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UNIQUENESS THEOREMS IN INVERSE SPECTRAL THEORY FOR ONE-DIMENSIONAL SCHRÖDINGER OPERATORS

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Abstract. New unique characterization results for the potential $V(x)$ in connection with Schrödinger operators on $\mathbb{R}$ and on the half-line $[0, \infty)$ are proven in terms of appropriate Krein spectral shift functions. Particular results obtained include a generalization of a well-known uniqueness theorem of Borg and Marchenko for Schrödinger operators on the half-line with purely discrete spectra to arbitrary spectral types and a new uniqueness result for Schrödinger operators with confining potentials on the entire real line.

1. Introduction

The purpose of this article is to prove a variety of new uniqueness theorems for potentials $V(x)$ in one-dimensional Schrödinger operators $-\frac{d^2}{dx^2} + V$ on $\mathbb{R}$ and on the half-line $\mathbb{R}_+ = [0, \infty)$ in terms of appropriate Krein spectral shift functions recently introduced in a series of papers describing new trace formulas for $V(x)$ on $\mathbb{R}$ [15],[17],[19],[20] and on $\mathbb{R}_+$ [14].

First we briefly recall these trace formulas for Schrödinger operators $H = -\frac{d^2}{dx^2} + V$ on the real line $\mathbb{R}$ assuming V to be real-valued, continuous, and bounded from below. In addition to H, one also considers the family of operators $H_y^\beta = -\frac{d^2}{dx^2} + V$, $\beta \in \mathbb{R} \cup \{\infty\}$, $y \in \mathbb{R}$, with an additional boundary condition of the type $g'(y_\pm) + \beta g(y_\pm) = 0$ for elements g in the domain of H_y^β; see (A.30) and (3.2) for detailed domain descriptions. Here, in obvious notation, $\beta = \infty$ denotes the corresponding operator H_y^∞ with an additional Dirichlet boundary condition at $y \in \mathbb{R}$. Denoting by $\xi^\beta(\lambda, y)$ Krein's spectral shift function for the pair (H_y^β, H), $\beta \in \mathbb{R} \cup \{\infty\}$, $y \in \mathbb{R}$ (see (3.12)–(3.18)), the following trace formulas have been derived in [15] in the Dirichlet case $\beta = \infty$ and in [20] for $\beta \in \mathbb{R}$:

$$(1.1) \qquad V(x) = E_0 + \lim_{z \to i\infty} \int_{E_0}^{\infty} d\lambda \, \frac{z^2}{(\lambda - z)^2} [1 - 2\xi^\infty(\lambda, x)],$$

$$E_0 = \inf\{\sigma(H)\}, \beta = \infty, x \in \mathbb{R},$$

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(1.2)

$$V(x) = 2\beta^2 + E_0^\beta(x) + \lim_{z\to i\infty} \int_{E_0^\beta(x)}^{\infty} d\lambda \, \frac{z^2}{(\lambda - z)^2} \, [1 + 2\xi^\beta(\lambda, x)],$$

$$E_0^\beta(x) = \inf\{\sigma H_x^\beta)\}, \beta \in \mathbb{R}, x \in \mathbb{R}.$$

(Here $\sigma(\,\cdot\,)$ denotes the spectrum.) These trace formulas extend previous results by [7–9],[12],[22],[26],[28],[29],[34],[35],[39],[40] in the short-range, periodic, and certain almost periodic cases.

A similar result can be derived for half-line Schrödinger operators. Assuming again V to be real-valued, continuous, and bounded from below, denote by $H_{+,\alpha} = -\frac{d^2}{dx^2} + V$, $\alpha \in [0, \pi)$, the family of Schrödinger operators on the half-line $\mathbb{R}_+ = [0, \infty)$ with the boundary condition $\sin(\alpha)g'(0_+) + \cos(\alpha)g(0_+) = 0$ for elements g in the domain of $H_{+,\alpha}$ (cf. (A.14)). For $\alpha_1, \alpha_2 \in (0, \pi)$, $\alpha_1 \neq \alpha_2$, let $\xi_{\alpha_1,\alpha_2}(\lambda)$ be Krein's spectral shift function for the pair $(H_{+,\alpha_2}, H_{+,\alpha_1})$ (cf. (2.8)–(2.10)). Then the following trace formula can be inferred from the results in [14]:

(1.3)

$$V(0) = \cot^2(\alpha) + \lim_{z\to i\infty} \left\{ -z - i\cot(\alpha) z^{1/2} + 2 \int_{\mathbb{R}} d\lambda \frac{z^2}{(\lambda - z)^2} \, \xi_{0,\alpha}(\lambda) \right\}, \quad \alpha \in (0, \pi).$$

A quick look at (1.1), (1.2), and (1.3) reveals the fact that $\xi^\beta(\lambda, x)$, $\lambda, x \in \mathbb{R}$, determines $V(x)$, $x \in \mathbb{R}$, and $\xi_{0,\alpha}(\lambda)$, $\lambda \in \mathbb{R}$, determines $V(0)$ in the half-line case. However, clearly both of these statements describe a mismatch and hence miss the point: $\xi^\beta(\lambda, x)$ depends on two real variables as opposed to one in $V(x)$ and, analogously, $\xi_{0,\alpha}(\lambda)$ depends on one real variable while $V(0)$ is just a constant. From the point of view of inverse spectral theory, the problems that need clarification appear to be the following: Does $\xi^\beta(\lambda, x_0)$ for fixed $x_0 \in \mathbb{R}$ and all $\lambda \in \mathbb{R}$ determine $V(x)$ for all $x \in \mathbb{R}$ and, similarly, does $\xi_{\alpha_1,\alpha_2}(\lambda)$, $\alpha_1 \neq \alpha_2$, for all $\lambda \in \mathbb{R}$ determine $V(x)$ for all $x \geq 0$ in the half-line case? The present paper provides complete solutions to these problems.

In Section 2 we treat the half-line case and provide an affirmative answer to the problem posed: $\xi_{\alpha_1,\alpha_2}(\lambda)$, $\alpha_1 \neq \alpha_2$, for a.e. $\lambda \in \mathbb{R}$ indeed uniquely determines $V(x)$ for a.e. $x \geq 0$ (cf. Theorem 2.4), extending a well-known result of Borg [5] and Marchenko [32], obtained independently from each other around 1952 for operators with purely discrete spectrum, to arbitrary spectral types (see Corollary 2.5). We conclude Section 2 with an application of our main Theorem 2.4 to three-dimensional Schrödinger operators with spherically symmetric potentials, and state a new uniqueness theorem in this context (cf. Theorem 2.6).

Section 3 is devoted to Schrödinger operators on the entire real line. While the corresponding question posed concerning $\xi^\beta(\lambda, x_0)$ turns out to have a negative answer, that is, $\xi^\beta(\lambda, x_0)$ for fixed $x_0 \in \mathbb{R}$ and a.e. $\lambda \in \mathbb{R}$ in general cannot determine V uniquely for a.e. $x \in \mathbb{R}$, Theorem 3.2 shows that $\xi^{\beta_1}(\lambda, x_0)$ and $\xi^{\beta_2}(\lambda, x_0)$, $\beta_1 \neq \beta_2$, for a.e. $\lambda \in \mathbb{R}$ uniquely determine V a.e. except in the Dirichlet and Neumann cases $\beta_1 = 0$, $\beta_2 = \infty$, respectively, $\beta_1 = \infty$, $\beta_2 = 0$. In the latter case, V is uniquely determined up to reflection symmetry with respect to x_0. When combining $\xi^\beta(\lambda, x_0)$, $\lambda \in \mathbb{R}$, with additional Dirichlet data and/or norming constants, further unique characterizations of V can be achieved. This is illustrated in connection with

Theorem 3.6, which provides a new uniqueness result for Schrödinger operators on $\mathbb{R}$ with purely discrete spectra.

Since our techniques rely heavily on the use of certain properties of Herglotz functions and especially on the Weyl-Titchmarsh theory, we collected a variety of pertinent results in Appendix A.

Perhaps we should emphasize at this point that we do not discuss explicit reconstruction procedures for $V(x)$ in this paper (the reader can find standard results on reconstruction techniques, e.g., in [13],[29],[30],[32], and [33]). Here we exclusively focus on deriving new minimal sets of spectral data which uniquely determine the potential V a.e. The basic outline of our philosophy of how to recover $V(x)$ from $\xi^\infty(\lambda, x_0)$, $\lambda \in \mathbb{R}$, and Dirichlet data is described in [15]. We shall return to this topic elsewhere.

Analogous results for second-order finite difference operators are in preparation [18].

2. Schrödinger operators on $[0, \infty)$

In this section we shall describe a uniqueness result for Schrödinger operators on the half-line $[0,\infty)$, which extends a well-known theorem of Borg [5] and Marchenko [32] in the special case of purely discrete spectra to arbitrary spectral types.

We shall freely exploit the notation introduced in Appendix A and recall τ_+, $H_{+,\alpha}$, ϕ_α, θ_α, $\psi_{+,\alpha}$, $m_{+,\alpha}$, $d\rho_{+,\alpha}$, and $G_{+,\alpha}(z,x,x')$ as introduced in (A.13)–(A.27). In particular, we shall assume hypothesis (A.12), that is,

$$V \in L^1([0,R]) \text{ for all } R>0, \qquad V \text{ real-valued} \tag{2.1}$$

throughout this section and recall that $H_{+,\alpha}$, defined in terms of separated boundary conditions, is a real operator of uniform spectral multiplicity one.

The basic uniqueness criterion for Schrödinger operators on the half-line $[0,\infty)$ we shall rely on repeatedly in the following can be stated as follows.

Theorem 2.1 (See, e.g., [32]). *Suppose $\alpha_1, \alpha_2 \in [0,\pi)$, $\alpha_1 \neq \alpha_2$, and define H_{+,j,α_j}, m_{+,j,α_j}, ρ_{+,j,α_j} associated with the differential expressions $\tau_j = -\frac{d^2}{dx^2} + V_j(x)$, $x \geq 0$, where $V_j, j=1,2$, satisfy hypothesis* (2.1). *Then the following are equivalent:*
(i) $m_{+,1,\alpha_1}(z) = m_{+,2,\alpha_2}(z)$, $z \in \mathbb{C}_+$.
(ii) $\rho_{+,1,\alpha_1}((-\infty,\lambda]) = \rho_{+,2,\alpha_2}((-\infty,\lambda])$, $\lambda \in \mathbb{R}$.
(iii) $\alpha_1 = \alpha_2$ *and* $V_1(x) = V_2(x)$ *for a.e.* $x \geq 0$.

We begin our analysis with a simple warm-up relating Green's functions for different boundary conditions at $x=0$. (We also recall our convention of Appendix A to fix the boundary condition (if any) at $x=+\infty$.)

