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 $(H_y^{\beta}, H), \beta \in \mathbb{R} \cup \{\infty\}, y \in \mathbb{R}$ (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)
$$V(x) = E_0 + \lim_{z \to i\infty} \int_{E_0}^{\infty} d\lambda \, \frac{z^2}{(\lambda - z)^2} \left[1 - 2\xi^{\infty}(\lambda, x)\right],$$
$$E_0 = \inf\{\sigma(H)\}, \beta = \infty, x \in \mathbb{R},$$

Received by the editors February 27, 1995.

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¹⁹⁹¹ Mathematics Subject Classification. Primary 34B24, 34L05, 81Q10; Secondary 34B20, 47A10.

 $Key\ words\ and\ phrases.$ Schrödinger operators, inverse spectral theory, Krein's spectral shift function.

This material is based upon work supported by the National Science Foundation under Grant No. DMS-9101715. The U.S. Government has certain rights in this material.

(1.2)

(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 threedimensional 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,

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

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 $H_{+,j,\alpha_j}, m_{+,j,\alpha_j}, \rho_{+,j,\alpha_j}$ 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. $x \ge 0$.

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 $z \in \mathbb{C} \setminus \{\sigma(H_{+,\alpha_1}) \cup \sigma(H_{+,\alpha_2})\}$. Then (i)

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

352 (ii)

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

(iii)

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

(2.6)
$$= \frac{d}{dz} \ln[\cot(\alpha_2 - \alpha_1) - m_{+,\alpha_2}(z)].$$

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 $z_1 \rightarrow z_2 = z$. (2.6) is clear from

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

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

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

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

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

(2.7) then implies

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

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. $\lambda \in \mathbb{R}$,

(2.11)
(2.12)
$$\xi_{\epsilon,1}(\lambda) = \begin{cases} \lim_{\epsilon \downarrow 0} \pi^{-1} \operatorname{Im} \{ \ln[\cot(\alpha_2 - \alpha_1) + m_{+,\alpha_1}(\lambda + i\epsilon)] \} \\ -\lim_{\epsilon \downarrow 0} \pi^{-1} \operatorname{Im} \{ \ln[\cot(\alpha_2 - \alpha_1) - m_{+,\alpha_2}(\lambda + i\epsilon)] \} \end{cases}$$

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

(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,

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

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

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

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

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

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

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

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

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

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

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

(2.19)

$$\cot(\alpha_{2} - \alpha_{1}) - m_{+,\alpha_{2}}(z) = \begin{cases} 0, & \alpha_{1} = 0, \\ \cot(\alpha_{2} - \alpha_{1}) - \cot(\alpha_{2}) > 0, & 0 < \alpha_{1} < \alpha_{2} < \pi, \end{cases}$$

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

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

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 $\tau_j = -\frac{d^2}{dx^2} + V_j(x)$, $x \ge 0$, j = 1, 2. Let $\alpha_{j,\ell} \in [0,\pi)$, $\ell = 1, 2$, suppose $0 \le \alpha_{1,1} < \alpha_{1,2} < \pi$, $0 \le \alpha_{2,1} < \alpha_{2,2} < \pi$, 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. $x \ge 0$.

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

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

Since by hypothesis $\alpha_{1,1} > 0$ if and only if $\alpha_{2,1} > 0$, 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

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

(2.23)
$$= \sum_{z \to i\infty} (\beta_{j,2} - \beta_{j,1}) i z^{-1/2} + (\beta_{j,1}^2 - \beta_{j,2}^2) 2^{-1} z^{-1} + o(z^{-1}),$$
$$\beta_{j,\ell} = \cot(\alpha_{j,\ell}), \qquad j, \ell = 1, 2.$$

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

(2.24)
$$\alpha_{1,1} = \alpha_{2,1}$$
 and $\alpha_{1,2} = \alpha_{2,2}$

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

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

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

(2.26)

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

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

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

$$= -\cot(\alpha_{j,2})iz^{-1/2} + o(z^{-1/2}), \quad j = 1, 2.$$

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

(2.28)
$$\alpha_{1,2} = \alpha_{2,2}$$

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

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

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

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

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,

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

Then the following are equivalent:

- (i) $\sigma(H_{+,1,\alpha_{1,1}}) = \sigma(\hat{H}_{+,2,\alpha_{2,1}}), \ \sigma(H_{+,1,\alpha_{1,2}}) = \sigma(H_{+,2,\alpha_{2,2}}), \ \alpha_{j,\ell} \in [0,\pi), \ j,\ell = 1,2, \ \sin(\alpha_{1,1} \alpha_{1,2}) \neq 0.$
- (ii) $\alpha_{1,1} = \alpha_{2,1}, \ \alpha_{1,2} = \alpha_{2,2}, \ and \ V_1(x) = V_2(x) \ for \ a.e. \ x \ge 0.$

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 threedimensional Schrödinger operators with spherically symmetric potentials.

