lambda,x)$, $\lambda > 0$ as in (5.4) with $V_0 = 0$. Consider

$$\psi_{\pm}(\lambda,x) = \Psi_{\pm}^{(0)}(\lambda,x) - \int_x^{\pm\infty} dx'\lambda^{-1/2}\sin[\lambda^{1/2}(x-x')]V(x')\psi_{\pm}(\lambda,x'), \quad \lambda > 0, \tag{5.9}$$

then

$$\Psi_{\pm}(\lambda,x) = -[2\pi i W(\psi_-(\lambda),\psi_+(\lambda))]^{-1}\psi_{\pm}(\lambda,x), \quad \lambda > 0, \tag{5.10}$$

$$\Sigma_1 = \Sigma_1^{\pm} = \emptyset,\ \Sigma_2 = (0,\infty), \tag{5.11}$$

$$\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ac}}(H) = [0,\infty),\ \sigma_{\mathrm{sc}}(H) = \sigma_p(H) \cap [0,\infty) = \emptyset \tag{5.12}$$

(where $\sigma_{\mathrm{ess}}(.)$ denotes the essential spectrum). The Volterra integral equation (5.9), in addition to (4.11), then leads to the representations

$$\begin{aligned} T(\lambda) &= -[2\pi i W(\psi_-(\lambda),\psi_+(\lambda))]^{-1} = [1 + 2\pi i \int_{\mathbb{R}} dx V(x)\Psi_{\pm}^{(0)}(\lambda,x)\psi_{\mp}(\lambda,x)]^{-1}, \\ R^{\substack{\ell \\ r}}(\lambda) &= -2\pi i T(\lambda)\int_{\mathbb{R}} dx V(x)\Psi_{\pm}^{(0)}(\lambda,x)\psi_{\pm}(\lambda,x), \quad \lambda \in \Sigma_2. \end{aligned} \tag{5.13}$$

The following example treats step potentials.

Example 5.3 (Step potentials). Suppose

$$V(x) = \begin{cases} V_0, & x > 0 \\ 0, & x < 0 \end{cases}, \quad V_0 > 0. \tag{5.14}$$

H is then defined on $H^{2,2}(\mathbb{R})$ and $\Psi^{\pm}_{\pm}(\lambda,x)$ are given by

$$\begin{aligned}
&\Psi^{-}_{-}(\lambda,x)=2^{-1}\pi^{-1/2}\lambda^{-1/4}e^{-i\lambda^{1/2}x}, \quad \lambda>0,\\
&\Psi^{+}_{+}(\lambda,x)=2^{-1}\pi^{-1/2}(\lambda-V_0)^{-1/4}e^{i(\lambda-V_0)^{1/2}x}, \quad \lambda>V_0,
\end{aligned} \tag{5.15}$$

$$W(\Psi^{\mp}_{\mp}(\lambda),\overline{\Psi^{\mp}_{\mp}(\lambda)})=\mp(2\pi i)^{-1}, \quad \lambda>\begin{cases}0\\ V_0\end{cases}. \tag{5.16}$$

Then

$$\Sigma_1^{-}=\emptyset,\ \Sigma_1^{+}=(0,V_0),\ \Sigma_2=(V_0,\infty), \tag{5.17}$$

$$\sigma(H)=\sigma_{\rm ac}(H)=[0,\infty),\ \sigma_{\rm sc}(H)=\sigma_p(H)=\emptyset, \tag{5.18}$$

$$m_-(z)=-iz^{1/2},\ m_+(z)=i(z-V_0)^{1/2}, \tag{5.19}$$

$$\begin{aligned}
&f_-(z,x)=\begin{cases} e^{-i\sqrt{z}x}, & x<0\\ \dfrac{(z-V_0)^{1/2}-z^{1/2}}{2(z-V_0)^{1/2}}e^{i(z-V_0)^{1/2}x}+\dfrac{(z-V_0)^{1/2}+z^{1/2}}{2(z-V_0)^{1/2}}e^{-i(z-V_0)^{1/2}x}, & x>0\end{cases},\\
&f_+(z,x)=\begin{cases} \dfrac{z^{1/2}+(z-V_0)^{1/2}}{2z^{1/2}}e^{iz^{1/2}x}+\dfrac{z^{1/2}-(z-V_0)^{1/2}}{2z^{1/2}}e^{-iz^{1/2}x}, & x<0\\ e^{i(z-V_0)^{1/2}x}, & x>0\end{cases},
\end{aligned} \tag{5.20}$$

$$\psi_{\mp}(\lambda,0)=\begin{cases}[2\pi^{1/2}\lambda^{1/4}]^{-1}, & \lambda>0\\ [2\pi^{1/2}(\lambda-V_0)^{1/4}]^{-1}, & \lambda>V_0\end{cases}, \tag{5.21}$$

