ON SPECTRAL THEORY FOR SCHRÖDINGER OPERATORS WITH STRONGLY SINGULAR POTENTIALS

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Abstract. We examine two kinds of spectral theoretic situations: First, we recall the case of self-adjoint half-line Schrödinger operators on $[a,\infty)$, $a \in \mathbb{R}$, with a regular finite end point a and the case of Schrödinger operators on the real line with locally integrable potentials, which naturally lead to Herglotz functions and 2×2 matrix-valued Herglotz functions representing the associated Weyl–Titchmarsh coefficients. Second, we contrast this with the case of self-adjoint half-line Schrödinger operators on (a,∞) with a potential strongly singular at the end point a. We focus on situations where the potential is so singular that the associated maximally defined Schrödinger operator is self-adjoint (equivalently, the associated minimally defined Schrödinger operator is essentially self-adjoint) and hence no boundary condition is required at the finite end point a. For this case we show that the Weyl–Titchmarsh coefficient in this strongly singular context still determines the associated spectral function, but ceases to posses the Herglotz property. However, as will be shown, Herglotz function techniques continue to play a decisive role in the spectral theory for strongly singular Schrödinger operators.

1. Introduction

The principal goal of this paper is to study singular Schrödinger operators on a half-line $[a,\infty)$, $a \in \mathbb{R}$, with strongly singular potentials at the finite end point a in the sense that

$$V \in L^1_{\mathrm{loc}}((a,\infty);dx), \;\; V \text{ real-valued}, V \notin L^1([a,b];dx), \quad b > a. \tag{1.1}$$

For previous studies of strongly singular Schrödinger operators we refer, for instance, to [3], [5], [6], [7], [8], [9], [10], [14], [15], [26] [27], [28], [29], [30], [31], [32], [33], [34], [35], [36], [37], [38], [39], [60], [62], [63], and the references therein. (Many of these references treat, in fact, a discrete set of singularities on $\mathbb{R}$ or on (a,b), $-\infty \le a < b \le \infty$.) Quite recently, singular potentials became again a popular object of study from various points of views: Some groups study singular interactions in connections with scales of Hilbert spaces (see, e.g., [19], [48], [49], [50] and the references therein), while other groups study strongly singular interactions in the context of Pontryagin spaces (we refer, e.g., to [11], [18], [20], [21], [67] and the references therein).

Our point of departure in connection with strongly singular potentials is quite different: We focus on the derivation of the spectral function for strongly singular

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half-line Schrödinger operators starting from the resolvent (and hence the Green's function). In stark contrast to the standard situation of Schrödinger operators on a half-line $[a,\infty)$, $a \in \mathbb{R}$, with a regular end point a, where the associated spectral function generates the measure in the Herglotz representation of the Weyl–Titchmarsh coefficient, we show that half-line Schrödinger operators with strongly singular potentials at the endpoint a lead to spectral functions which are related to the analog of a Weyl–Titchmarsh coefficient which ceases to be a Herglotz function. In fact, the strongly singular potentials studied in this paper are so singular at a that the associated maximally defined Schrödinger operator is self-adjoint (equivalently, the associated minimal Schrödinger operator is essentially self-adjoint) and hence no boundary condition is required at the finite endpoint a.

In Section 2 we recall the essential ingredients of standard spectral theory for self-adjoint Schrödinger operators on a half-line $[a,\infty)$, $a \in \mathbb{R}$, with a regular end point a and problems on the real line with locally integrable potentials. In either case the notion of a spectral function or 2×2 matrix spectral function is intimately connected with Herglotz functions and 2×2 Herglotz matrices representing the celebrated Weyl–Titchmarsh coefficients. This section is, in part, of an expository nature. In stark contrast to the half-line case with a regular finite endpoint a in Section 2, we will show in Section 3 in the case of strongly singular potentials V on (a,∞) with singularity concentrated at the endpoint a, that the corresponding spectral functions are no longer derived from associated Herglotz functions (although, certain Herglotz functions still play an important role in this context). We present and contrast two approaches in Section 3: First we discuss the case where the reference point x_0 coincides with the singular endpoint a, leading to a scalar Weyl–Titchmarsh coefficient and a scalar spectral function. Alternatively, we treat the case where the reference point x_0 belongs to the interior of the interval (a,∞), leading to a 2×2 matrix-valued Weyl–Titchmarsh and spectral function. Finally, in Section 4 we provide a detailed discussion of the explicitly solvable example $V(x) = [\gamma^2 - (1/4)]x^{-2}$, $x \in (0,\infty)$, $\gamma \in [1,\infty)$. Again we illustrate the two approaches with a choice of reference point $x_0 = 0$ and $x_0 \in (0,\infty)$.

2. Spectral Theory and Herglotz Functions

In this section we separately recall basic spectral theory for the case of half-line Schrödinger operators with a regular left endpoint and the case of full-line Schrödinger operators with locally integrable potentials and their relationship to Herglotz functions and matrices. The material of this section is standard and various parts of it can be found, for instance, in [12], [17, Ch. 9], [23, Sect. XIII.5], [24, Ch. 2], [25], [45, Ch. 10], [47], [54], [56], [58, Ch. 2], [61, Ch. VI], [64, Ch. 6], [70, Chs. II, III], [71, Sects. 7–10].

Starting with the half-line case (with a regular left endpoint) we introduce the following main assumption:

Hypothesis 2.1. (i) *Let $a \in \mathbb{R}$ and assume that*

$$V \in L^1([a,c];dx) \ \textit{ for all } c \in (a,\infty), \ V \textit{ real-valued.} \tag{2.1}$$

(ii) *Introducing the differential expression τ_+ given by*

$$\tau_+ = -\frac{d^2}{dx^2} + V(x), \quad x \in (a,\infty), \tag{2.2}$$

we assume τ_+ to be in the limit point case at $+\infty$.

Associated with the differential expression τ_+ one introduces the self-adjoint Schrödinger operator $H_{+,\alpha}$ in $L^2([a,\infty);dx)$ by

$$\begin{aligned}
&H_{+,\alpha}f = \tau_+ f, \quad \alpha \in [0,\pi),\\
&f \in \mathrm{dom}(H_{+,\alpha}) = \Big\{g \in L^2([a,\infty);dx)\,\Big|\, g, g' \in AC([a,c]) \text{ for all } c \in (a,\infty);\\
&\qquad \sin(\alpha)\lim_{\varepsilon\downarrow 0} g'(a+\varepsilon) + \cos(\alpha)\lim_{\varepsilon\downarrow 0} g(a+\varepsilon) = 0;\ \tau_+ g \in L^2([a,\infty);dx)\Big\}. \qquad (2.3)
\end{aligned}$$

Here (and in the remainder of this manuscript) $'$ denotes d/dx and $AC([c,d])$ denotes the class of absolutely continuous functions on the closed interval $[c,d]$.

Remark 2.2. For simplicity we chose the half-line $[a,\infty)$ rather than a finite interval $[a,b)$, $a < b < \infty$. Moreover, we chose the limit point hypothesis of τ_+ at the right end point to avoid having to consider any boundary conditions at that point. Both limitations can be removed.

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

$$(\tau_+\psi)(z,x) = z\psi(z,x), \quad x \in [a,\infty), \qquad (2.4)$$

satisfying the initial conditions at the point $x = a$,

$$\phi_\alpha(z,a) = -\theta'_\alpha(z,a) = -\sin(\alpha), \;\; \phi'_\alpha(z,a) = \theta_\alpha(z,a) = \cos(\alpha), \;\; \alpha \in [0,\pi). \qquad (2.5)$$

For future purpose we emphasize that for any fixed $x \in [a,\infty)$, $\phi_\alpha(z,x)$ and $\theta_\alpha(z,x)$ are entire with respect to z and that

$$W(\theta_\alpha(z,\cdot),\phi_\alpha(z,\cdot))(x) = 1, \quad z \in \mathbb{C}, \qquad (2.6)$$

where

$$W(f,g)(x) = f(x)g'(x) - f'(x)g(x) \qquad (2.7)$$

denotes the Wronskian of f and g.

A particularly important special solution of (2.4) is the *Weyl–Titchmarsh solution* $\psi_{+,\alpha}(z,\cdot)$, $z \in \mathbb{C}\backslash\mathbb{R}$, uniquely characterized by

$$\psi_{+,\alpha}(z,\cdot) \in L^2([a,\infty);dx), \quad \sin(\alpha)\psi'_{+,\alpha}(z,a) + \cos(\alpha)\psi_{+,\alpha}(z,a) = 1, \quad z \in \mathbb{C}\backslash\mathbb{R}. \qquad (2.8)$$

The second condition in (2.8) just determines the normalization of $\psi_{+,\alpha}(z,\cdot)$ and defines it uniquely. The crucial condition in (2.8) is the L^2-property which uniquely determines $\psi_{+,\alpha}(z,\cdot)$ up to constant multiples by the limit point hypothesis of τ_+ at ∞. In particular, for $\alpha, \beta \in [0,\pi)$,

$$\psi_{+,\alpha}(z,\cdot) = C(z,\alpha,\beta)\psi_{+,\beta}(z,\cdot) \text{ for some coefficient } C(z,\alpha,\beta) \in \mathbb{C}. \qquad (2.9)$$

The normalization in (2.8) shows that $\psi_{+,\alpha}(z,\cdot)$ is of the type

$$\psi_{+,\alpha}(z,x) = \theta_\alpha(z,x) + m_{+,\alpha}(z)\phi_\alpha(z,x), \quad z \in \mathbb{C}\backslash\mathbb{R},\ x \in [a,\infty) \qquad (2.10)$$

for some coefficient $m_{+,\alpha}(z)$, the *Weyl–Titchmarsh m-function* associated with τ_+ and α.

Next, we recall the fundamental identity

$$\int_a^\infty dx\,\psi_{+,\alpha}(z_1,x)\psi_{+,\alpha}(z_2,x) = \frac{m_{+,\alpha}(z_1) - m_{+,\alpha}(z_2)}{z_1 - z_2}, \quad z_1, z_2 \in \mathbb{C}\backslash\mathbb{R},\ z_1 \neq z_2. \qquad (2.11)$$

It is a consequence of the elementary fact

$$\frac{d}{dx} W(\psi(z_1,\cdot),\psi(z_2,\cdot))(x) = (z_1 - z_2)\psi(z_1,x)\psi(z_2,x) \tag{2.12}$$

for solutions $\psi(z_j,\cdot)$, $j = 1,2$, of (2.4), and the fact that τ_+ is assumed to be in the limit point case at ∞ which implies

$$\lim_{x\uparrow\infty} W(\psi_{+,\alpha}(z_1,\cdot),\psi_{+,\alpha}(z_2,\cdot))(x) = 0. \tag{2.13}$$

Moreover, since $\overline{\psi_{+,\alpha}(z,\cdot)}$ is the unique solution of $\tau_+\psi(\overline{z},x) = \overline{z}\psi(\overline{z},x)$, $x \in [a,\infty)$, satisfying

$$\overline{\psi_{+,\alpha}(z,\cdot)} \in L^2([a,\infty);dx), \quad \sin(\alpha)\overline{\psi'_{+,\alpha}(z,a)} + \cos(\alpha)\overline{\psi_{+,\alpha}(z,a)} = 1, \tag{2.14}$$

and since

$$\overline{\phi_\alpha(z,x)} = \phi_\alpha(\overline{z},x), \quad \overline{\theta_\alpha(z,x)} = \theta_\alpha(\overline{z},x), \quad z \in \mathbb{C},\ x \in [a,\infty), \tag{2.15}$$

one concludes that $\overline{\psi_{+,\alpha}(z,\cdot)}$ is the Weyl–Titchmarsh solution of $\tau_+\psi(\overline{z},x) = \overline{z}\psi(\overline{z},x)$, $x \geq a$, and hence

$$\overline{m_{+,\alpha}(z)} = m_{+,\alpha}(\overline{z}), \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{2.16}$$

Thus, choosing $z_1 = z$, $z_2 = \overline{z}$ in (2.9), one infers

$$\int_a^\infty dx\, |\psi_{+,\alpha}(z,x)|^2 = \frac{\operatorname{Im}(m_{+,\alpha}(z))}{\operatorname{Im}(z)}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{2.17}$$

Before we turn to the proper interpretation of formulas (2.16) and (2.17), we briefly take a look at the Green's function $G_{+,\alpha}(z,x,x')$ of $H_{+,\alpha}$. Using (2.5), (2.6), and (2.8) one obtains,

$$G_{+,\alpha}(z,x,x') = \begin{cases} \phi_\alpha(z,x)\psi_{+,\alpha}(z,x'), & a \leq x \leq x', \\ \phi_\alpha(z,x')\psi_{+,\alpha}(z,x), & a \leq x' \leq x, \end{cases} \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{2.18}$$

and thus,

$$\begin{aligned} ((H_{+,\alpha} - zI)^{-1}f)(x) &= \int_a^\infty dx'\, G_{+,\alpha}(z,x,x')f(x'), \\ &\qquad z \in \mathbb{C}\backslash\mathbb{R},\ x \in [a,\infty),\ f \in L^2([a,\infty);dx). \end{aligned} \tag{2.19}$$

Next we mention the following analyticity result (for the notion of Herglotz functions we refer to Appendix A). Here and in the remainder of this manuscript, $\chi_{\mathcal{M}}$ denotes the characteristic function of a set $\mathcal{M} \subset \mathbb{R}$.

Lemma 2.3. *Assume Hypothesis* 2.1 *and let* $\alpha \in [0,\pi)$. *Then* $m_{+,\alpha}$ *is analytic on* $\mathbb{C}\backslash\sigma(H_{+,\alpha})$, *moreover,* $m_{+,\alpha}$ *is a Herglotz function. In addition, for each* $x \in [a,\infty)$, $\psi_{+,\alpha}(\cdot,x)$ *and* $\psi'_{+,\alpha}(\cdot,x)$ *are analytic on* $\mathbb{C}\backslash\sigma(H_{+,\alpha})$.

Proof. Pick real numbers c and d such that $a \leq c < d < \infty$. Then, using (2.18) and (2.19) one computes

$$\begin{aligned}
\int_{\sigma(H_{+,\alpha})} & \frac{d\big\|E_{H_{+,\alpha}}(\lambda)\chi_{[c,d]}\big\|^2_{L^2([a,\infty);dx)}}{\lambda - z} = \big(\chi_{[c,d]}, (H_{+,\alpha} - zI)^{-1}\chi_{[c,d]}\big)_{L^2([a,\infty);dx)} \\
&= \int_c^d dx \int_c^x dx'\, \theta_\alpha(z,x)\phi_\alpha(z,x') + \int_c^d dx \int_x^d dx'\, \phi_\alpha(z,x)\theta_\alpha(z,x') \qquad (2.20) \\
&\quad + m_{+,\alpha}(z)\bigg[\int_c^d dx\, \phi_\alpha(z,x)\bigg]^2, \quad z \in \mathbb{C}\backslash\sigma(H_{+,\alpha}).
\end{aligned}$$

Since the left-hand side of (2.20) is analytic with respect to z on $\mathbb{C}\backslash\sigma(H_{+,\alpha})$ and since $\phi_\alpha(\cdot,x)$ and $\theta_\alpha(\cdot,x)$ are entire for fixed $x \in [a,\infty)$ with $\phi_\alpha(z,\cdot)$, $\theta_\alpha(z,\cdot)$, and their first x-derivatives being absolutely continuous on each interval $[a,b]$, $b > a$, one concludes that $m_{+,\alpha}$ is analytic in a sufficiently small open neighborhood $\mathcal{N}_{z_0}$ of a given point $z_0 \in \mathbb{C}\backslash\sigma(H_{+,\alpha})$, as long as we can guarantee the existence of $c(z_0), d(z_0) \in [a,\infty)$ such that

$$\int_{c(z_0)}^{d(z_0)} dx\, \phi_\alpha(z,x) \neq 0, \quad z \in \mathcal{N}_{z_0}. \qquad (2.21)$$

The latter is shown as follows: First, pick $z_0 \in \mathbb{C}\backslash\sigma(H_{+,\alpha})$. Then since $\phi_\alpha(z_0,\cdot)$ does not vanish identically, one can find $c(z_0), d(z_0) \in [a,\infty)$ such that

$$\int_{c(z_0)}^{d(z_0)} dx\, \phi_\alpha(z_0,x) \neq 0. \qquad (2.22)$$

Since

$$\int_{c(z_0)}^{d(z_0)} dx\, \phi_\alpha(z,x) \qquad (2.23)$$

is entire with respect to z, (2.22) guarantees the existence of an open neighborhood $\mathcal{N}_{z_0}$ of z_0 such that (2.21) holds. Since $z_0 \in \mathbb{C}\backslash\sigma(H_{+,\alpha})$ was chosen arbitrary, $m_{+,\alpha}$ is analytic on $\mathbb{C}\backslash\sigma(H_{+,\alpha})$. Together with (2.16) and (2.17) this proves that $m_{+,\alpha}$ is a Herglotz function. By (2.10) (and its x-derivative), $\psi_{+,\alpha}(\cdot,x)$ and $\psi'_{+,\alpha}(\cdot,x)$ are analytic on $\mathbb{C}\backslash\sigma(H_{+,\alpha})$ for each $x \in [a,\infty)$. ☐

Remark 2.4. Traditionally, one proves analyticity of $m_{+,\alpha}$ on $\mathbb{C}\backslash\mathbb{R}$ by first restricting $H_{+,\alpha}$ to the interval $[a,b]$ (introducing a self-adjoint boundary condition at the endpoint b) and then controls the uniform limit of a sequence of meromorphic Weyl–Titchmarsh coefficients analytic on $\mathbb{C}\backslash\mathbb{R}$ as $b \uparrow \infty$. We chose the somewhat roundabout proof of Lemma 2.3 based on the fundamental identity (2.20) in view of Section 3, in which we consider strongly singular potentials at $x = a$, where the traditional approach leading to a Weyl–Titchmarsh coefficient m_+ possessing the Herglotz property is not applicable, but the current method of proof relying on the family of spectral projections $\{E_{H_{+,\alpha}}\}_{\lambda\in\mathbb{R}}$, the Green's function $G_{+,\alpha}(z,x,x')$ of $H_{+,\alpha}$, and identity (2.20), remains in effect.

Moreover, we recall the following well-known facts on $m_{+,\alpha}$:

$$\lim_{\epsilon\downarrow 0} i\epsilon\, m_{+,\alpha}(\lambda+i\epsilon) = \begin{cases} 0, & \phi_\alpha(\lambda,\,\cdot\,) \notin L^2([a,\infty);dx), \\ -\|\phi_\alpha(\lambda,\,\cdot\,)\|^{-2}_{L^2([a,\infty);dx)}, & \phi_\alpha(\lambda,\,\cdot\,) \in L^2([a,\infty);dx), \end{cases} \tag{2.24}$$

$$\lambda\in\mathbb{R},\ \alpha\in[0,\pi),$$

$$m_{+,\alpha_1}(z) = \frac{-\sin(\alpha_1-\alpha_2)+\cos(\alpha_1-\alpha_2)m_{+,\alpha_2}(z)}{\cos(\alpha_1-\alpha_2)+\sin(\alpha_1-\alpha_2)m_{+,\alpha_2}(z)}, \quad \alpha_1,\alpha_2\in[0,\pi), \tag{2.25}$$

$$m_{+,\alpha}(z) \underset{z\to i\infty}{=} \begin{cases} \cot(\alpha)+\frac{i}{\sin^2(\alpha)}\,z^{-1/2}-\frac{\cos(\alpha)}{\sin^3(\alpha)}\,z^{-1}+o(z^{-1}), & \alpha\in(0,\pi), \\ iz^{1/2}+o(1), & \alpha=0. \end{cases} \tag{2.26}$$

The asymptotic behavior (2.26) then implies the Herglotz representation of $m_{+,\alpha}$ (cf. Theorem A.2 (iii)),

$$m_{+,\alpha}(z) = \begin{cases} c_{+,\alpha}+\int_{\mathbb{R}} d\rho_{+,\alpha}(\lambda)\Big[\frac{1}{\lambda-z}-\frac{\lambda}{1+\lambda^2}\Big], & \alpha\in[0,\pi), \\ \cot(\alpha)+\int_{\mathbb{R}} d\rho_{+,\alpha}(\lambda)\,(\lambda-z)^{-1}, & \alpha\in(0,\pi), \end{cases} \quad z\in\mathbb{C}\backslash\mathbb{R} \tag{2.27}$$

with

$$\int_{\mathbb{R}} \frac{d\rho_{+,\alpha}(\lambda)}{1+|\lambda|} \begin{cases} <\infty, & \alpha\in(0,\pi), \\ =\infty, & \alpha=0, \end{cases} \quad \int_{\mathbb{R}} \frac{d\rho_{+,0}(\lambda)}{1+\lambda^2}<\infty. \tag{2.28}$$

We note that in formulas (2.10)–(2.27) one can of course replace $z\in\mathbb{C}\backslash\mathbb{R}$ by $z\in\mathbb{C}\backslash\sigma(H_{+,\alpha})$.

For future purposes we also note the following result, a version of Stone's formula in the weak sense (cf., e.g., [23, p. 1203]).

Lemma 2.5. *Let T be a self-adjoint operator in a complex separable Hilbert space $\mathcal{H}$ (with scalar product denoted by $(\cdot,\cdot)_{\mathcal{H}}$, linear in the second factor) and denote by $\{E_T(\lambda)\}_{\lambda\in\mathbb{R}}$ the family of self-adjoint right-continuous spectral projections associated with T, that is, $E_T(\lambda)=\chi_{(-\infty,\lambda]}(T)$, $\lambda\in\mathbb{R}$. Moreover, let $f,g\in\mathcal{H}$, $\lambda_1,\lambda_2\in\mathbb{R}$, $\lambda_1<\lambda_2$, and $F\in C(\mathbb{R})$. Then,*

$$\begin{aligned} &\big(f,F(T)E_T((\lambda_1,\lambda_2])g\big)_{\mathcal{H}} \\ &\quad = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda)\big[\big(f,(T-(\lambda+i\varepsilon)I_{\mathcal{H}})^{-1}g\big)_{\mathcal{H}} \\ &\qquad\qquad - \big(f,(T-(\lambda-i\varepsilon)I_{\mathcal{H}})^{-1}g\big)_{\mathcal{H}}\big]. \end{aligned} \tag{2.29}$$

Proof. First, assume $F\geq 0$. Then

$$\begin{aligned} &\big(F(T)^{1/2}E_T((\lambda_1,\lambda_2])f,(T-zI_{\mathcal{H}})^{-1}F(T)^{1/2}E_T((\lambda_1,\lambda_2])f\big)_{\mathcal{H}} \\ &\quad = \int_{\mathbb{R}} d\big(f,E_T(\lambda)f\big)_{\mathcal{H}}\,F(\lambda)\chi_{(\lambda_1,\lambda_2]}(\lambda)(\lambda-z)^{-1} \\ &\quad = \int_{\mathbb{R}} \frac{d\big(F(T)^{1/2}\chi_{(\lambda_1,\lambda_2]}(T)f,E_T(\lambda)F(T)^{1/2}\chi_{(\lambda_1,\lambda_2]}(T)f\big)_{\mathcal{H}}}{(\lambda-z)}, \quad z\in\mathbb{C}_+ \end{aligned} \tag{2.30}$$

is a Herglotz function and hence (2.29) for $g=f$ follows from (A.4). If F is not nonnegative, one decomposes F as $F=(F_1-F_2)+i(F_3-F_4)$ with $F_j\geq 0$, $1\leq j\leq 4$ and applies (2.30) to each $j\in\{1,2,3,4\}$. The general case $g\neq f$ then follows from the case $g=f$ by polarization. $\square$

Next, we relate the family of spectral projections, $\{E_{H_{+,\alpha}}(\lambda)\}_{\lambda\in\mathbb{R}}$, of the self-adjoint operator $H_{+,\alpha}$ and the spectral function $\rho_{+,\alpha}(\lambda)$, $\lambda \in \mathbb{R}$, which generates the measure in the Herglotz representation (2.27) of $m_{+,\alpha}$.

We first note that for $F \in C(\mathbb{R})$,

$$
\begin{aligned}
&\big(f, F(H_{+,\alpha})g\big)_{L^2([a,\infty);dx)} = \int_{\mathbb{R}} d\big(f, E_{H_{+,\alpha}}(\lambda)g\big)_{L^2([a,\infty);dx)}\, F(\lambda), \\
&f, g \in \mathrm{dom}(F(H_{+,\alpha})) \qquad\qquad (2.31)\\
&\quad = \bigg\{h \in L^2([a,\infty); dx) \,\bigg|\, \int_{\mathbb{R}} d\big\|E_{H_{+,\alpha}}(\lambda)h\big\|^2_{L^2([a,\infty);dx)}\, |F(\lambda)|^2 < \infty\bigg\}.
\end{aligned}
$$

Equation (2.31) extends to measurable functions F and holds also in the strong sense, but the displayed weak version will suffice for our purpose.

