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# A note on reflectionless Jacobi matrices

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**Abstract.** The property that a Jacobi matrix is reflectionless is usually characterized either in terms of Weyl  $m$ -functions or the vanishing of the real part of the boundary values of the diagonal matrix elements of the resolvent. We introduce a characterization in terms of stationary scattering theory (the vanishing of the reflection coefficients) and prove that this characterization is equivalent to the usual ones. We also show that the new characterization is equivalent to the notion of being dynamically reflectionless, thus providing a short proof of an important result of [BRS]. The motivation for the new characterization comes from recent studies of the non-equilibrium statistical mechanics of the electronic black box model and we elaborate on this connection.

## 1 Introduction

The purpose of this paper is two fold. First, we wish to advertise a certain point of view regarding full-line Jacobi matrices that appears absent from the literature. Secondly, we shall use this point of view to give a new characterization of reflectionless Jacobi matrices.

The point of view we wish to describe has its origin in recent studies of the non-equilibrium statistical mechanics of the electronic black box model. We will need here only the simplest variant of this model. The simple electronic black box (SEBB) model describes a quantum dot  $\mathcal{S}$  coupled to two electronic reservoirs  $\mathcal{R}_{l/r}$  that we will colloquially call ‘left’ and ‘right.’ The system  $\mathcal{S}$  is described by the Hilbert space  $\mathbb{C}$  and energy  $\omega \in \mathbb{R}$ . The reservoir  $\mathcal{R}_{l/r}$  is described by a pair  $(\mathfrak{h}_{l/r}, h_{l/r})$ , where  $\mathfrak{h}_{l/r}$  is a single fermion Hilbert space and  $h_{l/r}$  is a single fermion Hamiltonian. We set

$$\mathfrak{h} = \mathfrak{h}_l \oplus \mathbb{C} \oplus \mathfrak{h}_r, \quad h_0 = h_l \oplus \omega \oplus h_r.$$

The fermionic second quantization of the pair  $(\mathfrak{h}, h_0)$  describes the uncoupled SEBB model  $\mathcal{R}_l + \mathcal{S} + \mathcal{R}_r$ . The junctions coupling  $\mathcal{S}$  to the reservoirs are specified by a choice of unit vectors  $\chi_{l/r} \in \mathfrak{h}_{l/r}$  and real numbers  $\lambda_{l/r}$  describing the strength of the coupling. The corresponding tunnelling Hamiltonian is

$$h_T = h_{T,l} + h_{T,r}, \quad h_{T,l/r} = \lambda_{l/r} (|1\rangle\langle\chi_{l/r}| + |\chi_{l/r}\rangle\langle 1|).$$

Finally, the coupled EBB model is obtained by the fermionic second quantization of the pair  $(\mathfrak{h}, h)$  where

$$h = h_0 + h_T.$$

In the literature, the Hamiltonian  $h$  is also known as the *Friedrichs model* or *Wigner-Weisskopf atom*.

In the study of the SEBB model it is no loss of generality to assume that  $\chi_{l/r}$  is a cyclic vector for  $h_{l/r}$ . We shall further assume that the operators  $h_{l/r}$  are bounded. The SEBB model is called non-trivial if the spectral measure  $\nu_{l/r}$  for  $h_{l/r}$  and  $\chi_{l/r}$  is not supported on a finite set.

The relevant transport phenomena in the SEBB model are linked to the choice of the initial state. Suppose that initially the reservoir  $\mathcal{R}_{l/r}$  is in equilibrium at inverse temperature  $\beta_{l/r}$  and chemical potential  $\mu_{l/r}$ . If either  $\beta_l \neq \beta_r$  or  $\mu_l \neq \mu_r$ , then, in the large time limit, the resulting temperature/chemical potential differential induces a non-trivial steady state energy/charge flux between the left and the right reservoirs. The Landauer-Büttiker formalism relates the transport theory of the SEBB model (the values of the steady state energy and charge fluxes, full counting statistics of the energy and charge fluxes, etc.) to the scattering theory of the pair  $(h, h_0)$ . For example, the steady state energy/charge flux is given by the Landauer-Büttiker formula that involves only the initial energy densities of the reservoirs and the scattering matrix of the pair  $(h, h_0)$ . The same is true for the Levitov-Lesovik formulas for the large deviation functionals associated to the full counting statistics of energy/charge flux. We refer the reader to the lecture notes [JKP, JOPP] for additional information and references to the vast literature on these subjects.

