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High-energy analysis and Levinson's theorem for the selfadjoint matrix Schrödinger operator on the half line

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The matrix Schrödinger equation with a selfadjoint matrix potential is considered on the half line with the general selfadjoint boundary condition at the origin. When the matrix potential is integrable, the high-energy asymptotics are established for the related Jost matrix, the inverse of the Jost matrix, and the scattering matrix. Under the additional assumption that the matrix potential has a first moment, Levinson's theorem is derived, relating the number of bound states to the change in the argument of the determinant of the scattering matrix. © *2013 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4773904]

I. INTRODUCTION

Consider the matrix Schrödinger equation on the half line

$$-\psi'' + V(x)\,\psi = k^2\psi, \qquad x \in \mathbf{R}^+, \tag{1.1}$$

where $\mathbf{R}^+ := (0,\ +\infty)$, the prime denotes the derivative with respect to the spatial coordinate x, and the potential V is a $n \times n$ selfadjoint matrix-valued function integrable in x. The integrability $V \in L^1(\mathbf{R}^+)$ means that each entry of the matrix V is Lebesgue measurable on $\mathbf{R}^+$ and

$$\int_0^\infty dx\, ||V(x)|| < +\infty, \tag{1.2}$$

where $||V(x)||$ denotes a matrix norm. Since all matrix norms are equivalent, without loss of generality, we can use the matrix norm defined as

$$||V(x)|| := \max_l \sum_{s=1}^n |V_{ls}(x)|, \qquad l = 1, \dots, n,$$

where $V_{ls}(x)$ denotes the (l, s)-entry of the matrix $V(x)$. Clearly, a matrix-valued function is integrable in x if and only if each entry of that matrix belongs to $L^1(\mathbf{R}^+)$.

Note that V is not assumed to be real valued but is assumed to be selfadjoint, i.e.,

$$V(x) = V(x)^\dagger, \qquad x \in \mathbf{R}^+, \tag{1.3}$$

where the dagger denotes the matrix adjoint (complex conjugate and matrix transpose). The wavefunction $\psi(k, x)$ appearing in (1.1) will be either an $n \times n$ matrix-valued function or it will be a column vector with n components.

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When the analysis of (1.1) is considered at or near $k = 0$, in addition to the integrability we require that the potential V has a first moment, i.e.,

$$\int_0^\infty dx\, x\, ||V(x)|| < +\infty. \tag{1.4}$$

All the results in our paper are valid under the assumption that the potential V is selfadjoint and belongs to $L^1_1(\mathbf{R}^+)$, i.e.,

$$\int_0^\infty dx\, (1+x)\, ||V(x)|| < +\infty. \tag{1.5}$$

We are interested in studying (1.1) with a selfadjoint potential V in $L^1_1(\mathbf{R}^+)$ under the general selfadjoint boundary condition at $x = 0$. As indicated in Ref. 2, without loss of generality, it is convenient to state the general selfadjoint boundary condition at $x = 0$ for (1.1) in terms of constant $n \times n$ matrices A and B such that

$$-B^\dagger \psi(0) + A^\dagger \psi'(0) = 0, \tag{1.6}$$

$$-B^\dagger A + A^\dagger B = 0, \tag{1.7}$$

$$A^\dagger A + B^\dagger B > 0, \tag{1.8}$$

i.e., $A^\dagger B$ is selfadjoint and the selfadjoint matrix $(A^\dagger A + B^\dagger B)$ is positive. There are various equivalent formulations[2,12–16] of the general selfadjoint boundary condition at $x = 0$. Let us also mention that it is possible to use some transformations on A and B without affecting (1.7) and (1.8). In Sec. IV we will elaborate on two such transformations, namely $(A, B) \mapsto (AT, BT)$, a right multiplication by an invertible matrix T, and a unitary transformation $(A, B) \mapsto (M^\dagger AM, M^\dagger BM)$, where M is a unitary matrix. A combination of such transformations as given in (4.10) will turn out to be useful.

We have two primary goals in this paper for the Schrödinger equation (1.1) with the selfadjoint boundary condition (1.6)–(1.8) when the potential V satisfies (1.3) and (1.5). Our first primary goal is, even when V satisfies the weaker condition (1.2) instead of (1.5), to establish the large-k asymptotics of various quantities related to (1.1) such as some relevant scattering solutions, the Jost matrix, the inverse of the Jost matrix, and the scattering matrix. Our second primary goal is, under the additional assumption (1.4), to derive so-called Levinson's theorem, namely to obtain the relationship between the number of bound states and the change in the phase of the determinant of the scattering matrix.

A bound state corresponds to a square-integrable column-vector solution to (1.1) satisfying the boundary condition (1.6)–(1.8). The selfadjointness (1.3) of V and the selfadjoint boundary condition (1.6)–(1.8) assure that the corresponding Schrödinger operator is selfadjoint on $L^2(\mathbf{R}^+)$, and hence its eigenvalues must be real. When $k^2 \geq 0$, it turns out that there are no square-integrable column-vector solutions to (1.1). As a result, a bound state, if it exists, occurs only when k^2 is negative, or equivalently when k appearing in (1.1) is on the positive imaginary axis in the complex plane $\mathbf{C}$. Thanks to the restriction (1.5), the number of such k-values turns out to be finite. We will see that, at each k-value corresponding to a bound state, the number of linearly independent square-integrable column-vector solutions (i.e., the multiplicity of the corresponding bound state) cannot exceed n. The number of bound states is defined as the number of bound states including the multiplicities.

The large-k analysis and Levinson's theorem for (1.1) with the selfadjoint boundary condition (1.6)–(1.8) are relevant in the study of the corresponding direct and inverse scattering problems. The direct scattering problem for (1.1) is to determine the scattering matrix and the bound-state information when the matrix potential V and the selfadjoint boundary condition are known. On the other hand, the inverse scattering problem is to recover the potential and the boundary condition from an appropriate set of scattering data.

Our paper complements the study[1] by Agranovich and Marchenko, where the large-k asymptotics and Levinson's theorem are provided only under the Dirichlet boundary condition. Our study also complements the study[12–14] by Harmer (see also Ref. 5), where the general selfadjoint boundary condition is used but the large-k asymptotics of the scattering matrix is obtained by only providing the leading term with the remaining terms specified as $o(1)$ as k becomes large. In our paper, we not only provide the leading term but we also specify the next-order term and establish the large-k asymptotics up to $O(1/k^2)$, which is crucial in establishing the Fourier transforms of various quantities relevant to the corresponding inverse scattering problem.

Our current paper also complements our own recent study,[2] where the rigorous small-k analysis for (1.1) is provided with the general selfadjoint boundary condition (1.6)–(1.8). The small-k analysis in Ref. 2 is crucial in the derivation of Levinson's theorem in our current paper. In fact, the only reason for needing (1.5) rather than merely (1.2) in our current paper is because of the fact that the small-k asymptotics are also needed to establish Levinson's theorem, and those asymptotics require (1.5).

The half-line matrix Schrödinger equation (1.1) has applications in quantum mechanical scattering involving particles of internal structures such as spins, in scattering on graphs,[4,6–11,17–21] and in quantum wires.[15,16] The consideration of the general selfadjoint boundary condition at $x = 0$ given in (1.6)–(1.8) rather than the Dirichlet boundary condition $\psi(0) = 0$ is relevant. For example, the half-line matrix Schrödinger equation (1.1) describes the behavior of n connected very thin quantum wires forming a one-vertex graph with open ends, and the boundary condition (1.6)–(1.8) imposes certain restrictions at the vertex. Such a problem is useful in designing elementary gates in quantum computing and nanotubes for microscopic electronic devices, where, for example, strings of atoms may form a star-shaped graph. For details we refer the reader to Refs. 15 and 16 and the references therein.

Our paper is organized as follows. In Sec. II we introduce various $n \times n$ matrix solutions to (1.1) that are needed later on. In Sec. III we introduce the Jost matrix $J(k)$ and the scattering matrix $S(k)$ and state some of their properties relevant to our study. In Sec. IV we introduce two key transformations on the boundary condition (1.6)–(1.8) and analyze how those transformations affect the Jost matrix and the scattering matrix. In Sec. V we provide the relevant properties of $J_0(k)$ and $S_0(k)$, which are, respectively, the Jost and scattering matrices corresponding to $V \equiv 0$; those properties are crucial in understanding similar properties when the potential is nonzero. In Sec. VI we analyze the behavior of the Jost matrix at $k = 0$, which is needed in establishing Levinson's theorem. In Sec. VII we analyze the large-k asymptotics of the Jost and scattering matrices. In Sec. VIII we analyze the bound states and the properties of the Jost matrix related to bound states. Finally, in Sec. IX we establish Levinson's theorem, showing how the change in the phase of the determinant of the scattering matrix is related to the number of bound states.

II. SCATTERING SOLUTIONS

In this section we introduce certain $n \times n$ matrix solutions to (1.1) and recall some of their properties relevant to our study. We use $\mathbf{C}^+$ to denote the upper-half complex plane and $\mathbf{R}$ for the real axis, and we let $\overline{\mathbf{C}^+} := \mathbf{C}^+ \cup \mathbf{R}$. Recall that we assume that the potential V appearing in (1.1) satisfies (1.3) and (1.5).

The Jost solution to (1.1) is the $n \times n$ matrix solution satisfying, for $k \in \overline{\mathbf{C}^+} \setminus \{0\}$, the asymptotics

$$f(k,x) = e^{ikx}[I_n + o(1/x)], \quad f'(k,x) = ik\, e^{ikx}[I_n + o(1/x)], \qquad x \to +\infty, \tag{2.1}$$

where I_n denotes the $n \times n$ identity matrix. It satisfies the integral equation

$$f(k,x) = e^{ikx} I_n + \frac{1}{k}\int_x^\infty dy\, \sin k(y-x)\, V(y)\, f(k,y), \tag{2.2}$$

and it is known[1,2] that $f(k,x)$ and $f'(k,x)$ are analytic in $k \in \mathbf{C}^+$ and continuous in $k \in \overline{\mathbf{C}^+}$ for each fixed x. We remark that $f(k,x)$ corresponds to the quantity $E(-k,x)$ described on p. 28 of Ref. 1.

From (2.1) it is seen that each of the n columns of $f(k,x)$ exponentially decays to zero as $x \to +\infty$ for each fixed $k \in \mathbf{C}^+$.

The matrix Schrödinger equation (1.1) has the $n \times n$ matrix solution $g(k,x)$ satisfying, for each $k \in \overline{\mathbf{C}^+} \setminus \{0\}$, the asymptotics

$$g(k,x) = e^{-ikx}[I_n + o(1/x)], \quad g'(k,x) = -ik\, e^{-ikx}[I_n + o(1/x)], \qquad x \to +\infty, \tag{2.3}$$

and $g(k,x)$ corresponds to the quantity $E^{(1)}(-k,x)$ described on p. 28 of Ref. 1. It is known[1] that $g(k,x)$ and $g'(k,x)$ are analytic in $k \in \mathbf{C}^+$ and continuous in $k \in \overline{\mathbf{C}^+} \setminus \{0\}$ for each fixed x. From (2.3) it is seen that each of the n columns of $g(k,x)$ exponentially grows as $x \to +\infty$ for each fixed $k \in \mathbf{C}^+$.

As indicated on p. 28 of Ref. 1, for each $k \in \overline{\mathbf{C}^+} \setminus \{0\}$, the combined $2n$ columns of $f(k,x)$ and $g(k,x)$ form a fundamental set of solutions to (1.1), and hence any column-vector solution $\omega(k,x)$ to (1.1) can be written as

$$\omega(k,x) = f(k,x)\,\xi + g(k,x)\,\eta, \tag{2.4}$$

for some constant column vectors ξ and η in $\mathbf{C}^n$.

The regular solution $\varphi(k,x)$ is the $n \times n$ matrix solution to (1.1) satisfying the initial conditions

$$\varphi(k,0) = A, \quad \varphi'(k,0) = B, \tag{2.5}$$

where A and B are the matrices appearing in (1.6)–(1.8). For each fixed $x \in \mathbf{R}^+$, it is known that $\varphi(k,x)$ is entire in k in the complex plane $\mathbf{C}$. Note that

$$\varphi(-k,x) = \varphi(k,x), \qquad k \in \mathbf{C}, \quad x \in \mathbf{R}^+, \tag{2.6}$$

because k appears as k^2 in (1.1) and the initial values given in (2.5) are independent of k.

We will use $[F; G] := FG' - F'G$ for the Wronskian and use an asterisk to denote complex conjugation. It can be verified directly that for any two $n \times n$ solutions $\phi(k,x)$ and $\psi(k,x)$ to (1.1), each of the Wronskians $[\phi(k^*,x)^\dagger; \psi(k,x)]$ and $[\phi(-k^*,x)^\dagger; \psi(k,x)]$ is independent of x. By evaluating the values of the Wronskians at two different x-values, say $x = 0$ and $x = +\infty$, we can obtain various useful identities. For example, we have

$$[f(\pm k,x)^\dagger; f(\pm k,x)] = \pm 2ikI_n, \qquad k \in \mathbf{R}, \tag{2.7}$$

$$[f(-k^*,x)^\dagger; f(k,x)] = 0, \qquad k \in \overline{\mathbf{C}^+}. \tag{2.8}$$

Let us add that, for each fixed $x \in \mathbf{R}^+$, if a solution $\phi(k,x)$ is analytic in $k \in \mathbf{C}^+$ then $\phi(-k^*,x)^\dagger$ becomes an analytic function of k in $\mathbf{C}^+$; on the other hand, $\phi(k^*,x)^\dagger$ becomes an analytic function of k in the lower-half complex plane $\mathbf{C}^-$.