Lemma 2.2. *Let $\alpha_j \in [0,\pi)$, $j=1,2$, $x,x' \in \mathbb{R}_+$, and $z \in \mathbb{C}\backslash\{\sigma(H_{+,\alpha_1}) \cup \sigma(H_{+,\alpha_2})\}$. Then*
(i)

$$G_{+,\alpha_2}(z,x,x') - G_{+,\alpha_1}(z,x,x') = -\frac{\psi_{+,\alpha_1}(z,x)\psi_{+,\alpha_1}(z,x')}{\cot(\alpha_2-\alpha_1) + m_{+,\alpha_1}(z)}. \tag{2.2}$$

(ii)

$$\frac{G_{+,\alpha_2}(z,0,0)}{G_{+,\alpha_1}(z,0,0)} = \frac{1}{(\beta_1-\beta_2)\sin^2(\alpha_1)[\cot(\alpha_2-\alpha_1)+m_{+,\alpha_1}(z)]} \tag{2.3}$$
$$= (\beta_1-\beta_2)\sin^2(\alpha_2)[\cot(\alpha_2-\alpha_1)-m_{+,\alpha_2}(z)],$$
$$\beta_j = \cot(\alpha_j), \qquad j=1,2. \tag{2.4}$$

(iii)

$$\mathrm{Tr}[(H_{+,\alpha_2}-z)^{-1}-(H_{+,\alpha_1}-z)^{-1}] = -\frac{d}{dz}\ln[\cot(\alpha_2-\alpha_1)+m_{+,\alpha_1}(z)] \tag{2.5}$$
$$= \frac{d}{dz}\ln[\cot(\alpha_2-\alpha_1)-m_{+,\alpha_2}(z)]. \tag{2.6}$$

Proof. (2.2) is a direct consequence of (A.16)–(A.18), (A.23), and (A.38). Similarly, (2.3) and (2.4) follow by combining (A.25) and (A.38). (2.5) follows from (2.2) and (A.44) in the limit $z_1 \to z_2 = z$. (2.6) is clear from

$$\cot(\alpha_2-\alpha_1)+m_{+,\alpha_1}(z) = [\sin(\alpha_2-\alpha_1)]^2[\cot(\alpha_2-\alpha_1)-m_{+,\alpha_2}(z)]^{-1}, \tag{2.7}$$

a simple consequence of (A.38). □

Since $m_{+,\alpha}(z)$ is a Herglotz function, we may now introduce Krein's spectral shift function [27] $\xi_{\alpha_1,\alpha_2}(\lambda)$ for the pair $(H_{+,\alpha_2}, H_{+,\alpha_1})$ according to (A.2), (A.4) by

$$\cot(\alpha_2-\alpha_1)+m_{+,\alpha_1}(z) = \exp\bigg\{\mathrm{Re}[\ln(\cot(\alpha_2-\alpha_1)+m_{+,\alpha_1}(i))] + \int_{\mathbb{R}}\bigg[\frac{1}{\lambda-z}-\frac{\lambda}{1+\lambda^2}\bigg]\xi_{\alpha_1,\alpha_2}(\lambda)\,d\lambda\bigg\}, \quad 0\le\alpha_1<\alpha_2<\pi, z\in\mathbb{C}\backslash\mathbb{R}. \tag{2.8}$$

This is extended to all $\alpha_1,\alpha_2\in[0,\pi)$ by

$$\xi_{\alpha,\alpha}(\lambda)=0, \qquad \xi_{\alpha_2,\alpha_1}(\lambda) = -\xi_{\alpha_1,\alpha_2}(\lambda) \qquad \text{for a.e. } \lambda\in\mathbb{R}. \tag{2.9}$$

(2.7) then implies

$$\cot(\alpha_2-\alpha_1)-m_{+,\alpha_2}(z) = \exp\bigg\{\mathrm{Re}[\ln(\cot(\alpha_2-\alpha_1)-m_{+,\alpha_2}(i))] - \int_{\mathbb{R}}\bigg[\frac{1}{\lambda-z}-\frac{\lambda}{1+\lambda^2}\bigg]\xi_{\alpha_1,\alpha_2}(\lambda)\,d\lambda\bigg\}, \quad 0\le\alpha_1<\alpha_2<\pi, z\in\mathbb{C}\backslash\mathbb{R}. \tag{2.10}$$

Next we summarize a few properties of $\xi_{\alpha_1,\alpha_2}(\lambda)$.

Lemma 2.3. (i) *Suppose* $0 \le \alpha_1 < \alpha_2 < \pi$. *Then for a.e.* $\lambda \in \mathbb{R}$,

$$\xi_{\alpha_1,\alpha_2}(\lambda) = \begin{cases} \lim_{\epsilon\downarrow 0} \pi^{-1}\mathrm{Im}\{\ln[\cot(\alpha_2-\alpha_1) + m_{+,\alpha_1}(\lambda+i\epsilon)]\} & (2.11) \\ -\lim_{\epsilon\downarrow 0} \pi^{-1}\mathrm{Im}\{\ln[\cot(\alpha_2-\alpha_1) - m_{+,\alpha_2}(\lambda+i\epsilon)]\} & (2.12) \\ \lim_{\epsilon\downarrow 0} \pi^{-1}\mathrm{Im}\{\ln\big[\frac{1}{\sin(\alpha_1)}\frac{G_{+,\alpha_1}(\lambda+i\epsilon,0,0)}{G_{+,\alpha_2}(\lambda+i\epsilon,0,0)}\big]\}. & (2.13) \end{cases}$$

(*For* $\alpha_1 = 0$, $G_{+,\alpha_1}(\lambda+i\epsilon,0,0)/\sin(\alpha_1)$ *has to be replaced by* -1 *in* (2.13) *according to* (A.25).) *Moreover,*

$$0 \le \xi_{\alpha_1,\alpha_2}(\lambda) \le 1 \ \text{a.e.} \tag{2.14}$$

(ii) *Let* $\alpha_j \in [0,\pi)$, $1 \le j \le 3$. *Then the "chain rule"*

$$\xi_{\alpha_1,\alpha_3}(\lambda) = \xi_{\alpha_1,\alpha_2}(\lambda) + \xi_{\alpha_2,\alpha_3}(\lambda) \tag{2.15}$$

holds for a.e. $\lambda \in \mathbb{R}$.

(iii) *For all* $\alpha_1, \alpha_2 \in [0,\pi)$,

$$\xi_{\alpha_1,\alpha_2} \in L^1(\mathbb{R}; (1+\lambda^2)^{-1}\, d\lambda). \tag{2.16}$$

(iv) *Assume* $\alpha_1, \alpha_2 \in [0,\pi)$, $\alpha_1 \ne \alpha_2$. *Then*

$$\xi_{\alpha_1,\alpha_2} \in L^1(\mathbb{R}; (1+|\lambda|)^{-1}\, d\lambda) \ \text{if and only if} \ \alpha_1,\alpha_2 \in (0,\pi). \tag{2.17}$$

(v) *For all* $\alpha_1, \alpha_2 \in [0,\pi)$,

$$\mathrm{Tr}[(H_{+,\alpha_2} - z)^{-1} - (H_{+,\alpha_1} - z)^{-1}] = -\int_{\mathbb{R}} (\lambda - z)^{-2}\xi_{\alpha_1,\alpha_2}(\lambda)\, d\lambda. \tag{2.18}$$

Proof. (i) (2.11)–(2.13) follow from (2.3), (2.4) (resp. (2.7)), (2.8), (A.2), and (A.4). (2.14) is clear from (A.4).

(ii) is a consequence of (2.13).

(iii) is obvious from $0 \le |\xi_{\alpha_1,\alpha_2}| \le 1$ a.e.

(iv) By (2.9) we may assume $0 \le \alpha_1 < \alpha_2 < \pi$. Then (A.39) yields

$$\cot(\alpha_2-\alpha_1) - m_{+,\alpha_2}(z) \underset{z\to i\infty}{=} \begin{cases} 0, & \alpha_1 = 0, \\ \cot(\alpha_2-\alpha_1) - \cot(\alpha_2) > 0, & 0 < \alpha_1 < \alpha_2 < \pi, \end{cases} \tag{2.19}$$

and it suffices to apply Theorem A.1(iii) to $\cot(\alpha_2 - \alpha_1) - m_{+,\alpha_2}(z)$ taking into account (2.10).

(v) follows from (2.5) and from applying $-\frac{d}{dz}\ln(\,\cdot\,)$ to (2.8). ☐

We note that $\xi_{\alpha_1,\alpha_2}(\lambda)$ (for $\alpha_1,\alpha_2 \in (0,\pi)$) has been introduced by Javrjan [23],[24]. In particular, he proved (2.5) and (2.18) in the non-Dirichlet cases where $0 < \alpha_1, \alpha_2 < \pi$. We also remark that (2.18) extends to more general situations of the type

$$\mathrm{Tr}[F(H_{+,\alpha_2}) - F(H_{+,\alpha_1})] = \int_{\mathbb{R}} F'(\lambda)\xi_{\alpha_1,\alpha_2}(\lambda)\, d\lambda \tag{2.20}$$

for appropriate functions F (see, e.g., [38]).

Given these preliminaries, we are now able to state our main uniqueness result for half-line Schrödinger operators.

Theorem 2.4. *Suppose V_j satisfy hypothesis* (2.1), *and introduce the differential expressions $\tau_j = -\frac{d^2}{dx^2} + V_j(x)$, $x \geq 0$, $j = 1, 2$. Let $\alpha_{j,\ell} \in [0, \pi)$, $\ell = 1, 2$, suppose $0 \leq \alpha_{1,1} < \alpha_{1,2} < \pi$, $0 \leq \alpha_{2,1} < \alpha_{2,2} < \pi$, and define $H_{+,j,\alpha_{j,\ell}}$ for $j, \ell = 1, 2$ associated with τ_j as in* (A.14). *In addition, let $\xi_{j,\alpha_{j,1},\alpha_{j,2}}$, $j = 1, 2$, be Krein's spectral shift function for the pair $(H_{+,j,\alpha_{j,1}}, H_{+,j,\alpha_{j,2}})$. Then the following are equivalent:*

(i) $\xi_{1,\alpha_{1,1},\alpha_{1,2}}(\lambda) = \xi_{2,\alpha_{2,1},\alpha_{2,2}}(\lambda)$ *for a.e.* $\lambda \in \mathbb{R}$.

(ii) $\alpha_{1,1} = \alpha_{2,1}$, $\alpha_{1,2} = \alpha_{2,2}$, *and* $V_1(x) = V_2(x)$ *for a.e.* $x \geq 0$.

Proof. We only need to prove that (i) implies (ii). From Lemma 2.3(iv), one infers that

$$\alpha_{j,1} \underset{(=)}{>} 0 \quad \text{if and only if} \quad \int_{\mathbb{R}} (1 + |\lambda|)^{-1} |\xi_{\alpha_{j,1},\alpha_{j,2}}(\lambda)| \, d\lambda \underset{(=)}{<} \infty, \quad j = 1, 2. \tag{2.21}$$

Since by hypothesis $\alpha_{1,1} \underset{(=)}{>} 0$ if and only if $\alpha_{2,1} \underset{(=)}{>} 0$, one is led to the following case distinction.

a) $0 < \alpha_{1,1} < \alpha_{1,2} < \pi$, $0 < \alpha_{2,1} < \alpha_{2,2} < \pi$. Then (2.10) and (A.39) imply

$$\int_z^{\infty} dz' \int_{\mathbb{R}} (\lambda - z')^{-2} \xi_{j,\alpha_{j,1},\alpha_{j,2}}(\lambda) \, d\lambda = \ln \left[\frac{\cot(\alpha_{j,2} - \alpha_{j,1}) - m_{+,j,\alpha_{j,2}}(z)}{\cot(\alpha_{j,2} - \alpha_{j,1}) - \cot(\alpha_{j,2})} \right] \tag{2.22}$$

$$\underset{z \to i\infty}{=} (\beta_{j,2} - \beta_{j,1}) i z^{-1/2} + (\beta_{j,1}^2 - \beta_{j,2}^2) 2^{-1} z^{-1} + o(z^{-1}), \tag{2.23}$$

$$\beta_{j,\ell} = \cot(\alpha_{j,\ell}), \qquad j, \ell = 1, 2.$$

Given (i), the asymptotic behavior (2.23) then yields

$$\alpha_{1,1} = \alpha_{2,1} \quad \text{and} \quad \alpha_{1,2} = \alpha_{2,2}. \tag{2.24}$$

Insertion of (2.24) into (2.22), still assuming (i), then yields

$$m_{+,1,\alpha_{1,2}}(z) = m_{+,2,\alpha_{1,2}}(z) \tag{2.25}$$

and hence $V_1 = V_2$ a.e. by Theorem 2.1.

b) $0 = \alpha_{1,1} < \alpha_{1,2} < \pi$, $0 = \alpha_{2,1} < \alpha_{2,2} < \pi$. Then (2.10) and (A.39) imply

$$\int_i^z dz' \int_{\mathbb{R}} (\lambda - z')^{-2} \xi_{j,0,\alpha_{j,2}}(\lambda) \, d\lambda$$

$$= -\ln \left[\frac{\cot(\alpha_{j,2}) - m_{+,j,\alpha_{j,2}}(z)}{\cot(\alpha_{j,2}) - m_{+,j,\alpha_{j,2}}(i)} \right] \tag{2.26}$$

$$\underset{z \to i\infty}{=} \ln(z^{1/2}) + \ln[i \sin^2(\alpha_{j,2})] + \ln[\cot(\alpha_{j,2}) - m_{+,j,\alpha_{j,2}}(i)]$$

$$- \cot(\alpha_{j,2}) i z^{-1/2} + o(z^{-1/2}), \qquad j = 1, 2. \tag{2.27}$$

Given (i), the $O(z^{-1/2})$-term in (2.27) then yields

$$\alpha_{1,2} = \alpha_{2,2} \tag{2.28}$$

and the $O(1)$-term in (2.27) yields

$$m_{+,1,\alpha_{1,2}}(i) = m_{+,2,\alpha_{1,2}}(i). \tag{2.29}$$

Inserting (2.28) and (2.29) into (2.26), still assuming (i), then yields

$$m_{+,1,\alpha_{1,2}}(z) = m_{+,2,\alpha_{1,2}}(z) \tag{2.30}$$

and hence again, $V_1 = V_2$ a.e. by Theorem 2.1. □

As a corollary, we obtain a well-known uniqueness result originally due to Borg [5] and Marchenko [32], obtained independently in 1952.