In the following, $C_0^\infty((c,d))$, $-\infty \le c < d \le \infty$, denotes the usual space of infinitely differentiable functions of compact support contained in (c,d).

Theorem 2.6. *Let $\alpha \in [0,\pi)$, $f, g \in C_0^\infty((a,\infty))$, $F \in C(\mathbb{R})$, and $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$. Then,*

$$
\big(f, F(H_{+,\alpha})E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} = \big(\widehat{f}_{+,\alpha}, M_F M_{\chi_{(\lambda_1,\lambda_2]}} \widehat{g}_{+,\alpha}\big)_{L^2(\mathbb{R};d\rho_{+,\alpha})}, \tag{2.32}
$$

where we introduced the notation

$$
\widehat{h}_{+,\alpha}(\lambda) = \int_a^\infty dx\, \phi_\alpha(\lambda,x)h(x), \quad \lambda \in \mathbb{R},\ h \in C_0^\infty((a,\infty)), \tag{2.33}
$$

and M_G denotes the maximally defined operator of multiplication by the $d\rho_{+,\alpha}$-measurable function G in the Hilbert space $L^2(\mathbb{R}; d\rho_{+,\alpha})$,

$$
\begin{aligned}
&(M_G\widehat{h})(\lambda) = G(\lambda)\widehat{h}(\lambda) \ \text{ for a.e. } \lambda \in \mathbb{R}, \\
&\widehat{h} \in \mathrm{dom}(M_G) = \{\widehat{k} \in L^2(\mathbb{R}; d\rho_{+,\alpha}) \,|\, G\widehat{k} \in L^2(\mathbb{R}; d\rho_{+,\alpha})\}.
\end{aligned} \tag{2.34}
$$

Here $d\rho_{+,\alpha}$ is the measure in the Herglotz representation of the Weyl–Titchmarsh function $m_{+,\alpha}$ (cf. (2.27)).

Proof. The point of departure for deriving (2.32) is Stone's formula (2.29) applied to $T = H_{+,\alpha}$,

$$
\begin{aligned}
&\big(f, F(H_{+,\alpha})E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} \\
&\quad = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0} \frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda)\big[\big(f, (H_{+,\alpha}-(\lambda+i\varepsilon)I)^{-1}g\big)_{L^2([a,\infty);dx)} \\
&\qquad\qquad - \big(f, (H_{+,\alpha}-(\lambda-i\varepsilon)I)^{-1}g\big)_{L^2([a,\infty);dx)}\big].
\end{aligned} \tag{2.35}
$$

Insertion of (2.18) and (2.19) into (2.35) then yields the following:

$$\begin{aligned}
\big(f, F(H_{+,\alpha})E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} &= \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda)\\
\times\bigg\{\int_a^\infty dx\,\bigg[&\overline{f(x)}\psi_{+,\alpha}(\lambda+i\varepsilon,x)\int_a^x dx'\,\phi_\alpha(\lambda+i\varepsilon,x')g(x')\\
&+\overline{f(x)}\phi_\alpha(\lambda+i\varepsilon,x)\int_x^\infty dx'\,\psi_{+,\alpha}(\lambda+i\varepsilon,x')g(x')\bigg]\\
-\bigg[&\overline{f(x)}\psi_{+,\alpha}(\lambda-i\varepsilon,x)\int_a^x dx'\,\phi_\alpha(\lambda-i\varepsilon,x')g(x')\\
&+\overline{f(x)}\phi_\alpha(\lambda-i\varepsilon,x)\int_x^\infty dx'\,\psi_{+,\alpha}(\lambda-i\varepsilon,x')g(x')\bigg]\bigg\}. \qquad (2.36)
\end{aligned}$$

Freely interchanging the dx and dx' integrals with the limits and the the $d\lambda$ integral (since all integration domains are finite and all integrands are continuous), and inserting expression (2.10) for $\psi_{+,\alpha}(z,x)$ into (2.36), one obtains

$$\begin{aligned}
\big(f, F(H_{+,\alpha})E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} &= \int_a^\infty dx\,\overline{f(x)}\bigg\{\int_a^x dx'\,g(x')\\
\times\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda)\Big[&\big[\theta_\alpha(\lambda,x)+m_{+,\alpha}(\lambda+i\varepsilon)\phi_\alpha(\lambda,x)\big]\phi_\alpha(\lambda,x')\\
&-\big[\theta_\alpha(\lambda,x)+m_{+,\alpha}(\lambda-i\varepsilon)\phi_\alpha(\lambda,x)\big]\phi_\alpha(\lambda,x')\Big]\\
+\int_x^\infty dx'\,g(x')\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} &d\lambda\, F(\lambda) \qquad (2.37)\\
\times\Big[&\phi_\alpha(\lambda,x)\big[\theta_\alpha(\lambda,x')+m_{+,\alpha}(\lambda+i\varepsilon)\phi_\alpha(\lambda,x')\big]\\
&-\phi_\alpha(\lambda,x)\big[\theta_\alpha(\lambda,x')+m_{+,\alpha}(\lambda-i\varepsilon)\phi_\alpha(\lambda,x')\big]\Big]\bigg\}.
\end{aligned}$$

Here we employed the fact that for fixed $x\in[a,\infty)$, $\theta_\alpha(z,x)$ and $\phi_\alpha(z,x)$ are entire with respect to z, that $\theta_\alpha(\lambda,x,x_0)$ and $\phi_\alpha(\lambda,x,x_0)$ are real-valued for $\lambda\in\mathbb{R}$, that $\theta_\alpha(z,\cdot),\phi_\alpha(z,\cdot)\in AC([a,c])$ for all $c>a$, and hence that

$$\begin{aligned}
\theta_\alpha(\lambda\pm i\varepsilon,x,x_0) &\underset{\varepsilon\downarrow 0}{=} \theta_\alpha(\lambda,x,x_0)+i\varepsilon(d/dz)\theta_\alpha(z,x,x_0)|_{z=\lambda}+O(\varepsilon^2),\\
\phi_\alpha(\lambda\pm i\varepsilon,x,x_0) &\underset{\varepsilon\downarrow 0}{=} \phi_\alpha(\lambda,x,x_0)+i\varepsilon(d/dz)\phi_\alpha(z,x,x_0)|_{z=\lambda}+O(\varepsilon^2)
\end{aligned} \qquad (2.38)$$

with $O(\varepsilon^2)$ being uniform with respect to (λ,x) as long as λ and x vary in compact subsets of $\mathbb{R}\times[a,\infty)$. Moreover, we used that

$$\begin{aligned}
&\varepsilon|m_{+,\alpha}(\lambda+i\varepsilon)|\le C(\lambda_1,\lambda_2,\varepsilon_0) \text{ for } \lambda\in[\lambda_1,\lambda_2],\ 0<\varepsilon\le\varepsilon_0,\\
&\varepsilon|\mathrm{Re}(m_{+,\alpha}(\lambda+i\varepsilon))| \underset{\varepsilon\downarrow 0}{=} o(1), \quad \lambda\in\mathbb{R}.
\end{aligned} \qquad (2.39)$$

In particular, utilizing (2.38) and (2.39), $\phi_\alpha(\lambda\pm i\varepsilon,x)$ and $\theta_\alpha(\lambda\pm i\varepsilon,x)$ have been replaced by $\phi_\alpha(\lambda,x)$ and $\theta_\alpha(\lambda,x)$ under the $d\lambda$ integrals in (2.37). Cancelling appropriate terms in (2.37), simplifying the remaining terms, and using (2.16) then yield

$$\begin{aligned}\big(f, F(H_{+,\alpha})E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} &= \int_a^\infty dx\,\overline{f(x)}\int_a^\infty dx'\,g(x') \\ &\times \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\,F(\lambda)\phi_\alpha(\lambda,x)\phi_\alpha(\lambda,x')\mathrm{Im}(m_{+,\alpha}(\lambda+i\varepsilon)).\end{aligned} \tag{2.40}$$

Using the fact that by (A.4)

$$\int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda) = \rho_{+,\alpha}((\lambda_1,\lambda_2]) = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\,\mathrm{Im}(m_{+,\alpha}(\lambda+i\varepsilon)), \tag{2.41}$$

and hence that

$$\int_{\mathbb{R}} d\rho_{+,\alpha}(\lambda)\,h(\lambda) = \lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\mathbb{R}} d\lambda\,\mathrm{Im}(m_{+,\alpha}(\lambda+i\varepsilon))\,h(\lambda), \quad h\in C_0(\mathbb{R}), \tag{2.42}$$

$$\int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\,k(\lambda) = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\,\mathrm{Im}(m_{+,\alpha}(\lambda+i\varepsilon))\,k(\lambda), \quad k\in C(\mathbb{R}), \tag{2.43}$$

(with $C_0(\mathbb{R})$ the space of continuous compactly supported functions on $\mathbb{R}$) one concludes

$$\begin{aligned}&\big(f, F(H_{+,\alpha})E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} \\ &\quad = \int_a^\infty dx\,\overline{f(x)}\int_a^\infty dx'\,g(x')\int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)F(\lambda)\phi_\alpha(\lambda,x)\phi_\alpha(\lambda,x') \\ &\quad = \int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)F(\lambda)\,\overline{\widehat{f}_{+,\alpha}(\lambda)}\,\widehat{g}_{+,\alpha}(\lambda),\end{aligned} \tag{2.44}$$

using (2.33) and interchanging the dx, dx' and $d\rho_{+,\alpha}$ integrals once more. ☐

Remark 2.7. Theorem 2.6 is of course well-known. We presented a detailed proof since this proof will serve as the model for generalizations to strongly singular potentials and hence pave the way into somewhat unchartered territory in Section 3. In this context it is worthwhile to examine the principal ingredients entering the proof of Theorem 2.6: Let $\lambda_j\in\mathbb{R}$, $j=0,1,2$, $\lambda_1<\lambda_2$, and $\varepsilon_0>0$. Then the following items played a crucial role in the proof of Theorem 2.6:

(i) For all $x\in[a,\infty)$, $\theta_\alpha(z,x)$ and $\phi_\alpha(z,x)$ are entire with respect to z and real-valued for $z\in\mathbb{R}$.

(ii) $m_{+,\alpha}$ is analytic on $\mathbb{C}\backslash\mathbb{R}$.

(iii) $\overline{m_{+,\alpha}(z)} = m_{+,\alpha}(\overline{z}), \quad z\in\mathbb{C}_+$.

(iv) $\varepsilon|m_{+,\alpha}(\lambda+i\varepsilon)|\leq C, \quad \lambda\in[\lambda_1,\lambda_2],\ 0<\varepsilon\leq\varepsilon_0.$ (2.45)

(v) $\varepsilon|\mathrm{Re}(m_{+,\alpha}(\lambda+i\varepsilon))| \underset{\varepsilon\downarrow 0}{=} o(1), \quad \lambda\in\mathbb{R}$.

(vi) $\rho_{+,\alpha}(\lambda)-\rho_{+,\alpha}(\lambda_0) = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_0+\delta}^{\lambda+\delta} d\mu\,\mathrm{Im}(m_{+,\alpha}(\mu+i\varepsilon))$.

defines a nondecreasing function $\rho_{+,\alpha}$ and hence a measure on $\mathbb{R}$.

Of course, properties (ii)–(vi) are satisfied by any Herglotz function. However, as we will see in Sections 3 and 4, properties (ii)–(vi) (possibly restricting z to a sufficiently small neighborhood of $\mathbb{R}$) are also crucial in connection with a class of strongly singular potentials at $x = a$, where the analog of the coefficient $m_{+,\alpha}$ will necessarily turn out to be a non-Herglotz function. In particular, one can (and we will in Section 3) use an analog of (2.20) to prove items (ii)–(vi) in (2.45) (for $|\mathrm{Im}(z)|$ sufficiently small) without ever invoking the Herglotz property of $m_{+,\alpha}$, by just using the fact that the left-hand side of (2.20) is a Herglotz function whether or not the potential V is strongly singular at the endpoint a. Thus, the mere existence of the family of spectral projections $\{E_{H_{+,\alpha}}(\lambda)\}_{\lambda\in\mathbb{R}}$ of the self-adjoint operator $H_{+,\alpha}$ implies properties of the type (ii)–(vi).

Remark 2.8. The effortless derivation of the link between the family of spectral projections $E_{H_{+,\alpha}}(\cdot)$ and the spectral function $\rho_{+,\alpha}(\cdot)$ of $H_{+,\alpha}$ in Theorem 2.6 applies equally well to half-line Dirac-type operators and Hamiltonian systems (see the extensive literature cited, e.g., in [16]) and to half-lattice Jacobi and CMV operators (cf. [13] and [42]). After circulating a first draft of this manuscript, it was kindly pointed out to us by Don Hinton that the idea of linking the family of spectral projections and the spectral function using Stone's formula as the starting point can already be found in a paper by Hinton and Schneider [47] published in 1998.

Actually, one can improve on Theorem 2.6 and remove the compact support restrictions on f and g in the usual way. To this end one considers the map

$$\widetilde{U}_{+,\alpha}\colon \begin{cases} C_0^\infty((a,\infty)) \to L^2(\mathbb{R};d\rho_{+,\alpha}) \\ \qquad\qquad h \mapsto \widehat{h}_{+,\alpha}(\cdot) = \int_a^\infty dx\, \phi_\alpha(\cdot,x)h(x). \end{cases} \tag{2.46}$$

Taking $f = g$, $F = 1$, $\lambda_1 \downarrow -\infty$, and $\lambda_2 \uparrow \infty$ in (2.32) then shows that $\widetilde{U}_{+,\alpha}$ is a densely defined isometry in $L^2([a,\infty);dx)$, which extends by continuity to an isometry on $L^2([a,\infty);dx)$. The latter is denoted by $U_{+,\alpha}$ and given by

$$U_{+,\alpha}\colon \begin{cases} L^2([a,\infty);dx) \to L^2(\mathbb{R};d\rho_{+,\alpha}) \\ \qquad\qquad h \mapsto \widehat{h}_{+,\alpha}(\cdot) = \operatorname{l.i.m.}_{b\uparrow\infty} \int_a^b dx\, \phi_\alpha(\cdot,x)h(x), \end{cases} \tag{2.47}$$

where l.i.m. refers to the $L^2(\mathbb{R};d\rho_{+,\alpha})$-limit.

The calculation in (2.44) also yields

$$(E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g)(x) = \int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\, \phi_\alpha(\lambda,x)\widehat{g}_{+,\alpha}(\lambda), \quad g \in C_0^\infty((a,\infty)) \tag{2.48}$$

and subsequently, (2.48) extends to all $g \in L^2([a,\infty);dx)$ by continuity. Moroever, taking $\lambda_1 \downarrow -\infty$ and $\lambda_2 \uparrow \infty$ in (2.48) using

$$\text{s-lim}_{\lambda\downarrow-\infty} E_{H_{+,\alpha}}(\lambda) = 0, \quad \text{s-lim}_{\lambda\uparrow\infty} E_{H_{+,\alpha}}(\lambda) = I_{L^2([a,\infty);dx)}, \tag{2.49}$$

where

$$E_{H_{+,\alpha}}(\lambda) = E_{H_{+,\alpha}}((-\infty,\lambda]), \tag{2.50}$$

then yields

$$g(\cdot) = \operatorname{l.i.m.}_{\mu_1\downarrow-\infty,\mu_2\uparrow\infty} \int_{\mu_1}^{\mu_2} d\rho_{+,\alpha}(\lambda)\, \phi_\alpha(\lambda,\cdot)\widehat{g}_{+,\alpha}(\lambda), \quad g \in L^2([a,\infty);dx), \tag{2.51}$$

where l.i.m. refers to the $L^2([a,\infty);dx)$-limit.

In addition, one can show that the map $U_{+,\alpha}$ in (2.47) is onto and hence that $U_{+,\alpha}$ is unitary (i.e., $U_{+,\alpha}$ and $U_{+,\alpha}^{-1}$ are isometric isomorphisms between $L^2([a,\infty);dx)$ and $L^2(\mathbb{R};d\rho_{+,\alpha})$) with

$$U_{+,\alpha}^{-1}\colon \begin{cases} L^2(\mathbb{R};d\rho_{+,\alpha}) \to L^2([a,\infty);dx) \\ \qquad \widehat{h} \mapsto \text{l.i.m.}_{\mu_1\downarrow-\infty,\mu_2\uparrow\infty} \int_{\mu_1}^{\mu_2} d\rho_{+,\alpha}(\lambda)\,\phi_\alpha(\lambda,\cdot)\widehat{h}(\lambda). \end{cases} \tag{2.52}$$

Indeed, consider an arbitrary function $f \in L^2(\mathbb{R};d\rho_{+,\alpha})$ such that

$$\big(f, U_{+,\alpha}h\big)_{L^2(\mathbb{R};d\rho_{+,\alpha})} = 0 \ \text{ for all } h \in L^2([a,\infty);dx). \tag{2.53}$$

Then, (2.53) holds for $h = E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g$, $\lambda_1,\lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$, $g \in C_0^\infty([a,\infty))$. Utilizing (2.48) one rewrites (2.53) as,

$$\begin{aligned} 0 &= \big(f, U_{+,\alpha}E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g\big)_{L^2(\mathbb{R};d\rho_{+,\alpha})} = \big(f, U_{+,\alpha}U_{+,\alpha}^{-1}\chi_{(\lambda_1,\lambda_2]}U_{+,\alpha}g\big)_{L^2(\mathbb{R};d\rho_{+,\alpha})} \\ &= \int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\,\overline{f(\lambda)} \int_{[a,\infty)} dx\,\phi_\alpha(\lambda,x)g(x) \\ &= \int_{[a,\infty)} dx\,g(x) \int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\,\phi_\alpha(\lambda,x)\overline{f(\lambda)}. \end{aligned} \tag{2.54}$$

Since $C_0^\infty([a,\infty))$ is dense in $L^2([a,\infty);dx)$ one concludes that

$$\int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\,\phi_\alpha(\lambda,x)\overline{f(\lambda)} = 0 \ \text{ for a.e. } x \in [a,\infty). \tag{2.55}$$

Differentiating (2.55) with respect to x leads to

$$\int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\phi_\alpha'(\lambda,x)\overline{f(\lambda)} = 0 \ \text{ for a.e. } x \in [a,\infty). \tag{2.56}$$

Using the dominated convergence theorem and the fact that $f \in L^2(\mathbb{R};d\rho_{+,\alpha}) \subseteq L^1((\lambda_1,\lambda_2];d\rho_{+,\alpha})$ and that $\phi_\alpha(\lambda,x), \phi_\alpha'(\lambda,x)$ are continuous in $(\lambda,x) \in \mathbb{R}\times[a,\infty)$, one concludes

$$\begin{aligned} &\int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\,\phi_\alpha(\lambda,x_0)\overline{f(\lambda)} = -\sin(\alpha)\int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\,\overline{f(\lambda)} = 0, \\ &\int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\,\phi_\alpha'(\lambda,x_0)\overline{f(\lambda)} = \cos(\alpha)\int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\,\overline{f(\lambda)} = 0. \end{aligned} \tag{2.57}$$

Since the interval $(\lambda_1,\lambda_2]$ was chosen arbitrary, (2.57) implies

$$f(\lambda) = 0 \ \ d\rho_{+,\alpha}\text{-a.e.}, \tag{2.58}$$

and hence $U_{+,\alpha}$ is onto.

We sum up these considerations in a variant of the spectral theorem for (functions of) $H_{+,\alpha}$.

Theorem 2.9. *Let $\alpha \in [0,\pi)$ and $F \in C(\mathbb{R})$. Then,*

$$U_{+,\alpha}F(H_{+,\alpha})U_{+,\alpha}^{-1} = M_F \tag{2.59}$$

in $L^2(\mathbb{R};d\rho_{+,\alpha})$ (cf. (2.34)). Moreover,

$$\sigma(F(H_{+,\alpha})) = \text{ess.ran}_{d\rho_{+,\alpha}}(F), \tag{2.60}$$

$$\sigma(H_{+,\alpha}) = \text{supp}\,(d\rho_{+,\alpha}), \tag{2.61}$$

and the spectrum of $H_{+,\alpha}$ is simple.

Here the essential range of F with respect to a measure $d\mu$ is defined by

$$\text{ess.ran}_{d\mu}(F) = \{z \in \mathbb{C} \,|\, \text{for all } \varepsilon > 0, \mu(\{\lambda \in \mathbb{R} \,|\, |F(\lambda) - z| < \varepsilon\}) > 0\}. \tag{2.62}$$

We conclude the half-line case by recalling the following elementary example of the Fourier-sine transform.

Example 2.10. *Let $\alpha = 0$ and $V(x) = 0$ for a.e. $x \in (0,\infty)$. Then,*

$$\begin{aligned} &\phi_0(\lambda, x) = \frac{\sin(\lambda^{1/2}x)}{\lambda^{1/2}}, \quad \lambda \geq 0, \ x \in (0,\infty), \\ &d\rho_{+,0}(\lambda) = \pi^{-1}\chi_{[0,\infty)}(\lambda)\lambda^{1/2}d\lambda, \quad \lambda \in \mathbb{R}, \end{aligned} \tag{2.63}$$

and hence,

$$\widehat{h}(\lambda) = \text{l.i.m.}_{y\uparrow\infty} \int_0^y dx\, \frac{\sin(\lambda^{1/2}x)}{\lambda^{1/2}} h(x), \quad h \in L^2([0,\infty); dx), \tag{2.64}$$
$$h(x) = \text{l.i.m.}_{\mu\uparrow\infty} \frac{1}{\pi}\int_0^\mu \lambda^{1/2}d\lambda\, \frac{\sin(\lambda^{1/2}x)}{\lambda^{1/2}}\, \widehat{h}(\lambda), \quad \widehat{h} \in L^2([0,\infty); \pi^{-1}\lambda^{1/2}d\lambda).$$

Introducing the change of variables

$$p = \lambda^{1/2} > 0, \quad \widehat{H}(p) = \left(\frac{2\lambda}{\pi}\right)^{1/2} \widehat{h}(\lambda), \tag{2.65}$$

the pair of equations in (2.64) *takes on the usual symmetric form of the Fourier-sine transform,*

$$\begin{aligned} &\widehat{H}(p) = \text{l.i.m.}_{y\uparrow\infty} \left(\frac{2}{\pi}\right)^{1/2} \int_0^y dx\, \sin(px)h(x), \quad h \in L^2([0,\infty); dx), \\ &h(x) = \text{l.i.m.}_{q\uparrow\infty} \left(\frac{2}{\pi}\right)^{1/2} \int_0^q dp\, \sin(px)\widehat{H}(p), \quad \widehat{H} \in L^2([0,\infty); dp). \end{aligned} \tag{2.66}$$

Next, we turn to the case of the entire real line and make the following basic assumption.

Hypothesis 2.11. (i) *Assume that*

$$V \in L^1_{\text{loc}}(\mathbb{R}; dx), \quad V \text{ real-valued.} \tag{2.67}$$

(ii) *Introducing the differential expression τ given by*

$$\tau = -\frac{d^2}{dx^2} + V(x), \quad x \in \mathbb{R}, \tag{2.68}$$

we assume τ to be in the limit point case at $+\infty$ and at $-\infty$.

Associated with the differential expression τ one introduces the self-adjoint Schrödinger operator H in $L^2(\mathbb{R}; dx)$ by

$$\begin{aligned} &Hf = \tau f, \\ &f \in \text{dom}(H) = \{g \in L^2(\mathbb{R}; dx) \,|\, g, g' \in AC_{\text{loc}}(\mathbb{R});\ \tau g \in L^2(\mathbb{R}; dx)\}. \end{aligned} \tag{2.69}$$

Here $AC_{\text{loc}}(\mathbb{R})$ denotes the class of locally absolutely continuous functions on $\mathbb{R}$.