III. THE JOST MATRIX AND THE SCATTERING MATRIX

In this section we introduce the Jost matrix $J(k)$ and the scattering matrix $S(k)$ for (1.1) with a selfadjoint matrix potential V in $L^1_1(\mathbf{R}^+)$ and with the selfadjoint boundary condition (1.6)–(1.8). We also recall or establish some of their properties relevant to our study.

The Jost matrix $J(k)$ is defined in terms of a Wronskian as

$$J(k) := [f(-k^*,x)^\dagger; \varphi(k,x)], \qquad k \in \overline{\mathbf{C}^+}, \tag{3.1}$$

where $f(k,x)$ is the Jost solution appearing in (2.1) and $\varphi(k,x)$ is the regular solution appearing in (2.5). Since the Wronskian in (3.1) is independent of x, by evaluating its value at $x = 0$, with the help of (2.5) we get

$$J(k) = f(-k^*,0)^\dagger B - f'(-k^*,0)^\dagger A, \tag{3.2}$$

where A and B are the matrices appearing in (1.6)–(1.8). Note that the domain of $J(k)$ is $\overline{\mathbf{C}^+}$ because $f(-k^*,0)^\dagger$ and $f'(-k^*,0)^\dagger$ are analytic in $k \in \mathbf{C}^+$ and continuous in $k \in \overline{\mathbf{C}^+}$, as $f(k,0)$ and $f'(k,0)$ are analytic in $k \in \mathbf{C}^+$ and continuous in $k \in \overline{\mathbf{C}^+}$.

We quote the following fundamental results from Ref. 2 regarding the Jost matrix and its inverse and their small-k behavior. We refer the reader to Theorems 4.1 and 6.3 of Ref. 2 for further details. These results are later needed in the derivation of Levinson's theorem.

Theorem 3.1: *Consider the selfadjoint matrix Schrödinger operator with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Then:*

(a) *$J(k)$ is analytic in $\mathbf{C}^+$ and continuous in $\overline{\mathbf{C}^+}$.*

(b) *As $k \to 0$ in $\overline{\mathbf{C}^+}$ we have*

$$J(k)=\mathcal{S}\,P_2^{-1}\begin{bmatrix} k\mathcal{A}_1+o(k) & k\mathcal{B}_1+o(k)\\ k\mathcal{C}_1+o(k) & \mathcal{D}_0+o(1)\end{bmatrix}P_1\mathcal{S}^{-1}, \tag{3.3}$$

where P_1 and P_2 are some permutation matrices, and $\mathcal{S}$ is a constant invertible matrix, and $\mathcal{A}_1, \mathcal{B}_1, \mathcal{C}_1,$ and $\mathcal{D}_0$ are some constant matrices of sizes $\mu\times\mu$, $\mu\times(n-\mu)$, $(n-\mu)\times\mu$, and $(n-\mu)\times(n-\mu)$, respectively, in such a way that $\mathcal{A}_1$ and $\mathcal{D}_0$ are both invertible. Here, μ is the geometric multiplicity of the zero eigenvalue of the zero-energy Jost matrix $J(0)$.

(c) *$J(k)$ is invertible for $k\in\mathbf{R}\setminus\{0\}$, and in fact $J(k)^{-1}$ is continuous for $k\in\mathbf{R}\setminus\{0\}$.*

(d) *As $k \to 0$ in $\overline{\mathbf{C}^+}$, we have*

$$J(k)^{-1}=\mathcal{S}\,P_1\begin{bmatrix} \dfrac{1}{k}\,\mathcal{A}_1^{-1}[I_\mu+o(1)] & -\mathcal{A}_1^{-1}\mathcal{B}_1\mathcal{D}_0^{-1}+o(1)\\ -\mathcal{D}_0^{-1}\mathcal{C}_1\mathcal{A}_1^{-1}+o(1) & \mathcal{D}_0^{-1}+o(1)\end{bmatrix}P_2\mathcal{S}^{-1}. \tag{3.4}$$

Hence, $J(k)^{-1}$ is either continuous at $k=0$, or it has a simple pole at $k=0$. In particular, $kJ(k)^{-1}$ has a well-defined limit at $k=0$.

The following result is already known, but we provide a brief proof for the reader's benefit, as the information contained in the proof is relevant to our study.

Proposition 3.2: Consider the selfadjoint matrix Schrödinger operator with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Then, the regular solution $\varphi(k,x)$ can be expressed in terms of the Jost solution $f(k,x)$ and the Jost matrix $J(k)$ as

$$\varphi(k,x)=\frac{1}{2ik}\,f(k,x)\,J(-k)-\frac{1}{2ik}\,f(-k,x)\,J(k),\qquad k\in\mathbf{R}\setminus\{0\}. \tag{3.5}$$

Proof: With the help of (2.1) we see that the combined $2n$ columns of $f(k,x)$ and $f(-k,x)$ form a fundamental set of column-vector solutions to (1.1) for any $k\in\mathbf{R}\setminus\{0\}$, and hence we can write the regular solution $\varphi(k,x)$ as

$$\varphi(k,x)=f(k,x)\,C_1(k)+f(-k,x)\,C_2(k),\qquad k\in\mathbf{R}\setminus\{0\}, \tag{3.6}$$

for some $n\times n$ matrices $C_1(k)$ and $C_2(k)$ depending only on k but not on x. Using (3.6) in the Wronskians $[f(\pm k,x)^\dagger;\varphi(k,x)]$, with the help of (2.7), (2.8), and (3.1) we obtain

$$C_1(k)=\frac{1}{2ik}\,J(-k),\quad C_2(k)=-\frac{1}{2ik}\,J(k),$$

yielding (3.5) for real nonzero values of k. ∎

Let us define the $n\times n$ physical solution $\Psi(k,x)$ to (1.1) as

$$\Psi(k,x):=-2ik\,\varphi(k,x)\,J(k)^{-1}, \tag{3.7}$$

where $\varphi(k,x)$ is the regular solution appearing in (2.5) and $J(k)$ is the Jost matrix defined in (3.1). The scattering matrix $S(k)$ is defined as[2,12–14]

$$S(k):=-J(-k)\,J(k)^{-1},\qquad k\in\mathbf{R}. \tag{3.8}$$

As we elaborate in Sec. VIII, $J(k)$ can uniquely be defined only up to a multiplication on the right by an invertible constant matrix. On the other hand, as seen from (3.8), such a postmultiplication of $J(k)$

by an invertible matrix does not affect $S(k)$. Hence, $S(k)$ is uniquely determined by the potential V and the boundary condition (1.6), independently of the particular parametrization used in (1.6)–(1.8). In general, $S(k)$ is defined only for real k because $J(-k)$ in general cannot be extended from $k \in \mathbf{R}$ to $k \in \mathbf{C}^+$. The continuity of $S(k)$ at $k = 0$ has recently been established.[2] Even when $J(k)^{-1}$ may not exist at $k = 0$, it has been shown[2] that the product on the right-hand side in (3.8) has a well-defined limit as $k \to 0$ in $\mathbf{R}$, and hence the domain of $S(k)$ is $k \in \mathbf{R}$. The small-k behavior of $S(k)$ is quoted from Ref. 2 in the following and hence a proof is omitted.

Proposition 3.3: Consider the selfadjoint matrix Schrödinger operator with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Then, the scattering matrix $S(k)$ defined in (3.8) is continuous for $k \in \mathbf{R}$ including $k = 0$, and we have $S(k) = S(0) + o(1)$ as $k \to 0$ in $\mathbf{R}$ with

$$S(0) = \mathcal{S} P_2^{-1} \begin{bmatrix} I_\mu & 0 \\ 2\mathcal{C}_1 \mathcal{A}_1^{-1} & -I_{n-\mu} \end{bmatrix} P_2 \mathcal{S}^{-1}, \tag{3.9}$$

where μ is the geometric multiplicity of the zero eigenvalue of the zero-energy Jost matrix $J(0)$, P_2 is an $n \times n$ permutation matrix, $\mathcal{S}$ is an $n \times n$ constant invertible matrix, $\mathcal{A}_1$ is a $\mu \times \mu$ constant invertible matrix, and $\mathcal{C}_1$ is an $(n - \mu) \times \mu$ constant matrix.

We note that the quantities μ, P_2, $\mathcal{S}$, $\mathcal{A}_1$, and $\mathcal{C}_1$ appearing in (3.9) are the same as those appearing in (3.3) and (3.4).

Proposition 3.4: Consider the selfadjoint matrix Schrödinger operator with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Then for each $x \in \mathbf{R}^+$ the physical solution given in (3.7) is continuous for $k \in \mathbf{R}$ and can be written as

$$\Psi(k, x) := f(-k, x) + f(k, x)\, S(k), \qquad k \in \mathbf{R}, \tag{3.10}$$

where $S(k)$ is the scattering matrix defined in (3.8).

Proof: Using (3.5) and (3.8) in (3.7) we get (3.10) for $k \in \mathbf{R} \setminus \{0\}$. From the continuity[2] of $f(k, x)$ and $S(k)$ for $k \in \mathbf{R}$ including $k = 0$, it follows that (3.10) also holds at $k = 0$, and hence $\Psi(k, x)$ is continuous in $k \in \mathbf{R}$ for each fixed $x \in \mathbf{R}^+$. We can verify the continuity of $\Psi(k, x)$ in $k \in \mathbf{R}$ in an alternate way. As stated in Theorem 3.1(d), even though $J(k)^{-1}$ may not exist at $k = 0$, the quantity $kJ(k)^{-1}$ is continuous for $k \in \mathbf{R}$. We recall that $\varphi(k, x)$ is entire in k for each $x \in \mathbf{R}^+$. Thus, for each fixed $x \in \mathbf{R}^+$, the physical solution $\Psi(k, x)$ defined in (3.7) is continuous in $k \in \mathbf{R}$. ■

Some useful properties of the scattering matrix $S(k)$ are provided in the following proposition. Thanks to the recent result[2] on the small-k limit of $S(k)$, the properties listed below hold for any real k, including $k = 0$.

Proposition 3.5: Consider the selfadjoint matrix Schrödinger operator with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Then the scattering matrix $S(k)$ defined in (3.8) is unitary for $k \in \mathbf{R}$ and satisfies

$$S(-k) = S(k)^{-1} = S(k)^\dagger, \qquad k \in \mathbf{R}. \tag{3.11}$$

Proof: Using (3.10) in the Wronskian $[\Psi(k, x)^\dagger; \Psi(k, x)]$, with the help of (2.7) and (2.8) we get

$$[\Psi(k, x)^\dagger; \Psi(k, x)] = -2ikI_n + 2ik\, S(k)^\dagger S(k), \qquad k \in \mathbf{R}. \tag{3.12}$$

On the other hand, using (3.7) in the same Wronskian, with the help of (1.7) and (2.5) we obtain

$$[\Psi(k, x)^\dagger; \Psi(k, x)] = -(2ik)^2 [J(k)^\dagger]^{-1} \left(A^\dagger B - B^\dagger A\right) J(k)^{-1} = 0, \qquad k \in \mathbf{R} \setminus \{0\}. \tag{3.13}$$

In fact, (3.13) holds also at $k = 0$ by letting $k \to 0$ and noting that $kJ(k)^{-1}$ has a well-defined limit[2] as $k \to 0$ in $\overline{\mathbf{C}^+}$, as stated in Theorem 3.1(d). Comparing (3.12) and (3.13) we then get $S(k)^\dagger S(k) = I_n$ for $k \in \mathbf{R}$, which yields $S(k)^{-1} = S(k)^\dagger$ for $k \in \mathbf{R}$. To establish $S(-k) = S(k)^\dagger$ for $k \in \mathbf{R}$ we proceed by evaluating the Wronskian $[\Psi(-k,x)^\dagger;\Psi(k,x)]$ in two different ways. First, using (3.10) in that Wronskian, with the help of (2.7) and (2.8) we get

$$[\Psi(-k,x)^\dagger;\Psi(k,x)] = 2ik\left(S(k)-S(-k)^\dagger\right), \qquad k\in\mathbf{R}. \tag{3.14}$$

On the other hand, using (3.7) in the same Wronskian, with the help of (1.7), (2.5), and (2.6) we obtain

$$[\Psi(-k,x)^\dagger;\Psi(k,x)] = (2ik)^2[J(-k)^\dagger]^{-1}\left(A^\dagger B - B^\dagger A\right)J(k)^{-1} = 0, \qquad k\in\mathbf{R}\setminus\{0\}. \tag{3.15}$$

For the same reason (3.13) holds at $k=0$, we conclude that (3.15) also holds at $k=0$. Thus, comparing (3.14) and (3.15) we conclude that $S(-k)=S(k)^\dagger$ for $k\in\mathbf{R}$. ■

IV. TRANSFORMATIONS

In this section we remark how the Jost solution and the regular solution to (1.1), the Jost matrix, and the scattering matrix change if the matrices A and B used in the parametrization of the boundary condition (1.6)–(1.8) undergo a transformation without affecting (1.7) and (1.8). In particular, we consider a multiplication on the right by an invertible matrix, a unitary transformation by a unitary matrix, and a combination of those two transformations. The results will be useful in analyzing the large-k asymptotics of various quantities and in the derivation of Levinson's theorem.