Consider now a full-line Jacobi matrix  $J$  acting on  $\mathcal{H} = \ell^2(\mathbb{Z})$  by

$$(Ju)_k = a_k u_{k+1} + a_{k-1} u_{k-1} + b_k u_k, \quad (1.1)$$

where  $\{a_k\}_{k \in \mathbb{Z}}$  and  $\{b_k\}_{k \in \mathbb{Z}}$  are bounded sequences of real numbers and  $a_k \neq 0$  for every  $k$ . To such a matrix one associates a SEBB model as follows. For fixed  $n \in \mathbb{Z}$ , let

$$\mathcal{H}_n^{(l)} = \ell^2((-\infty, n-1]), \quad \mathcal{H}_n^{(r)} = \ell^2([n+1, \infty)).$$

Let  $J_n^{(l)}$  and  $J_n^{(r)}$  be the half-line Jacobi matrices with Dirichlet boundary conditions obtained by restricting  $J$  to  $\mathcal{H}_n^{(l)}$  and  $\mathcal{H}_n^{(r)}$ , respectively. Setting  $\mathfrak{h}_{l/r} = \mathcal{H}_n^{(l/r)}$ ,  $h_{l/r} = J_n^{(l/r)}$ ,  $\omega = b_n$ ,  $\chi_l = \delta_{n-1}$ ,  $\chi_r = \delta_{n+1}$ ,  $\lambda_l = a_{n-1}$ ,  $\lambda_r = a_n$ , and

$$J_0 = J_n^{(l)} + J_n^{(r)} + b_n |\delta_n\rangle \langle \delta_n|, \quad (1.2)$$

one arrives at the SEBB model with

$$h_0 = J_0, \quad h = J.$$

Thus, a Jacobi matrix naturally induces a non-trivial SEBB model. In turn, a well-known orthogonal polynomial construction (see Theorem I.2.4 in [Si]) implies that *every* non-trivial SEBB model is unitarily equivalent to a Jacobi matrix SEBB model. This leads to the identification of the class of SEBB models with the class of Jacobi matrices.

This note is a first step in the exploration of this connection. We shall focus on the following point. Although the study of the scattering theory of the pair  $(h, h_0)$  is completely natural from the point of view of non-equilibrium statistical mechanics, the study of the scattering theory of the corresponding pair of Jacobi matrices  $(J, J_0)$  is, to the best of our knowledge, virtually absent in the literature on Jacobi matrices. We shall exploit this connection to determine when a Jacobi matrix is reflectionless, a property which has attracted considerable attention in the recent literature on Jacobi matrices (see Chapter 8 in [Te] and Chapter 7 in [Si]). Motivated by recent studies of the SEBB model (and in particular by [JLP]) we shall propose a definition of reflectionless based on the scattering matrix of the pair  $(J, J_0)$  that is, in our opinion, physically and mathematically natural. We show that this definition is equivalent to the standard definitions appearing in the literature and also to the dynamical definition introduced in [BRS]. A consequence is a short, transparent proof of the main result of [BRS] which has settled a 25 year old conjecture raised in [DeSi].

The paper is organized as follows. In Section 2 we recall the standard definitions of reflectionless Jacobi matrices and the result of [BRS]. In Section 3 we introduce stationary reflectionless Jacobi matrices and state our main result. Its proof is given in Section 4. The concepts introduced in this paper go beyond reflectionless and shed light on the notions of the dynamical reflection probability of [DaSi] and the spectral reflection probability of [BRS, GNP, GS] by identifying them with the scattering matrix reflection probability. This point is discussed in Section 5.

Finally, we remark that, as in [BRS], our results can be extended to Schrödinger operators on the real line and CMV matrices. The extension to Schrödinger operators is somewhat technical due to the lack of

convenient references to the stationary scattering theory of singular perturbations (induced by imposing boundary conditions). The details can be found in [Z]. The extension to CMV matrices can be found in [CLP].

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## 2 Three notions of reflectionless

The Green's function of the Jacobi matrix (1.1) is defined for  $z \in \mathbb{C} \setminus \mathbb{R}$  by

$$G_{nm}(z) = \langle \delta_n, (J - z)^{-1} \delta_m \rangle.$$

By general principles (see [J] or any book on harmonic analysis) the boundary values

$$G_{nm}(\lambda \pm i0) = \lim_{\varepsilon \downarrow 0} \langle \delta_n, (J - \lambda \mp i\varepsilon)^{-1} \delta_m \rangle \quad (2.3)$$

exist, are finite and non-vanishing for Lebesgue a.e.  $\lambda \in \mathbb{R}$ .

The Weyl  $m$ -functions are defined for  $z \in \mathbb{C} \setminus \mathbb{R}$  by

$$m_n^{(l)}(z) = \langle \delta_{n-1}, (J_n^{(l)} - z)^{-1} \delta_{n-1} \rangle, \quad m_n^{(r)}(z) = \langle \delta_{n+1}, (J_n^{(r)} - z)^{-1} \delta_{n+1} \rangle.$$

The boundary values  $m_n^{(l/r)}(\lambda \pm i0)$  are defined analogously to (2.3), and are also finite and non-vanishing for Lebesgue a.e.  $\lambda \in \mathbb{R}$ .

We recall the terminology of [BRS]. Let  $\epsilon \subset \mathbb{R}$  be a Borel set. A Jacobi matrix is called *measure theoretically reflectionless* on  $\epsilon$  if

$$\operatorname{Re} [G_{nn}(\lambda + i0)] = 0 \quad (2.4)$$

for Lebesgue a.e.  $\lambda \in \epsilon$  and every  $n$ . A Jacobi matrix is called *spectrally reflectionless* on  $\epsilon$  if

$$a_n^2 m_n^{(r)}(\lambda + i0) m_{n+1}^{(l)}(\lambda - i0) = 1 \quad (2.5)$$

for Lebesgue a.e.  $\lambda \in \epsilon$  and every  $n$ .