Corollary 2.5 (Borg [5], Theorem 1; Marchenko [32], Theorem 2.3.2; see also [30]). *Define τ_j and $H_{+,j,\alpha}$, $\alpha \in [0, \pi)$, as in Theorem 2.4. Assume in addition that $H_{+,1,\alpha_1}$ and $H_{+,2,\alpha_2}$ have purely discrete spectra for some* (*and hence for all*) *$\alpha_j \in [0, \pi)$, that is,*

$$\sigma_{\mathrm{ess}}(H_{+,j,\alpha_j}) = \emptyset \quad \textit{for some } \alpha_j \in [0, \pi), j = 1, 2. \tag{2.31}$$

Then the following are equivalent:

(i) $\sigma(H_{+,1,\alpha_{1,1}}) = \sigma(H_{+,2,\alpha_{2,1}})$, $\sigma(H_{+,1,\alpha_{1,2}}) = \sigma(H_{+,2,\alpha_{2,2}})$, $\alpha_{j,\ell} \in [0, \pi)$, $j, \ell = 1, 2$, $\sin(\alpha_{1,1} - \alpha_{1,2}) \neq 0$.

(ii) $\alpha_{1,1} = \alpha_{2,1}$, $\alpha_{1,2} = \alpha_{2,2}$, *and* $V_1(x) = V_2(x)$ *for a.e.* $x \geq 0$.

Proof. Without loss of generality, we may assume $0 \leq \alpha_{1,1} < \alpha_{1,2} < \pi$, $0 \leq \alpha_{2,1} < \alpha_{2,2} < \pi$, and hence we need to prove that (i) implies $\xi_{1,\alpha_{1,1},\alpha_{1,2}} = \xi_{2,\alpha_{2,1},\alpha_{2,2}}$ a.e. First we note that $\xi_{j,\alpha_{j,1},\alpha_{j,2}}(\lambda)$, being Krein's spectral shift function for the pair $(H_{+,j,\alpha_{j,2}}, H_{+,j,\alpha_{j,1}})$, $j = 1, 2$, increases (decreases) by 1 whenever λ passes an eigenvalue of $H_{+,j,\alpha_{j,1}}$ $(H_{+,j,\alpha_{j,2}})$ as λ increases from $-\infty$ to $+\infty$, and stays constant otherwise. (We recall that $\sigma(H_{+,\alpha})$ is simple.) This step-function behavior, together with $0 \leq \xi_{j,\alpha_{j,1},\alpha_{j,2}} \leq 1$ a.e., indeed yields $\xi_{1,\alpha_{1,1},\alpha_{1,2}} = \xi_{2,\alpha_{2,1},\alpha_{2,2}}$ a.e. and one can apply Theorem 2.4. □

Roughly speaking, Corollary 2.5 says that two sets of purely discrete spectra $\sigma(H_{+,\alpha_1}), \sigma(H_{+,\alpha_2})$ associated with distinct boundary conditions at $x = 0$ (but a fixed boundary condition (if any) at $+\infty$), that is, $\sin(\alpha_2 - \alpha_1) \neq 0$, uniquely determine V a.e. Our main result, Theorem 2.4, removes all a priori spectral hypotheses and shows that Krein's spectral shift function $\xi_{\alpha_1,\alpha_2}(\lambda)$ for the pair $(H_{+,\alpha_2}, H_{+,\alpha_1})$ with distinct boundary conditions at $x = 0$, $\sin(\alpha_2 - \alpha_1) \neq 0$, uniquely determines V a.e. This illustrates that Theorem 2.4 is the natural generalization of Borg's and Marchenko's theorem from the discrete spectrum case to arbitrary spectral types.

Finally, we give a simple application of Theorem 2.4 in the context of three-dimensional Schrödinger operators with spherically symmetric potentials.

Assuming hypothesis (2.1) for V, we introduce the potential

$$v(x) = V(|x|), \quad x \in \mathbb{R}^3, \tag{2.32}$$

and define the self-adjoint Schrödinger operator h in $L^2(\mathbb{R}^3)$ associated with the differential expression $-\Delta + v(x)$ by decomposition with respect to angular momenta, which represents h as an infinite direct sum of half-line operators in $L^2(\mathbb{R}_+; r^2\,dr)$ associated with differential expressions of the type

$$\widehat{\tau}_{+,\ell} = -\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + \frac{\ell(\ell+1)}{r^2} + V(r), \quad r = |x| > 0, \ell \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}. \tag{2.33}$$

A simple unitary transformation reduces (2.33) to

$$\tau_{+,\ell} = -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + V(r) \tag{2.34}$$

and associated Hilbert space $L^2(\mathbb{R}_+)$ (see, e.g., [37], Appendix to Sect. X.1).

Next, let $g(z, x, x')$, $x \neq x'$, denote the Green's function of h (i.e., the integral kernel of $(h-z)^{-1}$) and define another self-adjoint operator h_β in $L^2(\mathbb{R}^3)$ by

$$\begin{aligned} (h_\beta - z)^{-1} = (h-z)^{-1} + D_\beta(z)^{-1}(\overline{g(z,0,\cdot\,)}\,,\,\cdot\,)g(z,\,\cdot\,,0), \\ \beta \in \mathbb{R}, z \in \mathbb{C}\backslash\{\sigma(h_\beta) \cup \sigma(h)\}, \end{aligned} \tag{2.35}$$

where

$$D_\beta(z) = \beta - \lim_{|\epsilon|\downarrow 0}\,[g(z,0,\epsilon) - (4\pi|\epsilon|)^{-1}], \qquad z \in \mathbb{C}\backslash\sigma(h). \tag{2.36}$$

As shown, for example, in [1],[41], h_β models h plus an additional point (delta) interaction centered at $x = 0$ whose strength is parametrized by $\beta \in \mathbb{R}$. (Clearly, $h_\infty = h$.) The function $D_\beta(z)$ is Herglotz, and one computes (see [14])

$$\mathrm{Tr}[(h_\beta - z)^{-1} - (h-z)^{-1}] = -\frac{d}{dz}\ln[D_\beta(z)]. \tag{2.37}$$

This then allows one to define Krein's spectral shift function $\xi_\beta(\lambda)$ for the pair (h_β, h) by

$$\xi_\beta(\lambda) = \lim_{\epsilon\downarrow 0}\,\pi^{-1}\mathrm{Im}\{\ln[D_\beta(\lambda + i\epsilon)]\} \text{ a.e.}, \tag{2.38}$$

which yields

$$\mathrm{Tr}[(h_\beta - z)^{-1} - (h-z)^{-1}] = -\int_{\mathbb{R}} (\lambda - z)^{-2}\xi_\beta(\lambda)\,d\lambda. \tag{2.39}$$

Our uniqueness result for three-dimensional Schrödinger operators then reads as follows.

Theorem 2.6. *Define h_j, h_{j,β_j}, $\beta_j \in \mathbb{R}$, associated with $-\Delta + v_j(x)$, $x \in \mathbb{R}^3$, $j = 1, 2$, and introduce Krein's spectral shift function $\xi_{j,\beta_j}(\lambda)$ for the pair (h_{j,β_j}, h_j), $j = 1, 2$. Then the following are equivalent:*

(i) *$\xi_{1,\beta_1}(\lambda) = \xi_{2,\beta_2}(\lambda)$ for a.e. $\lambda \in \mathbb{R}$.*

(ii) *$\beta_1 = \beta_2$ and $v_1(x) = v_2(x)$ for a.e. $x \in \mathbb{R}^3$.*

Proof. Since $\tau_{+,\ell}$ is l.p. at $r = 0$ for all $\ell = \mathbb{N}$, the whole problem can be reduced to the angular momentum sector $\ell = 0$. For $\ell = 0$, however, h corresponds to $H_{+,\infty}$ and h_β to $H_{+,\alpha}$, $\beta = \cot(\alpha)$, in the notation of (A.14). In particular, $\xi_\beta(\lambda)$ introduced in (2.38) corresponds to $\xi_{0,\alpha}(\lambda)$ in our notation (2.8). Hence, an application of Theorem 2.4 completes the proof. □

An analogous result could be derived for two-dimensional Schrödinger operators with centrally symmetric potentials. Since this requires the replacement of $\tau_+ = -\frac{d^2}{dx^2} + V(x)$, $x \geq 0$, by

$$\tau_+ = -\frac{d^2}{dx^2} - \frac{1}{4x^2} + V(x), \quad x > 0, \tag{2.40}$$

a differential expression singular at $x = 0$, we omit further details at this point.

3. Schrödinger operators on $\mathbb{R}$

This section explores uniqueness results for Schrödinger operators on the whole real line.

As in Section 2, we shall rely on the notation introduced in Appendix A and hence recall τ, H, ϕ_α, θ_α, $\psi_{\pm,\alpha}$, $m_{\pm,\alpha}$, $d\rho_{\pm,\alpha}$, and $G(z,x,x')$ as introduced in (A.29)–(A.47). In particular, we shall assume hypothesis (A.28), that is,

$$V \in L^1_{\text{loc}}(\mathbb{R}), \quad V \text{ real-valued} \tag{3.1}$$

throughout this section. Following [20], we introduce, in addition, the following family of self-adjoint operators H_y^β in $L^2(\mathbb{R})$,

$$\begin{gathered} H_y^\beta f = \tau f, \qquad \beta \in \mathbb{R} \cup \{\infty\}, \quad y \in \mathbb{R}, \\ \mathcal{D}(H_y^\beta) = \{g \in L^2(\mathbb{R} \mid g, g' \in AC([y, \pm R]) \text{ for all } R > 0;\, g'(y_\pm) + \beta g(y_\pm) = 0; \\ \lim_{R\to\pm\infty} W(f_\pm(z_\pm), g)(R) = 0;\, \tau g \in L^2(\mathbb{R})\}. \end{gathered} \tag{3.2}$$

Thus $H_y^D := H_y^\infty (H_y^N := H_y^0)$ corresponds to the Schrödinger operator with an additional Dirichlet (Neumann) boundary condition at y. In obvious notation, H_y^β decomposes into the direct sum of half-line operators

$$H_y^\beta = H_{-,y}^\beta \oplus H_{+,y}^\beta \tag{3.3}$$

with respect to

$$L^2(\mathbb{R}) = L^2((-\infty, y]) \oplus L^2([y, \infty)). \tag{3.4}$$

In particular, $H_{+,y}^\beta$ equals $H_{+,\alpha}$ for $\beta = \cot(\alpha)$ and $y = 0$ in our notation (A.14), and, as indicated at the end of Appendix A, our (variable) reference point $x = y$ will be added as a subscript to obtain $\theta_{\alpha,y}(z,x)$, $\phi_{\alpha,y}(z,x)$, $\psi_{\pm,\alpha,y}(z,x)$, $m_{\pm,\alpha,y}(z)$, $M_{\alpha,y}(z)$, etc. H and H_y^β, defined in terms of separated boundary conditions, are real operators. Moreover, as observed in Appendix A, the point spectrum of H is simple.