Proposition 4.1: Consider the selfadjoint matrix Schrödinger operator with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Let A and B be the matrices appearing in (1.6)–(1.8), $f(k,x)$ be the Jost solution to (1.1) satisfying (2.1), $\varphi(k,x)$ be the regular solution to (1.1) satisfying (2.5), $J(k)$ be the Jost matrix defined in (3.1), and $S(k)$ be the scattering matrix defined in (3.8). Then:

(a) *Under the transformation $V\mapsto V$ and $(A,B)\mapsto(AT,BT)$, where T is an invertible $n\times n$ matrix, we have*

$$(f,\varphi,J,S)\mapsto(f,\varphi T,JT,S).$$

(b) *Under the unitary transformation $V\mapsto M^\dagger VM$ and $(A,B)\mapsto(M^\dagger AM, M^\dagger BM)$, where M is a unitary $n\times n$ matrix, we have*

$$(f,\varphi,J,S)\mapsto(M^\dagger fM, M^\dagger\varphi M, M^\dagger JM, M^\dagger SM).$$

(c) *Under the unitary transformation $V\mapsto M^\dagger VM$ with a unitary matrix M and the combination of three consecutive transformations $(A,B)\mapsto(M^\dagger AT_1MT_2, M^\dagger BT_1MT_2)$, first by a right multiplication by an invertible matrix T_1, then by the unitary transformation with M, followed by a right multiplication by an invertible matrix T_2, we have*

$$(f,\varphi,J,S)\mapsto(M^\dagger fM, M^\dagger\varphi T_1MT_2, M^\dagger JT_1MT_2, M^\dagger SM). \tag{4.1}$$

Proof: The proof is obtained by direct verification and by checking that the boundary condition (1.6)–(1.8), the Schrödinger equation (1.1), and the relevant conditions and definitions in (2.1), (2.5), (3.1), and (3.8) all remain satisfied. Finally, the transformation in (c) is obtained from the results in (a) and (b). ■

We note that the transformation $V\mapsto V$ and $(A,B)\mapsto(AT,BT)$ with an invertible matrix T is just a change of parametrization in the boundary condition (1.6)–(1.8). On the other hand, the unitary transformation $V\mapsto M^\dagger VM$ and $(A,B)\mapsto(M^\dagger AM, M^\dagger BM)$ with a unitary matrix M is a change of representation in the sense of quantum mechanics.

Motivated by the general selfadjoint boundary condition[3,22,23] in the scalar case, i.e., the case with $n=1$, we are interested in going from the pair A and B appearing in the selfadjoint boundary condition (1.6)–(1.8) to the special pair $\tilde A$ and $\tilde B$, where we have defined

$$\tilde A := -\mathrm{diag}\{\sin\theta_1,\ldots,\sin\theta_n\}, \qquad \tilde B := \mathrm{diag}\{\cos\theta_1,\ldots,\cos\theta_n\}, \tag{4.2}$$

with the real parameters θ_j taking values in the interval $(0, \pi]$. The special case $\theta_j = \pi$ corresponds to the Dirichlet boundary condition and the case $\theta_j = \pi/2$ corresponds to the Neumann boundary condition. We assume that there are $n_{\rm N}$ values with $\theta_j = \pi/2$ and $n_{\rm D}$ values with $\theta_j = \pi$, and hence there are $n_{\rm M}$ remaining values, with $n_{\rm M} := n - n_{\rm N} - n_{\rm D}$, such that those θ_j-values lie in the interval $(0, \pi/2)$ or $(\pi/2, \pi)$. Our analysis takes into consideration the special cases where any of $n_{\rm N}$, $n_{\rm D}$, and $n_{\rm M}$ may be zero or n. In our notation the subscripts M, D, and N refer to "mixed," "Dirichlet," and "Neumann," respectively. We assume that the θ_j-values in (4.2) are ordered in such a way that the first $n_{\rm M}$ values of θ_j correspond to the mixed conditions, the next $n_{\rm D}$ values correspond to the Dirichlet conditions, and the remaining $n_{\rm N}$ values correspond to the Neumann conditions.

We will provide the explicit steps to go from any pair of matrices A and B satisfying (1.6)–(1.8) to the diagonal-matrix pair $\tilde A$ and $\tilde B$ given in (4.2) and yet still satisfying (1.6)–(1.8) with $\tilde A$ and $\tilde B$ replacing A and B, respectively, there. For this, we need some auxiliary results.

Starting with A and B satisfying (1.6)–(1.8), let us define

$$E := (A^\dagger A + B^\dagger B)^{1/2}, \tag{4.3}$$

so that E is positive, and hence E is uniquely defined.

Proposition 4.2: Let A and B be a pair of matrices satisfying (1.6) and (1.7), and let E be the matrix defined in (4.3). Then:

(a) *The matrix E is invertible and satisfies*

$$E = E^\dagger, \quad E^{-1}(A^\dagger A + B^\dagger B)E^{-1} = I_n. \tag{4.4}$$

(b) *We have*

$$(B \pm iA)E^{-2}(B^\dagger \mp iA^\dagger) = I_n, \tag{4.5}$$

and hence the matrices $(B \pm iA)$ *and* $(B^\dagger \pm iA^\dagger)$ *are all invertible and in fact*

$$(B \pm iA)^{-1} = E^{-2}(B^\dagger \mp iA^\dagger). \tag{4.6}$$

(c) *The matrix U defined as*

$$U := (B - iA)E^{-2}(B^\dagger - iA^\dagger), \tag{4.7}$$

is unitary, and hence it satisfies $UU^\dagger = U^\dagger U = I_n$.

(d) *The matrix U defined in (4.7) can also be written as*

$$U = (B - iA)(B + iA)^{-1}, \tag{4.8}$$

and hence from $U^\dagger = U^{-1}$ *it follows that*

$$U^\dagger = (B + iA)(B - iA)^{-1}.$$

Proof: The proof of (a) readily follows from (4.3). To prove (b) we let

$$C := \begin{bmatrix} BE^{-1} & AE^{-1} \\ AE^{-1} & -BE^{-1} \end{bmatrix},$$

and, by using (1.7) and (4.4), we directly verify that $C^\dagger C = I_{2n}$, proving the unitarity of C. We must then also have $CC^\dagger = I_{2n}$, implying

$$AE^{-2}A^\dagger + BE^{-2}B^\dagger = I_n, \quad BE^{-2}A^\dagger - AE^{-2}B^\dagger = 0. \tag{4.9}$$

With the help of (4.9), from the identity

$$(B \pm iA)E^{-2}(B^\dagger \mp iA^\dagger) = (AE^{-2}A^\dagger + BE^{-2}B^\dagger) \mp i(BE^{-2}A^\dagger - AE^{-2}B^\dagger),$$

we obtain (4.5) and hence (b) is proved. Let us now turn to the proof of (c). With the help of (4.3) and (4.5) we directly verify that the matrix U defined in (4.7) satisfies $UU^\dagger = I_n$, and hence (c) is proved. From (4.6) and (4.7) we get (4.8) and hence (d) is also proved. ■

Proposition 4.3: Let A and B be a pair of matrices satisfying (1.7) and (1.8), and let $\tilde{A}$ and $\tilde{B}$ be the matrix pair appearing in (4.2). We then have

$$\tilde{A} = M^\dagger A T_1 M T_2, \quad \tilde{B} = M^\dagger B T_1 M T_2, \tag{4.10}$$

for some unitary matrix M and for some invertible matrices T_1 and T_2.

Proof: We can diagonalize the unitary matrix U appearing in (4.7) and (4.8) by using a unitary matrix M so that

$$M^\dagger U M = \text{diag}\{e^{2i\zeta_1}, \dots, e^{2i\zeta_n}\}, \tag{4.11}$$

where the constant parameters satisfy $\zeta_j \in (0, \pi]$. Let us define

$$Y := \text{diag}\{e^{i\zeta_1}, \dots, e^{i\zeta_n}\}. \tag{4.12}$$

With the help of a permutation matrix P, we can reorder ζ_j as θ_j in the manner described below (4.2), namely, the first n_{M} values of θ_j lie in $(0, \pi/2) \cup (\pi/2, \pi)$, the next n_{D} values of θ_j are all equal to π, and the remaining n_{N} values of θ_j are all equal to $\pi/2$. Thus, from (4.11) and (4.12) we obtain

$$\begin{cases} M^\dagger U M P = Y^2 P = \text{diag}\{e^{2i\theta_1}, \dots, e^{2i\theta_n}\}, \\ Y P = \text{diag}\{e^{i\theta_1}, \dots, e^{i\theta_n}\}, \\ Y^{-1} P = \text{diag}\{e^{-i\theta_1}, \dots, e^{-i\theta_n}\}. \end{cases} \tag{4.13}$$

On the other hand, from (4.2) we see that

$$\tilde{B} - i\tilde{A} = \text{diag}\{e^{i\theta_1}, \dots, e^{i\theta_n}\}, \tag{4.14}$$

and hence

$$(\tilde{B} - i\tilde{A})^{-1} = \tilde{B} + i\tilde{A} = \text{diag}\{e^{-i\theta_1}, \dots, e^{-i\theta_n}\}. \tag{4.15}$$

We are now ready to prove (4.10). The invertibility of $(B + iA)$ is assured by (4.6) and hence we have

$$(B + iA)(B + iA)^{-1} = I_n. \tag{4.16}$$

From (4.8) we have

$$(B - iA)(B + iA)^{-1} = U. \tag{4.17}$$

Let us premultiply (4.16) and (4.17) by $M^\dagger$ and postmultiply them by $MY^{-1}P$ in order to obtain

$$M^\dagger (B + iA)(B + iA)^{-1} M Y^{-1} P = Y^{-1} P, \tag{4.18}$$

$$M^\dagger (B - iA)(B + iA)^{-1} M Y^{-1} P = M^\dagger U M Y^{-1} P, \tag{4.19}$$

where we have used the unitarity property $M^\dagger M = I_n$. From (4.11) and (4.12) we know that $M^\dagger UM = Y^2$ and hence $M^\dagger UMY^{-1}P = YP$. Thus, we can rewrite (4.19) as

$$M^\dagger (B - iA)(B + iA)^{-1} M Y^{-1} P = Y P. \tag{4.20}$$

On the other hand, from (4.13)–(4.15) we see that

$$Y P = \tilde{B} - i\tilde{A}, \quad Y^{-1} P = \tilde{B} + i\tilde{A}. \tag{4.21}$$

Using (4.21) we can rewrite (4.18) and (4.20), respectively, as

$$M^\dagger (B + iA)(B + iA)^{-1} M(\tilde{B} + i\tilde{A}) = \tilde{B} + i\tilde{A}, \tag{4.22}$$

$$M^\dagger (B - iA)(B + iA)^{-1} M(\tilde{B} + i\tilde{A}) = \tilde{B} - i\tilde{A}. \tag{4.23}$$

Letting

$$T_1 := (B + iA)^{-1}, \quad T_2 := \tilde{B} + i\tilde{A}, \tag{4.24}$$

because of (4.6) and (4.15) we observe that T_1 and T_2 are invertible and in fact

$$T_1^{-1} = B + iA, \quad T_2^{-1} = \tilde{B} - i\tilde{A}. \tag{4.25}$$

Using (4.24) we can rewrite (4.22) and (4.23), respectively, as

$$M^\dagger (B + iA) T_1 M T_2 = \tilde{B} + i\tilde{A}, \tag{4.26}$$

$$M^\dagger (B - iA) T_1 M T_2 = \tilde{B} - i\tilde{A}. \tag{4.27}$$

By subtracting and adding, respectively, from (4.26) and (4.27) we obtain (4.10). ■

Because of Propositions 4.1 and 4.3, there is not much loss of generality in using the special boundary parametrization with $\tilde{A}$ and $\tilde{B}$ given in (4.2). The relevant results can then be transformed to obtain the corresponding results in the parametrization with A and B appearing in (1.6)–(1.8). Let us use a tilde to denote the quantities obtained under the transformation given in Proposition 4.1(c). With the help of (4.1) and (4.10), we can obtain the corresponding quantities in any boundary parametrization with A and B satisfying (1.7) and (1.8). In other words, when we have

$$V(x) = M\,\tilde{V}(x)\,M^\dagger, \quad A = M\tilde{A}T_2^{-1}M^\dagger T_1^{-1}, \quad B = M\tilde{B}T_2^{-1}M^\dagger T_1^{-1}, \tag{4.28}$$

we then get

$$f(k,x) = M\tilde{f}(k,x)\,M^\dagger, \quad J(k) = M\tilde{J}(k)\,T_2^{-1}M^\dagger T_1^{-1}, \quad S(k) = M\tilde{S}(k)\,M^\dagger, \tag{4.29}$$

where M is the unitary matrix appearing in (4.11) and T_1^{-1} and T_2^{-1} are the matrices specified in (4.25).