As in the half-line context we introduce the usual fundamental system of solutions $\phi_\alpha(z, \cdot, x_0)$ and $\theta_\alpha(z, \cdot, x_0)$, $z \in \mathbb{C}$, of

$$(\tau\psi)(z, x) = z\psi(z, x), \quad x \in \mathbb{R} \tag{2.70}$$

with respect to a fixed reference point $x_0 \in \mathbb{R}$, satisfying the initial conditions at the point $x = x_0$,

$$\begin{aligned} &\phi_\alpha(z,x_0,x_0) = -\theta'_\alpha(z,x_0,x_0) = -\sin(\alpha), \\ &\phi'_\alpha(z,x_0,x_0) = \theta_\alpha(z,x_0,x_0) = \cos(\alpha), \quad \alpha \in [0,\pi). \end{aligned} \tag{2.71}$$

Again we note that for any fixed $x, x_0 \in \mathbb{R}$, $\phi_\alpha(z,x,x_0)$ and $\theta_\alpha(z,x,x_0)$ are entire with respect to z and that

$$W(\theta_\alpha(z,\cdot,x_0), \phi_\alpha(z,\cdot,x_0))(x) = 1, \quad z \in \mathbb{C}. \tag{2.72}$$

Particularly important solutions of (2.70) are the *Weyl–Titchmarsh solutions* $\psi_{\pm,\alpha}(z,\cdot,x_0)$, $z \in \mathbb{C}\backslash\mathbb{R}$, uniquely characterized by

$$\begin{aligned} &\psi_{\pm,\alpha}(z,\cdot,x_0) \in L^2([x_0,\pm\infty);dx), \\ &\sin(\alpha)\psi'_{\pm,\alpha}(z,x_0,x_0) + \cos(\alpha)\psi_{\pm,\alpha}(z,x_0,x_0) = 1, \quad z \in \mathbb{C}\backslash\mathbb{R}. \end{aligned} \tag{2.73}$$

The crucial condition in (2.73) is again the L^2-property which uniquely determines $\psi_{\pm,\alpha}(z,\cdot,x_0)$ up to constant multiples by the limit point hypothesis of τ at $\pm\infty$. In particular, for $\alpha, \beta \in [0,\pi)$,

$$\begin{aligned} &\psi_{\pm,\alpha}(z,\cdot,x_0) = C_\pm(z,\alpha,\beta,x_0)\psi_{\pm,\beta}(z,\cdot,x_0) \\ &\quad \text{for some coefficients } C_\pm(z,\alpha,\beta,x_0) \in \mathbb{C}. \end{aligned} \tag{2.74}$$

The normalization in (2.73) shows that $\psi_{\pm,\alpha}(z,\cdot,x_0)$ are of the type

$$\psi_{\pm,\alpha}(z,x,x_0) = \theta_\alpha(z,x,x_0) + m_{\pm,\alpha}(z,x_0)\phi_\alpha(z,x,x_0), \quad z \in \mathbb{C}\backslash\mathbb{R},\ x \in \mathbb{R} \tag{2.75}$$

for some coefficients $m_{\pm,\alpha}(z,x_0)$, the *Weyl–Titchmarsh m-functions* associated with τ, α, and x_0.

Again we recall the fundamental identity

$$\begin{aligned} \int_{x_0}^{\pm\infty} dx\, \psi_{\pm,\alpha}(z_1,x,x_0)\psi_{\pm,\alpha}(z_2,x,x_0) &= \frac{m_{\pm,\alpha}(z_1,x_0) - m_{\pm,\alpha}(z_2,x_0)}{z_1 - z_2}, \\ &\qquad z_1, z_2 \in \mathbb{C}\backslash\mathbb{R},\ z_1 \neq z_2, \end{aligned} \tag{2.76}$$

and as before one concludes

$$\overline{m_{\pm,\alpha}(z,x_0)} = m_{\pm,\alpha}(\overline{z},x_0), \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{2.77}$$

Choosing $z_1 = z$, $z_2 = \overline{z}$ in (2.76), one infers

$$\int_{x_0}^{\pm\infty} dx\, |\psi_{\pm,\alpha}(z,x,x_0)|^2 = \frac{\mathrm{Im}(m_{\pm,\alpha}(z,x_0))}{\mathrm{Im}(z)}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{2.78}$$

Since $m_{\pm,\alpha}(\cdot,x_0)$ are analytic on $\mathbb{C}\backslash\mathbb{R}$, $\pm m_{\pm,\alpha}(\cdot,x_0)$ are Herglotz functions.

The Green's function $G(z,x,x')$ of H then reads

$$\begin{aligned} G(z,x,x') = &\frac{1}{W(\psi_{+,\alpha}(z,\cdot,x_0), \psi_{-,\alpha}(z,\cdot,x_0))} \\ &\times \begin{cases} \psi_{-,\alpha}(z,x,x_0)\psi_{+,\alpha}(z,x',x_0), & x \leq x', \\ \psi_{-,\alpha}(z,x',x_0)\psi_{+,\alpha}(z,x,x_0), & x' \leq x, \end{cases} \quad z \in \mathbb{C}\backslash\mathbb{R} \end{aligned} \tag{2.79}$$

with

$$W(\psi_{+,\alpha}(z,\cdot,x_0), \psi_{-,\alpha}(z,\cdot,x_0)) = m_{-,\alpha}(z,x_0) - m_{+,\alpha}(z,x_0), \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{2.80}$$

Thus,

$$((H - zI)^{-1}f)(x) = \int_{\mathbb{R}} dx' \, G(z,x,x') f(x'), \quad z \in \mathbb{C}\backslash\mathbb{R}, \ x \in \mathbb{R}, \ f \in L^2(\mathbb{R}; dx). \tag{2.81}$$

Given $m_\pm(z,x_0)$, we also introduce the 2×2 matrix-valued Weyl–Titchmarsh function

$$M_\alpha(z,x_0) = \begin{pmatrix} \frac{1}{m_{-,\alpha}(z,x_0) - m_{+,\alpha}(z,x_0)} & \frac{1}{2}\frac{m_{-,\alpha}(z,x_0)+m_{+,\alpha}(z,x_0)}{m_{-,\alpha}(z,x_0)-m_{+,\alpha}(z,x_0)} \\ \frac{1}{2}\frac{m_{-,\alpha}(z,x_0)+m_{+,\alpha}(z,x_0)}{m_{-,\alpha}(z,x_0)-m_{+,\alpha}(z,x_0)} & \frac{m_{-,\alpha}(z,x_0)m_{+,\alpha}(z,x_0)}{m_{-,\alpha}(z,x_0)-m_{+,\alpha}(z,x_0)} \end{pmatrix}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{2.82}$$

$M_\alpha(z,x_0)$ is a Herglotz matrix with representation

$$\begin{aligned} &M_\alpha(z,x_0) = C_\alpha(x_0) + \int_{\mathbb{R}} d\Omega_\alpha(\lambda,x_0)\bigg[\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\bigg], \quad z \in \mathbb{C}\backslash\mathbb{R}, \\ &C_\alpha(x_0) = C_\alpha(x_0)^*, \quad \int_{\mathbb{R}} \frac{\|d\Omega_\alpha(\lambda,x_0)\|}{1+\lambda^2} < \infty. \end{aligned} \tag{2.83}$$

The Stieltjes inversion formula for the 2×2 nonnegative matrix-valued measure $d\Omega_\alpha(\cdot,x_0)$ then reads

$$\Omega_\alpha((\lambda_1,\lambda_2],x_0) = \pi^{-1}\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda \, \mathrm{Im}(M_\alpha(\lambda+i\varepsilon,x_0)), \quad \lambda_1,\lambda_2 \in \mathbb{R}, \ \lambda_1 < \lambda_2. \tag{2.84}$$

In particular, this implies that the entries $d\Omega_{\alpha,\ell,\ell'}$, $\ell,\ell' = 0,1$, of the matrix-valued measure $d\Omega_\alpha$ are real-valued scalar measures. Moreover, since the diagonal entries of M_α are Herglotz functions, the diagonal entries of the measure $d\Omega_\alpha$ are nonnegative measures. The off-diagonal entries of the measure $d\Omega_\alpha$ equal a signed measure which naturally admits a decomposition into a difference of two nonnegative measures and hence the off-diagonal entries of M_α represent a difference of two Herglotz functions.

We note that in formulas (2.73)–(2.83) one can replace $z \in \mathbb{C}\backslash\mathbb{R}$ by $z \in \mathbb{C}\backslash\sigma(H)$.

Next, we relate the family of spectral projections, $\{E_H(\lambda)\}_{\lambda\in\mathbb{R}}$, of the self-adjoint operator H and the 2×2 matrix-valued increasing spectral function $\Omega_\alpha(\lambda,x_0)$, $\lambda \in \mathbb{R}$, which generates the matrix-valued measure in the Herglotz representation (2.83) of $M_\alpha(z,x_0)$.

We first note that for $F \in C(\mathbb{R})$,

$$\begin{aligned} &\big(f, F(H)g\big)_{L^2(\mathbb{R};dx)} = \int_{\mathbb{R}} d\big(f, E_H(\lambda)g\big)_{L^2(\mathbb{R};dx)} F(\lambda), \\ &f,g \in \mathrm{dom}(F(H)) = \bigg\{h \in L^2(\mathbb{R};dx) \,\bigg|\, \int_{\mathbb{R}} d\big\|E_H(\lambda)h\big\|^2_{L^2(\mathbb{R};dx)} |F(\lambda)|^2 < \infty\bigg\}. \end{aligned} \tag{2.85}$$

Given a 2×2 matrix-valued nonnegative measure $d\Omega = \big(d\Omega_{\ell,\ell'}\big)_{\ell,\ell'=0,1}$ on $\mathbb{R}$ with

$$d\Omega^{\mathrm{tr}} = d\Omega_{0,0} + d\Omega_{1,1} \tag{2.86}$$

its trace measure, the density matrix

$$\bigg(\frac{d\Omega_{\ell,\ell'}}{d\Omega^{\mathrm{tr}}}\bigg)_{\ell,\ell'=0,1} \tag{2.87}$$

is locally integrable on $\mathbb{R}$ with respect to $d\Omega^{\rm tr}$. One then introduces the vector-valued Hilbert space $L^2(\mathbb{R};d\Omega)$ in the following manner. Consider ordered pairs $f=(f_0,f_1)^\top$ of $d\Omega^{\rm tr}$-measurable functions such that

$$\sum_{\ell,\ell'=0}^{1} \overline{f_\ell(\cdot)}\,\frac{d\Omega_{\ell,\ell'}(\cdot)}{d\Omega^{\rm tr}(\cdot)}\,f_{\ell'}(\cdot) \tag{2.88}$$

is $d\Omega^{\rm tr}$-integrable on $\mathbb{R}$ and define $L^2(\mathbb{R};d\Omega)$ as the set of equivalence classes modulo $d\Omega$-null functions. Here $g=(g_0,g_1)^\top\in L^2(\mathbb{R};d\Omega)$ is defined to be a $d\Omega$-null function if

$$\int_{\mathbb{R}} d\Omega^{\rm tr}(\lambda)\sum_{\ell,\ell'=0}^{1}\overline{g_\ell(\lambda)}\,\frac{d\Omega_{\ell,\ell'}(\lambda)}{d\Omega^{\rm tr}(\lambda)}\,g_{\ell'}(\lambda)=0. \tag{2.89}$$

This space is complete with respect to the norm induced by the scalar product

$$(f,g)_{L^2(\mathbb{R};d\Omega)}=\int_{\mathbb{R}} d\Omega^{\rm tr}(\lambda)\sum_{\ell,\ell'=0}^{1}\overline{f_\ell(\lambda)}\,\frac{d\Omega_{\ell,\ell'}(\lambda)}{d\Omega^{\rm tr}(\lambda)}\,g_{\ell'}(\lambda),\quad f,g\in L^2(\mathbb{R};d\Omega). \tag{2.90}$$

For notational simplicity, expressions of the type (2.90) will usually be abbreviated by

$$(f,g)_{L^2(\mathbb{R};d\Omega)}=\int_{\mathbb{R}}\overline{f(\lambda)^\top}\,d\Omega(\lambda)\,g(\lambda),\quad f,g\in L^2(\mathbb{R};d\Omega). \tag{2.91}$$

(In this context we refer to [23, p. 1345–1346] for some peculiarities in connection with matrix-valued nonnegative measures.)

Theorem 2.12. *Let $\alpha\in[0,\pi)$, $f,g\in C_0^\infty(\mathbb{R})$, $F\in C(\mathbb{R})$, $x_0\in\mathbb{R}$, and $\lambda_1,\lambda_2\in\mathbb{R}$, $\lambda_1<\lambda_2$. Then,*

$$\begin{aligned}\big(f,F(H)E_H((\lambda_1,\lambda_2])g\big)_{L^2(\mathbb{R};dx)}&=\big(\widehat{f}_\alpha(\cdot,x_0),M_F M_{\chi_{(\lambda_1,\lambda_2]}}\widehat{g}_\alpha(\cdot,x_0)\big)_{L^2(\mathbb{R};d\Omega_\alpha(\cdot,x_0))}\\&=\int_{(\lambda_1,\lambda_2]}\overline{\widehat{f}_\alpha(\lambda,x_0)^\top}\,d\Omega_\alpha(\lambda,x_0)\,\widehat{g}_\alpha(\lambda,x_0)F(\lambda),\end{aligned} \tag{2.92}$$

where we introduced the notation

$$\begin{aligned}&\widehat{h}_{\alpha,0}(\lambda,x_0)=\int_{\mathbb{R}}dx\,\theta_\alpha(\lambda,x,x_0)h(x),\quad \widehat{h}_{\alpha,1}(\lambda,x_0)=\int_{\mathbb{R}}dx\,\phi_\alpha(\lambda,x,x_0)h(x),\\&\widehat{h}_\alpha(\lambda,x_0)=(\widehat{h}_{\alpha,0}(\lambda,x_0),\widehat{h}_{\alpha,1}(\lambda,x_0))^\top,\quad \lambda\in\mathbb{R},\ h\in C_0^\infty(\mathbb{R}),\end{aligned} \tag{2.93}$$

and M_G denotes the maximally defined operator of multiplication by the $d\Omega_\alpha^{\rm tr}$-measurable function G in the Hilbert space $L^2(\mathbb{R};d\Omega_\alpha(\cdot,x_0))$,

$$\begin{aligned}&(M_G\widehat{h})(\lambda)=G(\lambda)\widehat{h}(\lambda)=(G(\lambda)\widehat{h}_0(\lambda),G(\lambda)\widehat{h}_1(\lambda))^\top\ \text{for a.e. }\lambda\in\mathbb{R},\\&\widehat{h}\in\operatorname{dom}(M_G)=\{\widehat{k}\in L^2(\mathbb{R};d\Omega_\alpha(\cdot,x_0))\,|\,G\widehat{k}\in L^2(\mathbb{R};d\Omega_\alpha(\cdot,x_0))\}.\end{aligned} \tag{2.94}$$

Proof. The point of departure for deriving (2.92) is again Stone's formula (2.29) applied to $T=H$,

$$\begin{aligned}&\big(f,F(H)E_H((\lambda_1,\lambda_2])g\big)_{L^2(\mathbb{R};dx)}\\&\quad=\lim_{\delta\downarrow0}\lim_{\varepsilon\downarrow0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta}d\lambda\,F(\lambda)\big[\big(f,(H-(\lambda+i\varepsilon)I)^{-1}g\big)_{L^2(\mathbb{R};dx)}\\&\qquad\qquad-\big(f,(H-(\lambda-i\varepsilon)I)^{-1}g\big)_{L^2(\mathbb{R};dx)}\big].\end{aligned} \tag{2.95}$$

Insertion of (2.79) and (2.81) into (2.95) then yields the following:

$$
\begin{aligned}
&\big(f, F(H)E_H((\lambda_1,\lambda_2])g\big)_{L^2(\mathbb{R};dx)} = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda)\\
&\times\bigg\{\int_{\mathbb{R}} dx\,\frac{1}{W(\lambda+i\varepsilon)}\bigg[\overline{f(x)}\psi_{+,\alpha}(\lambda+i\varepsilon,x,x_0)\int_{-\infty}^{x} dx'\,\psi_{-,\alpha}(\lambda+i\varepsilon,x',x_0)g(x')\\
&\qquad + \overline{f(x)}\psi_{-,\alpha}(\lambda+i\varepsilon,x,x_0)\int_{x}^{\infty} dx'\,\psi_{+,\alpha}(\lambda+i\varepsilon,x',x_0)g(x')\bigg]\\
&\qquad - \frac{1}{W(\lambda-i\varepsilon)}\bigg[\overline{f(x)}\psi_{+,\alpha}(\lambda-i\varepsilon,x,x_0)\int_{-\infty}^{x} dx'\,\psi_{-,\alpha}(\lambda-i\varepsilon,x',x_0)g(x')\\
&\qquad + \overline{f(x)}\psi_{-,\alpha}(\lambda-i\varepsilon,x,x_0)\int_{x}^{\infty} dx'\,\psi_{+,\alpha}(\lambda-i\varepsilon,x',x_0)g(x')\bigg]\bigg\}, \qquad (2.96)
\end{aligned}
$$

where we used the abbreviation

$$
W(z) = W(\psi_{+,\alpha}(z,\cdot,x_0)),\psi_{-,\alpha}(z,\cdot,x_0)), \quad z\in\mathbb{C}\backslash\mathbb{R}. \tag{2.97}
$$

Freely interchanging the dx and dx' integrals with the limits and the $d\lambda$ integral (since all integration domains are finite and all integrands are continuous), and inserting the expressions (2.75) for $\psi_{\pm,\alpha}(z,x,x_0)$ into (2.96), one obtains

$$
\begin{aligned}
&\big(f, F(H)E_H((\lambda_1,\lambda_2])g\big)_{L^2(\mathbb{R};dx)} = \int_{\mathbb{R}} dx\,\overline{f(x)}\bigg\{\int_{-\infty}^{x} dx'\,g(x')\\
&\times\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda)\Big[\big[\theta_\alpha(\lambda,x,x_0)+m_{+,\alpha}(\lambda+i\varepsilon,x_0)\phi_\alpha(\lambda,x,x_0)\big]\\
&\qquad\times\big[\theta_\alpha(\lambda,x',x_0)+m_{-,\alpha}(\lambda+i\varepsilon,x_0)\phi_\alpha(\lambda,x',x_0)\big]W(\lambda+i\varepsilon)^{-1}\\
&\qquad-\big[\theta_\alpha(\lambda,x,x_0)+m_{+,\alpha}(\lambda-i\varepsilon,x_0)\phi_\alpha(\lambda,x,x_0)\big]\\
&\qquad\times\big[\theta_\alpha(\lambda,x',x_0)+m_{-,\alpha}(\lambda-i\varepsilon,x_0)\phi_\alpha(\lambda,x',x_0)\big]W(\lambda-i\varepsilon)^{-1}\Big]\\
&+\int_{x}^{\infty} dx'\,g(x')\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda) \qquad (2.98)\\
&\qquad\times\Big[\big[\theta_\alpha(\lambda,x,x_0)+m_{-,\alpha}(\lambda+i\varepsilon,x_0)\phi_\alpha(\lambda,x,x_0)\big]\\
&\qquad\times\big[\theta_\alpha(\lambda,x',x_0)+m_{+,\alpha}(\lambda+i\varepsilon,x_0)\phi_\alpha(\lambda,x',x_0)\big]W(\lambda+i\varepsilon)^{-1}\\
&\qquad-\big[\theta_\alpha(\lambda,x,x_0)+m_{-,\alpha}(\lambda-i\varepsilon,x_0)\phi_\alpha(\lambda,x,x_0)\big]\\
&\qquad\times\big[\theta_\alpha(\lambda,x',x_0)+m_{+,\alpha}(\lambda-i\varepsilon,x_0)\phi_\alpha(\lambda,x',x_0)\big]W(\lambda-i\varepsilon)^{-1}\Big]\bigg\}.
\end{aligned}
$$

Here we employed the fact that for fixed $x\in\mathbb{R}$, $\theta_\alpha(z,x,x_0)$ and $\phi_\alpha(z,x,x_0)$ are entire with respect to z, that $\theta_\alpha(\lambda,x,x_0)$ and $\phi_\alpha(\lambda,x,x_0)$ are real-valued for $\lambda\in\mathbb{R}$, that $\phi_\alpha(z,\cdot),\theta_\alpha(z,\cdot)\in AC_{\text{loc}}(\mathbb{R})$, and hence that

$$
\begin{aligned}
\theta_\alpha(\lambda\pm i\varepsilon,x,x_0) &\underset{\varepsilon\downarrow 0}{=} \theta_\alpha(\lambda,x,x_0)+i\varepsilon(d/dz)\theta_\alpha(z,x,x_0)|_{z=\lambda}+O(\varepsilon^2),\\
\phi_\alpha(\lambda\pm i\varepsilon,x,x_0) &\underset{\varepsilon\downarrow 0}{=} \phi_\alpha(\lambda,x,x_0)+i\varepsilon(d/dz)\phi_\alpha(z,x,x_0)|_{z=\lambda}+O(\varepsilon^2)
\end{aligned} \tag{2.99}
$$

with $O(\varepsilon^2)$ being uniform with respect to (λ, x) as long as λ and x vary in compact subsets of $\mathbb{R}^2$. Moreover, we used that

$$\begin{aligned}
&\varepsilon|M_{\alpha,\ell,\ell'}(\lambda+i\varepsilon,x_0)| \leq C(\lambda_1,\lambda_2,\varepsilon_0,x_0), \quad \lambda\in[\lambda_1,\lambda_2],\ 0<\varepsilon\leq\varepsilon_0,\ \ell,\ell'=0,1,\\
&\varepsilon|\mathrm{Re}(M_{\alpha,\ell,\ell'}(\lambda+i\varepsilon,x_0))| \underset{\varepsilon\downarrow 0}{=} o(1), \quad \lambda\in\mathbb{R},\ \ell,\ell'=0,1,
\end{aligned} \tag{2.100}$$

which follows from the properties of Herglotz functions since $M_{\alpha,\ell,\ell}$, $\ell=0,1$, are Herglotz and $M_{\alpha,0,1}=M_{\alpha,1,0}$ is a difference of two Herglotz functions. In particular, utilizing (2.77), (2.99), (2.100), and the elementary fact (cf. (2.80))

$$\mathrm{Im}\bigg[\frac{m_{\pm,\alpha}(\lambda+i\varepsilon,x_0)}{W(\lambda+i\varepsilon)}\bigg] = \frac{1}{2}\mathrm{Im}\bigg[\frac{m_{-,\alpha}(\lambda+i\varepsilon,x_0)+m_{+,\alpha}(\lambda+i\varepsilon,x_0)}{W(\lambda+i\varepsilon)}\bigg], \quad \lambda\in\mathbb{R},\ \varepsilon>0, \tag{2.101}$$

$\phi_\alpha(\lambda\pm i\varepsilon,x,x_0)$ and $\theta_\alpha(\lambda\pm i\varepsilon,x,x_0)$ under the $d\lambda$ integrals in (2.98) have been replaced by $\phi_\alpha(\lambda,x,x_0)$ and $\theta_\alpha(\lambda,x,x_0)$. Cancelling appropriate terms in (2.98) and simplifying the remaining terms then yield

$$\begin{aligned}
&\big(f,F(H)E_H((\lambda_1,\lambda_2])g\big)_{L^2(\mathbb{R};dx)}\\
&\quad=\int_{\mathbb{R}}dx\,\overline{f(x)}\int_{\mathbb{R}}dx'\,g(x')\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta}d\lambda\,F(\lambda)\\
&\qquad\times\bigg\{\theta_\alpha(\lambda,x,x_0)\theta_\alpha(\lambda,x',x_0)\mathrm{Im}\bigg[\frac{1}{m_{-,\alpha}(\lambda+i\varepsilon,x_0)-m_{+,\alpha}(\lambda+i\varepsilon,x_0)}\bigg]\\
&\qquad\quad+[\phi_\alpha(\lambda,x,x_0)\theta_\alpha(\lambda,x',x_0)+\theta_\alpha(\lambda,x,x_0)\phi_\alpha(\lambda,x',x_0)]\\
&\qquad\qquad\times\frac{1}{2}\mathrm{Im}\bigg[\frac{m_{-,\alpha}(\lambda+i\varepsilon,x_0)+m_{+,\alpha}(\lambda+i\varepsilon,x_0)}{m_{-,\alpha}(\lambda+i\varepsilon,x_0)-m_{+,\alpha}(\lambda+i\varepsilon,x_0)}\bigg]\\
&\qquad\quad+\phi_\alpha(\lambda,x,x_0)\phi_\alpha(\lambda,x',x_0)\mathrm{Im}\bigg[\frac{m_{-,\alpha}(\lambda+i\varepsilon,x_0)m_{+,\alpha}(\lambda+i\varepsilon,x_0)}{m_{-,\alpha}(\lambda+i\varepsilon,x_0)-m_{+,\alpha}(\lambda+i\varepsilon,x_0)}\bigg]\bigg\}.
\end{aligned} \tag{2.102}$$

Using the fact that by (2.84) ($\ell,\ell'=0,1$)

$$\begin{aligned}
\int_{(\lambda_1,\lambda_2]}d\Omega_{\alpha,\ell,\ell'}(\lambda,x_0)&=\Omega_{\alpha,\ell,\ell'}((\lambda_1,\lambda_2],x_0)\\
&=\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta}d\lambda\,\mathrm{Im}(M_{\alpha,\ell,\ell'}(\lambda+i\varepsilon,x_0)),
\end{aligned} \tag{2.103}$$

and hence that

$$\int_{\mathbb{R}}d\Omega_{\alpha,\ell,\ell'}(\lambda,x_0)\,h(\lambda)=\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\mathbb{R}}d\lambda\,\mathrm{Im}(M_{\alpha,\ell,\ell'}(\lambda+i\varepsilon,x_0))\,h(\lambda), \quad h\in C_0(\mathbb{R}), \tag{2.104}$$

$$\int_{(\lambda_1,\lambda_2]}d\Omega_{\alpha,\ell,\ell'}(\lambda,x_0)\,k(\lambda)=\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta}d\lambda\,\mathrm{Im}(M_{\alpha,\ell,\ell'}(\lambda+i\varepsilon,x_0))\,k(\lambda), \quad k\in C(\mathbb{R}), \tag{2.105}$$

one concludes

$$
\begin{aligned}
&\big(f, F(H)E_H((\lambda_1,\lambda_2])g\big)_{L^2(\mathbb{R};dx)} = \int_{\mathbb{R}} dx\, \overline{f(x)} \int_{\mathbb{R}} dx'\, g(x') \int_{(\lambda_1,\lambda_2]} F(\lambda) \\
&\quad \times \Big\{\theta_\alpha(\lambda,x,x_0)\theta_\alpha(\lambda,x',x_0)d\Omega_{\alpha,0,0}(\lambda,x_0) \\
&\qquad + [\phi_\alpha(\lambda,x,x_0)\phi_\alpha(\lambda,x',x_0) + \phi_\alpha(\lambda,x,x_0)\phi_\alpha(\lambda,x',x_0)]d\Omega_{\alpha,0,1}(\lambda,x_0) \\
&\qquad + \phi_\alpha(\lambda,x,x_0)\phi_\alpha(\lambda,x',x_0)d\Omega_{\alpha,1,1}(\lambda,x_0)\Big\} \\
&= \int_{(\lambda_1,\lambda_2]} \overline{\widehat{f}_\alpha(\lambda,x_0)^\top}\, d\Omega_\alpha(\lambda,x_0)\, \widehat{g}_\alpha(\lambda,x_0) F(\lambda),
\end{aligned} \tag{2.106}
$$

using (2.93), $d\Omega_{\alpha,0,1}(\cdot,x_0) = d\Omega_{\alpha,1,0}(\cdot,x_0)$, and interchanging the dx, dx' and $d\Omega_{\alpha,\ell,\ell'}(\cdot,x_0)$, $\ell,\ell'=0,1$, integrals once more. □

Remark 2.13. Again we emphasize that the idea of a straightforward derivation of the link between the family of spectral projections $E_H(\cdot)$ and the 2×2 matrix-valued spectral function $\Omega_\alpha(\cdot)$ of H in Theorem 2.12 can already be found in [47] as pointed out in Remark 2.8. It applies equally well to Dirac-type operators and Hamiltonian systems on $\mathbb{R}$ (see the extensive literature cited, e.g., in [16]) and to Jacobi and CMV operators on $\mathbb{Z}$ (cf. [13] and [42]).