From the first of the two formulas

$$G_{nn}(z) = -\frac{1}{a_n^2 m_n^{(r)}(z) - m_{n+1}^{(l)}(z)^{-1}} = -\frac{1}{a_{n-1}^2 m_n^{(l)}(z) - m_{n-1}^{(r)}(z)^{-1}}, \quad (2.6)$$

one derives that if (2.5) holds for  $\lambda$  and  $n$ , then (2.4) holds for the same  $\lambda$  and  $n$ . The following is the well-known converse (see [GKT, SY, Te] and Theorem 7.4.1 in [Si]).

**Theorem 2.1** *For Lebesgue a.e.  $\lambda \in \mathbb{R}$ , the following are equivalent.*

- (1)  $\operatorname{Re} [G_{nn}(\lambda + i0)] = 0$  for all  $n$ .
- (2)  $\operatorname{Re} [G_{nn}(\lambda + i0)] = 0$  for three consecutive  $n$ 's.
- (3) (2.5) holds for one  $n$ .
- (4) (2.5) holds for every  $n$ .

An immediate and well-known consequence is

**Corollary 2.2**  $J$  is measure theoretically reflectionless on  $\epsilon$  iff it is spectrally reflectionless on  $\epsilon$ .

Based on the ideas of Davies and Simon [DaSi], Breuer, Ryckman and Simon introduced in [BRS] the notion of being dynamically reflectionless. We first recall the setup of [DaSi] adapted to the Jacobi matrix case. For each  $n \in \mathbb{Z}$ , let  $\chi_n^{(l)}$  be the characteristic function of  $(-\infty, n-1]$  and  $\chi_n^{(r)}$  of  $[n+1, \infty)$ . Set

$$\mathcal{H}_l^\pm = \left\{ \varphi \in \mathcal{H}_{\text{ac}}(J) \mid \text{for all } n, \lim_{t \rightarrow \pm\infty} \|\chi_n^{(r)} e^{-itJ} \varphi\| = 0 \right\}.$$

The elements of  $\mathcal{H}_l^\pm$  are the states that are concentrated on the left in the distant future/past  $t \rightarrow \pm\infty$ . The sets  $\mathcal{H}_r^\pm$  are defined with  $\chi_n^{(l)}$  replacing  $\chi_n^{(r)}$ . The sets  $\mathcal{H}_{l/r}^+$  are related to  $\mathcal{H}_{l/r}^-$  by time-reversal, i.e.,

$$\mathcal{H}_{l/r}^+ = \left\{ \overline{\varphi} \mid \varphi \in \mathcal{H}_{l/r}^- \right\}. \quad (2.7)$$

In what follows  $\mathcal{H}_{\text{ac}}(A)$  denotes the absolutely continuous subspace for self-adjoint  $A$  and  $P_{\text{ac}}(A)$  the projection onto this subspace. The result of Davies and Simon [DaSi] is:

**Theorem 2.3**

$$\mathcal{H}_{\text{ac}}(J) = \mathcal{H}_l^+ \oplus \mathcal{H}_r^+ = \mathcal{H}_l^- \oplus \mathcal{H}_r^-. \quad (2.8)$$

**Remark.** In [DaSi] this theorem was proven in the context of Schrödinger operators on the real line. In the discrete setting considered here the argument is considerably simpler. For completeness and later reference, we sketch the proof.

**Proof.** By (2.7) it suffices to prove that  $\mathcal{H}_{\text{ac}}(J) = \mathcal{H}_l^+ \oplus \mathcal{H}_r^+$ . Since  $s - \lim_{t \rightarrow \infty} e^{itJ} C e^{-itJ} P_{\text{ac}}(J) = 0$  for any compact  $C$ , we have that for any  $n$

$$\mathcal{H}_{l/r}^+ = \left\{ \varphi \in \mathcal{H}_{\text{ac}}(J) \mid \lim_{t \rightarrow \infty} \|\chi_n^{(r/l)} e^{-itJ} \varphi\| = 0 \right\} = \left\{ \varphi \in \mathcal{H}_{\text{ac}}(J) \mid \lim_{t \rightarrow \infty} e^{itJ} \chi_n^{(l/r)} e^{-itJ} \varphi = \varphi \right\}.$$