$$\Psi_{\pm}(\lambda,0)=\pi^{-1/2}[(\lambda-V_0)^{1/2}+\lambda^{1/2}]^{-1}\begin{cases}\lambda^{1/4}, & \lambda>0\\ (\lambda-V_0)^{1/4}, & \lambda>V_0\end{cases}, \tag{5.22}$$

$$R^{\ell}(\lambda)=\frac{\lambda^{1/2}-i(V_0-\lambda)^{1/2}}{\lambda^{1/2}+i(V_0-\lambda)^{1/2}}, \quad \lambda\in\Sigma_1^{+}=(0,V_0), \tag{5.23}$$

$$T(\lambda)=\frac{2\lambda^{1/4}(\lambda-V_0)^{1/4}}{\lambda^{1/2}+(\lambda-V_0)^{1/2}},\ R^{\ell}_{r}(\lambda)=\pm\frac{\lambda^{1/2}-(\lambda-V_0)^{1/2}}{\lambda^{1/2}+(\lambda-V_0)^{1/2}}, \quad \lambda\in\Sigma_2. \tag{5.24}$$

Example 5.4 (Step-like potentials (see, e.g., [6], [16])). Let

$$V\in L^1_{\rm loc}(\mathbb{R}) \text{ be real-valued, } \int_{-\infty}^{0}dx(1+x^2)|V(x)|+\int_0^{\infty}dx(1+x^2)|V(x)-V_0|<\infty,$$
$$V_0>0, \tag{5.25}$$

define H as in (2.2), and $\Psi^{\mp}_{\mp}(\lambda,x)$, $\lambda > \begin{cases} 0 \\ V_0 \end{cases}$ as in (5.15). Consider

$$\psi_\pm(\lambda,x) = \Psi^{\pm}_{\pm}(\lambda,x) - \int_x^{\pm\infty} dx'(\lambda - V_\pm)^{-1/2}\sin[(\lambda - V_\pm)^{1/2}x][V(x') - V_\pm]\psi_\pm(\lambda,x'),$$
$$\lambda > \begin{cases} V_0 \\ 0 \end{cases}, \; V_\pm = \begin{cases} V_0 \\ 0 \end{cases}, \tag{5.26}$$

then

$$\Psi_\pm(\lambda,x) = (2\pi i)^{-1}\psi_\mp(\lambda,0)^{-1}[m_-(\lambda+i0) - m_+(\lambda+i0)]^{-1}f_\pm(\lambda,x), \quad \lambda > \begin{cases} 0 \\ V_0 \end{cases}, \tag{5.27}$$

$$\Sigma_1^- = \emptyset, \; \Sigma_1^+ = (0,V_0), \; \Sigma_2 = (V_0,\infty), \tag{5.28}$$

$$\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ac}}(H) = [0,\infty), \; \sigma_{\mathrm{sc}}(H) = \sigma_p(H) \cap [0,\infty) = \emptyset. \tag{5.29}$$

$R^\ell(\lambda)$, $\lambda \in \Sigma_1^+$ and $T(\lambda)$, $R^{\ell,r}(\lambda)$, $\lambda \in \Sigma_2$ are then given by (4.10) and (4.11).

The following example of periodic potentials plays the same role as a background potential in the subsequent Examples 5.6–5.8 as the constant potential in Example 5.1 for Examples 5.2–5.4.

Example 5.5 (Periodic potentials (see, e.g., [22] for the notation employed below)). Suppose

$$V^{(0)} \in L^1((0,\Omega)) \text{ is real-valued, } \Omega > 0, \; V^{(0)}(\cdot + \Omega) = V^{(0)}(\cdot) \text{ a.e.} \tag{5.30}$$

$H^{(0)}$ is then defined as in (2.2), $\theta^{(0)}(z,x)$, $\phi^{(0)}(z,x)$ are introduced as in (2.4),

$$m_\pm^{(0)}(z) = \{\Delta(z) \mp [\Delta(z)^2 - 1]^{1/2} - \theta^{(0)}(z,\Omega)\}/\phi^{(0)}(z,\Omega) \tag{5.31}$$

(choosing $[\Delta(\lambda)^2 - 1]^{1/2} > 0$ for $\lambda < 0$ sufficiently negative), where

$$\Delta(z) = [\theta^{(0)}(z,\Omega) + \phi^{(0)\prime}(z,\Omega)]/2 \tag{5.32}$$

denotes the Floquet discriminant and $f_\pm^{(0)}(z,x)$ are defined as in (2.5),

$$W(f_-^{(0)}(z), f_+^{(0)}(z)) = -2[\Delta(z)^2 - 1]^{1/2}/\phi^{(0)}(z,\Omega). \tag{5.33}$$