V. THE JOST AND SCATTERING MATRICES WITH ZERO POTENTIAL

In order to understand the large-k behavior of the Jost matrix $J(k)$, its inverse $J(k)^{-1}$, and the scattering matrix $S(k)$, we first need to understand those behaviors when the potential V appearing in (1.1) is identically zero. In that case, let us use the subscript 0 to denote the corresponding quantities and write $J_0(k)$ and $S_0(k)$ for the Jost and scattering matrices, respectively, corresponding to $V \equiv 0$.

When $V \equiv 0$, from (2.2) we get $f(k,x) = e^{ikx} I_n$, and hence (3.2) and (3.8) yield

$$J_0(k) = B - ikA, \quad J_0(k)^{-1} = (B - ikA)^{-1}, \quad S_0(k) = -(B + ikA)(B - ikA)^{-1}. \tag{5.1}$$

In the boundary parametrization with $\tilde{A}$ and $\tilde{B}$ in (4.2), the corresponding quantities are given by diagonal matrices, where we have

$$\tilde{J}_0(k) = \tilde{B} - ik\tilde{A} = \operatorname{diag}\{\cos\theta_1 + ik\sin\theta_1, \dots, \cos\theta_{n_{\rm M}} + ik\sin\theta_{n_{\rm M}}, -I_{n_{\rm D}}, ikI_{n_{\rm N}}\}, \tag{5.2}$$

$$\tilde{J}_0(k)^{-1} = \operatorname{diag}\left\{\frac{1}{\cos\theta_1 + ik\sin\theta_1}, \dots, \frac{1}{\cos\theta_{n_{\rm M}} + ik\sin\theta_{n_{\rm M}}}, -I_{n_{\rm D}}, \frac{1}{ik}\, I_{n_{\rm N}}\right\}, \tag{5.3}$$

$$\tilde{S}_0(k) = \operatorname{diag}\left\{\frac{-\cos\theta_1 + ik\sin\theta_1}{\cos\theta_1 + ik\sin\theta_1}, \dots, \frac{-\cos\theta_{n_{\rm M}} + ik\sin\theta_{n_{\rm M}}}{\cos\theta_{n_{\rm M}} + ik\sin\theta_{n_{\rm M}}}, -I_{n_{\rm D}}, I_{n_{\rm N}}\right\}. \tag{5.4}$$

Then, from (5.3) and (5.4) we see that, as $k \to \infty$ in $\mathbf{C}$,

$$\tilde{J}_0(k)^{-1} = \operatorname{diag}\{0_{n_{\rm M}}, -I_{n_{\rm D}}, 0_{n_{\rm N}}\} + \frac{1}{ik}\operatorname{diag}\{\csc\theta_1, \dots, \csc\theta_{n_{\rm M}}, 0_{n_{\rm D}}, I_{n_{\rm N}}\} + O(1/k^2), \tag{5.5}$$

$$\tilde{S}_0(k) = Z_0 + \frac{2i}{k}\, Z_1 + O(1/k^2), \tag{5.6}$$

where we have defined

$$Z_0 := \operatorname{diag}\{I_{n_\mathrm{M}}, -I_{n_\mathrm{D}}, I_{n_\mathrm{N}}\}, \quad Z_1 := \operatorname{diag}\{\cot\theta_1, \ldots, \cot\theta_{n_\mathrm{M}}, 0_{n_\mathrm{D}}, 0_{n_\mathrm{N}}\}, \tag{5.7}$$

with 0_j denoting the $j \times j$ zero matrix.

The results in the following proposition are needed in Sec. VII.

Proposition 5.1: The Jost matrix $J_0(k)$ appearing in (5.1) is invertible when $k \to \infty$ in $\mathbf{C}$. The matrix $J_0(k)^{-1}$and the scattering matrix $S_0(k)$ given in (5.1) satisfy, as $k \to \infty$ in $\mathbf{C}$,

$$J_0(k)^{-1} = T_1 M T_2 \operatorname{diag}\{0_{n_\mathrm{M}}, -I_{n_\mathrm{D}}, 0_{n_\mathrm{N}}\} M^\dagger + O(1/k), \tag{5.8}$$

$$A\, J_0(k)^{-1} = \frac{1}{ik} M \operatorname{diag}\{-I_{n_\mathrm{M}}, 0_{n_\mathrm{D}}, -I_{n_\mathrm{N}}\} M^\dagger + O(1/k^2), \tag{5.9}$$

$$S_0(k) = S_0(\infty) + \frac{2i}{k} M Z_1 M^\dagger + O(1/k^2), \quad S_0(\infty) := M Z_0 M^\dagger, \tag{5.10}$$

where T_1 and T_2 are the matrices in (4.24), M is the unitary matrix in (4.11), A and B are the matrices appearing in (1.6)–(1.8), $\tilde A$ and $\tilde B$ are the matrices defined in (4.2), and Z_0 and Z_1 are the matrices defined in (5.7). Thus, as $k \to \infty$ in $\mathbf{C}$ we have

$$J_0(k)^{-1} = O(1), \quad A J_0(k)^{-1} = O(1/k), \quad S_0(k) = S_0(\infty) + O(1/k). \tag{5.11}$$

Proof: Exploiting the unitarity properties $M^{-1} = M^\dagger$ and $M^\dagger M = I_n$, from (4.28) and (4.29) when $V \equiv 0$ we get

$$J_0(k)^{-1} = T_1 M T_2\, \tilde J_0(k)^{-1} M^\dagger, \quad A\, J_0(k)^{-1} = M \tilde A\, \tilde J_0(k)^{-1} M^\dagger, \quad S_0(k) = M \tilde S_0(k) M^\dagger. \tag{5.12}$$

From (5.3) we conclude that $\tilde J_0(k)$ is invertible when $k \to \infty$ in $\mathbf{C}$, and hence the first equality in (5.12) implies that $J_0(k)^{-1}$ exists when $k \to \infty$ in $\mathbf{C}$. Using (4.2), (5.5), and (5.6) in (5.12), we get the expansions (5.8)–(5.10) as $k \to \infty$ in $\mathbf{C}$. ■

VI. SMALL-*k* BEHAVIOR

The analysis of (1.1) near and at $k = 0$ deserves a separate attention and we refer the reader to Ref. 2 for such an analysis. Under the assumption that the potential V satisfies (1.3) and (1.5), we recall certain useful properties that will be needed in establishing Levinson's theorem.

When $k = 0$ from (1.1) we obtain the zero-energy matrix Schrödinger equation

$$\psi'' = V(x)\, \psi, \qquad x \in \mathbf{R}^+. \tag{6.1}$$

It is known[1,2] that the Jost solution $f(k, x)$ to (1.1) appearing in (2.1) satisfies (6.1) if we replace k by 0 in $f(k, x)$, and that $f(0, x)$ satisfies[1,2]

$$f(0, x) = I_n + o(1), \quad f'(0, x) = o(1/x), \qquad x \to +\infty. \tag{6.2}$$

It is also known[1,2] that $g(0, x)$, obtained by replacing k with 0 in the matrix-valued function $g(k, x)$ appearing in (2.3), is a solution to (6.1) and it satisfies

$$g(0, x) = x[I_n + o(1)], \quad g'(0, x) = I_n + o(1), \qquad x \to +\infty. \tag{6.3}$$

Thus, from (6.2) and (6.3) we see that the combined $2n$ columns of $f(0, x)$ and $g(0, x)$ form a fundamental set of solutions to (6.1), and hence (2.4) is valid even when $k = 0$. From (6.2) we see that the n columns of $f(0, x)$ form n linearly independent solutions to (6.1) that remain bounded as $x \to +\infty$. Similarly, (6.3) indicates that the n columns of $g(0, x)$ form n linearly independent solutions to (6.1) that become unbounded as $x \to +\infty$.

On the left-hand side of (2.4) with $k = 0$, let us use a linear combination of n columns of the zero-energy regular solution $\varphi(0, x)$, which itself is an $n \times n$ matrix solution to (6.1), and let us express such a column-vector solution as linear combinations of the $2n$ combined columns of $f(0, x)$ and $g(0, x)$, i.e., we let

$$\varphi(0, x)\, u = f(0, x)\, \xi + g(0, x)\, \eta, \tag{6.4}$$

for some nonzero constant column vectors u, ξ, η in $\mathbf{C}^n$. We know that the left-hand side in (6.4) satisfies (1.6) for any $u \in \mathbf{C}^n$ because $\varphi(0, x)$ itself satisfies (1.6). We are interested in knowing how many linearly independent bounded column-vector solutions to (6.1) we can form by using linear combinations of n columns of $\varphi(0, x)$. Equivalently, we are interested knowing how many of the n linearly independent bounded column-vector solutions to (6.1) also satisfy (1.6).

There are two possibilities for (6.4) with a nonzero column vector $u \in \mathbf{C}^n$; either $\varphi(0, x)\, u$ is bounded as $x \to +\infty$, in which case we must have $\xi \neq 0$ and $\eta = 0$, or $\varphi(0, x)\, u$ is unbounded as $x \to +\infty$, in which case we must have $\eta \neq 0$. In fact, the related results are known and quoted from Ref. 2 in the following proposition.

Proposition 6.1: Consider the selfadjoint matrix Schrödinger operator with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Then, we have:

(a) *The nonzero column vector $u \in \mathbf{C}^n$ is an eigenvector of the zero-energy Jost matrix $J(0)$ with the zero eigenvalue, i.e., $u \in$ Ker $[J(0)]$, if and only if $\varphi(0, x)\, u$ is bounded for $x \in \mathbf{R}^+$.*

(b) *For any column vector u in* Ker $[J(0)]$ *there exists a unique column vector ξ in* Ker $[J(0)^\dagger]$ *such that*

$$\varphi(0, x)\, u = f(0, x)\, \xi.$$

The map $u \mapsto \xi$ from Ker $[J(0)]$ to Ker $[J(0)^\dagger]$ *is a bijection.*

As in Theorem 3.1 let us use μ to denote the geometric multiplicity of the zero eigenvalue of $J(0)$. From Proposition 6.1 it follows that we can form exactly μ columns by using linear combinations of n columns of the zero-energy regular solution $\varphi(0, x)$ in such a way that those μ columns form linearly independent solutions to (6.1) and they remain bounded as $x \to +\infty$. Furthermore, each of such μ column-vector solutions to (6.1) can also be expressed as a linear combinations of columns of $f(0, x)$. In that sense, the integer μ indicates the maximal number of linearly independent bounded solutions to (6.1) that also satisfy (1.6), and hence μ acts as a "degree" of the exceptional case[2] for the Schrödinger equation (1.1) with the boundary condition (1.6)–(1.8). In the purely generic case, i.e., when $\mu = 0$, the $2n$ combined columns of $\varphi(0, x)$ and of $f(0, x)$ are all linearly independent. In that case, each column of $\varphi(0, x)$ can be expressed as a linear combination of n linearly independent columns of $g(0, x)$. In the purely exceptional case, i.e., when $\mu = n$, each column of $\varphi(0, x)$ can be expressed as a linear combination of n linearly independent columns of $f(0, x)$.

From (3.3), we have the following conclusion.

Corollary 6.2: Consider the selfadjoint matrix Schrödinger operator with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Then, the determinant of the Jost matrix $J(k)$ defined in (3.1) has the small-k behavior

$$\det J(k) = c_1 k^\mu [1 + o(1)], \qquad k \to 0 \text{ in } \overline{\mathbf{C}^+}, \tag{6.5}$$

where μ is the geometric multiplicity of the zero eigenvalue of the zero-energy Jost matrix $J(0)$ and c_1 is a nonzero constant. In fact, the value of c_1 is given by

$$c_1 := (\det P_1)(\det P_2)(\det \mathcal{A}_1)(\det \mathcal{D}_0),$$

where P_1 and P_2 are the $n \times n$ permutation matrices appearing in (3.3) and hence their determinants are either 1 or -1, and $\mathcal{A}_1$ and $\mathcal{D}_0$ are the invertible matrices appearing in (3.3) and hence their determinants are nonzero.

From (3.9) we see that the zero-energy scattering matrix $S(0)$ has only two eigenvalues, namely $+1$ and -1. In the next proposition we prove that the eigenvalue $+1$ of $S(0)$ has multiplicity (both geometric and algebraic) equal to μ and that the eigenvalue -1 has multiplicity (both geometric and algebraic) equal to $n - \mu$. Thus, the value of μ is uniquely determined from $S(0)$ alone.