Since the commutators  $[\chi_n^{(l/r)}, J]$  are finite rank, trace-class scattering theory implies that the limits

$$P_{l/r}^+ = s - \lim_{t \rightarrow \infty} e^{itJ} \chi_n^{(l/r)} e^{-itJ} P_{\text{ac}}(J)$$

exist, and are furthermore independent of  $n$ . From the fact that  $e^{itJ}$  commutes with  $P_{l/r}^+$ , we obtain that  $P_{\text{ac}}(J)$  commutes with  $P_{l/r}^+$ , and so

$$\begin{aligned} [P_{l/r}^+]^* &= \left[ s - \lim_{t \rightarrow \infty} e^{itJ} P_{\text{ac}}(J) \chi_n^{(l/r)} P_{\text{ac}}(J) e^{-itJ} \right]^* \\ &= s - \lim_{t \rightarrow \infty} e^{itJ} P_{\text{ac}}(J) \chi_n^{(l/r)} P_{\text{ac}}(J) e^{-itJ} = P_{l/r}^+, \end{aligned}$$

and

$$\begin{aligned} [P_{l/r}^+]^2 &= s - \lim_{t \rightarrow \infty} e^{itJ} \chi_0^{(l/r)} e^{-itJ} P_{\text{ac}}(J) e^{itJ} \chi_0^{(l/r)} e^{-itJ} P_{\text{ac}}(J) \\ &= s - \lim_{t \rightarrow \infty} e^{itJ} \chi_0^{(l/r)} e^{-itJ} e^{itJ} \chi_0^{(l/r)} e^{-itJ} P_{\text{ac}}(J) = P_{l/r}^+. \end{aligned}$$

Hence,  $P_{l/r}^+$  are the orthogonal projections onto  $\mathcal{H}_{l/r}^+$ . The statement now follows from the identity

$$P_{\text{ac}}(J) = e^{itJ} \chi_n^{(l)} e^{-itJ} P_{\text{ac}}(J) + e^{itJ} \chi_n^{(r)} e^{-itJ} P_{\text{ac}}(J) + e^{itJ} |\delta_n\rangle \langle \delta_n| e^{-itJ} P_{\text{ac}}(J).$$

□

In what follows  $P_\epsilon(A)$  denotes the spectral projection of a self-adjoint operator  $A$  onto a Borel set  $\epsilon$  and  $|S|$  the Lebesgue measure of a set  $S$ . In [BRS] the following notion was introduced.

**Definition 2.4** A Jacobi matrix is called *dynamically reflectionless* on  $\epsilon$  if for any Borel set  $\epsilon_1 \subset \epsilon$ ,

$$P_{\epsilon_1}(J)P_{\text{ac}}(J) = 0 \implies |\epsilon_1| = 0, \quad (2.9)$$

and

$$P_{\epsilon}(J)[\mathcal{H}_l^+] = P_{\epsilon}(J)[\mathcal{H}_r^-].$$

The result of [BRS] is

**Theorem 2.5**  $J$  is dynamically reflectionless on  $\epsilon$  iff it is spectrally reflectionless on  $\epsilon$ .

**Remark.** Theorem 2.5 verifies the conjecture of Deift and Simon [DeSi] that the a.c. spectrum of ergodic Jacobi matrices is dynamically reflectionless.

### 3 The notion of stationary reflectionless

Recall that  $J_0$  is given by (1.2). It follows from trace-class scattering theory that the wave operators

$$w_{\pm} = s - \lim_{t \rightarrow \pm\infty} e^{itJ} e^{-itJ_0} P_{\text{ac}}(J_0)$$

exist and are complete (here, completeness means that  $\text{Ran } w_{\pm} = \mathcal{H}_{\text{ac}}(J)$ ). Note that  $w_{\pm}$  depends on  $n$  (whenever this dependence is clear within the context, we shall not indicate it explicitly). By the spectral theorem we may identify  $\mathcal{H}_{\text{ac}}(J_0)$  with

$$\mathcal{H}_{\text{ac}}(J_0) = \mathcal{H}_{\text{ac}}(J_n^{(l)}) \oplus \mathcal{H}_{\text{ac}}(J_n^{(r)}) = L^2(\mathbb{R}, d\nu_{l,\text{ac}}) \oplus L^2(\mathbb{R}, d\nu_{r,\text{ac}})$$

where  $\nu_{l/r,\text{ac}}$  is the a.c. part of the spectral measure for  $J_0^{(l/r)}$  and  $\delta_{n-1}/\delta_{n+1}$ . We recall the well-known formula

$$\frac{d\nu_{l/r,\text{ac}}}{d\lambda}(\lambda) = \frac{1}{\pi} \text{Im} [m_n^{(l/r)}(\lambda + i0)]$$

(a pedagogical proof can be found in [J]). It follows from stationary scattering theory [Y] that the scattering matrix

$$s = w_+^* w_-$$

acts as multiplication by a unitary  $2 \times 2$  matrix

$$s(\lambda) = \begin{pmatrix} s_{ll}(\lambda) & s_{lr}(\lambda) \\ s_{rl}(\lambda) & s_{rr}(\lambda) \end{pmatrix}$$

on  $\mathcal{H}_{\text{ac}}(J_0)$  where

$$s_{jk}(\lambda) = \delta_{j,k} + 2ia_j a_k G_{nn}(\lambda + i0) \sqrt{\text{Im} [m_n^{(j)}(\lambda + i0)] \text{Im} [m_n^{(k)}(\lambda + i0)]}, \quad (3.10)$$

$j, k \in \{l, r\}$ ,  $a_l = a_{n-1}$  and  $a_r = a_n$ . In the current setting, the above formula can be also easily verified by a direct computation which we sketch in the appendix (see [La] for more details). Note that  $s_{lr}(\lambda) = s_{rl}(\lambda)$ .