Defining $\Psi_{\pm}^{(0)}(\lambda,x)$, $\lambda\in\Sigma_2$ in accordance with (2.17) and (2.26) (fixing the open phase factor conveniently) leads to

$$\Psi_{\pm}^{(0)}(\lambda,x)=2^{-1}\pi^{-1/2}|\Delta(\lambda)^2-1|^{-1/4}|\phi^{(0)}(\lambda,\Omega)|^{1/2}f_{\pm}^{(0)}(\lambda,x),\quad \lambda\in\Sigma_2, \tag{5.34}$$

$$W(\Psi_{\mp}^{(0)}(\lambda),\overline{\Psi_{\mp}^{(0)}(\lambda)})=\mp(2\pi i)^{-1},\quad \lambda\in\Sigma_2, \tag{5.35}$$

$$\Sigma_1=\Sigma_1^{\pm}=\emptyset,\ \Sigma_2=\bigcup_{n\in\mathbb{N}}(E_{2(n-1)}^{(0)},E_{2n-1}^{(0)}), \tag{5.36}$$

where

$$\begin{aligned}
&E_0^{(0)}<E_1^{(0)}\le E_2^{(0)}<E_3^{(0)}\le E_4^{(0)}<E_5^{(0)}\le\cdots,\\
&|\Delta(\lambda)|\le 1,\ \lambda\in[E_{2(n-1)}^{(0)},E_{2n-1}^{(0)}],\quad n\in\mathbb{N},\\
&\Delta(\lambda)>1,\ \lambda\in(-\infty,E_0^{(0)}),\ (E_{4n-1}^{(0)},E_{4n}^{(0)}),\quad n\in\mathbb{N},\\
&\Delta(\lambda)<-1,\ \lambda\in(E_{4n-3}^{(0)},E_{4n-2}^{(0)}),\quad n\in\mathbb{N},
\end{aligned} \tag{5.37}$$

$$\sigma(H^{(0)})=\sigma_{\rm ac}(H^{(0)})=\bigcup_{n\in\mathbb{N}}[E_{2(n-1)}^{(0)},E_{2n-1}^{(0)}],\ \sigma_{\rm sc}(H^{(0)})=\sigma_p(H^{(0)})=\emptyset. \tag{5.38}$$

The operator $H^{(0)}$ is reflectionless since $\Sigma_1=\emptyset$ and $m_+(\lambda+i0)=\overline{m_-(\lambda+i0)}$, $\lambda\in\Sigma_2$.

Next we briefly discuss impurity (defect) scattering off crystals assuming short-range interactions.

Example 5.6 (Short-range impurity (defect) scattering). Let

$$W\in L^1(\mathbb{R};(1+|x|)dx)\ \text{be real-valued}, \tag{5.39}$$

$$V(x)=V^{(0)}(x)+W(x), \tag{5.40}$$

where $V^{(0)}(x+\Omega)=V^{(0)}(x)$ is a fixed real-valued periodic potential considered in Example 5.5 and W models impurities (defects) in one-dimensional solids. H is then defined as in (2.2) and $\Psi_{\pm}^{\pm}(\lambda,x)=\Psi_{\pm}^{(0)}(\lambda,x)$, $\lambda\in\Sigma_2$ are defined as in (5.34). Consider

$$\begin{aligned}
\psi_{\pm}(\lambda,x)=\Psi_{\pm}^{(0)}(\lambda,x)+\int_x^{\pm\infty}dx'W(\Psi_{\pm}^{(0)}(\lambda),\overline{\Psi_{\pm}^{(0)}(\lambda)})^{-1}&\\
\times[\Psi_{\pm}^{(0)}(\lambda,x)\overline{\Psi_{\pm}^{(0)}(\lambda,x')}-\overline{\Psi_{\pm}^{(0)}(\lambda,x)}\Psi_{\pm}^{(0)}(\lambda,x')]W(x')\psi_{\pm}(\lambda,x'),\ \lambda\in\Sigma_2,&
\end{aligned} \tag{5.41}$$

then

$$\Psi_{\pm}(\lambda,x)=-[2\pi iW(\psi_-(\lambda),\psi_+(\lambda))]^{-1}\psi_{\pm}(\lambda,x),\quad \lambda\in\Sigma_2, \tag{5.42}$$

$$\Sigma_1 = \Sigma_1^{\pm} = \emptyset,\ \Sigma_2 = \bigcup_{n\in\mathbb{N}} (E^{(0)}_{2(n-1)}, E^{(0)}_{2n-1}), \tag{5.43}$$

$$\begin{aligned} &\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ac}}(H) = \sigma(H^{(0)}) = \bigcup_{n\in\mathbb{N}} [E^{(0)}_{2(n-1)}, E^{(0)}_{2n-1}], \\ &\sigma_{\mathrm{sc}}(H) = \sigma_p(H) \cap \sigma_{ac}(H) = \emptyset. \end{aligned} \tag{5.44}$$

Due to the Volterra integral equations (5.41) one obtains, in addition to (4.11), the representations

$$\begin{aligned} &T(\lambda) = -[2\pi i W(\psi_-(\lambda), \psi_+(\lambda))]^{-1} = [1 + 2\pi i \int_{\mathbb{R}} dx W(x)\Psi^{(0)}_{\pm}(\lambda,x)\psi_{\mp}(\lambda,x)]^{-1}, \\ &\overset{\ell}{R^r}(\lambda) = -2\pi i T(\lambda)\int_{\mathbb{R}} dx W(x)\Psi^{(0)}_{\pm}(\lambda,x)\psi_{\pm}(\lambda,x), \quad \lambda\in\Sigma_2. \end{aligned} \tag{5.45}$$

The next example considers half-crystals (see, e.g., [16]).