Proposition 6.3: Consider the selfadjoint matrix Schrödinger operator with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Let $J(k)$ and $S(k)$ be the corresponding Jost matrix and the scattering matrix defined in (3.1) and (3.8), respectively. Then:

(a) *$S(0)$ has two eigenvalues, which are $+1$ and -1.*
(b) *The geometric and algebraic multiplicities of the eigenvalue $+1$ of $S(0)$ are both equal to μ, which is the geometric multiplicity of the zero eigenvalue of $J(0)$.*
(c) *The geometric and algebraic multiplicities of the eigenvalue -1 of $S(0)$ are both equal to $n - \mu$.*

Proof: By (3.9), we see that $S(0)$ is similar to a lower-triangular matrix whose diagonal entries coincide with the diagonal entries of the diagonal matrix diag $\{I_\mu, -I_{n-\mu}\}$. Since a similarity transformation does not change the eigenvalues, we conclude that $S(0)$ has the eigenvalue $+1$ with the algebraic multiplicity μ and the eigenvalue -1 with the algebraic multiplicity $n - \mu$. We thus only need to determine the geometric multiplicity for each eigenvalue. By (3.11), we know that $S(0)$ is unitary and hence it can be diagonalized with a unitary matrix M_1. Thus, $S(0) = M_1 D M_1^\dagger$ for some diagonal matrix D, with μ of the diagonal entries being $+1$ and $n - \mu$ of them being -1. The algebraic and geometric multiplicities of eigenvalues remain invariant under a similarity transformation with a unitary matrix, and furthermore the algebraic and geometric multiplicities of each eigenvalue of a diagonal matrix are equal to each other. Thus, the geometric multiplicities of the eigenvalues $+1$ and -1 are given by μ and $n - \mu$, respectively. ■

VII. LARGE-*k* BEHAVIOR

In establishing the large-k behaviors of various quantities related to (1.1), it is sufficient for the potential to satisfy (1.2) rather than the stronger condition (1.5). The following matrices will be useful in our large-k analysis:

$$Q_1 := \frac{1}{2}\int_0^\infty dy\, V(y), \quad Q_2(k) := \frac{1}{2}\int_0^\infty dy\, e^{2iky} V(y), \tag{7.1}$$

$$Q_3 := \frac{1}{4}\int_0^\infty dz \int_0^z dy\, V(z)\, V(y), \quad Q_4(k) := \frac{1}{4}\int_0^\infty dz \int_0^z dy\, e^{2ikz} V(z)\, V(y), \tag{7.2}$$

$$Q_5(k) := \frac{1}{4}\int_0^\infty dz \int_0^z dy\, e^{2iky} V(z)\, V(y), \quad Q_6(k) := \frac{1}{4}\int_0^\infty dz \int_0^z dy\, e^{2ik(z-y)} V(z)\, V(y). \tag{7.3}$$

We emphasize that Q_1 and Q_3 are independent of k while the remaining four matrices are functions of k.

Proposition 7.1: Assume that V in (1.1) belongs to $L^1(\mathbf{R}^+)$. Then, Q_1 and Q_3 are well defined constant matrices. Furthermore, each of the four matrix quantities $Q_2(k)$, $Q_4(k)$, $Q_5(k)$, and $Q_6(k)$ is well defined for $k \in \overline{\mathbf{C}^+}$, and each one of them has the behavior of $o(1)$ as $k \to \infty$ in $\overline{\mathbf{C}^+}$.

Proof: The integrals defining Q_1 and Q_3 exist because $V \in L^1(\mathbf{R}^+)$. For $k \in \overline{\mathbf{C}^+}$, the coefficients of $2ik$ in the exponents appearing in $Q_2(k)$, $Q_4(k)$, $Q_5(k)$, and $Q_6(k)$ are all nonnegative, and hence each of those exponential terms are bounded by one in absolute value. Furthermore, $V \in L^1(\mathbf{R}^+)$, and hence we have the estimate

$$\left\| \int_0^x dz\, V(z) \right\| \le \int_0^x dz\, ||V(z)|| \le \int_0^\infty dz\, ||V(z)||,$$

where the integral on the right-hand side converges. Thus, we can establish that the integrals used in defining $Q_2(k)$, $Q_4(k)$, $Q_5(k)$, $Q_6(k)$ all exist for $k \in \overline{\mathbf{C}^+}$. Finally, the behavior of $o(1)$ as $k \to \infty$ in $\overline{\mathbf{C}^+}$ for $Q_2(k)$, $Q_4(k)$, $Q_5(k)$, $Q_6(k)$ is established with the help of the Riemann-Lebesgue lemma on the appropriate integrals. ∎

Proposition 7.2: Consider the matrix Schrödinger equation (1.1) with the selfadjoint potential V satisfying (1.2) and (1.3). Let $f(k,x)$ be the corresponding Jost solution satisfying (2.1). Then, we have as $k \to \infty$ in $\overline{\mathbf{C}^+}$

$$f(-k^*,0)^\dagger = I_n + \frac{1}{ik}[-Q_1 + Q_2(k)] + \frac{1}{k^2}[-Q_3 - Q_4(k) + Q_5(k) + Q_6(k)] + O(1/k^3), \tag{7.4}$$

$$f'(-k^*,0)^\dagger = ikI_n - Q_1 - Q_2(k) + \frac{1}{ik}[Q_3 - Q_4(k) + Q_5(k) - Q_6(k)] + O(1/k^2), \tag{7.5}$$

where Q_1, $Q_2(k)$, Q_3, $Q_4(k)$, $Q_5(k)$, $Q_6(k)$ are the matrices defined in (7.1)–(7.3) with the properties outlined in Proposition 7.1.

Proof: Writing the Jost solution $f(k,x)$ in terms of $m(k,x) := e^{-ikx} f(k,x)$, from (2.2) we obtain the integral relations

$$m(k,x) = I_n + \frac{1}{2ik}\int_x^\infty dy\, \left[e^{2ik(y-x)} - 1\right] V(y)\, m(k,y), \tag{7.6}$$

$$m'(k,x) = -\int_x^\infty dy\, e^{2ik(y-x)}\, V(y)\, m(k,y). \tag{7.7}$$

Iterating (7.6) and (7.7), for $k \to \infty$ in $\overline{\mathbf{C}^+}$ we obtain

$$\begin{aligned} m(k,x) = I_n &+ \frac{1}{2ik}\int_x^\infty dy\, \left[e^{2ik(y-x)} - 1\right] V(y) \\ &+ \frac{1}{(2ik)^2}\int_x^\infty dy\, \left[e^{2ik(y-x)} - 1\right] V(y) \int_y^\infty dz\, \left[e^{2ik(y-z)} - 1\right] V(z) + O(1/k^3), \end{aligned} \tag{7.8}$$

$$\begin{aligned} m'(k,x) = &-\int_x^\infty dy\, e^{2ik(y-x)}\, V(y) \\ &- \frac{1}{2ik}\int_x^\infty dy\, e^{2ik(y-x)}\, V(y) \int_y^\infty dz\, \left[e^{2ik(y-z)} - 1\right] V(z) + O(1/k^2). \end{aligned} \tag{7.9}$$

We evaluate (7.8) and (7.9) at $x = 0$, and we rewrite the double integrals in them by changing the order of integration. Then, with the help of

$$f(k,0) = m(k,0), \quad f'(k,0) = ik\, m(k,0) + m'(k,0), \tag{7.10}$$

we obtain the expansions for $f(k,0)$ and $f'(k,0)$ as $k \to \infty$ in $\overline{\mathbf{C}^+}$. Finally, by replacing k by $-k^*$, taking the adjoints, and using $[V(y)\,V(z)]^\dagger = V(z)\,V(y)$, with the help of (7.8)–(7.10) we obtain (7.4) and (7.5). ∎

Proposition 7.3: Consider the Schrödinger operator corresponding to (1.1) with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.2) and (1.3). Let $J(k)$ be the corresponding Jost matrix defined in (3.1). Then, we have as $k \to \infty$ in $\overline{\mathbf{C}^+}$

$$J(k) = -ikA + B + [Q_1 + Q_2(k)]A + \frac{1}{ik}P(k) + O(1/k^2), \tag{7.11}$$

where we have defined

$$P(k) := [-Q_1 + Q_2(k)]B + [-Q_3 + Q_4(k) - Q_5(k) + Q_6(k)]A,$$

with A and B being the matrices appearing in (1.6)–(1.8), and Q_1, $Q_2(k)$, Q_3, $Q_4(k)$, $Q_5(k)$, $Q_6(k)$ *being the matrices in (7.1)–(7.3).*

Proof: Using (7.4) and (7.5) in (3.2) we obtain (7.11). ∎

Proposition 7.4: Consider the Schrödinger operator corresponding to (1.1) with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.2) and (1.3). Let J(k) and $J_0(k)$ *be the corresponding Jost matrices appearing in (3.1) and (5.1), respectively,* Q_1 *and* $Q_2(k)$ *be the quantities in (7.1), and* $S_0(\infty)$ *be the constant matrix defined in (5.10). Then, as* $k \to \infty$ *in* $\overline{\mathbf{C}^+}$ *we have*

$$J(k)\, J_0(k)^{-1} = I_n - \frac{1}{ik}\,[Q_1 + Q_2(k)\, S_0(\infty)] + O(1/k^2), \tag{7.12}$$

$$J_0(k)\, J(k)^{-1} = I_n + \frac{1}{ik}\,[Q_1 + Q_2(k)\, S_0(\infty)] + O(1/k^2). \tag{7.13}$$

Proof: By replacing $B - ikA$ by $J_0(k)$, as given in (5.1), and replacing $B + ikA$ by $J_0(-k)$, from (7.11) we get, as $k \to \infty$ in $\overline{\mathbf{C}^+}$,

$$J(k)= J_0(k)-\frac{1}{ik}\, Q_1 J_0(k)+\frac{1}{ik}\, Q_2(k)\, J_0(-k)+\frac{1}{ik}[-Q_3 + Q_4(k) - Q_5(k) + Q_6(k)]A + O(1/k^2). \tag{7.14}$$

The invertibility of $J_0(k)$ as $k \to \infty$ in $\overline{\mathbf{C}^+}$ is assured by Proposition 5.1. Let us multiply (7.14) on the right by $J_0(k)^{-1}$ and use $J_0(-k)\, J_0(k)^{-1} = -S_0(k)$, which follows from (3.8). We then obtain, as $k \to \infty$ in $\overline{\mathbf{C}^+}$,

$$\begin{aligned} J(k)\, J_0(k)^{-1} =& I_n - \frac{1}{ik}\, Q_1 - \frac{1}{ik}\, Q_2(k)\, S_0(k) \\ &+ \frac{1}{ik}[-Q_3 + Q_4(k) - Q_5(k) + Q_6(k)]A\, J_0(k)^{-1} + O(1/k^2)\, J_0(k)^{-1}. \end{aligned} \tag{7.15}$$

Using (5.11) and (7.15), we get

$$J(k)\, J_0(k)^{-1} = I_n - \frac{1}{ik}\, Q_1 - \frac{1}{ik}\, Q_2(k)\, S_0(k) + O(1/k^2), \qquad k \to \infty \text{ in } \overline{\mathbf{C}^+},$$

which is also equivalent to (7.12) because of the third estimate in (5.11). The expansion in (7.13) is obtained by changing the signs of the $O(1/k)$-terms in (7.12). ∎

Proposition 7.5: Consider the Schrödinger operator corresponding to (1.1) with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.2) and (1.3). Then, the corresponding Jost matrix J(k) defined in (3.1) satisfies

$$J(k) = J_0(k)[I_n + O(1/k)], \qquad k \to \infty \text{ in } \overline{\mathbf{C}^+}, \tag{7.16}$$

$$\det J(k) = c_2 k^{n_{\mathrm{M}}+n_{\mathrm{N}}}[1 + O(1/k)], \qquad k \to \infty \text{ in } \overline{\mathbf{C}^+}, \tag{7.17}$$

where $J_0(k)$ *is the matrix in (5.1),* c_2 *is a nonzero constant, and* n_{M} *and* n_{N} *are the nonnegative integers defined after (4.2) and appearing in (5.2)–(5.4).*

Proof: Note that (7.16) is apparent from (7.15). With the help of the first equality in (5.12) we get

$$J_0(k) = M\, \tilde{J}_0(k)\, T_2^{-1} M^\dagger T_1^{-1}, \tag{7.18}$$

where T_1 and T_2 are the invertible matrices appearing in (4.24) and (4.25), M is the unitary matrix appearing in (4.11), and $\tilde{J}_0(k)$ is the matrix in (5.2). Using (5.2) and (7.18) we obtain

$$\det J_0(k) = c_2 k^{n_{\mathrm{M}}+n_{\mathrm{N}}}[1 + O(1/k)], \qquad k \to \infty \text{ in } \overline{\mathbf{C}^+}, \tag{7.19}$$

where we have defined

$$c_2 := \frac{(-1)^{n_D}(i)^{n_M+n_N}}{\det[T_1T_2]} \prod_{j=1}^{n_M} \sin\theta_j.$$

Note that c_2 is well defined and nonzero because T_1 and T_2 are invertible matrices and $\sin\theta_j \neq 0$ for $j = 1, \ldots, n_M$. The latter follows from the fact that those θ_j all lie in $(0, \pi/2) \cup (\pi/2, \pi)$, as stated above (4.13). From (7.16) and (7.19) we then get (7.17). ■

Next we present the large-k asymptotics of the scattering matrix.