As in the half-line case before, one can improve on Theorem 2.12 and remove the compact support restrictions on f and g in the usual way. To this end one considers the map

$$
\widetilde{U}_\alpha(x_0) \colon \begin{cases} C_0^\infty(\mathbb{R}) \to L^2(\mathbb{R}; d\Omega_\alpha(\cdot,x_0)) \\ \qquad h \mapsto \widehat{h}_\alpha(\cdot,x_0) = (\widehat{h}_{\alpha,0}(\lambda,x_0), \widehat{h}_{\alpha,1}(\lambda,x_0))^\top, \end{cases} \tag{2.107}
$$

$$
\widehat{h}_{\alpha,0}(\lambda,x_0) = \int_{\mathbb{R}} dx\, \theta_\alpha(\lambda,x,x_0)h(x), \quad \widehat{h}_{\alpha,1}(\lambda,x_0) = \int_{\mathbb{R}} dx\, \phi_\alpha(\lambda,x,x_0)h(x).
$$

Taking $f=g$, $F=1$, $\lambda_1 \downarrow -\infty$, and $\lambda_2 \uparrow \infty$ in (2.92) then shows that $\widetilde{U}_\alpha(x_0)$ is a densely defined isometry in $L^2(\mathbb{R};dx)$, which extends by continuity to an isometry on $L^2(\mathbb{R};dx)$. The latter is denoted by $U_\alpha(x_0)$ and given by

$$
U_\alpha(x_0) \colon \begin{cases} L^2(\mathbb{R};dx) \to L^2(\mathbb{R}; d\Omega_\alpha(\cdot,x_0)) \\ \qquad h \mapsto \widehat{h}_\alpha(\cdot,x_0) = (\widehat{h}_{\alpha,0}(\cdot,x_0), \widehat{h}_{\alpha,1}(\cdot,x_0))^\top, \end{cases} \tag{2.108}
$$

$$
\widehat{h}_\alpha(\cdot,x_0) = \begin{pmatrix} \widehat{h}_{\alpha,0}(\cdot,x_0) \\ \widehat{h}_{\alpha,1}(\cdot,x_0) \end{pmatrix} = \operatorname{l.i.m.}_{a\downarrow-\infty, b\uparrow\infty} \begin{pmatrix} \int_a^b dx\, \theta_\alpha(\cdot,x,x_0)h(x) \\ \int_a^b dx\, \phi_\alpha(\cdot,x,x_0)h(x) \end{pmatrix},
$$

where l.i.m. refers to the $L^2(\mathbb{R}; d\Omega_\alpha(\cdot,x_0))$-limit.

The calculation in (2.106) also yields

$$
\begin{aligned}
&(E_H((\lambda_1,\lambda_2])g)(x) = \int_{(\lambda_1,\lambda_2]} (\theta_\alpha(\lambda,x,x_0), \phi_\alpha(\lambda,x,x_0))\, d\Omega_\alpha(\lambda,x_0)\, \widehat{g}_\alpha(\lambda) \\
&\quad = \int_{(\lambda_1,\lambda_2]} \Big\{ d\Omega_{\alpha,0,0}(\lambda,x_0)\, \theta_\alpha(\lambda,x,x_0)\widehat{g}_{\alpha,0}(\lambda,x_0) \\
&\qquad + d\Omega_{\alpha,0,1}(\lambda,x_0)\, [\theta_\alpha(\lambda,x,x_0)\widehat{g}_{\alpha,1}(\lambda,x_0) + \phi_\alpha(\lambda,x,x_0)\widehat{g}_{\alpha,0}(\lambda,x_0)] \\
&\qquad + d\Omega_{\alpha,1,1}(\lambda,x_0)\, \phi_\alpha(\lambda,x,x_0)\widehat{g}_{\alpha,1}(\lambda,x_0)\Big\}, \quad g \in C_0^\infty(\mathbb{R})
\end{aligned} \tag{2.109}
$$

and subsequently, (2.109) extends to all $g \in L^2(\mathbb{R}; dx)$ by continuity. Moreover, taking $\lambda_1 \downarrow -\infty$ and $\lambda_2 \uparrow \infty$ in (2.109) and using

$$\operatorname{s-lim}_{\lambda\downarrow-\infty} E_H(\lambda) = 0, \quad \operatorname{s-lim}_{\lambda\uparrow\infty} E_H(\lambda) = I_{L^2(\mathbb{R};dx)}, \tag{2.110}$$

where

$$E_H(\lambda) = E_H((-\infty, \lambda]), \quad \lambda \in \mathbb{R}, \tag{2.111}$$

then yield

$$\begin{aligned} g(\cdot) &= \operatorname{l.i.m.}_{\mu_1\downarrow-\infty,\mu_2\uparrow\infty} \int_{(\mu_1,\mu_2]} (\theta_\alpha(\lambda,\cdot,x_0), \phi_\alpha(\lambda,\cdot,x_0))\, d\Omega_\alpha(\lambda,x_0)\, \widehat{g}_\alpha(\lambda) \\ &= \operatorname{l.i.m.}_{\mu_1\downarrow-\infty,\mu_2\uparrow\infty} \int_{\mu_1}^{\mu_2} \Big\{ d\Omega_{\alpha,0,0}(\lambda,x_0)\, \theta_\alpha(\lambda,\cdot,x_0)\widehat{g}_{\alpha,0}(\lambda,x_0) \\ &\quad + d\Omega_{\alpha,0,1}(\lambda,x_0)\, [\theta_\alpha(\lambda,\cdot,x_0)\widehat{g}_{\alpha,1}(\lambda,x_0) + \phi_\alpha(\lambda,\cdot,x_0)\widehat{g}_{\alpha,0}(\lambda,x_0)] \\ &\quad + d\Omega_{\alpha,1,1}(\lambda,x_0)\, \phi_\alpha(\lambda,\cdot,x_0)\widehat{g}_{\alpha,1}(\lambda,x_0) \Big\}, \quad g \in L^2(\mathbb{R}; dx), \end{aligned} \tag{2.112}$$

where l.i.m. refers to the $L^2(\mathbb{R}; dx)$-limit. In addition, one can show that the map $U_\alpha(x_0)$ in (2.108) is onto and hence that $U_\alpha(x_0)$ is unitary with

$$U_\alpha(x_0)^{-1} \colon \begin{cases} L^2(\mathbb{R}; d\Omega_\alpha(\cdot,x_0)) \to L^2(\mathbb{R}; dx) \\ \qquad\qquad \widehat{h}_\alpha(\cdot,x_0) \mapsto h, \end{cases} \tag{2.113}$$

$$h(\cdot) = \operatorname{l.i.m.}_{\mu_1\downarrow-\infty,\mu_2\uparrow\infty} \int_{\mu_1}^{\mu_2} (\theta_\alpha(\lambda,\cdot,x_0), \phi_\alpha(\lambda,\cdot,x_0))\, d\Omega_\alpha(\lambda,x_0)\, \widehat{h}_\alpha(\lambda,x_0).$$

Indeed, consider an arbitrary element $f = (f_0,\ f_1)^\top \in L^2(\mathbb{R}; d\Omega_\alpha(\cdot,x_0))$ such that

$$\big(f, U_\alpha(x_0)h\big)_{L^2(\mathbb{R};d\Omega_\alpha(\cdot,x_0))} = 0 \ \text{ for all } h \in L^2(\mathbb{R}; dx). \tag{2.114}$$

Then, (2.114) holds for $h = E_{H_\alpha}((\lambda_1,\lambda_2])g$, $\lambda_1,\lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$, $g \in C_0^\infty(\mathbb{R})$. Utilizing (2.109) one rewrites (2.114) as,

$$\begin{aligned} 0 &= \big(f, U_\alpha(x_0)E_{H_\alpha}((\lambda_1,\lambda_2])g\big)_{L^2(\mathbb{R};d\Omega_\alpha(\cdot,x_0))} && (2.115) \\ &= \big(f, U_\alpha(x_0)U_\alpha(x_0)^{-1}\chi_{(\lambda_1,\lambda_2]}U_\alpha(x_0)g\big)_{L^2(\mathbb{R};d\Omega_\alpha(\cdot,x_0))} \\ &= \int_{(\lambda_1,\lambda_2]} \overline{f(\lambda)^\top}\, d\Omega_\alpha(\lambda,x_0) \int_{\mathbb{R}} dx\, (\theta_\alpha(\lambda,x,x_0), \phi_\alpha(\lambda,x,x_0))^\top g(x) && (2.116) \\ &= \int_{\mathbb{R}} dx\, g(x) \int_{(\lambda_1,\lambda_2]} \overline{f(\lambda)^\top}\, d\Omega_\alpha(\lambda,x_0)(\theta_\alpha(\lambda,x,x_0), \phi_\alpha(\lambda,x,x_0))^\top. \end{aligned}$$

Since $C_0^\infty(\mathbb{R})$ is dense in $L^2(\mathbb{R}; dx)$ one concludes that

$$\int_{(\lambda_1,\lambda_2]} \overline{f(\lambda)^\top} d\Omega_\alpha(\lambda,x_0)(\theta_\alpha(\lambda,x,x_0), \phi_\alpha(\lambda,x,x_0))^\top = 0 \ \text{ for a.e. } x \in \mathbb{R}. \tag{2.117}$$

Differentiating (2.117) with respect to x leads to

$$\int_{(\lambda_1,\lambda_2]} \overline{f(\lambda)^\top} d\Omega_\alpha(\lambda,x_0)(\theta_\alpha'(\lambda,x,x_0), \phi_\alpha'(\lambda,x,x_0))^\top = 0 \ \text{ for a.e. } x \in \mathbb{R}. \tag{2.118}$$

Using the dominated convergence theorem and the fact that

$$f \in L^2(\mathbb{R}; d\Omega_\alpha(\cdot,x_0)) \subseteq L^1((\lambda_1,\lambda_2]; d\Omega_\alpha(\cdot,x_0)) \tag{2.119}$$

and that $\theta_\alpha(\lambda,x), \theta'_\alpha(\lambda,x), \phi_\alpha(\lambda,x), \phi'_\alpha(\lambda,x)$ are continuous with respect to $(\lambda,x)\in\mathbb{R}^2$, one concludes

$$\begin{aligned}
&\int_{(\lambda_1,\lambda_2]} \overline{f(\lambda)^\top} d\Omega_\alpha(\lambda,x_0)(\theta_\alpha(\lambda,x_0,x_0),\phi_\alpha(\lambda,x_0,x_0))^\top \\
&\quad = \int_{(\lambda_1,\lambda_2]} \overline{f(\lambda)^\top} d\Omega_\alpha(\lambda,x_0)(\cos(\alpha),-\sin(\alpha))^\top = 0, \\
&\int_{(\lambda_1,\lambda_2]} \overline{f(\lambda)^\top} d\Omega_\alpha(\lambda,x_0)(\theta'_\alpha(\lambda,x_0,x_0),\phi'_\alpha(\lambda,x_0,x_0))^\top \\
&\quad = \int_{(\lambda_1,\lambda_2]} \overline{f(\lambda)^\top} d\Omega_\alpha(\lambda,x_0)(\sin(\alpha),\cos(\alpha))^\top = 0.
\end{aligned} \tag{2.120}$$

Since the interval $(\lambda_1,\lambda_2]$ was chosen arbitrary, (2.120) implies

$$f(\lambda) = 0 \ \ d\Omega_\alpha(\cdot,x_0)\text{-a.e.}, \tag{2.121}$$

and hence $U_\alpha(x_0)$ is onto.

We sum up these considerations in a variant of the spectral theorem for (functions of) H.

Theorem 2.14. *Let $F\in C(\mathbb{R})$ and $x_0\in\mathbb{R}$. Then,*

$$U_\alpha(x_0)F(H)U_\alpha(x_0)^{-1} = M_F \tag{2.122}$$

in $L^2(\mathbb{R};d\Omega_\alpha(\cdot,x_0))$ (cf. (2.94)). Moreover,

$$\sigma(H) = \operatorname{supp}(d\Omega_\alpha(\cdot,x_0)) = \operatorname{supp}(d\Omega_\alpha^{\rm tr}(\cdot,x_0)). \tag{2.123}$$

Here $d\Omega_\alpha^{\rm tr}(\cdot,x_0) = d\Omega_{\alpha,0,0}(\cdot,x_0) + d\Omega_{\alpha,1,1}(\cdot,x_0)$ denotes the trace measure of $d\Omega_\alpha(\cdot,x_0)$.

3. The Case of Strongly Singular Potentials

In this section we extend our discussion to a class of strongly singular potentials V on the half-line (a,∞) with the singularity of V being concentrated at the endpoint a. We will present and contrast two approaches to this problem: One in which the reference point x_0 coincides with the singular endpoint a leading to a (scalar) spectral function, and one in which x_0 lies in the interior of the half-line (a,∞) and hence is a regular point for the half-line Schrödinger differential expression. The latter case naturally leads to a 2×2 matrix-valued spectral function which will be shown to be essentially equivalent to the scalar spectral function obtained from the former approach. While Herglotz functions still lie at the heart of the matter of spectral functions (resp., matrices), the direct analog of half-line Weyl–Titchmarsh coefficients will cease to be Herglotz functions in the first approach where the reference point x_0 coincides with the endpoint a.

Hypothesis 3.1. *(i) Let $a\in\mathbb{R}$ and assume that*

$$V \in L^1_{\rm loc}((a,\infty);dx), \quad V \text{ real-valued.} \tag{3.1}$$

(ii) Introducing the differential expression τ_+ given by

$$\tau_+ = -\frac{d^2}{dx^2} + V(x), \quad x\in(a,\infty), \tag{3.2}$$

we assume τ_+ to be in the limit point case at a and at $+\infty$.
(iii) Assume there exists an analytic Weyl–Titchmarsh solution $\widetilde{\phi}(z,\cdot)$ of

$$(\tau_+\psi)(z,x) = z\psi(z,x), \quad x \in (a,\infty), \tag{3.3}$$

for z in an open neighborhood $\mathcal{O}$ of $\mathbb{R}$ (containing $\mathbb{R}$) in the following sense:
- *(α) For all $x \in (a,\infty)$, $\widetilde{\phi}(z,x)$ is analytic with respect to $z \in \mathcal{O}$.*
- *(β) $\widetilde{\phi}(z,x)$, $x \in \mathbb{R}$, is real-valued for $z \in \mathbb{R}$.*
- *(γ) $\widetilde{\phi}(z,\cdot)$ satisfies an L^2-condition near the end point a*

$$\int_a^b dx\, \big|\widetilde{\phi}(z,x)\big|^2 < \infty \ \text{ for all } b \in (a,\infty) \tag{3.4}$$

for all $z \in \mathbb{C}\backslash\mathbb{R}$ with $|\mathrm{Im}(z)|$ sufficiently small.

Without loss of generality we assumed in Hypothesis 3.1 (iii) that the analytic Weyl–Titchmarsh solution satisfies the L^2-condition near the left end point a. One can replace this by the analogous L^2-condition at ∞.

A class of examples of strongly singular potentials satisfying Hypothesis 3.1 will be discussed in Examples 3.10 and 3.13 at the end of this section.

While we focus on strongly singular potentials with τ_+ in the limit point case at both endpoints a and ∞, the case of strongly singular potentials with τ_+ in the limit circle case at both endpoints has been studied by Fulton [30].

Associated with the differential expression τ_+ one introduces the self-adjoint Schrödinger operator H_+ in $L^2([a,\infty);dx)$ by

$$\begin{aligned} &H_+ f = \tau_+ f, \\ &f \in \mathrm{dom}(H_+) = \{g \in L^2([a,\infty);dx) \,|\, g, g' \in AC_{\mathrm{loc}}((a,\infty));\ \tau_+ g \in L^2([a,\infty);dx)\}. \end{aligned} \tag{3.5}$$

Next, we introduce the usual fundamental system of solutions $\phi(z,\cdot,x_0)$ and $\theta(z,\cdot,x_0)$, $z \in \mathbb{C}$, of (3.3) satisfying the initial conditions at the fixed reference point $x_0 \in (a,\infty)$,

$$\phi(z,x_0,x_0) = \theta'(z,x_0,x_0) = 0, \quad \phi'(z,x_0,x_0) = \theta(z,x_0,x_0) = 1. \tag{3.6}$$

Thus, for any fixed $x \in (a,\infty)$, the solutions $\phi(z,x,x_0)$ and $\theta(z,x,x_0)$ are entire with respect to z and

$$W(\theta(z,\cdot,x_0),\phi(z,\cdot,x_0))(x) = 1, \quad z \in \mathbb{C}. \tag{3.7}$$

We note, that Hypothesis 3.1 (iii) implies that for fixed $x \in (a,\infty)$, $\widetilde{\phi}'(z,x)$ is also analytic with respect to $z \in \mathcal{O}$. This follows from differentiating the identity

$$\widetilde{\phi}(z,x) = \widetilde{\phi}'(z,x_0)\phi(z,x,x_0) + \widetilde{\phi}(z,x_0)\theta(z,x,x_0), \quad x, x_0 \in (a,\infty) \tag{3.8}$$

for $z \in \mathcal{O}$.

Next, we also introduce the *Weyl–Titchmarsh solutions* $\psi_\pm(z,\cdot,x_0)$, $x_0 \in (a,\infty)$, $z \in \mathbb{C}\backslash\mathbb{R}$ of (3.3). Since by Hypothesis 3.1 (ii), τ_+ is assumed to be in the limit point case at a and at ∞, the Weyl–Titchmarsh solutions are uniquely characterized (up to constant multiples) by

$$\psi_-(z,\cdot,x_0) \in L^2([a,x_0];dx), \quad \psi_+(z,\cdot,x_0) \in L^2([x_0,\infty);dx), \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.9}$$

We fix the normalization of $\psi_\pm(z,\cdot,x_0)$ by requiring $\psi_\pm(z,x_0,x_0)=1$ and hence $\psi_\pm(z,\cdot,x_0)$ have the following structure,

$$\psi_\pm(z,x,x_0)=\theta(z,x,x_0)+m_\pm(z,x_0)\phi(z,x,x_0), \quad x,x_0\in(a,\infty),\ z\in\mathbb{C}\backslash\mathbb{R}, \tag{3.10}$$

where the coefficients $m_\pm(z,x_0)$ are given by

$$m_\pm(z,x)=\frac{\psi'_\pm(z,x,x_0)}{\psi_\pm(z,x,x_0)}, \quad x,x_0\in(a,\infty),\ z\in\mathbb{C}\backslash\mathbb{R}, \tag{3.11}$$

are Herglotz and anti-Herglotz functions, respectively.

Lemma 3.2. *Assume Hypothesis* 3.1 (i) *and* (ii)*. Then Hypothesis* 3.1 (iii) *is equivalent to the assumption that for any fixed $x\in(a,\infty)$, $m_-(z,x)$ is meromorphic with respect to $z\in\mathbb{C}$.*

Proof. In the following we fix $x\in(a,\infty)$. First, assume Hypothesis 3.1. By Hypothesis 3.1 (ii), the Weyl–Titchmarsh solutions are unique up to constant multiples and one concludes that $\psi_-(z,\cdot,x_0)=c(z,x_0)\widetilde\phi(z,\cdot)$. Hence by (3.11),

$$m_-(z,x)=\frac{\widetilde\phi'(z,x)}{\widetilde\phi(z,x)}, \quad x\in(a,\infty),\ z\in\mathbb{C}\backslash\mathbb{R}. \tag{3.12}$$

Since by Hypothesis 3.1 (iii), $\widetilde\phi(z,x)$ and $\widetilde\phi'(z,x)$ are analytic with respect to $z\in\mathcal{O}$ (cf. the paragraph preceding (3.8)), one concludes that $m_-(z,x)$ is meromorphic in $z\in\mathcal{O}$ and since m_- is analytic in $\mathbb{C}\backslash\mathbb{R}$, m_- is meromorphic on $\mathbb{C}$.