Example 5.7 (Half-crystals). Suppose $V^{\pm}(x+\Omega^{\pm}) = V^{\pm}(x)$, $\Omega^{\pm} > 0$ are two real-valued periodic potentials as in Example 5.5 and denote by H^{ϵ}, $\Psi^{\epsilon}_{\pm}(\lambda,x)$, Σ^{ϵ}_2, $f^{\epsilon}_{\pm}(z,x)$, $m^{\epsilon}_{\pm}(z)$, $\epsilon\in\{+,-\}$ the corresponding quantities. Define

$$V(x) = \begin{cases} V^+(x), & x>0 \\ V^-(x), & x<0 \end{cases}, \tag{5.46}$$

H as in (2.2), and the asymptotic solutions $\Psi^{\pm}_{\pm}(\lambda,x)$, $\lambda\in\Sigma^{\pm}_2$ as in (5.34) (with $V^{(0)}(x) = V^+(x)$, $V^-(x)$, respectively). Then

$$\Sigma_1^- = \Sigma_2^+\backslash\Sigma_2^-,\ \Sigma_1^+ = \Sigma_2^-\backslash\Sigma_2^+,\ \Sigma_2 = \Sigma_2^- \cap \Sigma_2^+, \tag{5.47}$$

$$\begin{aligned} &\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ac}}(H) = \sigma(H^-) \cup \sigma(H^+), \\ &\sigma_{\mathrm{sc}}(H) = \sigma_p(H)\cap\sigma_{ac}(H) = \emptyset, \end{aligned} \tag{5.48}$$

$$m_-(z) = m_-^-(z),\ m_+(z) = m_+^+(z), \tag{5.49}$$

$$\begin{aligned} &f_-(z,x) = \begin{cases} f_-^-(z,x), & x<0 \\ \dfrac{m_-^+(z)-m_-^-(z)}{m_-^+(z)-m_+^+(z)} f_+^+(z,x) + \dfrac{m_+^+(z)-m_-^-(z)}{m_+^+(z)-m_-^+(z)} f_-^+(z,x), & x>0 \end{cases}, \\ &f_+(z,x) = \begin{cases} \dfrac{m_-^-(z)-m_+^+(z)}{m_-^-(z)-m_+^-(z)} f_+^-(z,x) + \dfrac{m_+^-(z)-m_+^+(z)}{m_+^-(z)-m_-^-(z)} f_-^-(z,x), & x<0 \\ f_+^+(z,x), & x>0 \end{cases}, \end{aligned} \tag{5.50}$$

$$\psi_\mp(\lambda,0)=\Psi^\mp_\mp(\lambda,0),\quad \lambda\in\Sigma_2^\mp, \tag{5.51}$$

$$\Psi_\pm(\lambda,0)=(2\pi i)^{-1}\Psi^\mp_\mp(\lambda,0)^{-1}[m_-^-(\lambda+i0)-m_+^+(\lambda+i0)],\quad \lambda\in\Sigma_2^\mp. \tag{5.52}$$

Moreover,

$$R^{\ell}_{r}(\lambda)=-\frac{\overline{\Psi^\mp_\mp(\lambda,0)[m_-^-(\lambda+i0)-m_+^+(\lambda+i0)]}}{\Psi^\mp_\mp(\lambda,0)[m_-^-(\lambda+i0)-m_+^+(\lambda+i0)]},\quad \lambda\in\Sigma_1^\pm, \tag{5.53}$$

$$\begin{aligned}T(\lambda)&=2i\frac{|\Psi^-_-(\lambda,0)\Psi^+_+(\lambda,0)|}{\Psi^-_-(\lambda,0)\Psi^+_+(\lambda,0)}\frac{\{-\operatorname{Im}[m_-^-(\lambda+i0)]\operatorname{Im}[m_+^+(\lambda+i0)]\}}{m_-^-(\lambda+i0)-m_+^+(\lambda+i0)},\\ R^{\ell}_{r}(\lambda)&=\pm\frac{\overline{\Psi^\mp_\mp(\lambda,0)}[m^\pm_\pm(\lambda+i0)-\overline{m^\mp_\mp(\lambda+i0)}]}{\Psi^\mp_\mp(\lambda,0)[m_-^-(\lambda+i0)-m_+^+(\lambda+i0)]},\quad \lambda\in\Sigma_2,\end{aligned} \tag{5.54}$$

where the periodic background quantities $\Psi^\epsilon_\epsilon(\lambda,0)$, $m^\epsilon_\epsilon(\lambda+i0)$, $\epsilon\in\{+,-\}$ can be read off from (5.31), (5.32), and (5.34) (with $V^{(0)}(x)$ replaced by $V^\epsilon(x)$).