Theorem 7.6: *Consider the Schrödinger operator corresponding to (1.1) with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.2) and (1.3). Then the corresponding scattering matrix $S(k)$ defined in (3.8) satisfies*

$$S(k) = S_0(\infty) + \frac{G(k)}{ik} + O(1/k^2), \qquad k \to \pm\infty, \tag{7.20}$$

where $G(k)$ is the matrix defined as

$$G(k) := -2MZ_1M^\dagger + Q_1S_0(\infty) + S_0(\infty)\,Q_1 + S_0(\infty)Q_2(k)S_0(\infty) + Q_2(-k),$$

with M being the unitary matrix in (4.11), Z_1 the matrix in (5.7), $S_0(\infty)$ the matrix in (5.10), and Q_1 and $Q_2(k)$ the matrices in (7.1).

Proof: With the help of (3.8) we see that

$$S(k) = J(-k)\,J_0(-k)^{-1}S_0(k)J_0(k)\,J(k)^{-1}, \tag{7.21}$$

where $J_0(k)$ and $S_0(k)$ are the matrices defined in (5.1) and $J(k)$ is the Jost matrix appearing in (3.1). Using (7.12) and (7.13) in (7.21), with the help of the identity $S_0(-k)S_0(k) = I_n$, which follows from (3.11), we obtain

$$S(k) = S_0(k) + \frac{H(k)}{ik} + O(1/k^2), \qquad k \to \pm\infty, \tag{7.22}$$

where we have defined

$$H(k) := Q_1S_0(k) + S_0(k)Q_1 + S_0(k)Q_2(k)S_0(k) + Q_2(-k). \tag{7.23}$$

Finally, using (5.10) in (7.22) and (7.23), we obtain (7.20). ■

VIII. BOUND STATES

A bound state for the Schrödinger equation (1.1) with the boundary condition (1.6)–(1.8) at $x = 0$ corresponds to a square-integrable column-vector solution satisfying (1.6). Because of (1.3) and (1.6)–(1.8), the corresponding Schrödinger operator is selfadjoint, and hence a bound state must occur at a real value of k^2. From (2.1), (2.3), and (2.4), we see that we cannot have any bound states at any positive values of k^2 because none of the combined $2n$ linearly independent columns of $f(k, x)$ and $g(k, x)$ can be square integrable on $x \in \mathbf{R}^+$ when k is real. Similarly, from (6.2) and (6.3) we see that none of the combined $2n$ linearly independent columns of $f(0, x)$ and $g(0, x)$ can be square integrable on $x \in \mathbf{R}^+$, and since (2.4) also holds at $k = 0$, we can conclude that there cannot be a bound state when $k = 0$. Thus, a bound state, if it exists, can only occur when $k^2 < 0$, which corresponds to a value of k on the positive imaginary axis in $\mathbf{C}$.

Let us assume that $k = i\kappa$ for some positive κ corresponds to a bound state, and let $\omega(i\kappa, x)$ be a square-integrable column-vector solution satisfying (1.6). Then, (2.4) must hold at $k = i\kappa$ with $\eta = 0$ and for some nonzero column vector $\xi \in \mathbf{C}^n$, yielding

$$\omega(i\kappa, x) = f(i\kappa, x)\xi. \tag{8.1}$$

Let us show that ξ must belong to the kernel of $J(i\kappa)^\dagger$ because $\omega(i\kappa, x)$ must satisfy (1.6). Note that, from (1.6) and (8.1) we get

$$-B^\dagger f(i\kappa, 0)\xi + A^\dagger f'(i\kappa, 0)\xi = 0, \tag{8.2}$$

which is equivalent to

$$\left[-\varphi'(i\kappa, 0)^\dagger f(i\kappa, 0) + \varphi(i\kappa, 0)^\dagger f'(i\kappa, 0)\right]\xi = 0, \tag{8.3}$$

or equivalently, in terms of the Wronskian, (8.3) can be written as

$$[f(i\kappa, x)^\dagger, \varphi(i\kappa, x)]^\dagger \xi = 0. \tag{8.4}$$

Comparing (3.1) and (8.4), we see that (8.4) is equivalent to

$$J(i\kappa)^\dagger \xi = 0, \tag{8.5}$$

and hence ξ belongs to $\mathrm{Ker}[J(i\kappa)^\dagger]$. Thus, the determinant of $J(i\kappa)$ must be zero.

Conversely, consider any column vector of the form $f(i\kappa, x)\,\xi$, where $k = i\kappa$ corresponds to a zero of $\det J(k)$ on the positive imaginary axis and $\xi \in \mathbf{C}^n$ is a nonzero column vector belonging to $\mathrm{Ker}[J(i\kappa)^\dagger]$. Then, $f(i\kappa, x)\,\xi$ must be a bound-state column-vector solution to the corresponding Schrödinger operator. To verify this, we must prove that $f(i\kappa, x)\,\xi$ is a solution to (1.1), it is square integrable on $x \in \mathbf{R}^+$, and it satisfies the boundary condition (1.6)–(1.8). It is clearly a solution to (1.1) because $f(k, x)$ is a $n \times n$ matrix solution to (1.1). It is square integrable because $f(k, x)$ exponentially decays to zero for each $k \in \mathbf{C}^+$ as $x \to +\infty$, as apparent from (2.1). Finally, it satisfies the boundary condition (1.6) because

$$-B^\dagger f(i\kappa, 0)\xi + A^\dagger f'(i\kappa, 0)\xi = J(i\kappa)^\dagger \xi = 0,$$

as seen from (8.2)–(8.5). The multiplicity of the bound state at $k = i\kappa$ is equal to the dimension of the kernel of $J(i\kappa)^\dagger$, which is also equal to the dimension of the kernel of $J(i\kappa)$.

Let us now show that a bound-state column-vector solution at $k = i\kappa$ must have the form $\varphi(i\kappa, x)\alpha$ for some constant nonzero column vector $\alpha \in \mathbf{C}^n$ that belongs to the kernel of $J(i\kappa)$ in such a way that

$$\varphi(i\kappa, x)\alpha = f(i\kappa, x)\beta, \tag{8.6}$$

where $\beta \in \mathrm{Ker}[J(i\kappa)^\dagger]$. In other words, we must show that $\varphi(i\kappa, x)\alpha$ with $\alpha \in \mathrm{Ker}[J(i\kappa)]$ satisfies (1.6), is square integrable, and satisfies (8.6) for some column vector $\beta \in \mathrm{Ker}[J(i\kappa)^\dagger]$. Note that (1.6) is satisfied because with the help of (1.7) and (2.5) we get

$$-B^\dagger \varphi(i\kappa, 0)\alpha + A^\dagger \varphi'(i\kappa, 0)\alpha = (-B^\dagger A + A^\dagger B)\alpha = 0.$$

Next, let us show that $\varphi(i\kappa, x)\alpha$ exponentially decays to zero as $x \to +\infty$, and hence it is square integrable on $x \in \mathbf{R}^+$. From (2.4) we see that $\varphi(i\kappa, x)\alpha$ can be written as a linear combination of the $2n$ linearly independent columns of $f(i\kappa, x)$ and $g(i\kappa, x)$, i.e., there exist some constant column vectors β and γ in $\mathbf{C}^n$ such that

$$\varphi(i\kappa, x)\,\alpha = f(i\kappa, x)\,\beta + g(i\kappa, x)\,\gamma, \qquad x \in \mathbf{R}^+. \tag{8.7}$$

Let us now evaluate the Wronskian-related quantity $[f(i\kappa, x)^\dagger; \varphi(i\kappa, x)]\alpha$ using (8.7). With the help of (3.1) we get

$$[f(i\kappa, x)^\dagger; \varphi(i\kappa, x)]\alpha = J(i\kappa)\alpha = 0, \tag{8.8}$$

because $\alpha \in \mathrm{Ker}[J(i\kappa)]$. On the other hand, using (8.7) we get

$$\begin{aligned}\alpha &= [f(i\kappa, x)^\dagger; f(i\kappa, x)\,\beta + g(i\kappa, x)\,\gamma] \\ &= [f(i\kappa, x)^\dagger; f(i\kappa, x)]\,\beta + [f(i\kappa, x)^\dagger; g(i\kappa, x)]\,\gamma \\ &= [f(i\kappa, x)^\dagger; g(i\kappa, x)]\,\gamma \\ &= 2\kappa\gamma,\end{aligned} \tag{8.9}$$

where we have used (2.1) and (2.3) to evaluate the relevant Wronskians. Comparing (8.8) and (8.9) we see that $\gamma = 0$ and hence (8.6) is satisfied for some nonzero column vector β in $\mathbf{C}^n$. Because of (2.1), from (8.6) we conclude that $\varphi(i\kappa, x)\alpha$ decays exponentially to zero as $x \to +\infty$ and hence it is square integrable. Note that, β must belong to $\operatorname{Ker}[J(i\kappa)^\dagger]$ as a result of our earlier argument that if $f(i\kappa, x)\beta$ is a bound state then β must belong to the kernel of $J(i\kappa)^\dagger$.

Let us emphasize that (8.6) establishes a bijection $\alpha \mapsto \beta$ between $\operatorname{Ker}[J(i\kappa)]$ and $\operatorname{Ker}[J(i\kappa)^\dagger]$ for any $k = i\kappa$ that is a zero of $\det J(k)$ on the positive imaginary axis. Since $f(i\kappa, x)\xi$ corresponds to a bound state with $\xi \in \operatorname{Ker}[J(i\kappa)^\dagger]$, from (2.1) we conclude that there are as many linearly independent bound states at $k = i\kappa$ as the dimension of $\operatorname{Ker}[J(i\kappa)^\dagger]$. Since that is also equal to the dimension of $\operatorname{Ker}[J(i\kappa)]$, we can say that the multiplicity of the bound state at $k = i\kappa$ is given by the dimension of $\operatorname{Ker}[J(i\kappa)]$. Let us use m_κ to denote the multiplicity of the bound state at $k = i\kappa$. We thus have

$$m_\kappa = \dim \operatorname{Ker}[J(i\kappa)]. \tag{8.10}$$

Note that $1 \le m_\kappa \le n$ because the dimension of $\operatorname{Ker}[J(i\kappa)]$ cannot exceed n for the corresponding $n \times n$ matrix $J(k)$.

We summarize the above observations on bound states in the following theorem.

Theorem 8.1: *Consider the selfadjoint matrix Schrödinger operator with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Let $f(k, x)$, $\varphi(k, x)$, and $J(k)$ be the corresponding Jost solution, the regular solution, and the Jost matrix, appearing in (2.1), (2.5), and (3.1), respectively. Then:*

(a) *We have a bound state at $k = i\kappa$ for some positive κ if and only if $\operatorname{Ker}[J(i\kappa)]$ is nontrivial or equivalently if and only if $\det[J(i\kappa)] = 0$.*
(b) *The multiplicity m_κ of the bound state at $k = i\kappa$ is finite, and in fact it is equal to the dimension of $\operatorname{Ker}[J(i\kappa)]$.*
(c) *A bound-state column-vector solution to (1.1) at $k = i\kappa$ must be equal to $f(i\kappa, x)\,\beta$ for some nonzero column vector $\beta \in \operatorname{Ker}[J(i\kappa)^\dagger]$. Similarly, a bound-state column-vector solution to (1.1) at $k = i\kappa$ must be equal to $\varphi(i\kappa, x)\,\alpha$ for some nonzero column vector $\alpha \in \operatorname{Ker}[J(i\kappa)]$.*
(d) *If $k = i\kappa$ corresponds to a bound state, then there is a bijection $\alpha \mapsto \beta$ between $\operatorname{Ker}[J(i\kappa)]$ and $\operatorname{Ker}[J(i\kappa)^\dagger]$ in such a way that $\varphi(i\kappa, x)\,\alpha = f(i\kappa, x)\,\beta$.*

We will next analyze the behaviors of the Jost matrix $J(k)$ and of its inverse at a bound state $k = i\kappa$. One of our goals is to prove that the multiplicity m_κ of the bound state is equal to the multiplicity of the zero of $\det J(k)$ at $k = i\kappa$. We will use an overdot to indicate the derivative with respect to k.