Conversely, if $m_-(z,x)$ is meromorphic with respect to $z\in\mathbb{C}$, then it has the following structure,

$$m_-(z,x)=\frac{\eta_1(z,x)}{\eta_2(z,x)}, \tag{3.13}$$

where $\eta_1(z,x)$ and $\eta_2(z,x)$ can be chosen to be entire such that they do not have common zeros. Moreover, since the zeros of $\eta_j(\cdot,x)$, $j=1,2$, are necessarily all real, the Weierstrass factorization theorem (cf., e.g., Corollary 2 of Theorem II.10.1 in [59, p. 284–285]) shows that $\eta_1(z,x)$ and $\eta_2(z,x)$ can be chosen to be real for $z\in\mathbb{R}$. Thus, for $x_0\in(a,\infty)$,

$$\widetilde\phi(z,\cdot)=\eta_2(z,x_0)\psi_-(z,\cdot,x_0)=\eta_2(z,x_0)\theta(z,\cdot,x_0)+\eta_1(z,x_0)\phi(z,\cdot,x_0) \tag{3.14}$$

is entire in z, and moreover, it is a Weyl–Titchmarsh solution of (3.3) that satisfies Hypothesis 3.1 (iii). □

Lemma 3.3. *Assume Hypothesis* 3.1 (iii)*. Then, there is an open neighborhood $\mathcal{O}'$ of $\mathbb{R}$ (containing $\mathbb{R}$), $\mathcal{O}'\subseteq\mathcal{O}$, and a solution $\widetilde\theta(z,\cdot)$ of* (3.3)*, which, for each $x\in(a,\infty)$, is analytic with respect to $z\in\mathcal{O}'$, real-valued for $z\in\mathbb{R}$, such that,*

$$W(\widetilde\theta(z,\cdot),\widetilde\phi(z,\cdot))(x)=1, \quad z\in\mathcal{O}'. \tag{3.15}$$

Proof. Let $x_0\in(a,\infty)$ and consider the following solution of (3.3),

$$\widetilde\theta(z,x)=\frac{\widetilde\phi'(z,x_0)}{\widetilde\phi(z,x_0)^2+\widetilde\phi'(z,x_0)^2}\theta(z,x,x_0)-\frac{\widetilde\phi(z,x_0)}{\widetilde\phi(z,x_0)^2+\widetilde\phi'(z,x_0)^2}\phi(z,x,x_0), \quad x\in(a,\infty) \tag{3.16}$$

for z in a sufficiently small neighborhood of $\mathbb{R}$. Since for $x, x_0 \in (a,\infty)$, $\widetilde\phi(z,x)$, $\theta(z,x,x_0)$, and $\phi(z,x,x_0)$ are analytic with respect to $z \in \mathcal{O}$, real-valued for $z \in \mathbb{R}$, and $\widetilde\phi(z,x_0)$, $\widetilde\phi'(z,x_0)$ are not both zero for all z in a sufficiently small neighborhood of $\mathbb{R}$, $\widetilde\theta(z,x)$ in (3.16) is analytic with respect to $z \in \mathcal{O}'$, $\mathcal{O}' \subseteq \mathcal{O}$, for fixed $x \in (a,\infty)$ and real-valued for $z \in \mathbb{R}$. Moreover, $\widetilde\theta(z,x)$ satisfies (3.15) since for $z \in \mathcal{O}'$,

$$\begin{aligned} W(\widetilde\theta(z,\cdot),\widetilde\phi(z,\cdot))(x) &= W(\widetilde\theta(z,\cdot),\widetilde\phi(z,\cdot))(x_0) &(3.17)\\ &= \frac{\widetilde\phi'(z,x_0)}{\widetilde\phi(z,x_0)^2+\widetilde\phi'(z,x_0)^2}\widetilde\phi'(z,x_0) + \frac{\widetilde\phi(z,x_0)}{\widetilde\phi(z,x_0)^2+\widetilde\phi'(z,x_0)^2}\widetilde\phi(z,x_0) = 1. &(3.18)\end{aligned}$$

□

Having a system of two linearly independent solutions $\widetilde\phi(z,x)$ and $\widetilde\theta(z,x)$ we introduce a function $\widetilde m_+(z)$ such that the following solution of (3.3)

$$\widetilde\psi_+(z,x) = \widetilde\theta(z,x) + \widetilde m_+(z)\widetilde\phi(z,x), \quad x \in (a,\infty), \tag{3.19}$$

satisfies

$$\widetilde\psi_+(z,\cdot) \in L^2([b,\infty);dx) \text{ for all } b \in (a,\infty), \tag{3.20}$$

for $z \in \mathcal{O}'\backslash\mathbb{R}$. By Hypothesis 3.1 (ii), the solution $\widetilde\psi_+(z,\cdot)$ is proportional to $\psi_+(z,\cdot,x_0)$. Hence, using (3.11), one computes,

$$m_+(z,x) = \frac{\widetilde\theta'(z,x) + \widetilde m_+(z)\widetilde\phi'(z,x)}{\widetilde\theta(z,x)+\widetilde m_+(z)\widetilde\phi(z,x)}, \tag{3.21}$$

$$\begin{aligned} \widetilde m_+(z) &= \frac{\widetilde\theta(z,x)m_+(z,x) - \widetilde\theta'(z,x)}{\widetilde\phi'(z,x)-\widetilde\phi(z,x)m_+(z,x)} = \frac{W(\widetilde\theta(z,\cdot),\psi_+(z,\cdot,x_0))}{W(\psi_+(z,\cdot,x_0),\widetilde\phi(z,\cdot))} &(3.22)\\ &= \frac{\widetilde\theta(z,x)}{\widetilde\phi(z,x)}\frac{m_+(z,x)}{m_-(z,x)-m_+(z,x)} - \frac{\widetilde\theta'(z,x)}{\widetilde\phi(z,x)}\frac{1}{m_-(z,x)-m_+(z,x)}. &(3.23)\end{aligned}$$

By (3.22), $\widetilde m_+$ is independent of $x \in (a,\infty)$.

Having in mind the fact that $m_\pm(\cdot,x)$ are Herglotz and anti-Herglotz functions, that $\widetilde\phi(z,x) \neq 0$ for $z \in \mathbb{C}\backslash\mathbb{R}$, $|\mathrm{Im}(z)|$ sufficiently small, and that $\widetilde\theta(z,x)$ and $\widetilde\theta'(z,x)$ are analytic with respect to $z \in \mathcal{O}'$, one concludes from (3.23) that $\widetilde m_+$ is analytic in $\mathcal{O}'\backslash\mathbb{R}$. In contrast to m_+, the function $\widetilde m_+$, in general, is not a Herglotz function. Nevertheless, $\widetilde m_+$ shares some properties with Herglotz functions which are crucial for the proof of our main result, Theorem 3.5. Before we derive these properties we mention that by using Hypothesis 3.1 (iii), (3.15), and (3.20), a computation of the Green's function $G_+(z,x,x')$ of H_+ yields

$$G_+(z,x,x') = \begin{cases} \widetilde\phi(z,x)\widetilde\psi_+(z,x'), & a < x \le x', \\ \widetilde\phi(z,x')\widetilde\psi_+(z,x), & a < x' \le x \end{cases} \tag{3.24}$$

and thus,

$$\begin{gathered} ((H_+ - zI)^{-1}f)(x) = \int_a^\infty dx'\, G_+(z,x,x')f(x'), \\ x \in (a,\infty), \quad f \in L^2([a,\infty);dx) \end{gathered} \tag{3.25}$$

for $z \in \mathcal{O}'\backslash\mathbb{R}$.

The basic properties of $\widetilde m_+$ then read as follows:

Lemma 3.4. *Assume Hypothesis* 3.1. *Then the function* $\widetilde{m}_+$ *introduced in* (3.19) *satisfies the following properties:*

(*i*) $\widetilde{m}_+(z) = \overline{\widetilde{m}_+(\overline{z})}, \quad z \in \mathbb{C}_+,\ |\mathrm{Im}(z)|$ *sufficiently small.*
(*ii*) $\varepsilon|\widetilde{m}_+(\lambda + i\varepsilon)| \leq C(\lambda_1, \lambda_2, \varepsilon_0)$ *for* $\lambda \in [\lambda_1, \lambda_2],\ 0 < \varepsilon \leq \varepsilon_0$.
(*iii*) $\varepsilon|\mathrm{Re}(\widetilde{m}_+(\lambda + i\varepsilon))| \underset{\varepsilon\to 0}{=} o(1)$ *for* $\lambda \in [\lambda_1, \lambda_2],\ 0 < \varepsilon \leq \varepsilon_0$.
(*iv*) $-i\varepsilon \lim_{\varepsilon\downarrow 0} \widetilde{m}_+(\lambda + i\varepsilon) = \varepsilon \lim_{\varepsilon\downarrow 0} \mathrm{Im}(\widetilde{m}_+(\lambda + i\varepsilon))$ *exists for all* $\lambda \in \mathbb{R}$ *and is nonnegative.*
(*v*) $\widetilde{m}_+(\lambda + i0) = \lim_{\varepsilon\downarrow 0} \widetilde{m}_+(\lambda + i\varepsilon)$ *exists for a.e.* $\lambda \in [\lambda_1, \lambda_2]$ *and* $\mathrm{Im}(\widetilde{m}_+(\lambda + i0)) \geq 0$ *for a.e.* $\lambda \in [\lambda_1, \lambda_2]$.

Here $0 < \varepsilon_0 = \varepsilon(\lambda_1, \lambda_2)$ *is assumed to be sufficiently small. Moreover, one can introduce a nonnegative measure* $d\widetilde{\rho}_+$ *associated with* $\widetilde{m}_+$ *in a manner similar to the Herglotz situation* (A.4) *by*

$$\int_{(\lambda_1,\lambda_2]} d\widetilde{\rho}_+(\lambda) = \widetilde{\rho}_+((\lambda_1, \lambda_2]) = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0} \frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, \mathrm{Im}(\widetilde{m}_+(\lambda + i\varepsilon)). \tag{3.26}$$

Proof. Since $\widetilde{\phi}(\lambda, x)$ and $\widetilde{\theta}(\lambda, x)$ are real-valued for $(\lambda, x) \in \mathbb{R} \times (a, \infty)$, one obtains from (3.3) that

$$\begin{gathered} \widetilde{\phi}(z, x) = \overline{\widetilde{\phi}(\overline{z}, x)}, \quad \widetilde{\theta}(z, x) = \overline{\widetilde{\theta}(\overline{z}, x)}, \\ x \in (a, \infty),\ z \in \mathbb{C},\ |\mathrm{Im}(z)| \text{ sufficiently small.} \end{gathered} \tag{3.27}$$

Thus, picking real numbers c and d such that $a \leq c < d < \infty$, (3.24) and (3.25) imply for the analog of (2.20) in the present context of H_+,

$$\begin{aligned} &\int_{\sigma(H_+)} \frac{d\big\|E_{H_+}(\lambda)\chi_{[c,d]}\big\|^2_{L^2([a,\infty);dx)}}{\lambda - z} = \big(\chi_{[c,d]}, (H_+ - zI)^{-1}\chi_{[c,d]}\big)_{L^2([a,\infty);dx)} \\ &\quad = \int_c^d dx \int_c^x dx'\, \widetilde{\theta}(z, x)\widetilde{\phi}(z, x') + \int_c^d dx \int_x^d dx'\, \widetilde{\phi}(z, x)\widetilde{\theta}(z, x') \\ &\qquad + \widetilde{m}_+(z)\bigg[\int_c^d dx\, \widetilde{\phi}(z, x)\bigg]^2, \quad z \in \mathbb{C}\backslash\sigma(H_+). \end{aligned} \tag{3.28}$$

Choosing $c(z_0), d(z_0) \in [a, \infty)$ such that

$$\int_{c(z_0)}^{d(z_0)} dx\, \widetilde{\phi}(z, x) \neq 0 \tag{3.29}$$

for z in an open neighborhood $\mathcal{N}(z_0)$ of $z_0 \in \mathbb{C}\backslash\sigma(H_+)$ with $\mathrm{Im}(z_0)$ sufficiently small (cf. the proof of Lemma 2.3), items (*i*)–(*v*) follow from (3.28) since

$$\int_{\sigma(H_+)} \frac{d\big\|E_{H_+}(\lambda)\chi_{[c,d]}\big\|^2_{L^2([a,\infty);dx)}}{\lambda - z}, \quad z \in \mathbb{C}\backslash\sigma(H_+), \tag{3.30}$$

is a Herglotz function and $\widetilde{\phi}(z, x), \widetilde{\theta}(z, x)$ are analytic with respect to $z \in \mathcal{O}'$, where $\mathcal{O}' \subseteq \mathcal{O}$ is an open neighborhood of $\mathbb{R}$. In addition, $\widetilde{\phi}(z, x)$ and $\widetilde{\theta}(z, x)$ are real-valued for $(z, x) \in \mathbb{R} \times (a, \infty)$. Next, we pick $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$, such that for some $c_0, d_0 \in [a, \infty)$,

$$\int_{c_0}^{d_0} dx\, \widetilde{\phi}(z, x) \neq 0 \tag{3.31}$$

for all z in a complex neighborhood of the interval (λ_1, λ_2). Then (3.28) applied to $z = \lambda + i\varepsilon$, for real-valued λ in a neighborhood of (λ_1, λ_2), $0 < \varepsilon \leq \varepsilon_0$, implies that $\widetilde{\rho}_+$ defined in (3.26) satisfies

$$
\begin{aligned}
\widetilde{\rho}_+((\lambda_1, \lambda_2]) &= \lim_{\delta\downarrow 0} \lim_{\varepsilon\downarrow 0} \frac{1}{\pi} \int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda \, \operatorname{Im}(\widetilde{m}_+(\lambda + i\varepsilon)) \\
&= \lim_{\delta\downarrow 0} \lim_{\varepsilon\downarrow 0} \frac{1}{\pi} \int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda \, \operatorname{Im}\bigg\{ \int_{\sigma(H_+)} \frac{d\big\|E_{H_+}(\lambda')\chi_{[c_0,d_0]}\big\|^2_{L^2([a,\infty);dx)}}{\lambda' - \lambda - i\varepsilon} \\
&\quad \times \bigg[\bigg(\int_{c_0}^{d_0} dx \, \widetilde{\phi}(\lambda, x) \bigg)^2 + 2i\varepsilon \bigg(\int_{c_0}^{d_0} dx \, (d/dz)\widetilde{\phi}(z, x)|_{z=\lambda} \bigg) + O(\varepsilon^2) \bigg]^{-1} \\
&\quad + O(\varepsilon) \bigg\} \\
&= \int_{(\lambda_1,\lambda_2]} d\big\|E_{H_+}(\lambda)\chi_{[c_0,d_0]}\big\|^2_{L^2([a,\infty);dx)} \bigg[\int_{c_0}^{d_0} dx \, \widetilde{\phi}(\lambda, x) \bigg]^{-2}, \qquad (3.32)
\end{aligned}
$$

using item *(ii)*, item *(iii)*, the dominated convergence theorem, and the analog of (2.50) applied to the present context. Hence, $\widetilde{\rho}_+$ generates the nonnegative measure $d\widetilde{\rho}_+$. □

Next, we relate the family of spectral projections, $\{E_{H_+}(\lambda)\}_{\lambda\in\mathbb{R}}$, of the self-adjoint operator H_+ and the spectral function $\widetilde{\rho}_+(\lambda)$, $\lambda \in \mathbb{R}$, defined in (3.26).

We first note that for $F \in C(\mathbb{R})$,

$$
\begin{aligned}
&\big(f, F(H_+)g\big)_{L^2([a,\infty);dx)} = \int_{\mathbb{R}} d\big(f, E_{H_+}(\lambda)g\big)_{L^2([a,\infty);dx)} \, F(\lambda), \qquad (3.33) \\
&f, g \in \operatorname{dom}(F(H_+)) \\
&\quad = \bigg\{ h \in L^2([a,\infty); dx) \,\bigg|\, \int_{\mathbb{R}} d\big\|E_{H_+}(\lambda)h\big\|^2_{L^2([a,\infty);dx)} \, |F(\lambda)|^2 < \infty \bigg\}.
\end{aligned}
$$

Theorem 3.5. *Let $f, g \in C_0^\infty((a,\infty))$, $F \in C(\mathbb{R})$, and $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$. Then,*

$$
\big(f, F(H_+)E_{H_+}((\lambda_1, \lambda_2])g\big)_{L^2([a,\infty);dx)} = \big(\widehat{f}_+, M_F M_{\chi_{(\lambda_1,\lambda_2]}} \widehat{g}_+\big)_{L^2(\mathbb{R};d\widetilde{\rho}_+)}, \qquad (3.34)
$$

where we introduced the notation

$$
\widehat{h}_+(\lambda) = \int_a^\infty dx \, \widetilde{\phi}(\lambda, x)h(x), \quad \lambda \in \mathbb{R}, \ h \in C_0^\infty((a,\infty)), \qquad (3.35)
$$

and M_G denotes again the maximally defined operator of multiplication by the $d\widetilde{\rho}_+$-measurable function G in the Hilbert space $L^2(\mathbb{R}; d\widetilde{\rho}_+)$,

$$
\begin{aligned}
&(M_G\widehat{h})(\lambda) = G(\lambda)\widehat{h}(\lambda) \ \text{ for a.e. } \lambda \in \mathbb{R}, \\
&\widehat{h} \in \operatorname{dom}(M_G) = \{\widehat{k} \in L^2(\mathbb{R}; d\widetilde{\rho}_+) \,|\, G\widehat{k} \in L^2(\mathbb{R}; d\widetilde{\rho}_+)\}.
\end{aligned} \qquad (3.36)
$$

Proof. The point of departure for deriving (3.34) is again Stone's formula (2.29) applied to $T = H_+$,

$$\begin{aligned}&\big(f, F(H_+)E_{H_+}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)}\\&\quad=\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda)\big[\big(f,(H_+-(\lambda+i\varepsilon)I)^{-1}g\big)_{L^2([a,\infty);dx)}\\&\qquad\qquad-\big(f,(H_+-(\lambda-i\varepsilon)I)^{-1}g\big)_{L^2([a,\infty);dx)}\big].\end{aligned}\tag{3.37}$$

Insertion of (3.24) and (3.25) into (3.37) then yields the following:

$$\begin{aligned}&\big(f, F(H_+)E_{H_+}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)}=\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda)\\&\quad\times\bigg\{\int_a^\infty dx\,\bigg[\overline{f(x)}\widetilde\psi_+(\lambda+i\varepsilon,x)\int_a^x dx'\,\widetilde\phi(\lambda+i\varepsilon,x')g(x')\\&\qquad+\overline{f(x)}\widetilde\phi(\lambda+i\varepsilon,x)\int_x^\infty dx'\,\widetilde\psi_+(\lambda+i\varepsilon,x')g(x')\bigg]\\&\qquad-\bigg[\overline{f(x)}\widetilde\psi_+(\lambda-i\varepsilon,x)\int_a^x dx'\,\widetilde\phi(\lambda-i\varepsilon,x')g(x')\\&\qquad+\overline{f(x)}\widetilde\phi(\lambda-i\varepsilon,x)\int_x^\infty dx'\,\widetilde\psi_+(\lambda-i\varepsilon,x')g(x')\bigg]\bigg\}.\end{aligned}\tag{3.38}$$

Freely interchanging the dx and dx' integrals with the limits and the $d\lambda$ integral (since all integration domains are finite and all integrands are continuous), and inserting expression (3.19) for $\widetilde\psi_+(z,x)$ into (3.38), one obtains

$$\begin{aligned}&\big(f, F(H_+)E_{H_+}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)}=\int_a^\infty dx\,\overline{f(x)}\bigg\{\int_a^x dx'\,g(x')\\&\quad\times\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\,F(\lambda)\Big[\big[\widetilde\theta(\lambda,x)+\widetilde m_+(\lambda+i\varepsilon)\widetilde\phi(\lambda,x)\big]\widetilde\phi(\lambda,x')\\&\qquad-\big[\widetilde\theta(\lambda,x)+\widetilde m_+(\lambda-i\varepsilon)\widetilde\phi(\lambda,x)\big]\widetilde\phi(\lambda,x')\Big]\\&\quad+\int_x^\infty dx'\,g(x')\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\,F(\lambda)\\&\qquad\times\Big[\widetilde\phi(\lambda,x)\big[\widetilde\theta(\lambda,x')+\widetilde m_+(\lambda+i\varepsilon)\widetilde\phi(\lambda,x')\big]\\&\qquad-\widetilde\phi(\lambda,x)\big[\widetilde\theta(\lambda,x')+\widetilde m_+(\lambda-i\varepsilon)\widetilde\phi(\lambda,x')\big]\Big]\bigg\}.\end{aligned}\tag{3.39}$$

Here we employed the fact that for fixed $x\in(a,\infty)$, $\widetilde\phi(z,x)$, $\widetilde\theta(z,x)$ are analytic with respect to $z\in\mathcal{O}$ and real-valued for $z\in\mathbb{R}$, the fact that $\widetilde\phi(z,\cdot),\widetilde\theta(z,\cdot)\in AC_{\text{loc}}((a,\infty))$, and hence that

$$\begin{aligned}\widetilde\phi(\lambda\pm i\varepsilon,x,x_0)&\underset{\varepsilon\downarrow 0}{=}\widetilde\phi(\lambda,x,x_0)+i\varepsilon(d/dz)\widetilde\phi(z,x,x_0)|_{z=\lambda}+O(\varepsilon^2),\\\widetilde\theta(\lambda\pm i\varepsilon,x,x_0)&\underset{\varepsilon\downarrow 0}{=}\widetilde\theta(\lambda,x,x_0)+i\varepsilon(d/dz)\widetilde\theta(z,x,x_0)|_{z=\lambda}+O(\varepsilon^2),\end{aligned}\tag{3.40}$$

with $O(\varepsilon^2)$ being uniform with respect to (λ,x) as long as λ and x vary in compact subsets of $\mathbb{R}\times(a,\infty)$. Moreover, we used items *(ii)* and *(iii)* of Lemma 3.4 to replace $\widetilde\phi(\lambda\pm i\varepsilon,x)$ and $\widetilde\theta(\lambda\pm i\varepsilon,x)$ by $\widetilde\phi(\lambda,x)$ and $\widetilde\theta(\lambda,x)$ under the $d\lambda$ integrals in (3.39). Cancelling appropriate terms in (3.39), simplifying the remaining terms, and using item (i) of Lemma 3.4 then yield

$$\begin{aligned}\big(f, F(H_+)E_{H_+}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} &= \int_a^\infty dx\,\overline{f(x)}\int_a^\infty dx'\,g(x')\\ &\times \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\,F(\lambda)\widetilde\phi(\lambda,x)\widetilde\phi(\lambda,x')\mathrm{Im}(\widetilde m_+(\lambda+i\varepsilon)).\end{aligned} \tag{3.41}$$

Using (3.26),

$$\int_{\mathbb{R}} d\widetilde\rho_+(\lambda)\,h(\lambda) = \lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\mathbb{R}} d\lambda\,\mathrm{Im}(\widetilde m_+(\lambda+i\varepsilon))\,h(\lambda), \quad h\in C_0(\mathbb{R}), \tag{3.42}$$

$$\int_{(\lambda_1,\lambda_2]} d\widetilde\rho_+(\lambda)\,k(\lambda) = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\,\mathrm{Im}(\widetilde m_+(\lambda+i\varepsilon))\,k(\lambda), \quad k\in C(\mathbb{R}), \tag{3.43}$$

and hence

$$\begin{aligned}&\big(f, F(H_+)E_{H_+}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)}\\ &\quad= \int_a^\infty dx\,\overline{f(x)}\int_a^\infty dx'\,g(x')\int_{(\lambda_1,\lambda_2]} d\widetilde\rho_+(\lambda)F(\lambda)\widetilde\phi(\lambda,x)\widetilde\phi(\lambda,x')\\ &\quad= \int_{(\lambda_1,\lambda_2]} d\widetilde\rho_+(\lambda)F(\lambda)\,\overline{\widehat f_+(\lambda)}\,\widehat g_+(\lambda),\end{aligned} \tag{3.44}$$

using (3.35) and interchanging the dx, dx' and $d\widetilde\rho_+$ integrals once more. $\square$

Again one can improve on Theorem 3.5 and remove the compact support restrictions on f and g in the usual way. To this end we consider the map

$$\widetilde U_+ \colon \begin{cases} C_0^\infty((a,\infty)) \to L^2(\mathbb{R}; d\widetilde\rho_+) \\ \qquad\qquad h \mapsto \widehat h_+(\cdot) = \int_a^\infty dx\,\widetilde\phi(\cdot,x)h(x). \end{cases} \tag{3.45}$$

Taking $f = g$, $F = 1$, $\lambda_1 \downarrow -\infty$, and $\lambda_2 \uparrow \infty$ in (3.34) then shows that $\widetilde U_+$ is a densely defined isometry in $L^2([a,\infty); dx)$, which extends by continuity to an isometry on $L^2([a,\infty); dx)$. The latter is denoted by U_+ and given by

$$U_+ \colon \begin{cases} L^2([a,\infty); dx) \to L^2(\mathbb{R}; d\widetilde\rho_+) \\ \qquad\qquad h \mapsto \widehat h_+(\cdot) = \text{l.i.m.}_{b\uparrow\infty}\int_a^b dx\,\widetilde\phi(\cdot,x)h(x), \end{cases} \tag{3.46}$$

where l.i.m. refers to the $L^2(\mathbb{R}; d\widetilde\rho_+)$-limit.