The following example involving asymptotically periodic potentials has applications in modeling charge transport in quasi-one-dimensional mesoscopic quantum-interference devices (e.g., Zener diodes), see, e.g., [37] and the references therein.

Example 5.8 (Asymptotically periodic potentials). Let $V^\pm(x+\Omega^\pm)=V^\pm(x)$, $\Omega^\pm>0$ be two real-valued periodic potentials as in Example 5.5 (and 5.7) and denote by H^ϵ, $\Psi^\epsilon_\pm(\lambda,x)$, Σ_2^ϵ, $f^\epsilon_\pm(z,x)$, $\epsilon\in\{+,-\}$ the corresponding quantities. Suppose

$$\begin{aligned}&V\in L^1_{\text{loc}}(\mathbb{R})\text{ is real-valued},\\ &\int_{-\infty}^0 dx(1+x^2)|V(x)-V^-(x)|+\int_0^\infty dx(1+x^2)|V(x)-V^+(x)|<\infty.\end{aligned} \tag{5.55}$$

H is then defined as in (2.2) and the asymptotic solutions $\Psi^\pm_\pm(\lambda,x)$, $\lambda\in\Sigma_2^\pm$ as in (5.34) (with $V^{(0)}(x)=V^+(x)$, $V^-(x)$, respectively). Consider

$$\begin{aligned}\psi_\pm(\lambda,x)=\Psi^\pm_\pm(\lambda,x)+\int_x^{\pm\infty}dx'W(\Psi^\pm_\pm(\lambda),\overline{\Psi^\pm_\pm(\lambda)})^{-1}[\Psi^\pm_\pm(\lambda,x)\overline{\Psi^\pm_\pm(\lambda,x')}\\ -\overline{\Psi^\pm_\pm(\lambda,x)}\Psi^\pm_\pm(\lambda,x')][V(x')-V^\pm(x')]\psi_\pm(\lambda,x'),\ \lambda\in\Sigma_2^\pm,\end{aligned} \tag{5.56}$$

then

$$\Psi_\pm(\lambda,x)=(2\pi i)^{-1}\psi_\mp(\lambda,0)^{-1}[m_-(\lambda+i0)-m_+(\lambda+i0)]^{-1}f_\pm(\lambda,x),\quad \lambda\in\Sigma_2^\mp, \tag{5.57}$$

$$\Sigma_1^-=\Sigma_2^+\backslash\Sigma_2^-,\ \Sigma_1^+=\Sigma_2^-\backslash\Sigma_2^+,\ \Sigma_2=\Sigma_2^-\cap\Sigma_2^+, \tag{5.58}$$

$$\begin{aligned}&\sigma_{\text{ess}}(H)=\sigma_{\text{ac}}(H)=\sigma_{\text{ac}}(H^-)\cup\sigma_{\text{ac}}(H^+),\\&\sigma_{\text{sc}}(H)=\sigma_p(H)\cap\sigma_{ac}(H)=\emptyset.\end{aligned} \tag{5.59}$$

$\overset{\ell}{R^r}(\lambda)$, $\lambda\in\Sigma_1^\pm$ and $T(\lambda)$, $\overset{\ell}{R^r}(\lambda)$, $\lambda\in\Sigma_2$ are then given by (4.10) and (4.11).

Next we turn to a rather different situation where $V(x)\underset{x\to-\infty}{\longrightarrow}0$, $V(x)\underset{x\to+\infty}{\longrightarrow}+\infty$ (see, e.g., [16], [29]).

Example 5.9. Let

$$V\in L^1_{\text{loc}}(\mathbb{R})\text{ be real-valued, }\int_{-\infty}^0 dx(1+|x|)|V(x)|<\infty,\ \lim_{x\to+\infty}V(x)=+\infty, \tag{5.60}$$

define H as in (2.2), and $\Psi_-^-(\lambda,x)$, $\lambda>0$ as in (5.4) with $V_0=0$. Consider

$$\begin{aligned}\psi_-(\lambda,x)=\Psi_-^-(\lambda,x)+\int_x^{-\infty}dx'W(\Psi_-^-(\lambda),\Psi_-^-(\lambda))^{-1}[\Psi_-^-(\lambda,x)\overline{\Psi_-^-(\lambda,x')}\\-\overline{\Psi_-^-(\lambda,x)}\Psi_-^-(\lambda,x')]V(x')\psi_-(\lambda,x'),\ \lambda>0.\end{aligned} \tag{5.61}$$

Then

$$\Sigma_1^+=(0,\infty),\ \Sigma_1^-=\Sigma_2=\emptyset, \tag{5.62}$$

$$\sigma_{\text{ess}}(H)=\sigma_{\text{ac}}(H)=[0,\infty),\ \sigma_{\text{sc}}(H)=\sigma_p(H)\cap[0,\infty)=\emptyset, \tag{5.63}$$

and total reflection from the left at all energies $\lambda>0$ is described by R^ℓ in (4.10).