Next, we recall a few results from [20]. With $G(z,x,x')$ and $G_y^\beta(z,x,x')$ the Green's functions of H and H_y^β, one obtains

$$G_y^\beta(z,x,x') = G(z,x,x') - \frac{(\beta+\partial_2)G(z,x,y)(\beta+\partial_1)G(z,y,x')}{(\beta+\partial_1)(\beta+\partial_2)G(z,y,y)}, \quad \beta\in\mathbb{R}, z\in\mathbb{C}\backslash\{\sigma(H_y^\beta)\cup\sigma(H)\}, \tag{3.5}$$

$$G_y^\infty(z,x,x') = G(z,x,x') - G(z,y,y)^{-1}G(z,x,y)G(z,y,x'), \quad z\in\mathbb{C}\backslash\{\sigma(H_y^\infty)\cup\sigma(H)\}. \tag{3.6}$$

Here

$$\partial_1 G(z,y,x') := \partial_x G(z,x,x')\big|_{x=y}, \quad \partial_2 G(z,x,y) := \partial_{x'} G(z,x,x')\big|_{x'=y}, \quad \partial_1\partial_2 G(z,y,y) := \partial_x\partial_{x'} G(z,x,x')\big|_{x=y=x'}, \quad \text{etc.} \tag{3.7}$$

and

$$\partial_1 G(z,y,x) = \partial_2 G(z,x,y), \quad x\neq y. \tag{3.8}$$

As a consequence,

$$\operatorname{Tr}[(H_y^\beta - z)^{-1} - (H-z)^{-1}] = -\frac{d}{dz}\ln[(\beta+\partial_1)(\beta+\partial_2)G(z,y,y)], \quad \beta\in\mathbb{R}, \tag{3.9}$$

$$\operatorname{Tr}[(H_y^\infty - z)^{-1} - (H-z)^{-1}] = -\frac{d}{dz}\ln[G(z,y,y)]. \tag{3.10}$$

In analogy to $G(z,y,y)$ (cf. (A.47)), also

$$(\beta+\partial_1)(\beta+\partial_2)G(z,y,y) \text{ is Herglotz} \tag{3.11}$$

for each $y\in\mathbb{R}$. Hence, both admit exponential representations of the form

$$G(z,y,y) = \exp\biggl\{c_\infty(y) + \int_{\mathbb{R}} \biggl[\frac{1}{\lambda-z} - \frac{\lambda}{1+\lambda^2}\biggr]\xi^\infty(\lambda,y)\,d\lambda\biggr\}, \tag{3.12}$$

$$c_\infty(y)\in\mathbb{R}, \quad 0\le\xi^\infty(\lambda,y)\le 1 \text{ a.e.}, \tag{3.13}$$

$$\xi^\infty(\lambda,y) = \lim_{\epsilon\downarrow 0}\pi^{-1}\operatorname{Im}\{\ln[G(\lambda+i\epsilon,y,y)]\} \quad \text{for a.e. } \lambda\in\mathbb{R}, \tag{3.14}$$

$$(\beta+\partial_1)(\beta+\partial_2)G(z,y,y) = \exp\biggl\{c_\beta(y) + \int_{\mathbb{R}} \biggl[\frac{1}{\lambda-z} - \frac{\lambda}{1+\lambda^2}\biggr][\xi^\beta(\lambda,y)+1]\,d\lambda\biggr\}, \quad \beta\in\mathbb{R}, \tag{3.15}$$

$$c_\beta(y) \in \mathbb{R}, \quad -1 \le \xi^\beta(\lambda, y) \le 0 \text{ a.e.}, \quad \beta \in \mathbb{R}, \tag{3.16}$$

$$\xi^\beta(\lambda, y) = \lim_{\epsilon \downarrow 0} \pi^{-1} \mathrm{Im}\{\ln[(\beta + \partial_1)(\beta + \partial_2) G(\lambda + i\epsilon, y, y)]\} - 1, \quad \beta \in \mathbb{R}, \tag{3.17}$$

for each $y \in \mathbb{R}$. Moreover,

$$\mathrm{Tr}[(H_y^\beta - z)^{-1} - (H - z)^{-1}] = -\int_{\mathbb{R}} (\lambda - z)^{-2} \xi^\beta(\lambda, y)\, d\lambda, \quad \beta \in \mathbb{R} \cup \{\infty\}. \tag{3.18}$$

(Strictly speaking, the results (3.5)–(3.18) have been derived in [20] assuming τ to be in the l.p. case at $\pm\infty$. However, these results extend to our present setting without effort.)

For later purpose, we also note the identities (for each $y \in \mathbb{R}$),

$$G(z, y, y) = M_{0,y,2,2}(z) = [m_{-,0,y}(z) - m_{+,0,y}(z)]^{-1}, \tag{3.19}$$

$$\sin^2(\alpha)(\beta + \partial_1)(\beta + \partial_2) G(z, y, y) = M_{\alpha,y,2,2}(z) = [m_{-,\alpha,y}(z) - m_{+,\alpha,y}(z)]^{-1}, \quad \beta = \cot(\alpha), \alpha \in (0, \pi), \tag{3.20}$$

and especially

$$\begin{aligned} &m_{+,\alpha_2,y}(z)^2 + \{[m_{-,\alpha_2,y}(z) - m_{+,\alpha_2,y}(z)] + 2\cot(\alpha_1 - \alpha_2)\} m_{+,\alpha_2,y}(z) \\ &\quad + \cot^2(\alpha_1 - \alpha_2) + [m_{-,\alpha_2,y}(z) - m_{+,\alpha_2,y}(z)] \cot(\alpha_1 - \alpha_2) \\ &\quad - [\sin(\alpha_1 - \alpha_2)]^{-2} [m_{-,\alpha_2,y}(z) - m_{+,\alpha_2,y}(z)][m_{-,\alpha_1,y}(z) - m_{+,\alpha_1,y}(z)]^{-1} = 0, \\ &\qquad \alpha_1 \ne \alpha_2, z \in \mathbb{C}\backslash\mathbb{R}, \end{aligned} \tag{3.21}$$

following directly from (A.38).

As a consequence of Theorem 2.1, the basic uniqueness criterion for Schrödinger operators on $\mathbb{R}$ reads as follows.

Theorem 3.1. *Suppose $\alpha_1, \alpha_2 \in [0, \pi)$, $\alpha_1 \ne \alpha_2$, and assume V_j, $j = 1, 2$, satisfy hypothesis* (3.1). *Define H_j, $m_{\pm,j,\alpha_j,y}(z), M_{j,\alpha_j,y}(z)$ associated with $\tau_j = -\frac{d^2}{dx^2} + V_j(x)$, $x \in \mathbb{R}$, $j = 1, 2$. Then the following are equivalent:*

(i) *$m_{+,1,\alpha_1,y}(z) = m_{+,2,\alpha_2,y}(z)$, $m_{-,1,\alpha_1,y}(z) = m_{-,2,\alpha_2,y}(z)$, $z \in \mathbb{C}_+$.*
(ii) *$M_{1,\alpha_1,y}(z) = M_{2,\alpha_2,y}(z)$, $z \in \mathbb{C}_+$.*
(iii) *$\alpha_1 = \alpha_2$ and $V_1(x) = V_2(x)$ for a.e. $x \in \mathbb{R}$.*

The following is our principal characterization result for Schrödinger operators on $\mathbb{R}$.

Theorem 3.2. *Let $\beta_1, \beta_2 \in \mathbb{R} \cup \{\infty\}$, $\beta_1 \ne \beta_2$, and $x_0 \in \mathbb{R}$.*

(i) *$\xi^{\beta_1}(\lambda, x_0)$ and $\xi^{\beta_2}(\lambda, x_0)$ for a.e. $\lambda \in \mathbb{R}$ uniquely determine $V(x)$ for a.e. $x \in \mathbb{R}$ if the pair (β_1, β_2) differs from $(0, \infty)$, $(\infty, 0)$.*
(ii) *If $(\beta_1, \beta_2) = (0, \infty)$ or $(\infty, 0)$, assume in addition that τ is in the limit point case at $+\infty$ and $-\infty$. Then $\xi^\infty(\lambda, x_0)$ and $\xi^0(\lambda, x_0)$ for a.e. $\lambda \in \mathbb{R}$ uniquely determine V a.e. up to reflection symmetry with respect to x_0; that is, both $V(x)$, $V(2x_0 - x)$ for a.e. $x \in \mathbb{R}$ correspond to $\xi^\infty(\lambda, x_0)$ and $\xi^0(\lambda, x_0)$ for a.e. $\lambda \in \mathbb{R}$.*

Proof. (i) Identifying x_0 and y in (3.21), one can solve for $m_{+,\alpha_2,y}(z)$ to obtain

(3.22)
$$\begin{aligned} m_{+,\alpha_2,x_0}(z) = &-\frac{1}{2}[m_{-,\alpha_2,x_0}(z) - m_{+,\alpha_2,x_0}(z)] - \cot(\alpha_1-\alpha_2) \\ &\pm \bigg\{ \frac{1}{4}[m_{-,\alpha_2,x_0}(z) - m_{+,\alpha_2,x_0}(z)]^2 \\ &+ \frac{1}{\sin^2(\alpha_1-\alpha_2)} \frac{[m_{-,\alpha_2,x_0}(z) - m_{+,\alpha_2,x_0}(z)]}{[m_{-,\alpha_1,x_0}(z) - m_{+,\alpha_1,x_0}(z)]} \bigg\}^{1/2}, \qquad z \in \mathbb{C}\backslash\mathbb{R}. \end{aligned}$$

By (3.12), (3.15), (3.19), and (3.20), $[m_{-,\alpha_j,x_0}(z) - m_{+,\alpha_j,x_0}(z)]$ are both determined by $\xi^{\beta_j}(\lambda, x_0)$, $\beta_j = \cot(\alpha_j)$, $j = 1, 2$, respectively and hence the right-hand-side of (3.22) is determined up to the $+/-$ ambiguity. In order to resolve that ambiguity, we now consider the following case distinction:

a) $\alpha_j \in (0, \pi)$ (i.e., $\beta_j \in \mathbb{R}$), $j = 1, 2$. Then by (A.39),

$$m_{\pm,\alpha_2,x_0}(z) \underset{z\to i\infty}{=} \cot(\alpha_2) + o(z^{-1/2}), \tag{3.23}$$

which inserted into (3.22) results in
(3.24)
$$m_{+,\alpha_2,x_0}(z) \underset{z\to i\infty}{=} \cot(\alpha_2-\alpha_1) + o(z^{-1/2}) \pm \left\{ \frac{\sin^2(\alpha_1)}{\sin^2(\alpha_1-\alpha_2)\sin^2(\alpha_2)} + O(z^{-1}) \right\}^{1/2}.$$

A comparison of (3.23) and (3.24) reveals that only one choice of the sign (the $+$ sign, choosing the branch of $\sqrt{\cdot}$ such that $\sqrt{x} > 0$ for $x > 0$) in (3.24) can be compatible with the leading behavior $\cot(\alpha_2)$ in (3.23). This resolves the sign ambiguity in (3.24) and hence in (3.22), and thus determines $m_{+,\alpha_2,x_0}(z)$. Since $\xi^{\beta_2}(\lambda, x_0)$ determines $[m_{-,\alpha_2,x_0}(z) - m_{+,\alpha_2,x_0}(z)]$, $m_{-,\alpha_2,x_0}(z)$ is also determined. Thus, both Weyl m-functions $m_{\pm,\alpha_2,x_0}(z)$ are known, and this in turn determines V a.e. by Theorem 3.1.

b) $\alpha_2 = 0$ (i.e., $\beta_2 = \infty$), $\alpha_1 \neq \pi/2$ (i.e., $\beta_1 \neq 0$). Then by (A.40),

$$m_{\pm,0,x_0}(z) \underset{z\to i\infty}{=} \pm i z^{1/2} + o(1), \tag{3.25}$$

which inserted into (3.22) yields

$$m_{+,0,x_0}(z) \underset{z\to i\infty}{=} i z^{1/2} - \cot(\alpha_1) + o(1) \pm \{O(1)\}^{1/2}. \tag{3.26}$$

Since by (3.25) the $\{O(1)\}^{1/2}$-term must cancel $-\cot(\alpha_1)$, this again resolves the sign ambiguity in (3.26) (once more the $+$ sign turns out to be the right one) and hence in (3.22). Thus, $m_{+,0,x_0}(z)$ is determined. Since $\xi^{\infty}(\lambda, x_0)$ determines $[m_{-,0,x_0}(z) - m_{+,0,x_0}(z)]$, also $m_{-,0,x_0}(z)$ and hence V is determined a.e. as in part a).