The calculation in (3.44) also yields

$$(E_{H_+}((\lambda_1,\lambda_2])g)(\cdot) = \int_{(\lambda_1,\lambda_2]} d\widetilde\rho_+(\lambda)\,\widetilde\phi(\lambda,\cdot)\widehat g_+(\lambda), \quad g\in C_0^\infty((a,\infty)) \tag{3.47}$$

and subsequently, (3.47) extends to all $g \in L^2([a,\infty); dx)$ by continuity. Moreover, taking $\lambda_1 \downarrow -\infty$ and $\lambda_2 \uparrow \infty$ in (3.47) and using

$$\text{s-lim}_{\lambda\downarrow-\infty} E_{H_+}(\lambda) = 0, \quad \text{s-lim}_{\lambda\uparrow\infty} E_{H_+}(\lambda) = I_{L^2([a,\infty);dx)}, \tag{3.48}$$

where

$$E_{H_+}(\lambda) = E_{H_+}((-\infty,\lambda]), \tag{3.49}$$

then yield

$$g(\cdot) = \text{l.i.m.}_{\mu_1\downarrow-\infty,\mu_2\uparrow\infty} \int_{\mu_1}^{\mu_2} d\widetilde{\rho}_+(\lambda)\, \widetilde{\phi}(\lambda,\cdot)\widehat{g}_+(\lambda), \quad g\in L^2([a,\infty);dx), \tag{3.50}$$

where l.i.m. refers to the $L^2([a,\infty);dx)$-limit.

In addition, one can show that the map U_+ in (3.46) is onto and hence that U_+ is unitary (i.e., U_+ and U_+^{-1} are isometric isomorphisms between $L^2([a,\infty);dx)$ and $L^2(\mathbb{R};d\widetilde{\rho}_+)$) with

$$U_+^{-1}\colon \begin{cases} L^2(\mathbb{R};d\widetilde{\rho}_+)\to L^2([a,\infty);dx) \\ \qquad\qquad \widehat{h}\mapsto \text{l.i.m.}_{\mu_1\downarrow-\infty,\mu_2\uparrow\infty} \int_{\mu_1}^{\mu_2} d\widetilde{\rho}_+(\lambda)\, \widetilde{\phi}(\lambda,\cdot)\widehat{h}(\lambda). \end{cases} \tag{3.51}$$

Indeed, consider an arbitrary function $f\in L^2(\mathbb{R};d\widetilde{\rho}_+)$ such that

$$\big(f,U_+h\big)_{L^2(\mathbb{R};d\rho_{+,\alpha})} = 0 \text{ for all } h\in L^2([a,\infty);dx). \tag{3.52}$$

Then, (3.52) holds for $h=E_{H_+}((\lambda_1,\lambda_2])g$, $\lambda_1,\lambda_2\in\mathbb{R}$, $\lambda_1<\lambda_2$, $g\in C_0^\infty((a,\infty))$. Utilizing (3.47) one rewrites (3.52) as,

$$\begin{aligned} 0 &= \big(f,U_+E_{H_+}((\lambda_1,\lambda_2])g\big)_{L^2(\mathbb{R};d\widetilde{\rho}_+)} = \big(f,U_+U_+^{-1}\chi_{(\lambda_1,\lambda_2]}U_+g\big)_{L^2(\mathbb{R};d\widetilde{\rho}_+)} \\ &= \int_{(\lambda_1,\lambda_2]} d\widetilde{\rho}_+(\lambda)\,\overline{f(\lambda)} \int_{(a,\infty)} dx\, \widetilde{\phi}(\lambda,x)g(x) \\ &= \int_{(a,\infty)} dx\, g(x) \int_{(\lambda_1,\lambda_2]} d\widetilde{\rho}_+(\lambda)\, \widetilde{\phi}(\lambda,x)\overline{f(\lambda)}. \end{aligned} \tag{3.53}$$

Since $C_0^\infty((a,\infty))$ is dense in $L^2([a,\infty);dx)$ one concludes that

$$\int_{(\lambda_1,\lambda_2]} d\widetilde{\rho}_+(\lambda)\, \widetilde{\phi}(\lambda,x)\overline{f(\lambda)} = 0 \text{ for a.e. } x\in(a,\infty). \tag{3.54}$$

Differentiating (3.54) with respect to x leads to

$$\int_{(\lambda_1,\lambda_2]} d\widetilde{\rho}_+(\lambda)\, \widetilde{\phi}'(\lambda,x)\overline{f(\lambda)} = 0 \text{ for a.e. } x\in(a,\infty). \tag{3.55}$$

Using the dominated convergence theorem and the fact that $f\in L^2(\mathbb{R};d\widetilde{\rho}_+)\subseteq L^1((\lambda_1,\lambda_2];d\widetilde{\rho}_+)$ and that $\widetilde{\phi}(\lambda,x),\widetilde{\phi}'(\lambda,x)$ are continuous in $(\lambda,x)\in\mathbb{R}\times(a,\infty)$, one obtains (3.54) and (3.55) for all $x\in(a,\infty)$, in particular, for some fixed $x_0\in(a,\infty)$. Since the interval $(\lambda_1,\lambda_2]$ was chosen arbitrary (3.54) and (3.55) imply

$$\widetilde{\phi}(\lambda,x_0)\overline{f(\lambda)} = \widetilde{\phi}'(\lambda,x_0)\overline{f(\lambda)} = 0 \;\; d\widetilde{\rho}_+\text{-a.e.} \tag{3.56}$$

Finally, the fact that $\widetilde{\phi}(\lambda,x_0)$ and $\widetilde{\phi}'(\lambda,x_0)$ are not both zero for $\lambda\in\mathbb{R}$ implies

$$f(\lambda)=0 \;\; d\widetilde{\rho}_+\text{-a.e.}, \tag{3.57}$$

and hence U_+ is onto.

We sum up these considerations in a variant of the spectral theorem for (functions of) H_+.

Theorem 3.6. *Let $F\in C(\mathbb{R})$, Then,*

$$U_+F(H_+)U_+^{-1} = M_F \tag{3.58}$$

in $L^2(\mathbb{R}; d\widetilde{\rho}_+)$ (*cf.* (3.36)). *Moreover,*

$$\sigma(F(H_+)) = \text{ess.ran}_{d\widetilde{\rho}_+}(F), \tag{3.59}$$

$$\sigma(H_+) = \text{supp}\,(d\widetilde{\rho}_+), \tag{3.60}$$

and the spectrum of H_+ *is simple.*

Simplicity of the spectrum of H_+ is consistent with the observation that

$$\begin{aligned} &\det\left(\mathrm{Im}(M(\lambda + i0, x_0))\right) \\ &\quad = \det\left(\begin{pmatrix} \frac{\mathrm{Im}(m_+(\lambda+i0,x_0))}{|m_-(\lambda+i0,x_0)-m_+(\lambda+i0,x_0)|^2} & \frac{m_-(\lambda+i0,x_0)\mathrm{Im}(m_+(\lambda+i0,x_0))}{|m_-(\lambda+i0,x_0)-m_+(\lambda+i0,x_0)|^2} \\ \frac{m_-(\lambda+i0,x_0)\mathrm{Im}(m_+(\lambda+i0,x_0))}{|m_-(\lambda+i0,x_0)-m_+(\lambda+i0,x_0)|^2} & \frac{|m_-(\lambda+i0,x_0)|^2\mathrm{Im}(m_+(\lambda+i0,x_0))}{|m_-(\lambda+i0,x_0)-m_+(\lambda+i0,x_0)|^2} \end{pmatrix}\right) \\ &\quad = 0 \ \text{ for a.e. } \lambda \in \mathbb{R} \end{aligned} \tag{3.61}$$

since by Lemma 3.2, $m_-(z, x_0)$ is meromorphic and real-valued for $z \in \mathbb{R}$. In this context we also refer to [43], [44], [51], [52], where necessary and sufficient conditions for simplicity of the spectrum in terms of properties of $m_\pm(\cdot, x_0)$ can be found.

Next, we consider the alternative way of deriving the (matrix-valued) spectral function corresponding to a reference point $x_0 \in (a, \infty)$ and subsequently compare the two approaches.

As in the half-line context in Section 2 we introduce the usual fundamental system of solutions $\phi(z, \cdot, x_0)$ and $\theta(z, \cdot, x_0)$, $z \in \mathbb{C}$, of

$$(\tau_+\psi)(z, x) = z\psi(z, x), \quad x \in (a, \infty) \tag{3.62}$$

with respect to a fixed reference point $x_0 \in (a, \infty)$, satisfying the initial conditions at the point $x = x_0$,

$$\phi(z, x_0, x_0) = \theta'(z, x_0, x_0) = 0, \quad \phi'(z, x_0, x_0) = \theta(z, x_0, x_0) = 1. \tag{3.63}$$

Again we note that for any fixed $x, x_0 \in (a, \infty)$, $\phi(z, x, x_0)$ and $\theta(z, x, x_0)$ are entire with respect to z and that

$$W(\theta(z, \cdot, x_0), \phi(z, \cdot, x_0))(x) = 1, \quad z \in \mathbb{C}. \tag{3.64}$$

The *Weyl–Titchmarsh solutions* $\psi_{\pm,\alpha}(z, \cdot, x_0)$, $z \in \mathbb{C}\backslash\mathbb{R}$, of (3.62) are uniquely characterized by

$$\begin{aligned} &\psi_-(z, \cdot, x_0) \in L^2([a, x_0]; dx), \ \psi_+(z, \cdot, x_0) \in L^2([x_0, \infty); dx), \ z \in \mathbb{C}\backslash\mathbb{R}, \\ &\psi_\pm(z, x_0, x_0) = 1. \end{aligned} \tag{3.65}$$

The normalization in (3.65) shows that $\psi_\pm(z, \cdot, x_0)$ are of the type

$$\psi_\pm(z, x, x_0) = \theta(z, x, x_0) + m_\pm(z, x_0)\phi(z, x, x_0), \quad z \in \mathbb{C}\backslash\mathbb{R}, \ x \in \mathbb{R} \tag{3.66}$$

for some coefficients $m_\pm(z, x_0)$, the half-line *Weyl–Titchmarsh m-functions* associated with τ_+ and x_0. Again we recall the fundamental identity

$$\int_a^{x_0} dx\, \psi_-(z_1, x, x_0)\psi_-(z_2, x, x_0) = -\frac{m_-(z_1, x_0) - m_-(z_2, x_0)}{z_1 - z_2}, \tag{3.67}$$

$$\int_{x_0}^{\infty} dx\, \psi_+(z_1, x, x_0)\psi_+(z_2, x, x_0) = \frac{m_+(z_1, x_0) - m_+(z_2, x_0)}{z_1 - z_2}, \tag{3.68}$$

$$z_1, z_2 \in \mathbb{C}\backslash\mathbb{R}, \ z_1 \neq z_2,$$

and as before one concludes

$$\overline{m_\pm(z, x_0)} = m_\pm(\overline{z}, x_0), \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.69}$$

Choosing $z_1 = z$, $z_2 = \overline{z}$ in (3.67), (3.68) one infers

$$\begin{aligned} \int_a^{x_0} dx\, |\psi_-(z,x,x_0)|^2 &= -\frac{\operatorname{Im}(m_-(z,x_0))}{\operatorname{Im}(z)}, \\ \int_{x_0}^{\infty} dx\, |\psi_+(z,x,x_0)|^2 &= \frac{\operatorname{Im}(m_+(z,x_0))}{\operatorname{Im}(z)}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \end{aligned} \tag{3.70}$$

Since $m_\pm(\cdot,x_0)$ are analytic on $\mathbb{C}\backslash\mathbb{R}$, $\pm m_\pm(\cdot,x_0)$ are Herglotz functions.

The Green's function $G_+(z,x,x')$ of H_+ then admits the alternative representation (cf. also (3.24), (3.25))

$$G_+(z,x,x') = \frac{1}{W(\psi_+(z,\cdot,x_0),\psi_-(z,\cdot,x_0))} \begin{cases} \psi_-(z,x,x_0)\psi_+(z,x',x_0), & x \le x', \\ \psi_-(z,x',x_0)\psi_+(z,x,x_0), & x' \le x, \end{cases} \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{3.71}$$

with

$$W(\psi_+(z,\cdot,x_0),\psi_-(z,\cdot,x_0)) = m_-(z,x_0) - m_+(z,x_0), \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.72}$$

Thus,

$$\begin{aligned} ((H_+ - zI)^{-1} f)(x) &= \int_a^{\infty} dx'\, G_+(z,x,x') f(x'), \\ & z \in \mathbb{C}\backslash\mathbb{R},\ x \in [a,\infty),\ f \in L^2([a,\infty);dx). \end{aligned} \tag{3.73}$$

Given $m_\pm(z,x_0)$, we also introduce the 2×2 matrix-valued Weyl–Titchmarsh function

$$M(z,x_0) = \begin{pmatrix} \frac{1}{m_-(z,x_0)-m_+(z,x_0)} & \frac{1}{2}\frac{m_-(z,x_0)+m_+(z,x_0)}{m_-(z,x_0)-m_+(z,x_0)} \\ \frac{1}{2}\frac{m_-(z,x_0)+m_+(z,x_0)}{m_-(z,x_0)-m_+(z,x_0)} & \frac{m_-(z,x_0)m_+(z,x_0)}{m_-(z,x_0)-m_+(z,x_0)} \end{pmatrix}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.74}$$

$M(z,x_0)$ is a Herglotz matrix with representation

$$\begin{aligned} & M(z,x_0) = C(x_0) + \int_{\mathbb{R}} d\Omega(\lambda,x_0)\left[\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right], \quad z \in \mathbb{C}\backslash\mathbb{R}, \\ & C(x_0) = C(x_0)^*, \quad \int_{\mathbb{R}} \frac{\|d\Omega(\lambda,x_0)\|}{1+\lambda^2} < \infty, \end{aligned} \tag{3.75}$$

where

$$\Omega((\lambda_1,\lambda_2],x_0) = \frac{1}{\pi}\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, \operatorname{Im}(M(\lambda+i\varepsilon,x_0)), \quad \lambda_1,\lambda_2 \in \mathbb{R},\ \lambda_1 < \lambda_2. \tag{3.76}$$

Again one can of course replace $z \in \mathbb{C}\backslash\mathbb{R}$ by $z \in \mathbb{C}\backslash\sigma(H_+)$ in formulas (3.65)–(3.75).

Next, we relate once more the family of spectral projections, $\{E_{H_+}(\lambda)\}_{\lambda\in\mathbb{R}}$, of the self-adjoint operator H_+ and the 2×2 matrix-valued nondecreasing spectral function $\Omega(\lambda,x_0)$, $\lambda \in \mathbb{R}$, which generates the matrix-valued measure in the Herglotz representation (3.75) of $M(z,x_0)$.

Theorem 3.7. *Let $f, g \in C_0^\infty((a,\infty))$, $F \in C(\mathbb{R})$, $x_0 \in (a,\infty)$, and $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$. Then,*

$$\begin{aligned}\big(f, F(H_+)E_{H_+}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} &= \big(\widehat{f}(\cdot,x_0), M_F M_{\chi_{(\lambda_1,\lambda_2]}}\widehat{g}(\cdot,x_0)\big)_{L^2(\mathbb{R};d\Omega(\cdot,x_0))}\\ &= \int_{(\lambda_1,\lambda_2]} \overline{\widehat{f}(\lambda,x_0)^\top}\, d\Omega(\lambda,x_0)\,\widehat{g}(\lambda,x_0)F(\lambda),\end{aligned} \tag{3.77}$$

where we introduced the notation

$$\begin{aligned}&\widehat{h}_0(\lambda,x_0) = \int_a^\infty dx\,\theta(\lambda,x,x_0)h(x), \quad \widehat{h}_1(\lambda,x_0) = \int_a^\infty dx\,\phi(\lambda,x,x_0)h(x),\\ &\widehat{h}(\lambda,x_0) = (\widehat{h}_0(\lambda,x_0), \widehat{h}_1(\lambda,x_0))^\top, \quad \lambda \in \mathbb{R},\ h \in C_0^\infty((a,\infty)),\end{aligned} \tag{3.78}$$

and M_G denotes the maximally defined operator of multiplication by the $d\Omega^{\rm tr}(\cdot,x_0)$-measurable function G in the Hilbert space $L^2(\mathbb{R};d\Omega(\cdot,x_0))$,

$$\begin{aligned}&(M_G\widehat{h})(\lambda) = G(\lambda)\widehat{h}(\lambda) = (G(\lambda)\widehat{h}_0(\lambda), G(\lambda)\widehat{h}_1(\lambda))^\top \ \text{ for a.e. } \lambda \in \mathbb{R},\\ &\widehat{h} \in \mathrm{dom}(M_G) = \{\widehat{k} \in L^2(\mathbb{R};d\Omega(\cdot,x_0)) \,|\, G\widehat{k} \in L^2(\mathbb{R};d\Omega(\cdot,x_0))\}.\end{aligned} \tag{3.79}$$

We omit the proof of Theorem 3.7 since it parallels that of Theorem 2.12.

Repeating the proof of Theorem 2.14 one also obtains the following result.

Theorem 3.8. *Let $F \in C(\mathbb{R})$, $x_0 \in (a,\infty)$,*

$$\begin{aligned}&U(x_0)\colon \begin{cases} L^2([a,\infty);dx) \to L^2(\mathbb{R};d\Omega(\cdot,x_0))\\ \qquad h \mapsto \widehat{h}(\cdot,x_0) = (\widehat{h}_0(\cdot,x_0), \widehat{h}_1(\cdot,x_0))^\top,\end{cases}\\ &\widehat{h}(\cdot,x_0) = \begin{pmatrix}\widehat{h}_0(\cdot,x_0)\\ \widehat{h}_1(\cdot,x_0)\end{pmatrix} = \mathrm{l.i.m.}_{b\downarrow a, c\uparrow\infty} \begin{pmatrix}\int_b^c dx\,\theta(\cdot,x,x_0)h(x)\\ \int_b^c dx\,\phi(\cdot,x,x_0)h(x)\end{pmatrix},\end{aligned} \tag{3.80}$$

where l.i.m. *refers to the $L^2(\mathbb{R};d\Omega(\cdot,x_0))$-limit and*

$$\begin{aligned}&U(x_0)^{-1}\colon \begin{cases} L^2(\mathbb{R};d\Omega(\cdot,x_0)) \to L^2([a,\infty);dx)\\ \qquad \widehat{h} \mapsto h,\end{cases}\\ &h(\cdot) = \mathrm{l.i.m.}_{\mu_1\downarrow-\infty,\mu_2\uparrow\infty} \int_{\mu_1}^{\mu_2} (\theta(\lambda,\cdot,x_0), \phi(\lambda,\cdot,x_0))\, d\Omega(\lambda,x_0)\,\widehat{h}(\lambda,x_0),\end{aligned} \tag{3.81}$$

where l.i.m. *refers to the $L^2([a,\infty);dx)$-limit. Then,*

$$U(x_0)F(H_+)U(x_0)^{-1} = M_F \tag{3.82}$$

in $L^2(\mathbb{R};d\Omega(\cdot,x_0))$ (cf. (3.79)*). Moreover,*

$$\sigma(H_+) = \mathrm{supp}\,(d\Omega(\cdot,x_0)) = \mathrm{supp}\,(d\Omega^{\rm tr}(\cdot,x_0)). \tag{3.83}$$

Corollary 3.9. *The expansions in* (3.35) *and* (3.80) *are related by,*

$$\widehat{h}_+(\lambda) = \widetilde{\phi}(\lambda,x_0)\widehat{h}_0(\lambda,x_0) + \widetilde{\phi}'(\lambda,x_0)\widehat{h}_1(\lambda,x_0), \quad \lambda \in \sigma(H_+). \tag{3.84}$$

The measures $d\widetilde\rho_+$ *and* $d\Omega(\cdot,x_0)$ *are related by,*

$$\begin{aligned} d\widetilde\rho_+(\lambda) &= \frac{\widetilde\theta(\lambda,x_0)}{\widetilde\phi(\lambda,x_0)}d\Omega_{0,1}(\lambda,x_0) - \frac{\widetilde\theta'(\lambda,x_0)}{\widetilde\phi(\lambda,x_0)}d\Omega_{0,0}(\lambda,x_0) && (3.85)\\ &= \frac{\widetilde\phi'(\lambda,x_0)}{\widetilde\phi(\lambda,x_0)}\frac{1}{\widetilde\phi(\lambda,x_0)^2+\widetilde\phi'(\lambda,x_0)^2}d\Omega_{0,1}(\lambda,x_0)\\ &\quad + \frac{1}{\widetilde\phi(\lambda,x_0)^2+\widetilde\phi'(\lambda,x_0)^2}d\Omega_{0,0}(\lambda,x_0), \quad \lambda\in\sigma(H_+). && (3.86) \end{aligned}$$

Proof. (3.84) follows from (3.8), (3.35), and (3.78). (3.85) and (3.86) follow from (3.23), (3.26), (3.74), and (3.76). ☐

Finally, we illustrate the applicability of our approach to strongly singular potentials by verifying Hypothesis 3.1 under very general circumstances.

We start with a simple example first.

Example 3.10. *The class of potentials* V *of the form*

$$V(x) = \frac{\gamma^2-1/4}{x^2} + \widetilde V(x), \quad \gamma\in[1,\infty),\ x\in(0,\infty), \tag{3.87}$$

where $\widetilde V$ *is a real-valued measurable function on* $[0,\infty)$ *such that*

$$\widetilde V \in L^1([0,b];x\,dx) \ \textit{for all}\ b>0, \tag{3.88}$$

assuming that $\tau_+ = -d^2/dx^2 + [\gamma^2-(1/4)]x^{-2} + \widetilde V(x)$ *is in the limit point case at* ∞*, satisfies Hypothesis* 3.1*.*

To verify that the potential V in (3.87) indeed satisfies Hypothesis 3.1 we first state the following result. As kindly pointed out to us by Don Hinton, this is a special case of his Theorem 1 in [46]. For convenience of the reader we include the following elementary and short proof we found independently (and which differs from the proof in [46]).

Lemma 3.11. ([46].) Let $b\in(0,\infty)$. Then the differential expression τ_+ given by

$$\tau_+ = -\frac{d^2}{dx^2} + \frac{\gamma^2-(1/4)}{x^2} + \widetilde V(x), \quad x\in(0,b),\ \gamma\in[1,\infty), \tag{3.89}$$

with $\widetilde V$ a real-valued and measurable function on $[0,b]$ satisfying

$$\widetilde V \in L^1([0,b];x\,dx), \tag{3.90}$$

is in the limit point case at $x=0$.