Finally we consider reflectionless potentials (solitons) with respect to certain background potentials. The construction of such potentials (especially in the context of KdV and mKdV solutions) using the single and double commutation methods has been studied in great detail by [9], [11], [17], [19]–[21], [23]. Here we can only review these techniques very briefly. Our main aim will be a proof of the fact that potentials constructed by the single and double commutation method are reflectionless if and only if the underlying background potential is. What we call commutation methods in the following has its roots in factorizing H as a product of two first-order operators A, A^+, $H=AA^+$ and permuting these factors. For a detailed history of these techniques going back to Jacobi, Darboux, Crum, and Gelfand-Levitan, see [17] and the references therein.

We start with the single commutation or Crum-Darboux method (see, e.g., [9], [19], [21], [23]).

Example 5.10 (Single commutation method). Suppose $V_0 \in L^1_{\text{loc}}(\mathbb{R})$ is real-valued and the corresponding Schrödinger operator H_0 defined in (2.2) satisfies (H.2.1) and is bounded from below. Let $E_0 = \inf \sigma(H_0)$, pick $\lambda_1 < E_0$ and let $f_{0,\pm}(z,x)$, $m_{0,\pm}(z)$ be defined as in (2.5). Introduce

$$\psi_{0,\sigma_1}(\lambda_1, x) = \frac{1}{2}(1-\sigma_1)f_{0,-}(\lambda_1, x) + \frac{1}{2}(1+\sigma_1)f_{0,+}(\lambda, x), \quad \sigma_1 \in [-1,1], \tag{5.64}$$

$$V_{0,\sigma_1}(x) = V_0(x) - 2\frac{d^2}{dx^2}\ln[\psi_{0,\sigma_1}(\lambda_1, x)], \tag{5.65}$$

$$f_{0,\sigma_1,\pm}(z,x) = \frac{W(f_{0,\pm}(z), \psi_{0,\sigma_1}(\lambda_1))(x)\psi_{0,\sigma_1}(\lambda_1, 0)}{W(f_{0,\pm}(z), \psi_{0,\sigma_1}(\lambda_1))(0)\psi_{0,\sigma_1}(\lambda_1, x)}, \tag{5.66}$$

$$\tau_{0,\sigma_1} = -\frac{d^2}{dx^2} + V_{0,\sigma_1}(x), \quad \sigma_1 \in [-1,1]. \tag{5.67}$$

Then τ_{0,σ_1}, $\sigma_1(-1,1)$ satisfies (H.2.1) and

$$\tau_{0,\sigma_1} f_{0,\sigma_1,\pm}(z,x) = z f_{0,\sigma_1,\pm}(z,x), \tag{5.68}$$

$$f_{0,\sigma_1,\pm}(z,.) \in L^2((R,\pm\infty)),\ R \in \mathbb{R},\ z \in \mathbb{C}\backslash\sigma(H_{0,\sigma_1}),\ \sigma_1 \in (-1,1), \tag{5.69}$$

where H_{0,σ_1} is the operator associated with τ_{0,σ_1} defined according to (2.2) (see [9], [19]). Moreover,

$$\sigma(H_{0,\sigma_1}) = \sigma(H_0) \cup \{\lambda_1\}, \quad \sigma_1 \in (-1,1) \tag{5.70}$$

and H_{0,σ_1}, $\sigma_1 \in (-1,1)$, restricted to the orthogonal complement of the eigenfunction corresponding to λ_1, is unitarily equivalent to H_0 [9]. The corresponding asymptotic wave functions $\Psi^{\pm}_{0,\sigma_1,\pm}(\lambda, x)$ as $x \to \pm\infty$ can be identified with multiples of $f_{0,\pm1,\pm}(\lambda, x)$ [19]. Given (5.66)–(5.69) one computes for the Weyl m-functions $m_{0,\sigma_1,\pm}(z)$ of H_{0,σ_1} in terms of $m_{0,\pm}(z)$ of H_0,

$$\begin{aligned} m_{0,\sigma_1,\pm}(z) &= f'_{0,\sigma_1,\pm}(z,0) \\ &= (z-\lambda_1)[\psi'_{0,\sigma_1}(\lambda_1,0)\psi_{0,\sigma_1}(\lambda_1,0)^{-1} - m_{0,\pm}(z)]^{-1} - \psi'_{0,\sigma_1}(\lambda_1,0)\psi_{0,\sigma_1}(\lambda_1,0)^{-1}, \\ &\qquad \text{a.e. on } \sigma_1 \in (-1,1). \end{aligned} \tag{5.71}$$

In particular,

$$m_{0,\sigma_1,+}(\lambda+i0)=\overline{m_{0,\sigma_1,-}(\lambda+i0)} \quad \text{for a.e.} \quad \lambda\in\Sigma_2$$

$$\text{if and only if} \quad m_{0,+}(\lambda+i0)=\overline{m_{0,-}(\lambda+i0)} \quad \text{for a.e.} \quad \lambda\in\Sigma_2, \tag{5.72}$$

i.e., H_{0,σ_1}, $\sigma_1\in(-1,1)$ is reflectionless if and only if H_0 is (cf. Definition 4.6). This result can easily be iterated to insert N eigenvalues $\lambda_N<\lambda_{N-1}<\cdots<\lambda_1$.