(ii) In the exceptional case where $(\beta_1, \beta_2) = (0, \infty)$, $(\infty, 0)$, the exchange

$$V(x) \to V(2x_0 - x) \text{ implies } m_{\pm,0,x_0}(z) \to -m_{\mp,0,x_0}(z), \tag{3.27}$$

since we assumed the l.p. case at $\pm\infty$. This substitution leaves

$$[m_{-,0,x_0}(z) - m_{+,0,x_0}(z)]^{-1} = G(z, x_0, x_0) \tag{3.28}$$

and

$$\begin{aligned} m_{-,0,x_0}(z)m_{+,0,x_0}(z)[m_{-,0,x_0}(z) - m_{+,0,x_0}(z)]^{-1} \\ = [m_{-,\pi/2,x_0}(z) - m_{+,\pi/2,x_0}(z)]^{-1} = \partial_1\partial_2 G(z, x_0, x_0), \end{aligned} \tag{3.29}$$

and hence $\xi^{\infty}(\lambda, x_0)$ and $\xi^0(\lambda, x_0)$ invariant (cf. (3.19) and (3.20)). (Here we used that $m_{\pm,\pi/2,x_0}(z) = -[m_{\pm,0,x_0}(z)]^{-1}$, see (A.38).) □

Corollary 3.3. *Suppose τ is in the limit point case at $+\infty$ and $-\infty$, and let $\beta \in \mathbb{R} \cup \{\infty\}$ and $x_0 \in \mathbb{R}$. Then $\xi^{\beta}(\lambda, x_0)$ for a.e. $\lambda \in \mathbb{R}$ uniquely determines $V(x)$ for a.e. $x \in \mathbb{R}$ if and only if V is reflection symmetric with respect to x_0, that is, $V(2x_0 - x) = V(x)$ a.e.*

Proof. First suppose that $V(2x_0 - x) = V(x)$ a.e. Then (A.38) yields

$$m_{-,\alpha,x_0}(z) = -m_{+,\pi-\alpha,x_0}(z), \quad \alpha \in [0, \pi). \tag{3.30}$$

If $\beta \in \mathbb{R}\backslash\{0\}$ (i.e., $\alpha \in (0, \pi)\backslash\{\pi/2\}$, $\beta = \cot(\alpha)$), then (3.30) implies

$$[m_{-,\alpha,x_0}(z) - m_{+,\alpha,x_0}(z)]^{-1} = [m_{-,\pi-\alpha,x_0}(z) - m_{+,\pi-\alpha,x_0}(z)]^{-1}. \tag{3.31}$$

By (3.15), this yields $\xi^{\beta}(\lambda, x_0) = \xi^{-\beta}(\lambda, x_0)$ a.e., and hence V is uniquely determined a.e. by Theorem 3.2. On the other hand, if $\beta = \infty$ or 0 (i.e., $\alpha = 0$ or $\pi/2$), then (3.30) yields

$$m_{-,0,x_0}(z) = -m_{+,0,x_0}(z) \quad \text{or} \quad m_{-,\pi/2,x_0}(z) = -m_{+,\pi/2,x_0}(z). \tag{3.32}$$

This determines $m_{\pm,0,x_0}(z)$ or $m_{\pm,\pi/2,x_0}(z)$ and hence V a.e. by Theorem 3.1.

Conversely, suppose V is not reflection symmetric with respect to x_0. Define $\widehat{V}(x) = V(2x_0 - x)$ a.e. and denote by $\widehat{m}_{\pm,\alpha,x_0}(z_0)$, $\widehat{M}_{\alpha,x_0}(z)$, and $\widehat{\xi}^{\beta}(\lambda, x_0)$ the corresponding quantities associated with $\widehat{V}$. Then

$$\widehat{m}_{\pm,\pi-\alpha,x_0}(z) = -m_{\mp,\alpha,x_0}(z), \quad \alpha \in [0, \pi) \tag{3.33}$$

(identifying $\alpha = 0$ and π), and hence

$$\widehat{M}_{\pi-\alpha,x_0}(z) = \begin{pmatrix} M_{\alpha,x_0,1,1}(z) & -M_{\alpha,x_0,1,2}(z) \\ -M_{\alpha,x_0,2,1}(z) & M_{\alpha,x_0,2,2}(z) \end{pmatrix} \neq M_{\alpha,x_0}(z) \tag{3.34}$$

since $m_{-,\alpha,x_0}(z) \neq -m_{+,\alpha,x_0}(z)$ for all $\alpha \in [0, \pi)$. (The latter fact is obvious from the asymptotic behavior (A.39) for $\alpha \in (0, \pi)\backslash\{\pi/2\}$, and also follows from our hypothesis that V is not reflection symmetric w.r.t. x_0 for $\alpha = 0, \pi/2$. Alternatively, it also follows from our hypothesis and Theorem 3.1.) (3.34), however, shows that $\xi^{\beta}(\lambda, x_0) = \widehat{\xi}^{-\beta}(\lambda, x_0)$ is common to V and $\widehat{V} \neq V$. □

In view of Corollary 2.5, it seems appropriate to formulate Theorem 3.2 in the special case of purely discrete spectra.

Corollary 3.4. *Suppose H (and hence H_y^β for all $y \in \mathbb{R}$, $\beta \in \mathbb{R} \cup \{\infty\}$) has purely discrete spectrum, that is, $\sigma_{\text{ess}}(H) = \emptyset$, and let $\beta_1, \beta_2 \in \mathbb{R} \cup \{\infty\}$, $\beta_1 \neq \beta_2$, and $x_0 \in \mathbb{R}$.*

(i) *$\sigma(H)$, $\sigma(H_{x_0}^{\beta_j})$, $j = 1, 2$, uniquely determine V a.e. if the pair (β_1, β_2) differs from $(0, \infty)$ and $(\infty, 0)$.*

(ii) *If $(\beta_1, \beta_2) = (0, \infty)$ or $(\infty, 0)$, assume in addition that τ is in the limit point case at $+\infty$ and $-\infty$. Then $\sigma(H)$, $\sigma(H_{x_0}^\infty)$, and $\sigma(H_{x_0}^0)$ uniquely determine V a.e. up to reflection symmetry with respect to x_0, that is, both $V(x)$ and $\widehat{V}(x) = V(2x_0 - x)$ for a.e. $x \in \mathbb{R}$ correspond to $\sigma(H) = \sigma(\widehat{H})$, $\sigma(H_{x_0}^\infty) = \sigma(\widehat{H}_{x_0}^\infty)$, and $\sigma(H_{x_0}^0) = \sigma(\widehat{H}_{x_0}^0)$. Here, in obvious notation, $\widehat{H}$, $\widehat{H}_{x_0}^\infty$, $\widehat{H}_{x_0}^0$ correspond to $\widehat{\tau} = -\frac{d^2}{dx^2} + \widehat{V}(x)$, $x \in \mathbb{R}$.*

(iii) *Suppose τ is in the limit point case at $+\infty$ and $-\infty$, and let $\beta \in \mathbb{R} \cup \{\infty\}$. Then $\sigma(H)$ and $\sigma(H_{x_0}^\beta)$ uniquely determine V a.e. if and only if V is reflection symmetric with respect to x_0.*

(iv) *Suppose that V is reflection symmetric with respect to x_0 and τ is non-oscillatory at $+\infty$ and $-\infty$. Then V is uniquely determined a.e. by $\sigma(H)$ in the sense that V is the only potential symmetric with respect to x_0 with spectrum $\sigma(H)$.*

Proof. (i) We denote $\sigma(H) = \{e_n\}_{n \in J_0}$, $\sigma(H_{x_0}^\beta) = \{\lambda_n^\beta(x_0)\}_{n \in I^\beta}$, where $I^\beta = J_0$, $\beta \in \mathbb{R}$, and $I^\infty = J$, with $J_0 = \mathbb{N}_0$ or $\mathbb{Z}$ and $J = \mathbb{N}$ or $\mathbb{Z}$ depending on whether or not H is bounded from below. Moreover, we use the ordering $e_n < e_{n+1}$, $\lambda_n^\beta(x_0) \leq \lambda_{n+1}^\beta(x_0)$. By general principles,

$$\begin{aligned} &\lambda_0^\beta(x_0) \leq e_0, \quad \beta \in \mathbb{R} \text{ if } H \text{ is bounded from below,} \\ &\qquad e_n \leq \lambda_n^\beta(x_0) \leq e_{n+1}, \quad \beta \in \mathbb{R} \cup \{\infty\}. \end{aligned} \tag{3.35}$$

By hypothesis, $\xi^\beta(\lambda, x_0)$, $\beta \in \mathbb{R} \cup \{\infty\}$, is a pure step function which jumps by $+1$ at every (necessarily simple) eigenvalue of H (since $\psi_{+,\alpha,x_0}(e_m, x)$ and $\psi_{-,\tilde{\alpha},x_0}(e_m, x)$ for $e_m \in \sigma(H)$, $\alpha, \tilde{\alpha} \in [0, \pi)$, are unique up to constant multiples). Similarly, $\xi^\beta(\lambda, x_0)$ jumps by $-m(\lambda_n^\beta(x_0))$ ($m(\lambda)$ denotes the multiplicity of an eigenvalue λ) at any eigenvalue of $H_{x_0}^\beta$. As long as all multiplicities involved are equal to one, that is,

$$m(\lambda_n^{\beta_j}(x_0)) = 1, \quad n \in I^{\beta_j}, \tag{3.36}$$

$\sigma(H)$, $\sigma(H_{x_0}^{\beta_1})$, and $\sigma(H_{x_0}^{\beta_2})$ clearly determine $\xi^{\beta_j}(\lambda, x_0)$, $j = 1, 2$. The case where some eigenvalues of $H_{x_0}^{\beta_j}$ are degenerate needs a bit more care. Assume, for example,

$$\lambda_{m_0}^{\beta_1}(x_0) = \lambda_{m_0+1}^{\beta_1}(x_0) := e_{m_0}, \quad \text{i.e., } m(e_{m_0}) = 2 \tag{3.37}$$

for some $m_0 \in I^{\beta_1}$. Since half-line spectra are necessarily simple, (3.37) implies that $H_{+,x_0}^{\beta_1}$ and $H_{-,x_0}^{\beta_1}$, the corresponding half-line operators in $L^2((x_0, \pm\infty))$ (cf. (3.3), (3.4)) associated with $H_{x_0}^{\beta_1}$, have the same simple eigenvalue e_{m_0}. As a consequence, H itself has e_{m_0} as a (simple) eigenvalue, that is, $e_{m_0} \in \sigma(H)$. Thus, $\xi^{\beta_1}(\lambda, x_0)$ jumps by $-2 + 1 = -1$ at $\lambda_{m_0}^{\beta_1}(x_0)$ and stays -1 until $e_{m_0+1} \in \sigma(H)$.