Motivated by the non-equilibrium statistical mechanics of the SEBB model (and in particular by the work [JLP]) we introduce

**Definition 3.1** A Jacobi matrix  $J$  is called *stationary reflectionless* on a Borel set  $\epsilon$  if for one  $n$  the scattering matrix  $s(\lambda)$  is off-diagonal for Lebesgue a.e.  $\lambda \in \epsilon$ .

**Remark.** In other words,  $J$  is stationary reflectionless on  $\epsilon$  if, for one  $n$ ,  $|s_{lr}(\lambda)| = 1$  for Lebesgue a.e.  $\lambda \in \epsilon$ , or equivalently,  $s_{ll}(\lambda) = s_{rr}(\lambda) = 0$  for Lebesgue a.e.  $\lambda \in \epsilon$ .

Formulas (2.6), (3.10), and Theorem 2.1 immediately give:

**Proposition 3.2**  $J$  is spectrally reflectionless on  $\epsilon$  iff  $J$  is stationary reflectionless on  $\epsilon$ .

**Remark.** In particular, this proposition implies that if the scattering matrix  $s(\lambda)$  is off-diagonal for Lebesgue a.e.  $\lambda \in \epsilon$  and some  $n$ , then it is so for all  $n$ .

We shall prove

**Theorem 3.3**  $J$  is dynamically reflectionless on  $\epsilon$  iff it is stationary reflectionless on  $\epsilon$ .

This result combined with Proposition 3.2 implies Theorem 2.5.

The proof of Proposition 3.2 is very simple. As we shall see, the proof of Theorem 3.3 is also simple due to the direct connection with scattering theory. The notion of stationary reflectionless naturally links the notions of spectral and dynamical reflectionless and is likely to play a role in future developments.

## 4 Proof of Theorem 3.3

Let

$$\Sigma_{l/r,ac} = \left\{ \lambda \mid \frac{d\nu_{l/r,ac}}{d\lambda}(\lambda) > 0 \right\}, \quad \mathcal{E} = \Sigma_{l,ac} \cup \Sigma_{r,ac}.$$

The set  $\mathcal{E}$  is an essential support of the a.c. spectrum of  $J_0$ . From unitarity and symmetry of the scattering matrix, we see that for Lebesgue a.e.  $\lambda$ ,

$$s_{ll}(\lambda) = 0 \iff s_{rr}(\lambda) = 0.$$

Note also that if  $J$  is stationary reflectionless on  $\epsilon$ , then  $|\epsilon \setminus (\Sigma_{l,ac} \cap \Sigma_{r,ac})| = 0$ , and in particular  $|\epsilon \setminus \mathcal{E}| = 0$ . These two observations yield an equivalent formulation of stationary reflectionless that is more suitable for comparison with being dynamically reflectionless:

**Lemma 4.1**  $J$  is stationary reflectionless on  $\epsilon$  iff  $|\epsilon \setminus \mathcal{E}| = 0$  and, for some  $n$ ,

$$s_{ll}(\lambda) = 0 \text{ for Lebesgue a.e. } \lambda \in \epsilon \cap \Sigma_{l,ac}, \quad s_{rr}(\lambda) = 0 \text{ for Lebesgue a.e. } \lambda \in \epsilon \cap \Sigma_{r,ac}.$$

Since  $J - J_0$  is finite rank,  $\mathcal{E}$  is an essential support of the a.c. spectrum of  $J$ , and so the condition (2.9) in the definition of dynamical reflectionless can be replaced by the equivalent condition

$$|\epsilon \setminus \mathcal{E}| = 0. \tag{4.11}$$

The key observation is that the projections  $P_{l/r}^\pm$  on the subspaces  $\mathcal{H}_{l/r}^\pm$  (recall the proof of Theorem 2.3) satisfy

$$P_{l/r}^\pm = s \lim_{t \rightarrow \pm\infty} e^{itJ} e^{-itJ_0} \chi_n^{(l/r)} e^{itJ_0} e^{-itJ} P_{ac}(J) = w_\pm \chi_n^{(l/r)} w_\pm^*. \tag{4.12}$$

Above, we have used the fact that  $J_0$  commutes with  $\chi_n^{(l/r)}$  and that  $\text{Ran } w_\pm^* = \mathcal{H}_{ac}(J_0)$ . Note that the  $P_{l/r}^\pm$  commute with  $J$  and its spectral projections. For  $\varphi, \psi \in \mathcal{H}$ ,

$$\begin{aligned} \langle \varphi, P_\epsilon(J) P_l^+ P_l^- \psi \rangle &= \langle \varphi, P_\epsilon(J) P_l^+ P_\epsilon(J) P_l^- \psi \rangle = \langle w_+^* P_\epsilon(J) \varphi, \chi_n^{(l)} w_+^* w_- \chi_n^{(l)} w_-^* P_\epsilon(J) \psi \rangle \\ &= \langle w_+^* \varphi, P_\epsilon(J_0) \chi_n^{(l)} s \chi_n^{(l)} P_\epsilon(J_0) w_-^* \psi \rangle, \end{aligned} \tag{4.13}$$

where the last line follows by the intertwining property of the wave operators. We write

$$w_+^* \varphi = \tilde{\varphi}_l(\lambda) \oplus \tilde{\varphi}_r(\lambda) \in L^2(\mathbb{R}, d\nu_{l,ac}) \oplus L^2(\mathbb{R}, d\nu_{r,ac}),$$

and the same for  $w_{\pm}^* \psi$ . With this notation, the last line of (4.13) becomes

$$\int_{\mathfrak{e}} \overline{\varphi_l}(\lambda) s_{ll}(\lambda) \tilde{\psi}_l(\lambda) d\nu_{l,ac}(\lambda).$$