The single commutation method just described requires H_0 to be bounded from below and insertion of eigenvalues below the spectrum of H_0. The following double commutation method (see [17], [19], [20]) removes these restrictions.

Example 5.11 (Double commutation method). Let $V_0\in L^1_{\text{loc}}(\mathbb{R})$ be real-valued and suppose H_0 defined as in (2.2) satisfies (H.2.1). Assume H_0 has a spectral gap, pick $\lambda_1\in\mathbb{R}\backslash\sigma(H_0)$, and let $f_{0,\pm}(z,x)$, $m_{0,\pm}(z)$ be defined as in (2.5). Introduce

$$V_{\gamma_1,\epsilon_1}(x)=V_0(x)-2\frac{d^2}{dx^2}\ln\Big[1-\epsilon_1\gamma_{1,\epsilon_1}\int_{\epsilon_1\infty}^x dx' f_{0,\epsilon_1}(\lambda_1,x')^2\Big],\ \epsilon_1\in\{+,-\},\ 0\leq\gamma_{1,\epsilon_1}\leq\infty, \tag{5.73}$$

$$\begin{aligned}\psi_{\gamma_1,\epsilon_1,\epsilon}(z,x)=f_{0,\epsilon}(z,x)+\epsilon_1\Big[1-\epsilon_1\gamma_{1,\epsilon_1}\int_{\epsilon_1\infty}^x dx' f_{0,\epsilon_1}(\lambda_1,x')^2\Big]^{-1} f_{0,\epsilon_1}(\lambda_1,x)\\ \times(z-\lambda_1)^{-1}W(f_{0,\epsilon}(z),f_{0,\epsilon_1}(\lambda_1))(x),\end{aligned} \tag{5.74}$$

$$\begin{aligned}&f_{\gamma_1,\epsilon_1,\epsilon}(z,x)=\psi_{\gamma_1,\epsilon_1,\epsilon}(z,x)\psi_{\gamma_1,\epsilon_1,\epsilon}(z,0)^{-1}, \quad \epsilon\in\{+,-\},\\ &\tau_{\gamma_1,\epsilon_1}=-\frac{d^2}{dx^2}+V_{\gamma_1,\epsilon_1}(x),\ \epsilon_1\in\{+,-\},\ 0\leq\gamma_{1,\epsilon_1}\leq\infty.\end{aligned} \tag{5.75}$$

Then $\tau_{\gamma_1,\epsilon_1}$, $0<\gamma_{1,\epsilon_1}<\infty$ satisfies (H.2.1) and

$$\tau_{\gamma_1,\epsilon_1}\psi_{\gamma_1,\epsilon_1,\epsilon}(z,x)=z\psi_{\gamma_1,\epsilon_1,\epsilon}(z,x), \tag{5.76}$$

$$\psi_{\gamma_1,\epsilon_1,\epsilon}(z,.)\in L^2((R,\epsilon\infty)),\ R\in\mathbb{R},\ z\in\mathbb{C}\backslash\sigma(H_{\gamma_1,\epsilon_1}),\ 0<\gamma_{1,\epsilon_1}<\infty, \tag{5.77}$$

where H_{γ_1,ϵ_1} is the operator associated with $\tau_{\gamma_1,\epsilon}$ defined as in (2.2) (see [17]). Moreover,

$$\sigma(H_{\gamma_1,\epsilon_1})=\sigma(H_0)\cup\{\lambda_1\}, \quad 0<\gamma_{1,\epsilon_1}<\infty \tag{5.78}$$

and H_{γ_1,ϵ_1}, $0<\gamma_{1,\epsilon_1}<\infty$, restricted to the orthogonal complement of the eigenfunction corresponding to λ_1, is unitarily equivalent to H_0 [17]. The corresponding asymptotic wave functions $\Psi^{\pm}_{\gamma_1,\epsilon_1,\pm}(\lambda,x)$ as $x\to\pm\infty$ can be identified with multiples of $f_{\substack{0\\ \infty,+,\pm}}(\lambda,x)$ for $\epsilon_1=+$