Proof. Consider a solution θ of

$$\begin{aligned} &(\tau_+\theta)(x) = 0, \quad x\in(0,b),\\ &\theta(x_0) = x_0^{1/2-\gamma},\ \theta'(x_0) = (1/2-\gamma)x_0^{-1/2-\gamma} \quad \text{for some } x_0\in(0,b). \end{aligned} \tag{3.91}$$

By the "variation of constants" formula, θ satisfies

$$\theta(x) = x^{1/2-\gamma} + \frac{1}{2\gamma}\int_{x_0}^x dt\big[x^{1/2+\gamma}t^{1/2-\gamma} - x^{1/2-\gamma}t^{1/2+\gamma}\big]\widetilde V(t)\theta(t). \tag{3.92}$$

Introducing

$$\theta_0(x) = x^{1/2-\gamma},$$
$$\theta_k(x) = \frac{1}{2\gamma}\int_{x_0}^{x} dt\big[x^{1/2+\gamma}t^{1/2-\gamma} - x^{1/2-\gamma}t^{1/2+\gamma}\big]\widetilde{V}(t)\theta_{k-1}(t), \quad k \in \mathbb{N}, \tag{3.93}$$

and estimating θ_k by

$$|\theta_k(x)| \le x^{1/2-\gamma}\frac{1}{k!}\left(\frac{1}{2\gamma}\int_0^{x_0} dt\, t\big|\widetilde{V}(t)\big|\right)^k, \quad x \in (0, x_0),\ k \ge 0, \tag{3.94}$$

then imply

$$\theta(x) = \sum_{k=0}^{\infty}\theta_k(x), \tag{3.95}$$

where the sum converges absolutely and uniformly on any compact subset of $(0, x_0)$. In addition,

$$|\theta(x)| \le \sum_{k=0}^{\infty}|\theta_k(x)| \le x^{1/2-\gamma}\exp\left(\frac{1}{2\gamma}\int_0^{x_0} dt\, t\big|\widetilde{V}(t)\big|\right), \quad x \in (0, x_0). \tag{3.96}$$

Since $\widetilde{V} \in L^1([0,b]; x\,dx)$, there exists $x_0 \in (0,b)$ such that

$$\frac{1}{2\gamma}\int_0^{x_0} dt\, t\big|\widetilde{V}(t)\big| \le \ln(3/2), \tag{3.97}$$

and hence by (3.93), (3.95), (3.96), and (3.97),

$$\theta(x) \ge 2\theta^{(0)} - \sum_{k=0}^{\infty}\big|\theta^{(k)}(x)\big| \ge x^{1/2-\gamma}\Big(2 - e^{\ln(3/2)}\Big) \ge \frac{1}{2}x^{1/2-\gamma}, \quad x \in (0, x_0). \tag{3.98}$$

Thus, $\theta \notin L^2((0,x_0); dx)$ and hence τ_+ is in the limit point case at $x = 0$. $\square$

Moreover, by the "variation of constants" formula, the Weyl–Titchmarsh solution $\widetilde{\phi}(z,\cdot)$ of

$$-\psi''(z,x) + V(x)\psi(z,x) = z\psi(z,x), \quad x \in (0,\infty), \tag{3.99}$$
$$\psi(z,\cdot) \in L^2((0,b); dx) \text{ for some } b \in (0,\infty),\ z \in \mathbb{C} \tag{3.100}$$

satisfies the Volterra integral equation

$$\widetilde{\phi}(z,x) = x^{1/2+\gamma} + \frac{1}{2\gamma}\int_0^x dt\,\big[x^{1/2+\gamma}t^{1/2-\gamma} - t^{1/2+\gamma}x^{1/2-\gamma}\big]U(z,t)\widetilde{\phi}(z,t), \tag{3.101}$$

where

$$U(z,x) = \widetilde{V}(x) - z. \tag{3.102}$$

To verify this claim one iterates (3.101) to obtain a solution $\widetilde{\phi}(z,x)$ of (3.99) in the form

$$\widetilde{\phi}(z,x) = \sum_{k=0}^{\infty}\widetilde{\phi}_k(z,x), \quad z \in \mathbb{C},\ x \in (0,\infty), \tag{3.103}$$

where

$$\begin{aligned}
&\widetilde{\phi}_0(z,x) = x^{1/2+\gamma}, \\
&\widetilde{\phi}_k(z,x) = \frac{1}{2\gamma}\int_0^x dx' \big[x^{1/2+\gamma}(x')^{1/2-\gamma} - (x')^{1/2+\gamma}x^{1/2-\gamma}\big]U(z,x')\widetilde{\phi}_{k-1}(z,x'), \\
&\hspace{6cm} k\in\mathbb{N},\ z\in\mathbb{C},\ x\in(0,\infty). \qquad (3.104)
\end{aligned}$$

Since $\widetilde{\phi}_k(z,x)$, $k\in\mathbb{N}$, is continuous in $(z,x)\in\mathbb{C}\times(0,\infty)$, entire with respect to z for all fixed $x\in(0,\infty)$, and since

$$\big|\widetilde{\phi}_k(z,x)\big| \le \frac{x^{1/2+\gamma}}{k!}\bigg(\frac{1}{\gamma}\int_0^x dx'x'\,|U(z,x')|\bigg)^k, \quad (z,x)\in K, \qquad (3.105)$$

where K is any compact subset of $\mathbb{C}\times(0,\infty)$, the series in (3.103) converges absolutely and uniformly on K, and hence $\widetilde{\phi}(z,x)$ is continuous in $(z,x)\in\mathbb{C}\times(0,\infty)$ and entire in z for all fixed $x\in(0,\infty)$. Moreover, it follows from (3.103) and (3.105) that

$$\big|\widetilde{\phi}(z,x)\big| \le x^{1/2+\gamma}\exp\bigg(\frac{1}{\gamma}\int_0^x dx'x'\,|U(z,x')|\bigg), \quad (z,x)\in K, \qquad (3.106)$$

and hence, $\widetilde{\phi}(z,\cdot)$ satisfies (3.100). Summarizing these considerations, $\widetilde{\phi}(z,\cdot)$ satisfies Hypotheses 3.1 (ii) $(\alpha)-(\gamma)$.

While this represents just an elementary example, we now turn to a vast class of singular potentials.

We first state the following auxiliary result.

Lemma 3.12. *Let $b\in(0,\infty)$ and $f,f'\in AC_{\rm loc}((0,b))$, f real-valued, and $f(x)\neq 0$ for all $x\in(0,b)$.*
(i) Introduce

$$\eta_\pm(x) = 2^{-1/2}f(x)\exp\bigg(\pm\int_x^{x_0} dx'\,f(x')^{-2}\bigg), \quad x,x_0\in(0,b). \qquad (3.107)$$

Then $\eta_\pm$ are a fundamental system of solutions of

$$-\psi''(x) + \bigg[\frac{f''(x)}{f(x)} + \frac{1}{f(x)^4}\bigg]\psi(x) = 0, \quad x\in(0,b) \qquad (3.108)$$

and

$$W(\eta_+,\eta_-)(x) = 1. \qquad (3.109)$$

(ii) Assume in addition that $f\in L^2([0,b'];dx)$ for some $b'\in(0,b)$ and $\widetilde{V}\in L^1([0,c];f^2dx)$ for all $c\in(0,b)$. Then there exists an entire Weyl–Titchmarsh solution $\widetilde{\phi}(z,\cdot)$ of

$$-\phi''(z,x) + \bigg[\frac{f''(x)}{f(x)} + \frac{1}{f(x)^4} + \widetilde{V}(x)\bigg]\phi(z,x) = z\phi(z,x), \quad z\in\mathbb{C},\ x\in(0,b) \qquad (3.110)$$

in the following sense:

(α) *For all $x\in(0,b)$, $\widetilde{\phi}(\cdot,x)$ is entire.*

(β) *$\widetilde{\phi}(z,x)$, $x\in(0,b)$, is real-valued for $z\in\mathbb{R}$.*

(γ) *$\widetilde{\phi}(z,\cdot)$ satisfies the L^2-condition near the end point 0 and hence*

$$\widetilde{\phi}(z,\cdot)\in L^2([0,c];dx) \ \text{ for all } z\in\mathbb{C} \text{ and all } c\in(0,b). \qquad (3.111)$$

Proof. Verifying item (i) is a straightforward computation. To verify item (ii), consider the Volterra integral equation

$$\widetilde{\phi}(z,x) = \eta_-(x) + \int_0^x dx' \, [\eta_+(x')\eta_-(x) - \eta_+(x)\eta_-(x')]\big[\widetilde{V}(x') - z\big]\widetilde{\phi}(z,x'), \quad z \in \mathbb{C}, \ x \in (0,b). \tag{3.112}$$

Again, iterating (3.112) then yields

$$\widetilde{\phi}(z,x) = \sum_{k=0}^{\infty} \widetilde{\phi}_k(z,x), \quad \widetilde{\phi}_0(z,x) = \eta_-(x), \tag{3.113}$$

$$\widetilde{\phi}_k(z,x) = \int_0^x dx' \, [\eta_+(x')\eta_-(x) - \eta_+(x)\eta_-(x')]\big[\widetilde{V}(x') - z\big]\widetilde{\phi}_{k-1}(z,x'), \quad k \in \mathbb{N}. \tag{3.114}$$

The elementary estimate

$$\left| \frac{\eta_+(x)}{\eta_-(x)} \frac{\eta_-(x')}{\eta_+(x')} \right| \leq \exp\bigg(- \int_{x'}^x dy \, f(y)^{-2} \bigg) \leq 1, \quad 0 \leq x' \leq x < b \tag{3.115}$$

then yields

$$\begin{aligned} \big|\widetilde{\phi}_1(z,x)\big| &\leq |\eta_-(x)| \int_0^x dx' \, |\eta_+(x')\eta_-(x')| \left| 1 + \frac{\eta_+(x)}{\eta_-(x)} \frac{\eta_-(x')}{\eta_+(x')} \right| \big|\widetilde{V}(x') - z\big| \\ &\leq 2|\eta_-(x)| \int_0^x dx' f(x')^2 |\widetilde{V}(x') - z| \end{aligned} \tag{3.116}$$

and hence

$$\big|\widetilde{\phi}_k(z,x)\big| \leq |\eta_-(x)| \frac{1}{k!} \bigg(2 \int_0^x dx' f(x')^2 \big|\widetilde{V}(x) - z\big| \bigg)^k, \quad k \in \mathbb{N}, \ z \in \mathbb{C}, \ x \in (0,b). \tag{3.117}$$

Thus,

$$\big|\widetilde{\phi}(z,x)\big| \leq |\eta_-(x)| \exp\bigg(2 \int_0^x dx' f(x')^2 \big|\widetilde{V}(x) - z\big| \bigg), \quad k \in \mathbb{N}, \ z \in \mathbb{C}, \ x \in (0,b). \tag{3.118}$$

This proves items $(ii)\,(\alpha)$ and $(ii)\,(\beta)$. Since by hypothesis, $f \in L^2([0,b']; dx)$ for some $b' \in (0,b)$ and hence $\eta_- \in L^2([0,c]; dx)$ for all $c \in (0,b)$, item $(ii)\,(\gamma)$ holds as well. ☐

A general class of examples of strongly singular potentials satisfying Hypothesis 3.1 (iii) is then described in the following example.

Example 3.13. *Let $b \in (0,\infty)$. Then the class of potentials V such that*

$$V, V' \in AC_{\rm loc}((0,b)), \ V \in L^1_{\rm loc}((0,\infty); dx), \ \ V \ \text{real-valued}, \tag{3.119}$$

$$V(x) > 0, \quad x \in (0,b), \tag{3.120}$$

$$V^{-1/2} \in L^1([0,b]; dx), \tag{3.121}$$

$$V'V^{-5/4} \in L^2([0,b]; dx), \tag{3.122}$$

$$\text{either } V^{-3/2}V'' \in L^1([0,b]; dx), \text{ or else,} \tag{3.123}$$

$$V'' > 0 \text{ a.e. on } (0,b) \text{ and } \lim_{x \downarrow 0} V'(x)V(x)^{-3/2} \text{ exists and is finite,} \tag{3.124}$$

satisfies Hypothesis 3.1 (*iii*) (α)–(γ) *in the following sense: There exists an entire Weyl–Titchmarsh solution* $\widetilde{\phi}(z,\cdot)$ *of*

$$-\psi''(z,x) + V(x)\psi(z,x) = z\psi(z,x), \quad z \in \mathbb{C},\ x \in (0,\infty) \tag{3.125}$$

satisfying the following conditions (α)–(β)*:*

(α) *For all* $x \in (0,\infty)$, $\widetilde{\phi}(\cdot,x)$ *is entire.*

(β) $\widetilde{\phi}(z,x)$, $x \in (0,\infty)$, *is real-valued for* $z \in \mathbb{R}$.

(γ) $\widetilde{\phi}(z,\cdot)$ *satisfies the* L^2*-condition near the end point* 0 *and hence*

$$\widetilde{\phi}(z,\cdot) \in L^2([0,c];dx) \ \textit{ for all } z \in \mathbb{C} \textit{ and all } c \in (0,\infty). \tag{3.126}$$

Since V is strongly singular at most at $x = 0$, it suffices to discuss this example for $x \in (0,b)$ only. Moreover, for simplicity, we focus only on sufficient conditions for Hypotheses 3.1 (*iii*) (α)–(γ) to hold. The additional limit point assumptions on V at zero and at infinity can easily be supplied. Moreover, we made no efforts to optimize the conditions on V. The point of the example is just to show the wide applicability of our approach based on Hypothesis 3.1.

In order to reduce Example 3.13 to Lemma 3.12, one can argue as follows: Introduce

$$f(x) = V(x)^{-1/4}, \tag{3.127}$$

$$\widetilde{V}(x) = -f''(x)/f(x). \tag{3.128}$$

Then $f, f' \in AC_{\rm loc}((0,b))$, $f \neq 0$ on $(0,b)$, and $f \in L^2([0,c];dx)$ for all $c \in (0,b)$. Moreover, since

$$f^2\widetilde{V} = -ff'' = -\frac{5}{16}\big[V^{-5/4}V'\big]^2 + \frac{1}{4}V^{-3/2}V'', \tag{3.129}$$

$\widetilde{V} \in L^1([0,c];f^2dx)$ for some $c \in (0,b)$. (This is clear from (3.122) if condition in (3.123) is assumed. In case (3.124) is assumed, a straightforward integration by parts, using (3.122), yields $\widetilde{V} \in L^1([0,c];f^2dx)$ for some $c \in (0,b)$.) Thus, Lemma 3.12 applies to

$$V = f^{-4} = [(f''/f) + f^{-4}] + \widetilde{V}. \tag{3.130}$$

Remark 3.14. We focused on the strongly singular case where τ_+ is in the limit point case at the singular endpoint $x = a$. The singular case, where V is not integrable at the endpoint a and τ_+ is in the limit circle case at a is similar to the regular case (associated with a Weyl–Titchmarsh coefficient having the Herglotz property) considered in Section 2. For pertinent references to this case see [30], [34].

4. An Illustrative Example

In this section we provide a detailed treatment of the following well-known singular potential example,

$$V(x,\gamma) = \frac{\gamma^2 - (1/4)}{x^2}, \quad x \in (0,\infty),\ \gamma \in [1,\infty) \tag{4.1}$$

with associated differential expression

$$\tau_+(\gamma) = -\frac{d^2}{dx^2} + V(x,\gamma), \quad x \in (0,\infty),\ \gamma \in [1,\infty). \tag{4.2}$$

Numerous references have been devoted to this example, we refer, for instance, to [20], [21], [23, p. 1532–1536], [26], [34], [35], [60], [61, p. 142–144], [62], [70, p. 87–90], and the literature therein. The corresponding maximally defined self-adjoint Schrödinger operator $H_+(\gamma)$ in $L^2([0,\infty);dx)$ is then defined by

$$\begin{aligned} &H_+(\gamma)f = \tau_+(\gamma)f, \\ &f \in \operatorname{dom}(H_+(\gamma)) = \{g \in L^2([0,\infty);dx) \,|\, g, g' \in AC_{\mathrm{loc}}((0,\infty)); \\ &\hspace{6cm} \tau_+(\gamma)g \in L^2([0,\infty);dx)\}. \end{aligned} \tag{4.3}$$

The potential $V(\cdot,\gamma)$ in (4.1) is so strongly singular at the finite end point $x=0$ that $H_+(\gamma)$ (in stark contrast to cases regular at $x=0$, cf. (2.3)) is self-adjoint in $L^2([0,\infty);dx)$ without imposing any boundary condition at $x=0$. Equivalently, the corresponding minimal Schrödinger operator $\widetilde{H}_+(\gamma)$, defined by

$$\begin{aligned} &\widetilde{H}_+(\gamma)f = \tau_+(\gamma)f, \\ &f \in \operatorname{dom}(\widetilde{H}_+(\gamma)) = \{g \in L^2([0,\infty);dx) \,|\, g, g' \in AC_{\mathrm{loc}}((0,\infty)); \\ &\hspace{2cm} \operatorname{supp}(g) \subset (0,\infty) \text{ compact}; \tau_+(\gamma)g \in L^2([0,\infty);dx)\}, \end{aligned} \tag{4.4}$$

is essentially self-adjoint in $L^2([0,\infty);dx)$.

A fundamental system of solutions of

$$(\tau_+(\gamma)\psi)(z,x) = z\psi(z,x), \quad x \in (0,\infty) \tag{4.5}$$

is given by

$$x^{1/2}J_\gamma(z^{1/2}x),\ x^{1/2}Y_\gamma(z^{1/2}x), \quad z \in \mathbb{C}\backslash\{0\},\ x \in (0,\infty),\ \gamma \in [1,\infty) \tag{4.6}$$

with $J_\gamma(\cdot)$ and $Y_\gamma(\cdot)$ the usual Bessel functions of order γ (cf. [1, Ch. 9]). We first treat the case where

$$\gamma \in (1,\infty), \quad \gamma \notin \mathbb{N}, \tag{4.7}$$

in which case

$$x^{1/2}J_\gamma(z^{1/2}x),\ x^{1/2}J_{-\gamma}(z^{1/2}x), \quad z \in \mathbb{C}\backslash\{0\},\ x \in (0,\infty),\ \gamma \in (1,\infty)\backslash\mathbb{N} \tag{4.8}$$

is a fundamental system of solutions of (4.5). Since the system of solutions in (4.8) exhibits the branch cut $[0,\infty)$ with respect to z, we slightly change it into the following system,

$$\begin{aligned} &\phi(z,x,\gamma) = C^{-1}\pi[2\sin(\pi\gamma)]^{-1}z^{-\gamma/2}x^{1/2}J_\gamma(z^{1/2}x), \\ &\theta(z,x,\gamma) = Cz^{\gamma/2}x^{1/2}J_{-\gamma}(z^{1/2}x), \quad z \in \mathbb{C},\ x \in (0,\infty),\ \gamma \in (1,\infty)\backslash\mathbb{N}, \end{aligned} \tag{4.9}$$

which for each $x \in (0,\infty)$ represents entire functions with respect to z. Here $C \in \mathbb{R}\backslash\{0\}$ is a normalization constant to be discussed in Remark 4.4. One verifies that (cf. [1, p. 360])

$$W(\theta(z,\cdot,\gamma),\phi(z,\cdot,\gamma)) = 1, \quad z \in \mathbb{C},\ \gamma \in (1,\infty)\backslash\mathbb{N} \tag{4.10}$$

and that (cf. [1, p. 360])

$$\begin{aligned} z^{\mp\gamma/2}x^{1/2}J_{\pm\gamma}(z^{1/2}x) = 2^{-\gamma}x^{(1/2)\pm\gamma}\sum_{k=0}^{\infty}\frac{(-zx^2/4)^k}{k!\Gamma(k+1\pm\gamma)}&, \\ z \in \mathbb{C},\ x \in (0,\infty),\ \gamma \in (1,\infty)\backslash\mathbb{N}&. \end{aligned} \tag{4.11}$$

Hence the fundamental system $\phi(z,\cdot,\gamma),\theta(z,\cdot,\gamma)$ in (4.9) of solutions of (4.5) is entire with respect to z and real-valued for $z \in \mathbb{R}$.

The corresponding solution of (4.5), square integrable in a neighborhood of infinity, is given by

$$\begin{aligned} x^{1/2}H_\gamma^{(1)}(z^{1/2}x) = \frac{i}{\sin(\pi\gamma)} x^{1/2}\big[e^{-i\pi\gamma}J_\gamma(z^{1/2}x) - J_{-\gamma}(z^{1/2}x)\big],& \\ z\in\mathbb{C}\backslash[0,\infty),\ x\in(0,\infty),\ \gamma\in(1,\infty)\backslash\mathbb{N}& \end{aligned} \tag{4.12}$$

with $H_\gamma^{(1)}(\cdot)$ the usual Hankel function of order γ (cf. [1, Ch. 9]). In order to be compatible with our modified system ϕ,θ of solutions of (4.5), we replace it by

$$\begin{aligned} \psi_+(z,x,\gamma) &= Cz^{\gamma/2}x^{1/2}J_{-\gamma}(z^{1/2}x) - C^2e^{-i\pi\gamma}z^\gamma C^{-1}z^{-\gamma/2}x^{1/2}J_\gamma(z^{1/2}x) \\ &= \theta(z,x,\gamma) + m_+(z,\gamma)\phi(z,x,\gamma), \\ &\quad z\in\mathbb{C}\backslash[0,\infty),\ x\in(0,\infty),\ \gamma\in(1,\infty)\backslash\mathbb{N}, \end{aligned} \tag{4.13}$$

where

$$m_+(z,\gamma) = -C^2(2/\pi)\sin(\pi\gamma)e^{-i\pi\gamma}z^\gamma, \quad z\in\mathbb{C}\backslash[0,\infty),\ \gamma\in(1,\infty)\backslash\mathbb{N} \tag{4.14}$$

and

$$\overline{m_+(z,\gamma)} = m_+(\overline{z},\gamma), \quad z\in\mathbb{C}\backslash[0,\infty). \tag{4.15}$$

Next, we consider the case,

$$\gamma = n\in\mathbb{N}, \tag{4.16}$$

in which

$$x^{1/2}J_n(z^{1/2}x),\ x^{1/2}Y_n(z^{1/2}x), \quad z\in\mathbb{C}\backslash\{0\},\ x\in(0,\infty),\ n\in\mathbb{N}, \tag{4.17}$$

is a fundamental system of solutions of (4.5). As before, we slightly change it into the following system,

$$\begin{aligned} &\phi(z,x,n) = C^{-1}(\pi/2)z^{-n/2}x^{1/2}J_n(z^{1/2}x), \\ &\theta(z,x,n) = Cz^{n/2}x^{1/2}\big[-Y_n(z^{1/2}x) + \pi^{-1}\ln(z)J_n(z^{1/2}x)\big], \\ &\qquad\qquad z\in\mathbb{C},\ x\in(0,\infty),\ n\in\mathbb{N}. \end{aligned} \tag{4.18}$$

Here $C\in\mathbb{R}\backslash\{0\}$ is a normalization constant to be discussed in Remark 4.4. One verifies that (cf. [1, p. 360])

$$W(\theta(z,\cdot,n),\phi(z,\cdot,n))(x) = 1, \quad z\in\mathbb{C},\ n\in\mathbb{N}, \tag{4.19}$$

and that the fundamental system of solutions of (4.5), $\phi(z,\cdot,n),\theta(z,\cdot,n)$ in (4.18), is entire with respect to z and real-valued for $z\in\mathbb{R}$.

The corresponding solution of (4.5), square integrable in a neighborhood of infinity, is given by

$$\begin{aligned} x^{1/2}H_n^{(1)}(z^{1/2}x) = x^{1/2}\big[J_n(z^{1/2}x) + iY_n(z^{1/2}x)\big],& \\ z\in\mathbb{C}\backslash[0,\infty), x\in(0,\infty),\ n\in\mathbb{N}& \end{aligned} \tag{4.20}$$

with $H_n^{(1)}(\cdot)$ the usual Hankel function of order n (cf. [1, Ch. 9]). In order to be compatible with our modified system ϕ,θ of solutions of (4.5), we replace it by

$$\begin{aligned} \psi_+(z,x,n) &= Cz^{n/2}x^{1/2}iH_n(z^{1/2}x) = Cz^{1/2}x^{1/2}\big[-Y_n(z^{1/2}x) + iJ_n(z^{1/2}x)\big] \\ &= \theta(z,x,n) + m_+(z,n)\phi(z,x,n), \\ &\quad z\in\mathbb{C}\backslash[0,\infty),\ x\in(0,\infty),\ n\in\mathbb{N}, \end{aligned} \tag{4.21}$$

where

$$m_+(z,n) = C^2(2/\pi)z^n\big[i - (1/\pi)\ln(z)\big], \quad z \in \mathbb{C}\backslash[0,\infty),\ n \in \mathbb{N} \tag{4.22}$$

and

$$\overline{m_+(z,n)} = m_+(\overline{z},n), \quad z \in \mathbb{C}\backslash[0,\infty). \tag{4.23}$$

Remark 4.1. (i) We emphasize that in stark contrast to the case of regular half-line Schrödinger operators in Section 2, $m_+(\cdot,\gamma)$ in (4.14) and (4.22) is not a Herglotz function for $\gamma \in [1,\infty)$.
(ii) After finishing our paper, we received a manuscript by Everitt and Kalf [26] in which the Friedrichs extension and the associated Hankel eigenfunction transform are treated in detail for the case $\gamma \in [0,1)$ in (4.1). In this case the corresponding Weyl–Titchmarsh coefficient turns out to be a Herglotz function.

Since $\tau_+(\gamma)$ is in the limit point case at $x = 0$ and at $x = \infty$, (4.5) has a unique solution (up to constant multiples) that is L^2 near 0 and L^2 near ∞. Indeed, that unique L^2-solution near 0 (up to normalization) is precisely $\phi(z,\cdot,\gamma)$; similarly, the unique L^2-solution near ∞ (up to normalization) is $\psi_+(z,\cdot,\gamma)$.