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

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

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

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

A simple unitary transformation reduces (2.33) to

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

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

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

where

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

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])

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

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

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

which yields

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

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 $\tau_{+} = -\frac{d^2}{dx^2} + V(x), x \ge 0$, by

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

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,

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

throughout this section. Following [20], we introduce, in addition, the following family of self-adjoint operators H_y^β in $L^2(\mathbb{R})$, (3.2)

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

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

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

with respect to

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

In particular, $H_{\pm,y}^{\beta}$ equals $H_{\pm,\alpha}$ 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 = ywill 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

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

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

Here

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

and

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

As a consequence,

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

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

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

(3.11)
$$(\beta + \partial_1)(\beta + \partial_2)G(z, y, y)$$
 is Herglotz

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

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

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

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

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

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

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

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

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

(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 $y \in \mathbb{R}$),

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

(3.20)

$$\sin^{2}(\alpha)(\beta + \partial_{1})(\beta + \partial_{2})G(z, y, y) = M_{\alpha, y, 2, 2}(z) = [m_{-, \alpha, y}(z) - m_{+, \alpha, y}(z)]^{-1}$$

$$\beta = \cot(\alpha), \alpha \in (0, \pi)$$

and especially

$$(3.21)^{(3.21)} m_{+,\alpha_{2},y}(z)^{2} + \{[m_{-,\alpha_{2},y}(z) - m_{+,\alpha_{2},y}(z)] + 2\cot(\alpha_{1} - \alpha_{2})\}m_{+,\alpha_{2},y}(z) + \cot^{2}(\alpha_{1} - \alpha_{2}) + [m_{-,\alpha_{2},y}(z) - m_{+,\alpha_{2},y}(z)]\cot(\alpha_{1} - \alpha_{2}) - [\sin(\alpha_{1} - \alpha_{2})]^{-2}[m_{-,\alpha_{2},y}(z) - m_{+,\alpha_{2},y}(z)][m_{-,\alpha_{1},y}(z) - m_{+,\alpha_{1},y}(z)]^{-1} = 0, \alpha_{1} \neq \alpha_{2}, z \in \mathbb{C} \backslash \mathbb{R},$$

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 $\alpha_1, \alpha_2 \in [0, \pi)$, $\alpha_1 \neq \alpha_2$, 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 $\beta_1, \beta_2 \in \mathbb{R} \cup \{\infty\}, \beta_1 \neq \beta_2, and x_0 \in \mathbb{R}$.

- (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 (β₁, β₂) = (0, ∞) or (∞, 0), assume in addition that τ is in the limit point case at +∞ and -∞. Then ξ[∞](λ, x₀) and ξ⁰(λ, x₀) for a.e. λ ∈ ℝ uniquely determine V a.e. up to reflection symmetry with respect to x₀; that is, both V(x), V(2x₀ x) for a.e. x ∈ ℝ correspond to ξ[∞](λ, x₀) and ξ⁰(λ, x₀) for a.e. λ ∈ ℝ.

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

$$(3.22)$$

$$m_{+,\alpha_{2},x_{0}}(z) = -\frac{1}{2}[m_{-,\alpha_{2},x_{0}}(z) - m_{+,\alpha_{2},x_{0}}(z)] - \cot(\alpha_{1} - \alpha_{2})$$

$$\pm \left\{ \frac{1}{4}[m_{-,\alpha_{2},x_{0}}(z) - m_{+,\alpha_{2},x_{0}}(z)]^{2} + \frac{1}{\sin^{2}(\alpha_{1} - \alpha_{2})} \frac{[m_{-,\alpha_{2},x_{0}}(z) - m_{+,\alpha_{2},x_{0}}(z)]}{[m_{-,\alpha_{1},x_{0}}(z) - m_{+,\alpha_{1},x_{0}}(z)]} \right\}^{1/2}, \qquad z \in \mathbb{C} \backslash \mathbb{R}.$$