Since  $\text{Ran } w_{\pm}^* = \mathcal{H}_{ac}(J_0)$ , we conclude

$$P_{\mathfrak{e}}(J)P_l^+P_l^- = 0 \iff s_{ll}(\lambda) = 0 \text{ for Lebesgue a.e. } \lambda \in \mathfrak{e} \cap \Sigma_{l,ac}.$$

A similar computation yields

$$P_{\mathfrak{e}}(J)P_l^-P_l^+ = 0 \iff \overline{s_{ll}}(\lambda) = 0 \text{ for Lebesgue a.e. } \lambda \in \mathfrak{e} \cap \Sigma_{l,ac},$$

and two similar statements where  $P_l^{\pm}$  is replaced by  $P_r^{\pm}$  and  $s_{ll}$  by  $s_{rr}$ . This, together with Lemma 4.1 and (4.11), yields the theorem.

## 5 Remarks

The arguments used in the proof of Theorem 3.3 go beyond reflectionless and shed light on the notions of dynamical and spectral reflection probability.

*Dynamical reflection probability.* In [DaSi] (see also [BRS]) Davies and Simon introduced the concept of dynamical reflection probability (also called reflection modulus) as follows. Recall that the projections  $P_{l/r}^{\pm}$  satisfy (4.12).  $J$  commutes with  $P_l^+P_l^-P_l^+$  and, since  $J \upharpoonright \text{Ran } P_l^+$  has simple spectrum, there exists a Borel function  $R_l^+$  on  $\text{sp}(J \upharpoonright \text{Ran } P_l^+)$  such that

$$P_l^+P_l^-P_l^+ = R_l^+(J) \upharpoonright \text{Ran } P_l^+.$$

$R_l^+$  is unique (up to sets of Lebesgue measure zero) and satisfies  $0 \leq R_l^+(\lambda) \leq 1$ . One extends  $R_l^+$  to  $\mathbb{R}$  by setting  $R_l^+(\lambda) = 1$  for  $\lambda \notin \text{sp}(J \upharpoonright \text{Ran } P_l^+)$  and defines  $R_l^-$ ,  $R_r^{\pm}$  analogously. The functions  $R_{l/r}^{\pm}$  are discussed in Section 4 of [DaSi] in the Schrödinger case (their proofs easily extend to the Jacobi case). In this context, the main observation of this note is that the formula (4.12) implies the identity

$$R_{l/r}^{\pm}(\lambda) = |s_{ll}(\lambda)|^2 = |s_{rr}(\lambda)|^2.$$

*Spectral reflection probability.* To the best of our knowledge, the link between reflection probability and half-line  $m$ -functions was first observed in [GNP, GS] in the context of Schrödinger operators on the line. The definition of the spectral reflection probability of [GNP, GS] was based on suitable generalized eigenfunctions and was extended to Jacobi matrices in [BRS] as follows. Consider the case  $n = 0$ . For  $z \in \mathbb{C}_+$ , let  $\psi^{l/r}(z) = \{\psi_k^{(l/r)}(z)\}_{k \in \mathbb{Z}}$  be the unique solution of the equation

$$a_k \psi_{k+1} + a_{k-1} \psi_{k-1} + b_k \psi_k = z \psi_k \tag{5.14}$$

that is square summable at  $\mp\infty$  and normalized by  $\psi_0^{(l/r)} = 1$ . These solutions are related to  $m$ -functions as

$$m_0^{(r)}(z) = -\frac{\psi_1^{(r)}(z)}{a_0}, \quad m_1^{(l)}(z) = -\frac{1}{a_0 \psi_1^{(l)}(z)}. \tag{5.15}$$

For all  $k$  and Lebesgue a.e.  $\lambda$  the limit

$$\lim_{\epsilon \downarrow 0} \psi_k^{(l/r)}(\lambda + i\epsilon) = \psi_k^{(l/r)}(\lambda + i0)$$

exists and  $\psi^{(l/r)}(\lambda + i0)$  solves (5.14) with  $z = \lambda$ . For Lebesgue a.e.  $\lambda \in \Sigma_{r,ac}$  the solution  $\psi^{(r)}(\lambda + i0)$  is not a multiple of a real solution and so  $\overline{\psi^{(r)}(\lambda + i0)}$  is also a solution linearly independent of  $\psi^{(r)}(\lambda + i0)$ . Hence, for Lebesgue a.e.  $\lambda \in \Sigma_{r,ac}$  we can expand

$$\psi^{(l)}(\lambda + i0) = \alpha(\lambda) \overline{\psi^{(r)}(\lambda + i0)} + \beta(\lambda) \psi^{(r)}(\lambda + i0). \tag{5.16}$$