By (4.10) and (4.19), a computation of the Green's function $G_+(z,x,x',\gamma)$ of $H_+(\gamma)$ yields

$$G_+(z,x,x',\gamma) = \frac{i\pi}{2}\begin{cases} x^{1/2}J_\gamma(z^{1/2}x)x'^{1/2}H_\gamma^{(1)}(z^{1/2}x'), & 0 < x \le x', \\ x'^{1/2}J_\gamma(z^{1/2}x')x^{1/2}H_\gamma^{(1)}(z^{1/2}x), & 0 < x' \le x, \end{cases} \tag{4.24}$$

$$= \begin{cases} \phi(z,x,\gamma)\psi_+(z,x',\gamma), & 0 < x \le x', \\ \phi(z,x',\gamma)\psi_+(z,x,\gamma), & 0 < x' \le x, \end{cases} \tag{4.25}$$

$$z \in \mathbb{C}\backslash[0,\infty),\ \gamma \in [1,\infty).$$

Thus,

$$\begin{gathered}((H_+(\gamma) - zI)^{-1}f)(x) = \int_0^\infty dx'\, G_+(z,x,x',\gamma)f(x'), \\ z \in \mathbb{C}\backslash[0,\infty),\ x \in (0,\infty),\ f \in L^2([0,\infty);dx),\ \gamma \in [1,\infty).\end{gathered} \tag{4.26}$$

Given $m_+(z,\gamma)$ in (4.14), we define the associated measure $\rho_+(\cdot,\gamma)$ by

$$\rho_+((\lambda_1,\lambda_2],\gamma) = \pi^{-1}\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, \mathrm{Im}(m_+(\lambda + i\varepsilon,\gamma)) \tag{4.27}$$

$$= C^2\frac{\lambda_2^{\gamma+1} - \lambda_1^{\gamma+1}}{\gamma+1}\frac{2}{\pi^2}\begin{cases} \sin^2(\pi\gamma), & \gamma \notin \mathbb{N}, \\ 1, & \gamma \in \mathbb{N}, \end{cases} \tag{4.28}$$

$$0 \le \lambda_1 < \lambda_2,\ \gamma \in [1,\infty),$$

generated by the function

$$\rho_+(\lambda,\gamma) = C^2\chi_{[0,\infty)}(\lambda)\frac{\lambda^{\gamma+1}}{\gamma+1}\frac{2}{\pi^2}\begin{cases} \sin^2(\pi\gamma), & \gamma \notin \mathbb{N}, \\ 1, & \gamma \in \mathbb{N}, \end{cases} \quad \lambda \in \mathbb{R},\ \gamma \in [1,\infty). \tag{4.29}$$

Even though $m_+(\cdot,\gamma)$ is not a Herglotz function for $\gamma \in [1,\infty)$, $d\rho_+(\cdot,\gamma)$ is defined as in (3.26), in analogy to the case of Herglotz functions discussed in Appendix A (cf. (A.4)).

Next, we introduce the family of spectral projections, $\{E_{H_+(\gamma)}(\lambda)\}_{\lambda\in\mathbb{R}}$, of the self-adjoint operator $H_+(\gamma)$ and note that for $F \in C(\mathbb{R})$,

$$\begin{aligned}
&\big(f, F(H_+(\gamma))g\big)_{L^2([0,\infty);dx)} = \int_{\mathbb{R}} d\big(f, E_{H_+(\gamma)}(\lambda)g\big)_{L^2([0,\infty);dx)}\, F(\lambda), \\
&f, g \in \mathrm{dom}(F(H_+(\gamma))) \qquad (4.30)\\
&\quad = \bigg\{h \in L^2([0,\infty);dx) \,\bigg|\, \int_{\mathbb{R}} d\big\|E_{H_+(\gamma)}(\lambda)h\big\|^2_{L^2([0,\infty);dx)}\, |F(\lambda)|^2 < \infty\bigg\}.
\end{aligned}$$

The connection between $\{E_{H_+(\gamma)}(\lambda)\}_{\lambda\in\mathbb{R}}$ and $\rho_+(\lambda,\gamma)$, $\lambda \geq 0$, is described in the next result.

Lemma 4.2. *Let $\gamma \in [1,\infty)$, $f, g \in C_0^\infty((0,\infty))$, $F \in C(\mathbb{R})$, and $\lambda_1, \lambda_2 \in [0,\infty)$, $\lambda_1 < \lambda_2$. Then,*

$$\begin{aligned}
&\big(f, F(H_+(\gamma))E_{H_+(\gamma)}((\lambda_1,\lambda_2])g\big)_{L^2([0,\infty);dx)} \\
&\quad = \big(\widehat{f}_+(\gamma), M_F M_{\chi_{(\lambda_1,\lambda_2]}} \widehat{g}_+(\gamma)\big)_{L^2(\mathbb{R};d\rho_+(\cdot,\gamma))},
\end{aligned} \tag{4.31}$$

where

$$\widehat{h}_+(\gamma)(\lambda) = \int_0^\infty dx\, \phi(\lambda,x,\gamma)h(x), \quad \lambda \in [0,\infty),\ h \in C_0^\infty((0,\infty)) \tag{4.32}$$

and M_G denotes the operator of multiplication by the $d\rho_+(\cdot,\gamma)$-measurable function G in the Hilbert space $L^2(\mathbb{R};d\rho_+(\cdot,\gamma))$.

The proof of Lemma 4.2 is a special case of that of Theorem 3.5 and hence ommitted.

As in Section 3 one can remove the compact support restrictions on f and g in Lemma 4.2. To this end one considers the map

$$U_+(\gamma)\colon \begin{cases} L^2([0,\infty);dx) \to L^2(\mathbb{R};d\rho_+(\cdot,\gamma)) \\ \qquad h \mapsto \widehat{h}_+(\cdot,\gamma) = \text{l.i.m.}_{b\uparrow\infty} \int_0^b dx\, \phi(\cdot,x,\gamma)h(x), \end{cases} \tag{4.33}$$

where l.i.m. refers to the $L^2(\mathbb{R};d\rho_+(\cdot,\gamma))$-limit.

In addition, it is of course known (cf., e.g., [23, p. 1535]) that the Bessel transform $U_+(\gamma)$ in (4.33) is onto and hence that $U_+(\gamma)$ is unitary with

$$U_+(\gamma)^{-1}\colon \begin{cases} L^2(\mathbb{R};d\rho_+(\cdot,\gamma)) \to L^2([0,\infty);dx) \\ \qquad \widehat{h} \mapsto \text{l.i.m.}_{\mu_1\downarrow-\infty,\mu_2\uparrow\infty} \int_{\mu_1}^{\mu_2} d\rho_+(\lambda,\gamma)\, \phi(\lambda,\cdot,\gamma)\widehat{h}(\lambda), \end{cases} \tag{4.34}$$

where l.i.m. refers to the $L^2([0,\infty);dx)$-limit.

Again we sum up these considerations in a variant of the spectral theorem for (functions of) $H_+(\gamma)$.

Theorem 4.3. *Let $\gamma \in [1,\infty)$, $F \in C(\mathbb{R})$. Then,*

$$U_+(\gamma)F(H_+(\gamma))U_+(\gamma)^{-1} = M_F \tag{4.35}$$

in $L^2(\mathbb{R};d\rho_+(\cdot,\gamma))$. Moreover,

$$\sigma(F(H_+(\gamma))) = \text{ess.ran}_{d\rho_+(\cdot,\gamma)}(F), \tag{4.36}$$

$$\sigma(H_+(\gamma)) = \operatorname{supp}(d\rho_+(\cdot,\gamma)), \tag{4.37}$$

and the spectrum of $H_+(\gamma)$ is simple.

Next, we reconsider spectral theory for $H_+(\gamma)$ by choosing a reference point $x_0 \in (0,\infty)$ away from the singularity of $V(\cdot,\gamma)$ at $x=0$.

Consider a system $\phi(z,\cdot,x_0,\gamma)$, $\theta(z,\cdot,x_0,\gamma)$ of solutions of (4.5) with the following initial conditions at the reference point $x_0 \in (0,\infty)$,

$$\phi(z,x_0,x_0,\gamma)=\theta'(z,x_0,x_0,\gamma)=0, \quad \phi'(z,x_0,x_0,\gamma)=\theta(z,x_0,x_0,\gamma)=1.$$

Denote by $m_\pm(z,x_0,\gamma)$ two Weyl–Titchmarsh m-functions corresponding to the restriction of our problem to the intervals $(0,x_0]$ and $[x_0,\infty)$, respectively. Then the Weyl–Titchmarsh solutions $\psi_\pm(z,\cdot,x_0,\gamma)$ and the 2×2 matrix-valued Weyl–Titchmarsh M-function $M(z,x_0,\gamma)$ are given by

$$\psi_\pm(z,x,x_0,\gamma)=\theta(z,x,x_0,\gamma)+m_\pm(z,x_0,\gamma)\phi(z,x,x_0,\gamma), \tag{4.38}$$

$$M(z,x_0,\gamma)=\begin{pmatrix} \frac{1}{m_-(z,x_0,\gamma)-m_+(z,x_0,\gamma)} & \frac{1}{2}\frac{m_-(z,x_0,\gamma)+m_+(z,x_0,\gamma)}{m_-(z,x_0,\gamma)-m_+(z,x_0,\gamma)} \\ \frac{1}{2}\frac{m_-(z,x_0,\gamma)+m_+(z,x_0,\gamma)}{m_-(z,x_0,\gamma)-m_+(z,x_0,\gamma)} & \frac{m_-(z,x_0,\gamma)m_+(z,x_0,\gamma)}{m_-(z,x_0,\gamma)-m_+(z,x_0,\gamma)} \end{pmatrix}. \tag{4.39}$$

Since any L^2-solution near 0 and near ∞ (i.e., any Weyl–Titchmarsh solution) is necessarily proportional to $x^{1/2}J_\gamma(z^{1/2}x)$ and $x^{1/2}H^{(1)}_\gamma(z^{1/2}x)$, respectively, one explicitly computes for $m_\pm(z,x_0,\gamma)$,

$$m_-(z,x_0,\gamma)=\frac{1}{2x_0}+z^{1/2}\frac{J'_\gamma(z^{1/2}x_0)}{J_\gamma(z^{1/2}x_0)}, \tag{4.40}$$

$$m_+(z,x_0,\gamma)=\frac{1}{2x_0}+z^{1/2}\frac{H^{(1)\prime}_\gamma(z^{1/2}x_0)}{H^{(1)}_\gamma(z^{1/2}x_0)}, \tag{4.41}$$

and for $M(z,x_0,\gamma)$,

$$M_{0,0}(z,x_0,\gamma)=\frac{i\pi x_0}{2}J_\gamma(z^{1/2}x_0)H^{(1)}_\gamma(z^{1/2}x_0), \tag{4.42}$$

$$\begin{aligned} M_{0,1}(z,x_0,\gamma)=M_{1,0}(z,x_0,\gamma)=\frac{i\pi}{4}\bigg[&J_\gamma(z^{1/2}x_0)H^{(1)}_\gamma(z^{1/2}x_0)+x_0z^{1/2} \\ &\times\Big(J_\gamma(z^{1/2}x_0)H^{(1)\prime}_\gamma(z^{1/2}x_0)+J'_\gamma(z^{1/2}x_0)H^{(1)}_\gamma(z^{1/2}x_0)\Big)\bigg], \end{aligned} \tag{4.43}$$

$$\begin{aligned} M_{1,1}(z,x_0,\gamma)=\frac{i\pi}{8x_0}\bigg[&J_\gamma(z^{1/2}x_0)H^{(1)}_\gamma(z^{1/2}x_0)+2x_0z^{1/2} \\ &\times\Big(J_\gamma(z^{1/2}x_0)H^{(1)\prime}_\gamma(z^{1/2}x_0)+J'_\gamma(z^{1/2}x_0)H^{(1)}_\gamma(z^{1/2}x_0)\Big) \\ &+4x_0^2zJ'_\gamma(z^{1/2}x_0)H^{(1)\prime}_\gamma(z^{1/2}x_0)\bigg]. \end{aligned} \tag{4.44}$$

Using (4.12), (4.20), and the calculation above, one can also compute the 2×2 spectral measure $d\Omega(\cdot, x_0, \gamma)$ and its density $d\Omega(\cdot, x_0, \gamma)/d\lambda$,

$$\frac{d\Omega(\lambda, x_0, \gamma)}{d\lambda} = \frac{1}{\pi} \lim_{\varepsilon\downarrow 0} \operatorname{Im}(M(\lambda + i\varepsilon, x_0)), \quad \lambda \in \mathbb{R}, \tag{4.45}$$

$$\frac{d\Omega_{0,0}(\lambda, x_0, \gamma)}{d\lambda} = \begin{cases} \frac{x_0}{2} J_\gamma(\lambda^{1/2} x_0)^2, & \lambda > 0, \\ 0, & \lambda \leq 0, \end{cases} \tag{4.46}$$

$$\begin{aligned} \frac{d\Omega_{0,1}(\lambda, x_0, \gamma)}{d\lambda} &= \frac{d\Omega_{1,0}(\lambda, x_0)}{d\lambda} \\ &= \begin{cases} \frac{1}{4}\left[J_\gamma(\lambda^{1/2} x_0)^2 + 2x_0 \lambda^{1/2} J_\gamma(\lambda^{1/2} x_0) J_\gamma'(\lambda^{1/2} x_0)\right], & \lambda > 0, \\ 0, & \lambda \leq 0, \end{cases} \end{aligned} \tag{4.47}$$

$$\frac{d\Omega_{1,1}(\lambda, x_0, \gamma)}{d\lambda} = \begin{cases} \frac{1}{8x_0}\left[J_\gamma(\lambda^{1/2} x_0) + 2x_0 \lambda^{1/2} J_\gamma'(\lambda^{1/2} x_0)\right]^2, & \lambda > 0, \\ 0, & \lambda \leq 0. \end{cases} \tag{4.48}$$

Moreover, one verifies that,

$$\operatorname{rank}\left(\frac{d\Omega(\lambda, x_0, \gamma)}{d\lambda}\right) = \begin{cases} 1, & \lambda > 0, \\ 0, & \lambda \leq 0. \end{cases} \tag{4.49}$$

Finally, we will show that the results of Section 3 which let one obtain a scalar spectral measure $d\widetilde{\rho}_+(\lambda, \gamma)$ from the 2×2 spectral measure $d\Omega(\lambda, x_0, \gamma)$ lead to the measure equivalent to $d\rho_+(\lambda, \gamma)$ obtained in the first part of this section.

Let

$$\widetilde{\phi}(z, x, \gamma) = z^{-\gamma/2} x^{1/2} J_\gamma(z^{1/2} x) \tag{4.50}$$

be the Weyl–Titchmarsh solution satisfying Hypothesis 3.1 (iii). Inserting (4.46), (4.47), and (4.50) into (3.86) then yields

$$\frac{d\widetilde{\rho}_+(\lambda, \gamma)}{d\lambda} = \begin{cases} \frac{1}{2}\lambda^\gamma, & \lambda > 0, \\ 0, & \lambda \leq 0, \end{cases} \tag{4.51}$$

which, up to a constant multiple, is the same as $d\rho_+(\lambda, \gamma)/d\lambda$ in (4.29).

Of course the analogs of Theorem 3.7, Theorem 3.8, and Corollary 3.9 all hold in the present context of the potential (4.1); we omit the details.

Remark 4.4. We explicitly introduced the normalization constant $C \in \mathbb{R}\backslash\{0\}$ in (4.9) and (4.18) to determine its effect on (the analog of) the Weyl–Titchmarsh coefficient m_+ (cf. (4.14) and (4.22)) and the associated spectral function ρ_+ (cf. (4.29)). As C enters quadratically in m_+ and ρ_+, it clearly has an effect on their asymptotic behavior as $|z| \to \infty$, respectively, $|\lambda| \to \infty$. The same observation applies of course in the regular half-line case considered in the first half of Section 2. It just so happens that in this case the standard normalization of the fundamental system of solutions ϕ_α and θ_α of (2.4) in (2.5) represents a canonical choice and the normalization dependence can safely be ignored. In the strongly singular case in Sections 3 and 4 no such canonical choice of normalization exists. Of course, the actual spectral properties of the corresponding half-line Schrödinger operator are independent of such a choice of normalization.

Appendix A. Basic Facts on Herglotz Functions

In this appendix we recall the definition and basic properties of Herglotz functions.

Definition A.1. Let $\mathbb{C}_\pm = \{z \in \mathbb{C} \mid \mathrm{Im}(z) \gtrless 0\}$. $m : \mathbb{C}_+ \to \mathbb{C}$ is called a *Herglotz* function (or *Nevanlinna* or *Pick* function) if m is analytic on $\mathbb{C}_+$ and $m(\mathbb{C}_+) \subseteq \mathbb{C}_+$.

One then extends m to $\mathbb{C}_-$ by reflection, that is, one defines

$$m(z) = \overline{m(\overline{z})}, \quad z \in \mathbb{C}_-. \tag{A.1}$$

Of course, generally, (A.1) does not represent the analytic continuation of $m\big|_{\mathbb{C}_+}$ into $\mathbb{C}_-$.

The fundamental result on Herglotz functions and their representations on Borel transforms, in part due to Fatou, Herglotz, Luzin, Nevanlinna, Plessner, Privalov, de la Vallée Poussin, Riesz, and others, then reads as follows.

Theorem A.2. ([2], Sect. 69, [4], [22], Chs. II, IV, [53], [55], Ch. 6, [65], Chs. II, IV, [66], Ch. 5.) Let m be a Herglotz function. Then,
(i) $m(z)$ has finite normal limits $m(\lambda \pm i0) = \lim_{\varepsilon\downarrow 0} m(\lambda \pm i\varepsilon)$ for a.e. $\lambda \in \mathbb{R}$.
(ii) Suppose $m(z)$ has a zero normal limit on a subset of $\mathbb{R}$ having positive Lebesgue measure. Then $m \equiv 0$.
(iii) There exists a Borel measure $d\omega$ on $\mathbb{R}$ satisfying

$$\int_{\mathbb{R}} \frac{d\omega(\lambda)}{1+\lambda^2} < \infty \tag{A.2}$$

such that the Nevanlinna, respectively, Riesz-Herglotz representation

$$m(z) = c + dz + \int_{\mathbb{R}} d\omega(\lambda)\left[\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right], \quad z \in \mathbb{C}_+, \tag{A.3}$$

$$c = \mathrm{Re}(m(i)), \quad d = \lim_{\eta\uparrow\infty} m(i\eta)/(i\eta) \geq 0$$

holds. Conversely, any function m of the type (A.3) is a Herglotz function.
(iv) Let $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$. Then the Stieltjes inversion formula for $d\omega$ reads

$$\omega((\lambda_1, \lambda_2]) = \pi^{-1} \lim_{\delta\downarrow 0} \lim_{\varepsilon\downarrow 0} \int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, \mathrm{Im}(m(\lambda + i\varepsilon)). \tag{A.4}$$

(v) The absolutely continuous (ac) part $d\omega_{ac}$ of $d\omega$ with respect to Lebesgue measure $d\lambda$ on $\mathbb{R}$ is given by

$$d\omega_{ac}(\lambda) = \pi^{-1}\mathrm{Im}(m(\lambda + i0))\, d\lambda. \tag{A.5}$$

(vi) Local singularities of m and m^{-1} are necessarily real and at most of first order in the sense that

$$\lim_{\epsilon\downarrow 0}(-i\epsilon)\, m(\lambda + i\epsilon) \geq 0, \quad \lambda \in \mathbb{R}, \tag{A.6}$$

$$\lim_{\epsilon\downarrow 0}(i\epsilon)\, m(\lambda + i\epsilon)^{-1} \geq 0, \quad \lambda \in \mathbb{R}. \tag{A.7}$$

Further properties of Herglotz functions are collected in the following theorem. We denote by

$$d\omega = d\omega_{\mathrm{ac}} + d\omega_{\mathrm{sc}} + d\omega_{\mathrm{pp}} \tag{A.8}$$

the decomposition of $d\omega$ into its absolutely continuous (ac), singularly continuous (sc), and pure point (pp) parts with respect to Lebesgue measure on $\mathbb{R}$.

Theorem A.3. ([4], [41], [53], [68], [69].) Let m be a Herglotz function with representation (A.3). Then,
(i)

$$\begin{aligned}
&d = 0 \text{ and } \int_{\mathbb{R}} d\omega(\lambda)(1+|\lambda|^s)^{-1} < \infty \text{ for some } s \in (0,2) \\
&\text{if and only if } \int_1^\infty d\eta\, \eta^{-s}\, \mathrm{Im}(m(i\eta)) < \infty.
\end{aligned} \tag{A.9}$$

(ii) Let $(\lambda_1, \lambda_2) \subset \mathbb{R}$, $\eta_1 > 0$. Then there is a constant $C(\lambda_1, \lambda_2, \eta_1) > 0$ such that

$$\eta |m(\lambda + i\eta)| \le C(\lambda_1, \lambda_2, \eta_1), \quad (\lambda, \eta) \in [\lambda_1, \lambda_2] \times (0, \eta_1). \tag{A.10}$$

(iii)

$$\sup_{\eta>0} \eta |m(i\eta)| < \infty \text{ if and only if } m(z) = \int_{\mathbb{R}} d\omega(\lambda)(\lambda - z)^{-1} \text{ and } \int_{\mathbb{R}} d\omega(\lambda) < \infty. \tag{A.11}$$

In this case,

$$\int_{\mathbb{R}} d\omega(\lambda) = \sup_{\eta>0} \eta |m(i\eta)| = -i \lim_{\eta \uparrow \infty} \eta m(i\eta). \tag{A.12}$$

(iv) For all $\lambda \in \mathbb{R}$,

$$\lim_{\varepsilon \downarrow 0} \varepsilon \mathrm{Re}(m(\lambda + i\varepsilon)) = 0, \tag{A.13}$$

$$\omega(\{\lambda\}) = \lim_{\varepsilon \downarrow 0} \varepsilon \mathrm{Im}(m(\lambda + i\varepsilon)) = -i \lim_{\varepsilon \downarrow 0} \varepsilon m(\lambda + i\varepsilon). \tag{A.14}$$

(v) Let $L > 0$ and suppose $0 \le \mathrm{Im}(m(z)) \le L$ for all $z \in \mathbb{C}_+$. Then $d = 0$, $d\omega$ is purely absolutely continuous, $d\omega = d\omega_{ac}$, and

$$0 \le \frac{d\omega(\lambda)}{d\lambda} = \pi^{-1} \lim_{\varepsilon \downarrow 0} \mathrm{Im}(m(\lambda + i\varepsilon)) \le \pi^{-1} L \text{ for a.e. } \lambda \in \mathbb{R}. \tag{A.15}$$

(vi) Let $p \in (1, \infty)$, $[\lambda_3, \lambda_4] \subset (\lambda_1, \lambda_2)$, $[\lambda_1, \lambda_2] \subset (\lambda_5, \lambda_6)$. If

$$\sup_{0<\varepsilon<1} \int_{\lambda_1}^{\lambda_2} d\lambda\, |\mathrm{Im}(m(\lambda + i\varepsilon))|^p < \infty, \tag{A.16}$$

then $d\omega = d\omega_{ac}$ is purely absolutely continuous on (λ_1, λ_2), $\frac{d\omega_{ac}}{d\lambda} \in L^p((\lambda_1, \lambda_2); d\lambda)$, and

$$\lim_{\varepsilon \downarrow 0} \left\| \pi^{-1} \mathrm{Im}(m(\cdot + i\varepsilon)) - \frac{d\omega_{ac}}{d\lambda} \right\|_{L^p((\lambda_3, \lambda_4); d\lambda)} = 0. \tag{A.17}$$

Conversely, if $d\omega$ is purely absolutely continuous on (λ_5, λ_6), and if $\frac{d\omega_{ac}}{d\lambda} \in L^p((\lambda_5, \lambda_6); d\lambda)$, then (A.16) holds.
(vii) Let $(\lambda_1, \lambda_2) \subset \mathbb{R}$. Then a local version of Wiener's theorem reads for $p \in (1, \infty)$,

$$\begin{aligned}
&\lim_{\varepsilon \downarrow 0} \varepsilon^{p-1} \int_{\lambda_1}^{\lambda_2} d\lambda\, |\mathrm{Im}(m(\lambda + i\varepsilon))|^p \\
&\quad = \frac{\Gamma(\frac{1}{2})\Gamma(p - \frac{1}{2})}{\Gamma(p)} \bigg[\frac{1}{2} \omega(\{\lambda_1\})^p + \frac{1}{2} \omega(\{\lambda_2\})^p + \sum_{\lambda \in (\lambda_1, \lambda_2)} \omega(\{\lambda\})^p \bigg].
\end{aligned} \tag{A.18}$$

Moreover, for $0 < p < 1$,

$$\lim_{\varepsilon \downarrow 0} \int_{\lambda_1}^{\lambda_2} d\lambda \, |\pi^{-1} \mathrm{Im}(m(\lambda + i\varepsilon))|^p = \int_{\lambda_1}^{\lambda_2} d\lambda \left| \frac{d\omega_{ac}(\lambda)}{d\lambda} \right|^p. \tag{A.19}$$

It should be stressed that Theorems A.2 and A.3 record only the tip of an iceberg of results in this area. A substantial number of additional references relevant in this context can be found in [41].

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