Similarly, suppose $\lambda_{m_0}^{\beta_1}(x_0) = e_{m_0-1}$ for some $m_0 \in I^{\beta_1}$ and let $\psi_{+,\alpha_1,x_0}(e_{m_0}, x) = \text{const.}\psi_{-,\alpha_1,x_0}(e_{m_0-1}, x)$, $\beta_1 = \cot(\alpha_1)$, be the unique eigenfunction of H associated with e_{m_0-1}. Then also $\lambda_{m_0-1}^{\beta_1}(x_0) = e_{m_0-1}$, since the restrictions of

$\psi_{\pm,\alpha_1,x_0}(e_{m_0-1},x)$ to $x \le x_0$ and $x \ge x_0$ are eigenfunctions of $H^{\beta_1}_{-,x_0}$ and $H^{\beta_1}_{+,x_0}$, respectively. Hence $\sigma(H)$, $\sigma(H^{\beta_1}_{x_0})$, and $\sigma(H^{\beta_2}_{x_0})$ determine $\xi^{\beta_j}(\lambda,x_0)$, $j=1,2$, and we may apply Theorem 3.2(i).

(ii) now follows from Theorem 3.2(ii), and (iii) is clear from Corollary 3.3. (iv) is a consequence of (iii), the fact that τ being non-oscillatory at $\pm\infty$ implies the l.p. case at $\pm\infty$, and the ordering

$$\begin{aligned} \lambda^0_0(x_0) = e_0, \quad \lambda^\infty_{2m+1}(x_0) = e_{2m+1} = \lambda^\infty_{2m+2}(x_0),\\ \lambda^0_{2m+1}(x_0) = e_{2m+2} = \lambda^0_{2m+2}(x_0), \quad m \in \mathbb{N}_0. \qquad \square \end{aligned} \tag{3.38}$$

We emphasize that Corollary 3.4(iii) is, of course, implied by the result of Borg [5] and Marchenko [32] (see Corollary 2.5 with $\alpha_1 = 0$, $\alpha_2 = \pi/2$).

So far, we have exclusively dealt with ξ-functions and spectra in connection with uniqueness theorems. A variety of further uniqueness results can be obtained by invoking alternative information such as the left/right distribution of $\lambda^\beta_n(x_0)$ (i.e., whether $\lambda^\beta_n(x_0)$ is an eigenvalue of H^β_{-,x_0} in $L^2((-\infty,x_0])$ or of H^β_{+,x_0} in $L^2([x_0,\infty))$) and/or associated norming constants. For brevity we concentrate on only one such case, the Dirichlet boundary condition $\beta=\infty$.

We start by introducing *Dirichlet data* instead of merely Dirichlet eigenvalues. For notational convenience we now denote the Dirichlet eigenvalues $\lambda^\infty_n(x_0)$ by

$$\mu_n(x_0), \quad n \in J, \tag{3.39}$$

with $J \subseteq \mathbb{N}$ or $\mathbb{Z}$ an appropriate index set. Let $(a,b) \subseteq \mathbb{R}\backslash\sigma(H)$ be a spectral gap of H and assume $\mu_n(x_0) \in (a,b)$. The corresponding Dirichlet datum is then defined by

$$(\mu_n(x_0), \sigma_n(x_0)), \quad \sigma_n(x_0) \in \{-,+\}, \tag{3.40}$$

where $\sigma_n(x_0) = -/+$ records whether $\mu_n(x_0)$ is a left/right Dirichlet eigenvalue (i.e., an eigenvalue of H^∞_{-,x_0}, respectively H^∞_{+,x_0}).

A combination of ξ-functions and Dirichlet data allows one to rephrase the celebrated uniqueness theorem of Borg [4] for periodic potentials as follows. Assume in addition to hypothesis (3.1) that V is periodic with period $\Omega > 0$. Then Floquet theory yields that the spectra of H and $H^\infty_{x_0}$ are of the type

$$\sigma(H) = \bigcup_{n\in\mathbb{N}} [E_{2(n-1)}, E_{2n-1}], \quad E_0 < E_1 \le E_2 < E_3 \le \cdots, \tag{3.41}$$

$$\sigma(H^\infty_{x_0}) = \sigma(H) \cup \{\mu_n(x_0)\}_{n\in\mathbb{N}}, \quad E_{2n-1} \le \mu_n(x_0) \le E_{2n}, n \in \mathbb{N}. \tag{3.42}$$

Let $I(x_0) \subseteq \mathbb{N}$ denote the set of all indices j such that

$$\mu_j(x_0) \notin \{E_n\}_{n\in\mathbb{N}_0} \quad (\text{i.e., } \mu_j(x_0) \notin \sigma(H)). \tag{3.43}$$

Then Borg's result can be rephrased as follows.

Theorem 3.5 (Borg [4], see also [34],[35]). *Let $V \in L^1_{\text{loc}}(\mathbb{R})$ be real-valued and periodic of period $\Omega > 0$. Then $\xi^\infty(\lambda, x_0)$ for a.e. $\lambda \in \mathbb{R}$ and $\sigma_j(x_0)$, $j \in I(x_0)$, uniquely determine V for a.e. $x \in \mathbb{R}$.*

For the proof, it suffices to note that (cf., e.g., [15],[20],[26])

$$\xi^\infty(\lambda, x_0) = \begin{cases} \frac{1}{2}, & \lambda \in (E_{2(n-1)}, E_{2n-1}), n \in \mathbb{N}, \\ 1, & \lambda \in (E_{2n-1}, \mu_n(x_0)), n \in \mathbb{N}, \\ 0, & \lambda \in (-\infty, E_0), (\mu_n(x_0), E_{2n}), n \in \mathbb{N}, \end{cases} \tag{3.44}$$

in connection with the periodic case (3.41), (3.42). This result extends to algebro-geometric quasi-periodic finite-gap potentials and certain classes of almost-periodic potentials; we omit further details at this point.

After this warm-up we turn to a new uniqueness result for operators with purely discrete spectra. Assume

$$\sigma_{\text{ess}}(H) = \emptyset \quad \text{and denote } \sigma(H) = \{e_n\}_{n \in J_0} \tag{3.45}$$

such that

$$\sigma(H^\infty_{x_0}) = \{\mu_n(x_0)\}_{n \in J}, \quad e_{n-1} \le \mu_n(x_0) \le e_n, n \in J, \tag{3.46}$$

where $J_0 = \mathbb{N}_0$ or $\mathbb{Z}$ and $J = \mathbb{N}$ or $\mathbb{Z}$ are appropriate index sets depending on whether or not H is bounded from below.

Next we divide the spectrum of $H^\infty_{x_0}$ into simple and (twice) degenerate Dirichlet eigenvalues, that is, those which are disjoint from $\sigma(H)$ and those which coincide with an element of $\sigma(H)$,

$$\begin{gathered} J = I(x_0) \cup I'(x_0), \quad I(x_0) \cap I'(x_0) = \emptyset, \\ \{\mu_j(x_0)\}_{j \in I(x_0)} \cap \sigma(H) = \emptyset, \quad \{\mu_{j'}(x_0)\}_{j' \in I'(x_0)} \subset \sigma(H) \end{gathered} \tag{3.47}$$

(i.e., $\mu_{j'}(x_0) \in \{e_{j'-1}, e_{j'}\}$ for $j' \in I'(x_0)$). As a last ingredient we need the norming constants associated with the (twice) degenerate Dirichlet eigenvalues $\{\mu_{j'}(x_0)\}_{j' \in I'(x_0)}$ denoted by

$$c_{\pm, j'}(x_0) > 0, \quad j' \in I'(x_0). \tag{3.48}$$

Quite generally, the norming constant $c_{+,n}(x_0) > 0$ (respectively $c_{-,n}(x_0) > 0$) associated with $\mu_n(x_0) \in \sigma(H^\infty_{+,x_0})$ (respectively $\mu_n(x_0) \in \sigma(H^\infty_{-,x_0})$) is given by minus (respectively plus) the residue of the corresponding Weyl m-function $m_{+,0,x_0}(z)$ (respectively $m_{-,0,x_0}(z)$) at $z = \mu_n(x_0)$. Equivalently, one has

$$c_{\pm,n}(x_0) = \|\phi_{0,x_0}(\mu_n(x_0), \cdot\,)\|^{-2}_{L^2(\mathbb{R}_\pm)} \tag{3.49}$$

(cf. (A.37)).

Given these preparations we can state the following result.

Theorem 3.6. *Let $x_0 \in \mathbb{R}$ and suppose H has purely discrete spectrum, that is, $\sigma_{\rm ess}(H) = \emptyset$, $\sigma(H) = \{e_n\}_{n \in J_0}$. Then $\xi^\infty(\lambda, x_0)$ for a.e. $\lambda \in \mathbb{R}$, $\sigma_j(x_0)$, $j \in I(x_0)$, and $c_{+,j'}(x_0)$, $c_{-,j'}(x_0)$, $j' \in I'(x_0)$, uniquely determine V for a.e. $x \in \mathbb{R}$.*

Proof. The step function $\xi^\infty(\lambda, x_0)$ determines the Green's function $G(z, x_0, x_0)$ of H by (3.12), and hence

$$[m_{-,0,x_0}(z) - m_{+,0,x_0}(z)] = G(z, x_0, x_0)^{-1} \tag{3.50}$$

is determined. Since $\sigma_{\rm ess}(H) = \emptyset$, both $m_{\pm,0,x_0}(z)$ are meromorphic (on $\mathbb{C}$) with first-order poles (and zeros) on $\mathbb{R}$. Since by hypothesis we know the left/right distribution of all simple Dirichlet eigenvalues $\{\mu_j(x_0)\}_{j \in I(x_0)}$, we can infer the corresponding residue of $m_{-,0,x_0}(z)$ (respectively $m_{+,0,x_0}(z)$) from the knowledge of $G(z, x_0, x_0)^{-1} = [m_{-,0,x_0}(z) - m_{+,0,x_0}(z)]$. But for the remaining (twice) degenerate Dirichlet eigenvalues $\{\mu_{j'}(x_0)\}_{j' \in I'(x_0)}$ of $H^\infty_{x_0}$, the residue of $m_{\pm,-,x_0}(z)$ at $z = \mu_{j'}(x_0)$, $j' \in I'(x_0)$, equals $\mp c_{\pm,j'}(x_0)$ and hence is known as well. Thus, the principal parts of $m_{\pm,0,x_0}(z)$ are determined. Since the corresponding half-line spectral measures $d\rho_{\pm,0,x_0}(\lambda)$ associated with $H^\infty_{\pm,x_0} = H_{\pm,0,x_0}$ are pure point measures supported on $\sigma(H_{\pm,0,x_0})$ of corresponding mass $c_{\pm,n}(x_0)$, they are completely determined under our hypothesis. But $d\rho_{\pm,0,x_0}(\lambda)$ uniquely determines V a.e. on $[x_0, \pm\infty)$ by Theorem 2.1. □

If in addition V is symmetric with respect to x_0 and τ is in the limit point case at $+\infty$ and $-\infty$, then $I(x_0) = \emptyset$, $I'(x_0) = J$, $m_{+,0,x_0}(z) = -m_{-,0,x_0}(z)$, and hence $\xi^\infty(\lambda, x_0)$ alone uniquely determines V a.e., recovering again the result of Borg [5] and Marchenko [32] recorded in Corollary 3.4(iii).