The spectral reflection probability of [GNP, GS, BRS] is

$$\mathcal{R}_r(\lambda) = \left| \frac{\beta(\lambda)}{\alpha(\lambda)} \right|^2.$$

One extends  $\mathcal{R}_r(\lambda)$  to  $\mathbb{R}$  by setting  $\mathcal{R}_r(\lambda) = 1$  for  $\lambda \notin \Sigma_{r,\text{ac}}$  and defines  $\mathcal{R}_l(\lambda)$  analogously. Using (5.15) and (5.16) one computes

$$|\mathcal{R}_r(\lambda)|^2 = \left| \frac{\overline{a_0^2 m_0^{(r)}(\lambda + i0) m_1^{(l)}(\lambda + i0) - 1}}{a_0^2 m_0^{(r)}(\lambda + i0) m_1^{(l)}(\lambda + i0) - 1} \right|^2.$$

In this context the main observation of this note is that the formulas (2.6) and (3.10) yield the identity

$$\mathcal{R}_r(\lambda) = |s_{rr}(\lambda)|^2.$$

Similarly,

$$\mathcal{R}_l(\lambda) = |s_{ll}(\lambda)|^2.$$

These identities clarify the meaning of the spectral reflection probability and yield

$$\mathcal{R}_{l/r} = R_{l/r}^\pm. \quad (5.17)$$

Much of the technical work in [BRS] was devoted to a direct proof of (5.17) via an implicit rederivation of the scattering matrix.

## A Computation of the scattering matrix

We briefly sketch the derivation of the formula (3.10) for the scattering matrix of the pair  $(J, J_0)$ . For details, we refer the reader to [La].

It suffices to consider the case  $n = 0$  (recall 1.1). First, we shall show that for  $\varphi \in \mathcal{H}$ ,

$$w_\pm^* \varphi = \varphi_l^{(\pm)} \oplus \varphi_r^{(\pm)} \in \mathcal{H}_{\text{ac}}(J_0^{(l)}) \oplus \mathcal{H}_{\text{ac}}(J_0^{(r)}),$$

where (recalling that  $a_l = a_{-1}$  and  $a_r = a_0$ ),

$$\varphi_{l/r}^{(\pm)}(\lambda) = P_{\text{ac}}(J_0^{(l/r)})\varphi(\lambda) - a_{l/r} \langle \delta_0, (J - \lambda \mp i0)^{-1} \varphi \rangle.$$

For any  $\psi = \psi_l \oplus \psi_r \in \mathcal{H}_{\text{ac}}(J_0^{(l)}) \oplus \mathcal{H}_{\text{ac}}(J_0^{(r)})$  we have,

$$\langle \psi, w_+^* \varphi \rangle = \langle w_+ \psi, \varphi \rangle = \lim_{t \rightarrow \infty} \langle e^{itJ} e^{-itJ_0} \psi, \varphi \rangle = \lim_{t \rightarrow \infty} \langle \psi, e^{itJ_0} e^{-itJ} \varphi \rangle$$

By an abelian limit and the definition of  $J - J_0$  we can rewrite the RHS as

$$\lim_{t \rightarrow \infty} \langle \psi, e^{itJ_0} e^{-itJ} \varphi \rangle = \langle \psi, \varphi \rangle - i \lim_{t \rightarrow \infty} \int_0^t \langle \psi, e^{isJ_0} (J - J_0) e^{-isJ} \varphi \rangle ds = \langle \psi, \varphi \rangle - \lim_{\varepsilon \downarrow 0} (L_l(\varepsilon) + L_r(\varepsilon)),$$

where

$$L_{l/r}(\varepsilon) = i \int_0^\infty e^{-\varepsilon s} a_{l/r} \langle \psi, e^{isJ_0} \delta_{-1/1} \rangle \langle \delta_0, e^{-isJ} \varphi \rangle ds.$$

Expanding the first inner product in the above integrand yields

$$\begin{aligned} L_{l/r}(\varepsilon) &= i a_{l/r} \int_{\mathbb{R}} \overline{\psi}_{l/r}(\lambda) \left[ \int_0^\infty \langle \delta_0, e^{-is(J - \lambda - i\varepsilon)} \varphi \rangle ds \right] d\nu_{l/r,\text{ac}}(\lambda) \\ &= a_{l/r} \int_{\mathbb{R}} \overline{\psi}_{l/r}(\lambda) \langle \delta_0, (J - \lambda - i\varepsilon)^{-1} \varphi \rangle d\nu_{l/r,\text{ac}}(\lambda). \end{aligned}$$

For  $\psi$  in a judiciously chosen dense set (see [La] or Proposition 7 in [JKP]) one can take the limit  $\varepsilon \rightarrow 0^+$  inside the integral. This yields the formula for  $w_+^*$ . The computation for  $w_-^*$  is identical.