Proposition 8.2: Consider the selfadjoint matrix Schrödinger operator with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Let $f(k, x)$ and $J(k)$ be the corresponding Jost solution and the Jost matrix, appearing in (2.1) and (3.2), respectively. Assume that there is a bound state at $k = i\kappa$ for some positive κ. Then, for each fixed $x \in \mathbf{R}^+$ we have

$$f(-k^*, x)^\dagger\Big|_{k=i\kappa} = f(i\kappa, x)^\dagger, \qquad \left.\frac{df(-k^*, x)^\dagger}{dk}\right|_{k=i\kappa} = -\dot f(i\kappa, x)^\dagger, \tag{8.11}$$

$$\left.\frac{df'(-k^*, x)^\dagger}{dk}\right|_{k=i\kappa} = -\dot f'(i\kappa, x)^\dagger, \qquad \left.\frac{df''(-k^*, x)^\dagger}{dk}\right|_{k=i\kappa} = -\dot f''(i\kappa, x)^\dagger, \tag{8.12}$$

$$\dot J(i\kappa) = \dot f'(i\kappa)^\dagger A - \dot f(i\kappa, 0)^\dagger B. \tag{8.13}$$

Proof: As stated in Sec. II, $f(k, x)$ is analytic in $k \in \mathbf{C}^+$ for each fixed $x \in \mathbf{R}^+$. Thus, we have the Taylor series expansion

$$f(k, x) = f(i\kappa, x) + (k - i\kappa)\, \dot f(i\kappa, x) + O((k - i\kappa)^2)), \qquad k \to i\kappa. \tag{8.14}$$

Replacing k by $-k^*$ in (8.14) and by taking the adjoint of both sides of the resulting expansion, we get

$$f(-k^*, x)^\dagger = f(i\kappa, x)^\dagger - (k - i\kappa)\,\dot{f}(i\kappa, x)^\dagger + O((k - i\kappa)^2)), \qquad k \to i\kappa. \tag{8.15}$$

The first and second terms in the expansion on the right-hand side in (8.15) yield the equalities in (8.11). The equalities in (8.12) are established in a similar manner by exploiting the analyticity of $f'(k, x)$ and $f''(k, x)$ in $k \in \mathbf{C}^+$ for each fixed $x \in \mathbf{R}^+$. By taking the k-derivative of both sides of (3.2) and using the second equality in (8.11) and the first equality in (8.12), we obtain (8.13). ■

Theorem 8.3: *Consider the selfadjoint matrix Schrödinger operator with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Let $f(k, x)$, $\varphi(k, x)$, and $J(k)$ be the corresponding Jost solution, the regular solution, and the Jost matrix, appearing in (2.1), (2.5), and (3.1), respectively. Assume that there is a bound state at $k = i\kappa$ for some positive κ. For any constant column vector $\alpha \in \mathrm{Ker}[J(i\kappa)]$, let β be the corresponding unique constant column vector indicated in Theorem 8.1(d). Then*

$$i\beta^\dagger \dot{J}(i\kappa)\alpha = 2\kappa \int_0^\infty dx\, [\varphi(i\kappa, x)\alpha]^\dagger [\varphi(i\kappa, x)\alpha], \tag{8.16}$$

and hence $\beta^\dagger \dot{J}(i\kappa)\alpha \neq 0$ unless $\alpha = 0$.

Proof: The Jost solution $f(k, x)$ satisfies (1.1) and hence

$$f''(k, x) + k^2 f(k, x) = V(x)\, f(k, x). \tag{8.17}$$

By taking the k-derivative, from (8.17) we get

$$\dot{f}''(k, x) + k^2 \dot{f}(k, x) + 2k f(k, x) = V(x)\, \dot{f}(k, x), \tag{8.18}$$

and by replacing k by $-k^*$ in (8.17) and then taking the adjoint we get

$$f''(-k^*, x)^\dagger + k^2 f(-k^*, x)^\dagger = f(-k^*, x)^\dagger V(x), \tag{8.19}$$

where we have used the selfadjointness of V given in (1.3). Evaluating (8.18) and (8.19) at $k = i\kappa$, with the help of (8.11), we get

$$\dot{f}''(i\kappa, x) - \kappa^2 \dot{f}(i\kappa, x) + 2i\kappa f(i\kappa, x) = V(x)\, \dot{f}(i\kappa, x), \tag{8.20}$$

$$f''(i\kappa, x)^\dagger - \kappa^2 f(i\kappa, x)^\dagger = f(i\kappa, x)^\dagger V(x). \tag{8.21}$$

Premultiplying (8.20) by $f(i\kappa, x)^\dagger$ and postmultiplying (8.21) by $\dot{f}(i\kappa, x)$ and taking the difference of the resulting equations, we obtain

$$\frac{d}{dx}\left[f(i\kappa, x)^\dagger \dot{f}'(i\kappa, x) - f'(i\kappa, x)^\dagger \dot{f}(i\kappa, x)\right] = -2i\kappa f(i\kappa, x)^\dagger f(i\kappa, x). \tag{8.22}$$

Premultiplying (8.22) by $\beta^\dagger$ and postmultiplying it by β, we integrate the resulting equation over $x \in \mathbf{R}^+$. We then get

$$-\beta^\dagger f(i\kappa, 0)^\dagger \dot{f}'(i\kappa, 0)\beta + \beta^\dagger f'(i\kappa, 0)^\dagger \dot{f}(i\kappa, 0)\beta = -2i\kappa \int_0^\infty dx\, [f(i\kappa, x)\beta]^\dagger [f(i\kappa, x)\beta], \tag{8.23}$$

where we have used Theorem 8.1(c) with the fact that $f(i\kappa, x)\beta$ is a bound-state column-vector solution and hence it is square integrable, and we have also used the fact that the quantity inside the brackets in (8.22) vanishes as $x \to +\infty$. The latter property is a consequence of the exponential decay to zero of $f(i\kappa, x)\beta$ and of $f'(i\kappa, x)\beta$ and can be established with the help of (2.1) at $k = i\kappa$. Multiplying (8.23) on both sides by i and using (8.6) we get

$$-i\left[\alpha^\dagger \varphi(i\kappa, 0)^\dagger \dot{f}'(i\kappa, 0)\beta - \alpha^\dagger \varphi'(i\kappa, 0)^\dagger \dot{f}(i\kappa, 0)\beta\right] = 2\kappa \int_0^\infty dx\, [\varphi(i\kappa, x)\alpha]^\dagger [\varphi(i\kappa, x)\alpha]. \tag{8.24}$$

Using (2.5) and by taking the adjoint of both sides in (8.24) we get

$$i\beta^\dagger \left[\dot{f}'(i\kappa,0)^\dagger A - \dot{f}(i\kappa,0)^\dagger B\right]\alpha = 2\kappa \int_0^\infty dx\, [\varphi(i\kappa,x)\alpha]^\dagger [\varphi(i\kappa,x)\alpha]. \tag{8.25}$$

Comparing the left-hand side of (8.25) with (8.13), we obtain (8.16). Finally, since $\kappa > 0$ we see that the right-hand side in (8.16) is positive if $\alpha \neq 0$ and is equal to zero if $\alpha = 0$. Thus, from the left-hand side of (8.16) we conclude that $\beta^\dagger \dot{J}(i\kappa)\alpha = 0$ only when $\alpha = 0$. ■

Theorem 8.4: *Consider the selfadjoint matrix Schrödinger operator with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Let $f(k,x)$, $\varphi(k,x)$, and $J(k)$ be the corresponding Jost solution, the regular solution, and the Jost matrix, appearing in (2.1), (2.5), and (3.1), respectively. Assume that there is a bound state at $k = i\kappa$ for some positive κ. Then, $J(k)^{-1}$ has a simple pole at $k = i\kappa$.*

Proof: By Theorem 8.1(a), the determinant of $J(k)$ vanishes at $k = i\kappa$, and hence Theorem 3.1(a) implies that $J(k)^{-1}$ is analytic in a deleted neighborhood of $k = i\kappa$ with a pole of some finite order p at $k = i\kappa$. If the pole at $k = i\kappa$ were not simple, then for $p \geq 2$, in some neighborhood of $k = i\kappa$ we would have the expansions

$$J(k) = J(i\kappa) + (k - i\kappa)\, \dot{J}(i\kappa) + O((k - i\kappa)^2), \tag{8.26}$$

$$J(k)^{-1} = \frac{N_{-p}}{(k-i\kappa)^p} + \frac{N_{-p+1}}{(k-i\kappa)^{p-1}} + \cdots + \frac{N_{-1}}{k-i\kappa} + N_0 + (k-i\kappa)\, N_1 + O((k-i\kappa)^2). \tag{8.27}$$

Using (8.26) and (8.27) in $J(k)J(k)^{-1} = I_n$, we would obtain

$$J(i\kappa)\, N_{-p} = 0, \quad J(i\kappa)\, N_{-p+1} + \dot{J}(i\kappa)\, N_{-p} = 0. \tag{8.28}$$

From the first equation in (8.28) we see that each column of N_{-p} would have to belong to Ker$[J(i\kappa)]$. For each nonzero column of N_{-p}, by denoting that nonzero column with α as in Theorem 8.3, from (8.28) we would get the column-vector equation

$$J(i\kappa)\zeta + \dot{J}(i\kappa)\alpha = 0, \tag{8.29}$$

where $\alpha \in$ Ker$[J(i\kappa)]$ and ζ is some column vector in $\mathbf{C}^n$. Let $\beta \in$ Ker$[J(i\kappa)^\dagger]$ be the unique column vector corresponding to α as stated in Theorem 8.3. Thus we would have $J(i\kappa)^\dagger \beta = 0$ or equivalently

$$\beta^\dagger J(i\kappa) = 0. \tag{8.30}$$

Let us premultiply (8.29) by $\beta^\dagger$ and use (8.30) in order to obtain

$$\beta^\dagger \dot{J}(i\kappa)\alpha = 0. \tag{8.31}$$

Using Theorem 8.3 in (8.31) we see that we must have $\alpha = 0$ and hence $N_{-p} = 0$ for $p \geq 2$. Thus, from (8.27) we conclude that $J(k)^{-1}$ must have a simple pole at $k = i\kappa$. ■

Having established that the expansion (8.27) contains only a simple pole as

$$J(k)^{-1} = \frac{N_{-1}}{k-i\kappa} + N_0 + (k-i\kappa)\, N_1 + O((k-i\kappa)^2), \qquad k \to i\kappa, \tag{8.32}$$

we would like investigate the term N_{-1} further. One of our goals is to relate the multiplicity of the bound state at $k = i\kappa$ to the multiplicity of the zero of $\det J(k)$ at $k = i\kappa$ and to show that those two multiplicities are equal to each other. Recall that the multiplicity m_κ of the bound state at $k = i\kappa$ is defined as the number of linearly independent column vectors that are square-integrable column-vector solutions to (1.1) at $k = i\kappa$ and that also satisfy the boundary condition (1.6)–(1.8). From (8.10) we see that m_κ is equal to the dimension of the kernel of $J(i\kappa)$. Our goal is to prove that m_κ is also equal to the multiplicity of the zero of $\det J(k)$ at $k = i\kappa$.

Theorem 8.5: *Consider the selfadjoint matrix Schrödinger operator with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Let $J(k)$ be the* *corresponding Jost matrix appearing in (3.1). Assume that there is a bound state at $k = i\kappa$ for some positive κ. Then, we have*

$$\det J(k) = c_3(k - i\kappa)^{m_\kappa}[1 + O(k - i\kappa)], \qquad k \to i\kappa, \tag{8.33}$$

where c_3 is a nonzero constant and m_κ is the positive integer appearing in (8.10) and denoting the multiplicity of the bound state at $k = i\kappa$. Consequently, the order of the zero of $\det J(k)$ *at $k = i\kappa$ is equal to m_κ.*

Proof: From (8.10) we know that the geometric multiplicity of the zero-eigenvalue of $J(i\kappa)$ is equal to m_κ. We will proceed as in Section 6 of Ref. 2, and hence we will omit some of the details by referring the reader to Ref. 2. Using a similarity transformation $J(i\kappa) \mapsto \mathcal{S}_1^{-1} J(i\kappa)\mathcal{S}_1$ with an appropriate invertible matrix $\mathcal{S}_1$, we will transform $J(i\kappa)$ to a Jordan canonical form. Let us assume that there are ν_κ Jordan chains and hence the Jordan canonical form of $J(i\kappa)$ contains ν_κ Jordan blocks. Let us use λ_s to denote the eigenvalue of $J(i\kappa)$ associated with the sth Jordan chain, where we realize that the eigenvalues may be repeated and hence there may be more than one Jordan block for a given eigenvalue λ_s. Let us use $J_{n_s}(\lambda_s)$ to denote the sth Jordan block, where we assume that the matrix size of that block is $n_s \times n_s$. Without loss of generality we can assume that the first m_κ Jordan chains all belong to the zero eigenvalue of $J(i\kappa)$. Let us use μ_κ to denote the algebraic multiplicity of the zero eigenvalue of $J(i\kappa)$. Thus, we assume that the number of nonzero eigenvalues (including multiplicities) of $J(i\kappa)$ is $n - \mu_\kappa$. As a result, the first m_κ Jordan blocks each have the form

$$J_{n_s}(\lambda_s) = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & 0 & \dots & 0 & 0 \end{bmatrix}, \qquad s = 1, \dots, m_\kappa, \tag{8.34}$$

and the remaining Jordan blocks associated with the nonzero eigenvalues of $J(i\kappa)$ have the form

$$J_{n_s}(\lambda_s) = \begin{bmatrix} \lambda_s & 1 & 0 & \dots & 0 & 0 \\ 0 & \lambda_s & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \lambda_s & 1 \\ 0 & 0 & 0 & \dots & 0 & \lambda_s \end{bmatrix}, \qquad s = m_\kappa + 1, \dots, \nu_\kappa,$$

with nonzero diagonal entries λ_s. The Jordan canonical form of $J(i\kappa)$ is then given by

$$\mathcal{S}_1^{-1} J(i\kappa)\,\mathcal{S}_1 = \oplus_{s=1}^{\nu_\kappa} J_{n_s}(\lambda_s).$$