The reader might want to compare our method of proof of Theorem 3.6 with the inverse spectral approach to confining potentials on the half-line $\mathbb{R}_+$ as presented in [21].

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Appendix A. Herglotz functions and Weyl-Titchmarsh theory

We briefly summarize a few basic facts on Herglotz functions and then recall some of the essential elements of the Weyl-Titchmarsh theory for Schrödinger operators on the half-line $[0, \infty)$ as well as on $\mathbb{R}$ relevant in Sections 2 and 3.

We start with Herglotz functions (also called Pick or Nevanlinna-Pick functions). Denoting $\mathbb{C}_\pm := \{z \in \mathbb{C} \mid \pm\text{Im}(z) > 0\}$, any analytic map $m : \mathbb{C}_+ \to \mathbb{C}_+$ is called Herglotz. One conveniently defines m on $\mathbb{C}_-$ by $m(\bar{z}) = \overline{m(z)}$ for $z \in \mathbb{C}_+$. Herglotz functions admit particular representations (Borel transforms) in terms of certain measures on $\mathbb{R}$. Since this aspect is of fundamental importance in the context of inverse spectral theory of Schrödinger operators, we recall the following classical results of Aronszajn and Donoghue [2].

Theorem A.1 [2]. *Let m be a Herglotz function. Then,*

(i) *There exist a measure $d\rho$ on $\mathbb{R}$ and a real-valued $\xi \in L^1_{\mathrm{loc}}(\mathbb{R})$ such that*

$$m(z) = a + bz + \int_{\mathbb{R}} \left[\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right] d\rho(\lambda) \tag{A.1}$$

$$= \exp\left\{c + \int_{R} \left[\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right] \xi(\lambda)\, d\lambda\right\}, \tag{A.2}$$

where

$$\int_{\mathbb{R}} \frac{d\rho(\lambda)}{1+\lambda^2} < \infty, \quad a = \mathrm{Re}[m(i)], b \geq 0 \tag{A.3}$$

and

$$0 \leq \xi \leq 1 \ \text{a.e.}, \quad c = \mathrm{Re}\{\ln[m(i)]\}. \tag{A.4}$$

(ii) (*Fatou's lemma*)

$$\rho((\lambda, \mu]) = \lim_{\delta \downarrow 0} \lim_{\epsilon \downarrow 0} \pi^{-1} \int_{\lambda+\delta}^{\mu+\delta} d\nu \, \mathrm{Im}[m(\nu + i\epsilon)], \tag{A.5}$$

$$\xi(\lambda) = \lim_{\epsilon \downarrow 0} \pi^{-1} \mathrm{Im}\{\ln[m(\lambda + i\epsilon)]\} \ \text{a.e.} \tag{A.6}$$

(iii) *Let $m, n \in \mathbb{N}$ and $b = 0$. Then*

$$\int_{-\infty}^{0} (1+\lambda^2)^{-1} |\lambda|^m |\xi(\lambda)| \, d\lambda + \int_{0}^{\infty} (1+\lambda^2)^{-1} |\lambda|^n |\xi(\lambda)| \, d\lambda < \infty \tag{A.7}$$

if and only if

$$\begin{gathered} \int_{-\infty}^{0} (1+\lambda^2)^{-1} |\lambda|^m \, d\rho(\lambda) + \int_{0}^{\infty} (1+\lambda^2)^{-1} |\lambda|^n \, d\rho(\lambda) < \infty \\ \text{and} \quad \lim_{z \to i\infty} m(z) = a - \int_{\mathbb{R}} (1+\lambda^2)^{-1} \lambda \, d\rho(\lambda) > 0. \end{gathered} \tag{A.8}$$

(iv)

$$m(z) = 1 + \int_{\mathbb{R}} (\lambda - z)^{-1} \, d\rho(\lambda) \quad \text{with} \int_{\mathbb{R}} d\rho(\lambda) < \infty \tag{A.9}$$

if and only if

$$m(z) = \exp\left[\int_{\mathbb{R}} (\lambda - z)^{-1} \xi(\lambda) \, d\lambda\right] \quad \text{with } 0 \leq \xi \leq 1 \ \text{ a.e. and } \xi \in L^1(\mathbb{R}). \tag{A.10}$$

In this case

$$\int_{\mathbb{R}} d\rho(\lambda) = \int_{\mathbb{R}} \xi(\lambda)\, d\lambda. \tag{A.11}$$

(v) *Any poles and zeros of* m *are simple and located on the real axis, the residues at poles being negative.*

The link between Herglotz functions and rank-one perturbations of self-adjoint operators is developed in detail in [38]. In particular, its universal applicability and unifying aspects in connection with the spectral theory of ordinary differential operators and finite-difference operators are amply illustrated in [16],[25],[38].

Next we turn to Schrödinger operators on the half-line $\mathbb{R}_+ := [0,\infty)$. The following material can be found, for example, in [6],[31], and [36]. Suppose

$$V \in L^1([0,R]) \text{ for all } R>0, \quad V \text{ real-valued} \tag{A.12}$$

and introduce the differential expression

$$\tau_+ = -\frac{d^2}{dx^2} + V(x), \quad x \geq 0. \tag{A.13}$$

Associated with τ_+ we introduce the following self-adjoint operator $H_{+,\alpha}$ in $L^2(\mathbb{R}_+)$. Pick a $z_+ \in \mathbb{C}\backslash\mathbb{R}$ and a solution $f_+(z_+,\,\cdot\,) \in L^2(\mathbb{R}_+)$ of $\tau_+\psi = z_+\psi$ (the existence of such an $f_+(z_+,x)$ is a fundamental result of Weyl's theory), and define

$$\begin{gathered} H_{+,\alpha} f = \tau_+ f, \quad \alpha \in [0,\pi), \\ f \in \mathcal{D}(H_{+,\alpha}) = \{g \in L^2(\mathbb{R}_+) \mid g, g' \in AC([0,R]) \text{ for all } R>0; \\ \sin(\alpha) g'(0_+) + \cos(\alpha) g(0_+) = 0;\ \lim_{R\to\infty} W(f_+(z_+), g)(R) = 0;\ \tau_+ g \in L^2(\mathbb{R}_+)\}. \end{gathered} \tag{A.14}$$

Here $W(f,g)(x) = f(x)g'(x) - f'(x)g(x)$ denotes the Wronskian of f and g and the boundary condition $\lim_{R\to\infty} W(f_+(z_+),g) = 0$ at $x = +\infty$ can be omitted if and only if τ_+ is in the limit point (l.p.) case at $+\infty$, that is, if and only if $f_+(z_+,x)$ is unique (up to constant multiples). If τ_+ is in the limit circle (l.c.) case at $+\infty$, $H_{+,\alpha}$ depends on the choice of $f_+(z_+,x)$ and for definiteness we shall "fix the boundary condition at $+\infty$," that is, always employ the same $f_+(z_+,\,\cdot\,)$ in the definition (A.14) of $H_{+,\alpha}$ for all values of $\alpha \in [0,\pi)$. Due to our choice of (symmetric) separated boundary conditions in (A.14), $H_{+,\alpha}$ is a real operator (i.e., $g \in \mathcal{D}(H_{+,\alpha})$ implies $\bar{g} \in \mathcal{D}(H_{+,\alpha})$ and $H_{+,\alpha}\bar{g} = \overline{(H_{+,\alpha}g)}$), see, for example, [36], Section 6.4, with uniform spectral multiplicity one, cf. [10], Corollary XIII.5.5.

Next we introduce the fundamental system $\phi_\alpha(z,x)$, $\theta_\alpha(z,x)$, $z \in \mathbb{C}$, of solutions of

$$\tau_+\psi(z,x) = z\psi(z,x), \quad x \geq 0, \tag{A.15}$$

satisfying

$$\phi_\alpha(z,0) = -\theta'_\alpha(z,0) = -\sin(\alpha), \quad \phi'_\alpha(x,0) = \theta_\alpha(z,0) = \cos(\alpha) \tag{A.16}$$

such that $W(\theta_\alpha(z), \phi_\alpha(z)) = 1$. Furthermore, let $\psi_{+,\alpha}(z,x)$, $z \in \mathbb{C}\backslash\mathbb{R}$, be the unique solution of (A.15) which satisfies

$$\text{(A.17)} \qquad \begin{gathered} \psi_{+,\alpha}(z,\,\cdot\,) \in L^2(\mathbb{R}_+), \quad \sin(\alpha)\psi'_{+,\alpha}(z,0_+) + \cos(\alpha)\psi_{+,\alpha}(z,0_+) = 1, \\ \lim_{R\to\infty} W(f_+(z_+), \psi_{+,\alpha}(z))(R) = 0, \quad z \in \mathbb{C}\backslash\mathbb{R} \end{gathered}$$

(the latter condition being superfluous, i.e., automatically fulfilled, if τ_+ is l.p. at $+\infty$). Uniqueness of $\psi_{+,\alpha}(z,x)$ is a consequence of Weyl's theory and the fact that we are imposing conditions separately at 0 and ∞ in (A.17); see, for example, [10], Theorem XIII.2.32. $\psi_{+,\alpha}(z,x)$ is of the form

$$\text{(A.18)} \qquad \psi_{+,\alpha}(z,x) = \theta_\alpha(z,x) + m_{+,\alpha}(z)\phi_\alpha(z,x)$$

with $m_{+,\alpha}(z)$ being Weyl's m-function. $m_{+,\alpha}(z)$ is well known to be a Herglotz function (cf. also the comment following (A.27)). To avoid repetitions, we list properties of $m_{+,\alpha}(z)$ a bit later (together with those of $m_{-,\alpha}(z)$). Here we just note that the Herglotz property of $m_{+,\alpha}(z)$ together with the asymptotic behavior (A.39), (A.40) yields the existence of a measure $d\rho_{+,\alpha}$ such that

$$\text{(A.19)} \qquad m_{+,\alpha} = a_{+,\alpha} + \int_{\mathbb{R}} \left[\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right] d\rho_{+,\alpha}(\lambda), \quad \alpha \in [0,\pi),$$

$$\text{(A.20)} \qquad = \cot(\alpha) + \int_{\mathbb{R}} (\lambda - z)^{-1} d\rho_{+,\alpha}(\lambda), \qquad \alpha \in (0,\pi),$$

with

$$\text{(A.21)} \qquad \int_{\mathbb{R}} \frac{d\rho_{+,\alpha}(\lambda)}{1+|\lambda|} \begin{cases} < \infty, & \alpha \in (0,\pi), \\ = \infty, & \alpha = 0. \end{cases}$$

The Green's function $G_{+,\alpha}(z,x,x')$ of $H_{+,\alpha}$ finally reads

$$\text{(A.22)} \qquad \begin{gathered} ((H_{+,\alpha} - z)^{-1} f)(x) = \int_0^\infty dx' G_{+,\alpha}(z,x,x') f(x'), \\ z \in \mathbb{C}\backslash\sigma(H_{+,\alpha}), f \in L^2(\mathbb{R}_+), \end{gathered}$$

$$\text{(A.23)} \qquad G_{+,\alpha}(z,x,x') = \begin{cases} \phi_\alpha(z,x)\psi_{+,\alpha}(z,x'), & 0 \le x \le x', \\ \phi_\alpha(z,x')\psi_{+,\alpha}(z,x), & 0 \le x' \le x, \end{cases}$$

$$\text{(A.24)} \qquad = \int_{\mathbb{R}} (\lambda - z)^{-1} \phi_\alpha(\lambda,x)\phi_\alpha(\lambda,x')\, d\rho_{+,\alpha}(\lambda),$$

where $\sigma(\,\cdot\,)$ denotes the spectrum. In particular, (A.18), (A.23), and (A.24) yield

$$\text{(A.25)} \qquad G_{+,\alpha}(z,0,0) = -\sin(\alpha)[\cos(\alpha) - m_{+,\alpha}(z)\sin(\alpha)], \quad \alpha \in [0,\pi),$$

$$\text{(A.26)} \qquad = \sin^2(\alpha) \int_{\mathbb{R}} (\lambda - z)^{-1}\, d\rho_{+,\alpha}(\lambda), \qquad \alpha \in (0,\pi),$$

and for each $x \geq 0$,

$$G_{+,\alpha}(z,x,x) \text{ is Herglotz.} \tag{A.27}$$

While the latter result is obvious from (A.24) (note we have $\phi_\alpha(\lambda,x) \underset{|\lambda|\to\infty}{=} O(1)$ for $\alpha \in (0,\pi)$ and $\phi_0(\lambda,x) \underset{|\lambda|\to\infty}{=} O(|\lambda|^{-1/2})$ for fixed $x \in \mathbb{R}$), the fact (A.27) is easily proved directly using the first resolvent equation and self-adjointness of $H_{+,\alpha}$. (This statement holds quite generally for the diagonal integral kernel of resolvents of self-adjoint operators in connection with general measure spaces as long as the diagonal kernel is well-defined. In particular, it holds for the diagonal Green's function of finite difference operators.) Together with (A.25) this yields a direct proof that $m_{+,\alpha}(z)$ is Herglotz too.