To compute the scattering matrix, note that for  $\psi = \psi_l \oplus \psi_r$  and  $\varphi = \varphi_l \oplus \varphi_r$  in  $\mathcal{H}_{\text{ac}}(J_0)$ ,

$$\begin{aligned} \langle \psi, (s - \mathbb{1})\varphi \rangle &= \langle \psi, (w_+^* w_- - w_-^* w_+) \varphi \rangle \\ &= \langle (w_+ - w_-)\psi, w_- \varphi \rangle \\ &= \lim_{t \rightarrow \infty} \langle (e^{itJ} e^{-itJ_0} - e^{-itJ} e^{itJ_0})\psi, w_- \varphi \rangle \\ &= \lim_{t \rightarrow \infty} -i \int_{-t}^t \langle e^{isJ} (J - J_0) e^{-isJ_0} \psi, w_- \varphi \rangle ds \\ &= \lim_{\varepsilon \downarrow 0} -i \int_{\mathbb{R}} e^{-\varepsilon|s|} \langle e^{isJ} (J - J_0) e^{-isJ_0} \psi, w_- \varphi \rangle ds. \end{aligned}$$

The inner product in the above integrand equals

$$a_l \langle e^{-isJ_0} \psi, \delta_{-1} \rangle \langle w_-^* \delta_0, e^{-isJ_0} \varphi \rangle + a_r \langle e^{-isJ_0} \psi, \delta_1 \rangle \langle w_-^* \delta_0, e^{-isJ_0} \varphi \rangle,$$

where we have used the intertwining property of the wave operators. We use our formula for  $w_-^*$  to compute

$$\langle \psi, (s - \mathbb{1})\varphi \rangle = \lim_{\varepsilon \downarrow 0} i(H_{ll}(\varepsilon) + H_{rl}(\varepsilon) + H_{lr}(\varepsilon) + H_{rr}(\varepsilon)),$$

where

$$H_{jk}(\varepsilon) = a_j a_k \int_{\mathbb{R}} e^{-\varepsilon|s|} \left[ \int_{\mathbb{R}} e^{is\lambda} \overline{\psi_j}(\lambda) d\nu_{j,\text{ac}}(\lambda) \right] \left[ \int_{\mathbb{R}} e^{-is\lambda'} G_{00}(\lambda' + i0) \varphi_k(\lambda') d\nu_{k,\text{ac}}(\lambda') \right] ds,$$

for  $j, k \in \{l, r\}$ . Formally, the computation is completed by noting that

$$H_{jk}(\varepsilon) = a_j a_k \int_{\mathbb{R}} \int_{\mathbb{R}} \overline{\psi_j}(\lambda) \varphi_k(\lambda') G_{00}(\lambda' + i0) \left[ \int_{\mathbb{R}} e^{is(\lambda - \lambda') - \varepsilon|s|} ds \right] d\nu_{j,\text{ac}}(\lambda) d\nu_{k,\text{ac}}(\lambda'),$$

and that

$$\int_{\mathbb{R}} e^{is(\lambda - \lambda') - \varepsilon|s|} ds \rightarrow 2\pi\delta(\lambda - \lambda')$$

as  $\varepsilon \rightarrow 0^+$ . For a suitable dense set of  $\psi$  and  $\varphi$ , this formal computation can be easily justified (see [La]).

Finally, we remark that the scattering matrix formula (3.10) is valid only after a ‘unitarity’ transformation which we describe now. For any  $\psi \in \mathcal{H}_{\text{ac}}(J_0)$ , let  $\psi(\lambda)$  denote the vector  $(\psi_l(\lambda), \psi_r(\lambda)) \in \mathbb{C}^2$ . For  $\psi$  and  $\varphi$  in  $\mathcal{H}_{\text{ac}}(J_0)$ , we have

$$\langle \psi, \varphi \rangle = \int_{\mathbb{R}} \langle V(\lambda)\psi(\lambda), V(\lambda)\varphi(\lambda) \rangle_2 d\lambda$$

where  $\langle \cdot, \cdot \rangle_2$  denotes the standard inner product on  $\mathbb{C}^2$  and  $V(\lambda)$  is the  $2 \times 2$  matrix

$$V(\lambda) = \begin{pmatrix} \sqrt{\frac{d\nu_{l,\text{ac}}}{d\lambda}}(\lambda) & 0 \\ 0 & \sqrt{\frac{d\nu_{r,\text{ac}}}{d\lambda}}(\lambda) \end{pmatrix}.$$

Multiplication by the matrix  $V(\lambda)$  is a unitary operator  $V : \mathcal{H}_{\text{ac}}(J_0) \rightarrow L^2(\mathbb{R}, \rho_l(\lambda)d\lambda) \oplus L^2(\mathbb{R}, \rho_r(\lambda)d\lambda)$ , with  $\rho_{l/r}$  the characteristic function of  $\Sigma_{l/r,\text{ac}}$ . Our computation shows that the operator  $VsV^{-1}$  acts as multiplication by the  $2 \times 2$  matrix  $s(\lambda)$  given by (3.10) on  $V\mathcal{H}_{\text{ac}}(J_0)$ . In particular, this transformation ensures that  $s(\lambda)$  is unitary w.r.t. the standard inner product on  $\mathbb{C}^2$ .

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