and $f_{\substack{\infty\\0,-,\pm}}(\lambda,x)$ for $\epsilon_1=-$ (cf. [19], [20]). Given (5.74)–(5.77), one computes for the Weyl m-functions $m_{\gamma_1,\epsilon_1,\pm}(z)$ of H_{γ_1,ϵ_1} in terms of $m_{0,\pm}(z)$ of H_0,

$$\begin{aligned}
m_{\gamma_1,\epsilon_1,\epsilon}(z) &= f'_{\gamma_1,\epsilon_1,\epsilon}(z,0)\\
&= \Big\{1-\epsilon_1\gamma_{1,\epsilon_1}\Big(1-\epsilon_1\gamma_{1,\epsilon_1}\int_{\epsilon_1\infty}^0 dx f_{0,\epsilon_1}(\lambda_1,x)^2\Big)^{-1}(z-\lambda_1)^{-1}[m_{0,\epsilon}(z)-m_{0,\epsilon_1}(\lambda_1)]\Big\}^{-1}\\
&\times\Big\{m_{0,\epsilon}(z)-\epsilon_1\gamma_{1,\epsilon_1}(z-\lambda_1)^{-1}\Big[m_{0,\epsilon_1}(\lambda_1)\Big(1-\epsilon_1\gamma_{1,\epsilon_1}\int_{\epsilon_1\infty}^0 dx f_{0,\epsilon_1}(\lambda_1,x)^2\Big)^{-1}\\
&+\epsilon_1\gamma_{1,\epsilon_1}\Big(1-\epsilon_1\gamma_{1,\epsilon_1}\int_{\epsilon_1\infty}^0 dx f_{0,\epsilon_1}(\lambda_1,x)^2\Big)^{-2}\Big][m_{0,\epsilon}(z)-m_{0,\epsilon_1}(\lambda_1)]\\
&+\epsilon_1\gamma_{1,\epsilon_1}\Big(1-\epsilon_1\gamma_{1,\epsilon_1}\int_{\epsilon_1\infty}^0 dx f_{0,\epsilon_1}(\lambda_1,x)^2\Big)^{-1}\Big\},\\
&\qquad\qquad \epsilon_1,\epsilon\in\{+,-\},\ 0<\gamma_{1,\epsilon_1}<\infty,\ m_{0,\epsilon_1}(\lambda_1)\neq\infty,
\end{aligned}\tag{5.79}$$

$$\begin{aligned}
m_{\gamma_1,\epsilon_1,\epsilon}(z) &= m_{0,\epsilon}(z)+\epsilon_1\gamma_{1,\epsilon_1}f'_{0,\epsilon_1}(\lambda_1,0)^2(z-\lambda_1)^{-1}\Big(1-\epsilon_1\gamma_{1,\epsilon_1}\int_{\epsilon_1\infty}^0 dx f_{0,\epsilon_1}(\lambda_1,x)^2\Big)^{-1},\\
&\qquad\qquad \epsilon_1,\epsilon\in\{+,-\},\ 0<\gamma_{1,\epsilon_1}<\infty,\ m_{0,\epsilon_1}(\lambda_1)=\infty.
\end{aligned}\tag{5.80}$$

The case distinctions $m_{0,\epsilon_1}(\lambda_1)\neq 0$ and $m_{0,\epsilon_1}(\lambda_1)=\infty$ in (5.79) and (5.80) are equivalent to $f_{0,\epsilon_1}(\lambda_1,0)\neq 0$ and $f_{0,\epsilon_1}(\lambda_1,0)=0$, respectively. Again one concludes that

$$\begin{aligned}
&m_{\gamma_1,\epsilon_1,+}(\lambda+i0)=\overline{m_{\gamma_1,\epsilon_1,-}(\lambda_1+i0)} \text{ for a.e. } \lambda\in\Sigma_2\\
&\text{if and only if}\quad m_{0,+}(\lambda+i0)=\overline{m_{0,-}(\lambda+i0)}\quad\text{for a.e.}\quad \lambda\in\Sigma_2,
\end{aligned}\tag{5.81}$$

i.e., H_{γ_1,ϵ_1}, $0<\gamma_{1,\epsilon_1}<\infty$ is reflectionless if and only if H_0 is. This result can be iterated to insert a finite number of eigenvalues into any given spectral gap of H_0 in a straightforward manner.

We summarize these findings in

Theorem 5.12. *Under the hypotheses in Examples 5.10 and 5.11, repeated applications of the single and double commutation methods yield reflectionless potentials if and only if the corresponding background operator H_0 is reflectionless.*

The results of Example 5.10 and (5.11) can be combined with Section 4 to determine all scattering data of H_{0,σ_1}, $\sigma_1\in(-1,1)$ and H_{γ_1,ϵ_1}, $0<\gamma_{1,\epsilon_1}<\infty$ in terms of those of H_0 (whether or not H_0 is reflectionless). Further investigations, especially in the particularly interesting case where the background H_0 is associated with algebro-geometric quasi-periodic finite-gap potentials and the scattering data can be expressed in terms of Abelian functions, are in preparation [18].

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