Finally, we recall a few facts in connection with Schrödinger operators on $\mathbb{R}$. Assuming

$$V \in L^1_{\text{loc}}(\mathbb{R}), \quad V \text{ real-valued,} \tag{A.28}$$

one introduces the differential expression

$$\tau = -\frac{d^2}{dx^2} + V(x), \quad x \in \mathbb{R}, \tag{A.29}$$

and picks $z_\pm \in \mathbb{C}\backslash\mathbb{R}$ and solutions $f_\pm(z_\pm,\,\cdot\,) \in L^2(\mathbb{R}_\pm)$ ($\mathbb{R}_- := (-\infty,0]$) of $\tau\psi(z) = z\psi(z)$ for $z = z_+$, respectively z_-. One then defines a self-adjoint operator H in $L^2(\mathbb{R})$ by

$$\begin{aligned} &Hf = \tau f, \\ &f \in \mathcal{D}(H) = \{g \in L^2(\mathbb{R}) \mid g, g' \in AC_{\text{loc}}(\mathbb{R}); \\ &\qquad \lim_{R\to\pm\infty} W(f_\pm(z_\pm), g)(R) = 0;\, \tau g \in L^2(\mathbb{R})\}, \end{aligned} \tag{A.30}$$

where again, the boundary condition at $+\infty$ (or $-\infty$) can be omitted if and only if τ is l.p. at $+\infty$ (or $-\infty$), that is, if and only if $f_+(z_+,\,\cdot\,)$ (or $f_-(z_-,\,\cdot\,)$) is unique up to constant multiples. Again, when considering restrictions of τ to $\mathbb{R}_\pm$, we shall fix the boundary condition at $+\infty$ and/or $-\infty$ if τ is l.c. at $+\infty$ and/or $-\infty$. As in the half-line case (A.14), the separated boundary conditions in (A.30) imply that H is a real operator (see, e.g., [36], Section 6.4). Moreover, the point spectrum $\sigma_p(H)$ of H (the set of eigenvalues of H) is simple (this follows, e.g., from [10], Theorem XIII.2.32).

Next we define $\phi_\alpha(z,x)$, $\theta_\alpha(z,x)$ as in (A.15), (A.16) (replacing τ_+ by τ) and introduce the uniquely determined solutions $\psi_{\pm,\alpha}(z,x)$ of

$$\tau\psi(z,x) = z\psi(z,x), \quad x \in \mathbb{R}, \tag{A.31}$$

satisfying

$$\begin{aligned} &\psi_{\pm,\alpha}(z,\,\cdot\,) \in L^2(\mathbb{R}_\pm), \quad \sin(\alpha)\psi'_{\pm,\alpha}(z,0) + \cos(\alpha)\psi_{\pm,\alpha}(z,0) = 1, \\ &\lim_{R\to\pm\infty} W(f_\pm(z_\pm), \psi_{\pm,\alpha}(z))(R) = 0, \quad z \in \mathbb{C}\backslash\mathbb{R} \end{aligned} \tag{A.32}$$

(the latter condition being superfluous at $+\infty$ and/or $-\infty$, i.e., automatically fulfilled if τ is l.p. at $+\infty$ and/or $-\infty$). Existence and uniqueness of $\psi_{\pm,\alpha}(z,x)$ follows from Theorem XIII.2.32 in [10]; they admit the representation

$$\psi_{\pm,\alpha}(z,x) = \theta_\alpha(z,x) + m_{\pm,\alpha}(z)\phi_\alpha(z,x) \tag{A.33}$$

in terms of the Weyl m-functions $m_{\pm,\alpha}(z)$. With our conventions

$$\pm m_{\pm,\alpha}(z) \text{ is Herglotz}, \quad \pm\mathrm{Im}[m_{\pm,\alpha}(z)] > 0, \quad \pm z \in \mathbb{C}_+, \tag{A.34}$$

$$\overline{m_{\pm,\alpha}(z)} = m_{\pm,\alpha}(\bar z), \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{A.35}$$

$$W(\psi_{+,\alpha}(z), \psi_{-,\alpha}(z)) = m_{-,\alpha}(z) - m_{+,\alpha}(z). \tag{A.36}$$

Moreover, we recall the following facts:

$$\pm \lim_{\epsilon\downarrow 0} i\epsilon\, m_{\pm,\alpha}(\lambda + i\epsilon) = \begin{cases} 0, & \phi_\alpha(\lambda,\,\cdot\,) \notin L^2(\mathbb{R}_\pm), \\ -\|\phi_\alpha(\lambda,\,\cdot\,)\|_2^{-2}, & \phi_\alpha(\lambda,\,\cdot\,) \in L^2(\mathbb{R}_\pm), \lambda \in \mathbb{R}, \end{cases} \tag{A.37}$$

$$m_{\pm,\alpha_1}(z) = \frac{-\sin(\alpha_1-\alpha_2) + \cos(\alpha_1-\alpha_2)m_{\pm,\alpha_2}(z)}{\cos(\alpha_1-\alpha_2) + \sin(\alpha_1-\alpha_2)m_{\pm,\alpha_2}(z)}, \tag{A.38}$$

$$m_{\pm,\alpha}(z) \underset{z\to i\infty}{=} \cot(\alpha) \pm \frac{i}{\sin^2(\alpha)}\, z^{-1/2} - \frac{\cos(\alpha)}{\sin^3(\alpha)}\, z^{-1} + o(z^{-1}), \quad \alpha \in (0,\pi), \tag{A.39}$$

$$m_{\pm,0}(z) \underset{z\to i\infty}{=} \pm i z^{1/2} + o(1), \tag{A.40}$$

$$m_{\pm,\alpha}(z) = a_{\pm,\alpha} \pm \int_{\mathbb{R}} \left[\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right] d\rho_{\pm,\alpha}(\lambda), \quad \alpha \in [0,\pi), \tag{A.41}$$

$$= \cot(\alpha) \pm \int_{\mathbb{R}} (\lambda - z)^{-1}\, d\rho_{\pm,\alpha}(\lambda), \quad \alpha \in (0,\pi), \tag{A.42}$$

with

$$\int_{\mathbb{R}} \frac{d\rho_{\pm,\alpha}(\lambda)}{1+|\lambda|} \begin{cases} < \infty, & \alpha \in (0,\pi), \\ = \infty, & \alpha = 0, \end{cases} \tag{A.43}$$

$$\begin{aligned} \pm \int_0^{\pm\infty} dx\, \psi_{\pm,\alpha}(z_1,x)\psi_{\pm,\alpha}(z_2,x) &= \pm \frac{m_{\pm,\alpha}(z_1) - m_{\pm,\alpha}(z_2)}{z_1 - z_2} \\ &= \int_{\mathbb{R}} (\lambda - z_1)^{-1}(\lambda - z_2)^{-1}\, d\rho_{\pm,\alpha}(\lambda). \end{aligned} \tag{A.44}$$

While the meaning of (A.38) is clear whenever τ is l.p. at $\pm\infty$, its interpretation in the l.c. case is as follows: Pick an $m_{+,\alpha_2}(z)$ (respectively $m_{-,\alpha_2}(z)$) on the corresponding limit circle of τ at $+\infty$ (respectively $-\infty$) for α_2. Then the left-hand-side of (A.38) defines a point $m_{+,\alpha_1}(z)$ (respectively $m_{-,\alpha_1}(z)$) on the corresponding limit circle of τ at $+\infty$ (respectively $-\infty$) for α_1. As a consequence, a more sophisticated notation for $\psi_{\pm,\alpha}(z,x)$, $m_{\pm,\alpha}(z)$, $d\rho_{\pm,\alpha}(\lambda)$, etc. would have to include an additional subscript $\varphi_\pm(\alpha) \in [0,\pi)$ parametrizing points on the limit circle at $\pm\infty$ for α. For simplicity, we decided to omit this additional subscript in the limit circle case.

Perhaps the asymptotic expansions (A.39) and (A.40) also warrant a comment. Under our general hypothesis (A.12), the standard literature usually provides somewhat weaker asymptotic formulas. The actual results (A.39), (A.40) appear to be due to Everitt [11] (see also [3]).

The Green's function $G(z,x,x')$ of H is then characterized by

(A.45)
$$((H-z)^{-1}f)(x) = \int_{\mathbb{R}} dx'\, G(z,x,x')f(x'), \quad z \in \mathbb{C}\backslash\sigma(H), f \in L^2(\mathbb{R}),$$

(A.46)
$$G(z,x,x') = \frac{1}{m_{-,\alpha}(z) - m_{+,\alpha}(z)} \begin{cases} \psi_{-,\alpha}(z,x)\psi_{+,\alpha}(z,x'), & x \le x', \\ \psi_{-,\alpha}(z,x')\psi_{+,\alpha}(z,x), & x' \le x. \end{cases}$$

Again (cf. the paragraph following (A.27)), for each $x \in \mathbb{R}$, the diagonal Green's function

$$G(z,x,x) \text{ is Herglotz.} \tag{A.47}$$

We emphasize that our choice of reference point $x = 0$ in (A.16) was purely a matter of convenience. In Section 3 it turns out to be advantageous to introduce a (variable) reference point $x = y$ instead. Without going into further details at this point, we agree to add the subscript y in this case and hence use the notation $\theta_{\alpha,y}(z,x)$, $\phi_{\alpha,y}(z,x)$, $\psi_{\pm,\alpha,y}(z,x)$, $m_{\pm,\alpha,y}(z)$, $d\rho_{\pm,\alpha,y}(\lambda)$, etc. The Weyl M-matrix for H is then defined by

(A.48)
$$\begin{aligned} M_{\alpha,y}(z) &= (M_{\alpha,y,p,q}(z))_{1\le p,q\le 2} \\ &= [m_{-,\alpha,y}(z) - m_{+,\alpha,y}(z)]^{-1} \\ &\quad\times \begin{pmatrix} m_{-\alpha,y}(z)m_{+,\alpha,y}(z) & [m_{-,\alpha,y}(z) + m_{+,\alpha,y}(z)]/2 \\ [m_{-,\alpha,y}(z) + m_{+,\alpha,y}(z)]/2 & 1 \end{pmatrix}. \end{aligned}$$

By inspection,

$$\det[M_{\alpha,y}(z)] = -\frac{1}{4} \tag{A.49}$$

and

$$M_{\alpha,y,p,p}(z) \text{ are Herglotz}, \quad p = 1,2. \tag{A.50}$$

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