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),

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

which inserted into (3.22) results in (3.24)

$$m_{+,\alpha_2,x_0}(z) = \cot(\alpha_2 - \alpha_1) + o(z^{-1/2}) \pm \left\{ \frac{\sin^2(\alpha_1)}{\sin^2(\alpha_1 - \alpha_2)\sin^2(\alpha_2)} + O(z^{-1}) \right\}^{1/2}.$$

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),

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

which inserted into (3.22) yields

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

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

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

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

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

and

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

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

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

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

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

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

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

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

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

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

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

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 $\alpha \in (0,\pi) \setminus \{\pi/2\}$, 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 $\xi^{\beta}(\lambda, x_0) = \hat{\xi}^{-\beta}(\lambda, x_0)$ is common to V and $\hat{V} \neq V$.

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 (β₁, β₂) = (0, ∞) or (∞, 0), assume in addition that τ is in the limit point case at +∞ and -∞. Then σ(H), σ(H[∞]_{x0}), and σ(H⁰_{x0}) uniquely determine V a.e. up to reflection symmetry with respect to x₀, that is, both V(x) and Ŷ(x) = V(2x₀ x) for a.e. x ∈ ℝ correspond to σ(H) = σ(Ĥ), σ(H[∞]_{x0}) = σ(Ĥ[∞]_{x0}), and σ(H⁰_{x0}) = σ(Ĥ⁰_{x0}). Here, in obvious notation, Ĥ, Ĥ[∞]_{x0}, Ĥ⁰_{x0} correspond to τ̂ = d²/dx² + Ŷ(x), x ∈ ℝ.
 (iii) Suppose τ is in the limit point case at +∞ and -∞, and let β ∈ 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 nonoscillatory 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 $\sigma(H) = \{e_n\}_{n \in J_0}, \ \sigma(H_{x_0}^{\beta}) = \{\lambda_n^{\beta}(x_0)\}_{n \in I^{\beta}}, \text{ where } I^{\beta} = J_0, \beta \in \mathbb{R}, \text{ and } I^{\infty} = J, \text{ with } J_0 = \mathbb{N}_0 \text{ or } \mathbb{Z} \text{ and } J = \mathbb{N} \text{ or } \mathbb{Z} \text{ depending on whether or not } H \text{ is bounded from below. Moreover, we use the ordering } e_n < e_{n+1}, \lambda_n^{\beta}(x_0) \leq \lambda_{n+1}^{\beta}(x_0).$ By general principles,

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

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,

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

 $\sigma(H)$, $\sigma(H_{x_0}^{\beta_1})$, 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,

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

for some $m_0 \in I^{\beta_1}$. Since half-line spectra are necessarily simple, (3.37) implies that $H^{\beta_1}_{+,x_0}$ and $H^{\beta_1}_{-,x_0}$, the corresponding half-line operators in $L^2((x_0, \pm \infty))$ (cf. (3.3), (3.4)) associated with $H^{\beta_1}_{x_0}$, 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 $\lambda^{\beta_1}_{m_0}(x_0)$ 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 $\psi_{+,\alpha_1,x_0}(e_{m_0},x) = \text{const.}\psi_{-,\alpha_1,x_0}(e_{m_0-1},x), \ \beta_1 = \text{cot}(\alpha_1)$, 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 $x \leq x_0$ and $x \geq x_0$ 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

(3.38)
$$\lambda_{0}^{0}(x_{0}) = e_{0}, \quad \lambda_{2m+1}^{\infty}(x_{0}) = e_{2m+1} = \lambda_{2m+2}^{\infty}(x_{0}), \\ \lambda_{2m+1}^{0}(x_{0}) = e_{2m+2} = \lambda_{2m+2}^{0}(x_{0}), \quad m \in \mathbb{N}_{0}. \quad \Box$$

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 $\lambda_n^{\beta}(x_0)$ (i.e., whether $\lambda_n^{\beta}(x_0)$ is an eigenvalue of H_{-,x_0}^{β} in $L^2((-\infty, x_0])$ or of H_{+,x_0}^{β} 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 $\lambda_n^{\infty}(x_0)$ by

$$(3.39) \qquad \qquad \mu_n(x_0), \quad n \in J,$$

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

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

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 $H_{x_0}^{\infty}$ are of the type

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

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

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

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

Then Borg's result can be rephrased as follows.

Theorem 3.5 (Borg [4], see also [34],[35]). Let $V \in L^1_{loc}(\mathbb{R})$ 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])

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

in connection with the periodic case (3.41), (3.42). This result extends to algebrogeometric 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

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

such that

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

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 $H_{x_0}^{\infty}$ into simple and (twice) degenerate Dirichlet eigenvalues, that is, those which are disjoint from $\sigma(H)$ and those which coincide with an element of $\sigma(H)$,

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

(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

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

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

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

(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, $\sigma_{ess}(H) = \emptyset$, $\sigma(H) = \{e_n\}_{n \in J_0}$. 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

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

is determined. Since $\sigma_{ess}(H) = \emptyset$, 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 $H_{x_0}^{\infty}$, 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 $H_{\pm,x_0}^{\infty} = H_{\pm,0,x_0}$ 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].

Acknowledgment

F.G. is indebted to the Department of Mathematics at Caltech for its hospitality and support during the summers of 1993 and 1994 where some of this work was done.

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 $\mathbb{C}_{\pm} := \{z \in \mathbb{C} \mid \pm \operatorname{Im}(z) > 0\}$, any analytic map $m : \mathbb{C}_{+} \to \mathbb{C}_{+}$ is called Herglotz. One conveniently defines m on \mathbb{C}_{-} by $m(\overline{z}) = \overline{m(z)}$ 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].

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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 $\xi \in L^1_{loc}(\mathbb{R})$ such that

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

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

where

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

and

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

(ii) (Fatou's lemma)

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

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

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

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

if and only if

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

(iv)

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

if and only if

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

In this case

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

(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

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

and introduce the differential expression

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

Associated with τ_+ we introduce the following self-adjoint operator $H_{+,\alpha}$ in $L^2(\mathbb{R}_+)$. Pick a $z_+ \in \mathbb{C} \setminus \mathbb{R}$ 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 (A.14)

$$H_{+,\alpha}f = \tau_{+}f, \quad \alpha \in [0,\pi),$$

$$f \in \mathcal{D}(H_{+,\alpha}) = \{g \in L^{2}(\mathbb{R}_{+}) \mid g, g' \in AC([0,R]) \text{ for all } R > 0;$$

$$\sin(\alpha)g'(0_{+}) + \cos(\alpha)g(0_{+}) = 0; \lim_{R \to \infty} W(f_{+}(z_{+}),g)(R) = 0; \tau_{+}g \in L^{2}(\mathbb{R}_{+})\}.$$

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 $H_{+,\alpha}\bar{g} = (H_{+,\alpha}g)$), 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

(A.15)
$$\tau_+\psi(z,x) = z\psi(z,x), \quad x \ge 0,$$

satisfying

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

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

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

(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

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

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

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

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

with

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

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

(A.22)
$$((H_{+,\alpha} - z)^{-1}f)(x) = \int_{0}^{\infty} dx' G_{+,\alpha}(z, x, x')f(x'), \\ z \in \mathbb{C} \setminus \sigma(H_{+,\alpha}), f \in L^{2}(\mathbb{R}_{+}),$$

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

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

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

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

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

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

While the latter result is obvious from (A.24) (note we have $\phi_{\alpha}(\lambda, x) = O(1)$ for $\alpha \in (0, \pi)$ and $\phi_0(\lambda, x) = O(|\lambda|^{-1/2})$ 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

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

one introduces the differential expression

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

and picks $z_{\pm} \in \mathbb{C} \setminus \mathbb{R}$ 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

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

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

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

satisfying

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

(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

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

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

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

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

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

Moreover, we recall the following facts:

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

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

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

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

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

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

with

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

(A.44)
$$\pm \int_{0}^{\pm \infty} dx \, \psi_{\pm,\alpha}(z_1, x) \psi_{\pm,\alpha}(z_2, x) = \pm \frac{m_{\pm,\alpha}(z_1) - m_{\pm,\alpha}(z_2)}{z_1 - z_2} \\ = \int_{\mathbb{R}} (\lambda - z_1)^{-1} (\lambda - z_2)^{-1} \, d\rho_{\pm,\alpha}(\lambda).$$

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

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

(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

(A.47)
$$G(z, x, x)$$
 is Herglotz

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)

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

By inspection,

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

and

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

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