Next, let us move all the entries with 1 appearing in the superdiagonal in the first m_κ Jordan blocks in (8.34) and collect those entries into the $(\mu_\kappa - m_\kappa) \times (\mu_\kappa - m_\kappa)$ identity matrix $I_{\mu_\kappa - m_\kappa}$. This can be achieved by using the matrices P_4 and P_5 given by

$$P_4 = \begin{bmatrix} \Pi_4 & 0 \\ 0 & I_{n-\mu_\kappa} \end{bmatrix}, \quad P_5 = \begin{bmatrix} \Pi_5 & 0 \\ 0 & I_{n-\mu_\kappa} \end{bmatrix},$$

for some permutation matrices Π_4 and Π_5 that affect only the first μ_κ columns and μ_κ rows, respectively, of the matrices on which they operate. The combined matrix transformation $J(i\kappa) \mapsto P_5\mathcal{S}_1^{-1} J(i\kappa)\mathcal{S}_1 P_4$ results in the upper-triangular matrix given by

$$P_5\mathcal{S}_1^{-1} J(i\kappa)\mathcal{S}_1 P_4 = \operatorname{diag}\{0_{m_\kappa}, I_{\mu_\kappa - m_\kappa}, J_{n_{\mu_\kappa+1}}(\lambda_{\mu_\kappa+1}), \dots, J_{n_{\nu_\kappa}}(\lambda_{\nu_\kappa})\}, \tag{8.35}$$

where we recall that 0_{m_κ} denotes the $m_\kappa \times m_\kappa$ zero matrix. Let us define the $(n - \mu_\kappa) \times (n - \mu_\kappa)$ matrix $\mathbf{d}_0$ as

$$\mathbf{d}_0 := \operatorname{diag}\{I_{\mu_\kappa - m_\kappa}, J_{n_{\mu_\kappa+1}}(\lambda_{\mu_\kappa+1}), \dots, J_{n_{\nu_\kappa}}(\lambda_{\nu_\kappa})\}. \tag{8.36}$$

The matrix $\mathbf{d}_0$ is invertible because it is an upper-triangular matrix with nonzero diagonal entries. Using (8.36) in (8.35) we obtain the block decomposition

$$P_5\mathcal{S}_1^{-1}J(i\kappa)\mathcal{S}_1P_4 = \text{diag}\{0_{m_\kappa}, \mathbf{d}_0\}. \tag{8.37}$$

Comparing (8.26) and (8.37) we see that

$$P_5\mathcal{S}_1^{-1}J(k)\mathcal{S}_1P_4 = \text{diag}\{0_{m_\kappa}, \mathbf{d}_0\} + (k - i\kappa)\begin{bmatrix} \mathbf{a}_1 & \mathbf{b}_1 \\ \mathbf{c}_1 & \mathbf{d}_1 \end{bmatrix} + O((k - i\kappa)^2), \qquad k \to i\kappa, \tag{8.38}$$

where we have let

$$\begin{bmatrix} \mathbf{a}_1 & \mathbf{b}_1 \\ \mathbf{c}_1 & \mathbf{d}_1 \end{bmatrix} := P_5\mathcal{S}_1^{-1}\dot{J}(i\kappa)\mathcal{S}_1P_4.$$

From Theorem 8.4 we know that $J(k)^{-1}$ has a simple pole at $k = i\kappa$ and hence with the help of (8.32) we get

$$\left(P_5\mathcal{S}_1^{-1}J(k)\mathcal{S}_1P_4\right)^{-1} = \frac{1}{k - i\kappa}\begin{bmatrix} \mathbf{n}_1 & \mathbf{n}_2 \\ \mathbf{n}_3 & \mathbf{n}_4 \end{bmatrix} + \begin{bmatrix} \mathbf{m}_1 & \mathbf{m}_2 \\ \mathbf{m}_3 & \mathbf{m}_4 \end{bmatrix} + O(k - i\kappa), \qquad k \to i\kappa, \tag{8.39}$$

where we have defined

$$\begin{bmatrix} \mathbf{n}_1 & \mathbf{n}_2 \\ \mathbf{n}_3 & \mathbf{n}_4 \end{bmatrix} := P_4^{-1}\mathcal{S}_1^{-1}N_{-1}\mathcal{S}_1P_5^{-1}, \qquad \begin{bmatrix} \mathbf{m}_1 & \mathbf{m}_2 \\ \mathbf{m}_3 & \mathbf{m}_4 \end{bmatrix} := P_4^{-1}\mathcal{S}_1^{-1}N_0\mathcal{S}_1P_5^{-1},$$

with N_{-1} and N_0 being the matrices appearing in (8.32), with some $m_\kappa \times m_\kappa$ block matrices $\mathbf{n}_1$ and $\mathbf{m}_1$, some $(n - m_\kappa) \times (n - m_\kappa)$ block matrices $\mathbf{n}_4$ and $\mathbf{m}_4$, and the remaining block matrices of appropriate sizes. Using (8.38) and (8.39) in the matrix identities

$$\begin{cases} \left(P_5\mathcal{S}_1^{-1}J(k)\mathcal{S}_1P_4\right)^{-1}\left(P_5\mathcal{S}_1^{-1}J(k)\mathcal{S}_1P_4\right) = I_n, \\ \left(P_5\mathcal{S}_1^{-1}J(k)\mathcal{S}_1P_4\right)\left(P_5\mathcal{S}_1^{-1}J(k)\mathcal{S}_1P_4\right)^{-1} = I_n, \end{cases}$$

we obtain

$$\begin{bmatrix} \mathbf{n}_1 & \mathbf{n}_2 \\ \mathbf{n}_3 & \mathbf{n}_4 \end{bmatrix}\text{diag}\{0_{m_\kappa}, \mathbf{d}_0\} = 0_n, \quad \text{diag}\{0_{m_\kappa}, \mathbf{d}_0\}\begin{bmatrix} \mathbf{n}_1 & \mathbf{n}_2 \\ \mathbf{n}_3 & \mathbf{n}_4 \end{bmatrix} = 0_n, \tag{8.40}$$

$$\begin{bmatrix} \mathbf{n}_1 & \mathbf{n}_2 \\ \mathbf{n}_3 & \mathbf{n}_4 \end{bmatrix}\begin{bmatrix} \mathbf{a}_1 & \mathbf{b}_1 \\ \mathbf{c}_1 & \mathbf{d}_1 \end{bmatrix} + \begin{bmatrix} \mathbf{m}_1 & \mathbf{m}_2 \\ \mathbf{m}_3 & \mathbf{m}_4 \end{bmatrix}\text{diag}\{0_{m_\kappa}, \mathbf{d}_0\} = I_n, \tag{8.41}$$

$$\begin{bmatrix} \mathbf{a}_1 & \mathbf{b}_1 \\ \mathbf{c}_1 & \mathbf{d}_1 \end{bmatrix}\begin{bmatrix} \mathbf{n}_1 & \mathbf{n}_2 \\ \mathbf{n}_3 & \mathbf{n}_4 \end{bmatrix} + \text{diag}\{0_{m_\kappa}, \mathbf{d}_0\}\begin{bmatrix} \mathbf{m}_1 & \mathbf{m}_2 \\ \mathbf{m}_3 & \mathbf{m}_4 \end{bmatrix} = I_n. \tag{8.42}$$

Because $\mathbf{d}_0$ is invertible, from (8.40) we see that

$$\mathbf{n}_2 = 0, \quad \mathbf{n}_3 = 0, \quad \mathbf{n}_4 = 0, \tag{8.43}$$

for some zero matrices of appropriate sizes. Using (8.43) in (8.41) and (8.42) we get

$$\mathbf{n}_1\mathbf{a}_1 = I_{m_\kappa}, \quad \mathbf{n}_1\mathbf{b}_1 + \mathbf{m}_2\mathbf{d}_0 = 0, \quad \mathbf{m}_4\mathbf{d}_0 = I_{n-m_\kappa}, \quad \mathbf{c}_1\mathbf{n}_1 + \mathbf{d}_0\mathbf{m}_3 = 0,$$

which establishes the invertibility of the block matrix $\mathbf{a}_1$ and also implies

$$\mathbf{n}_1 = \mathbf{a}_1^{-1}, \quad \mathbf{m}_2 = -\mathbf{a}_1^{-1}\mathbf{b}_1\mathbf{d}_0^{-1}, \quad \mathbf{m}_4 = \mathbf{d}_0^{-1}, \quad \mathbf{m}_3 = -\mathbf{d}_0^{-1}\mathbf{c}_1\mathbf{a}_1^{-1}. \tag{8.44}$$

Using (8.44) in (8.39) we obtain the expansion

$$\left(P_5\mathcal{S}_1^{-1}J(k)\mathcal{S}_1P_4\right)^{-1} = \begin{bmatrix} \dfrac{\mathbf{a}_1^{-1}[I_{m_\kappa} + O(k - i\kappa)]}{k - i\kappa} & -\mathbf{a}_1^{-1}\mathbf{b}_1\mathbf{d}_0^{-1} \\ -\mathbf{d}_0^{-1}\mathbf{c}_1\mathbf{a}_1^{-1} & \mathbf{d}_0^{-1} \end{bmatrix} + O(k - i\kappa), \qquad k \to i\kappa. \tag{8.45}$$

From (8.45) we see that

$$\det\left(\left(P_5\mathcal{S}_1^{-1}J(k)\mathcal{S}_1P_4\right)^{-1}\right)=\frac{\left(\det\mathbf{a}_1^{-1}\right)\left(\det\mathbf{d}_0^{-1}\right)}{(k-i\kappa)^{m_\kappa}}\,[1+O(k-i\kappa)]\,,\qquad k\to i\kappa,$$

or equivalently

$$\det J(k)=\frac{\det(\mathbf{a}_1\mathbf{d}_0)}{\det(P_4P_5)}(k-i\kappa)^{m_\kappa}\,[1+O(k-i\kappa)]\,,\qquad k\to i\kappa. \tag{8.46}$$

Thus, (8.46) establishes (8.33) with c_3 given by

$$c_3:=(\det P_4)(\det P_5)(\det\mathbf{a}_1)(\det\mathbf{d}_0),$$

which is nonzero due to the fact that P_4 and P_5 are some $n\times n$ permutation matrices and hence their determinants are either 1 or -1, and the matrices $\mathbf{a}_1$ and $\mathbf{d}_0$ are invertible and hence their determinants are nonzero. ■

We remark the similarity between Theorem 8.5 and Corollary 6.2 and the similarity between (8.33) and (6.5).

Let us note that the transformation specified in Proposition 4.1(a) on the boundary parameters A and B does not affect the boundary condition (1.6)–(1.8). This is because $(A,B)\mapsto(AT,BT)$ for an invertible matrix T results in a premultiplication of both sides of (1.6) by $T^\dagger$ as well as a premultiplication by $T^\dagger$ and a postmultiplication by T of both sides of (1.7) and (1.8). Thus, as seen from (3.2), the potential V and the boundary parameters A and B cannot uniquely determine the Jost matrix $J(k)$, but they determine $J(k)$ uniquely up to a postmultiplication by an invertible matrix T. However, such a nonuniqueness does not affect the zeros in $\mathbf{C}^+$ of the determinant of $J(k)$ because $\det J(k)$ and $\det[J(k)\,T]$ have the same set of zeros. Hence, the bound states are not affected by such a nonuniqueness, and the bound states are uniquely determined by the potential V and the boundary parameters A and B appearing in (1.6)–(1.8).

The following result is relevant in establishing the finiteness of the number of bound states.

Theorem 8.6: *Consider the Schrödinger operator corresponding to (1.1) with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Let J(k) be the corresponding Jost matrix defined in (3.1). Then, the zeros of* $\det J(k)$ *in* $\overline{\mathbf{C}^+}\setminus\{0\}$ *can only occur on the positive imaginary axis, and the number of such zeros, which we denote by N (without counting multiplicities), is finite.*

Proof: By Theorem 3.1(a) we know that $J(k)$ is analytic in $\mathbf{C}^+$ and continuous in $\overline{\mathbf{C}^+}$. Thus, $\det J(k)$ possesses the same properties. Because of the selfadjointness of the Schrödinger operator, the bound-state k-values, i.e., the zeros of $\det J(k)$ in $\overline{\mathbf{C}^+}\setminus\{0\}$, can occur either on the real axis or on the positive imaginary axis. By Proposition 3.1(c), $J(k)$ is invertible for $k\in\mathbf{R}\setminus\{0\}$ and hence those zeros can only occur on the positive imaginary axis. Let us use $\mathcal{H}$ to denote the set of zeros of $\det J(k)$ on the positive imaginary axis. Because of (7.17), $\mathcal{H}$ is a bounded set. Furthermore, (6.5) implies that $\det J(i\zeta)\neq 0$ for $0<\zeta<\kappa_0$ for some positive κ_0-value. Thus, it follows that $\mathcal{H}\subset[i\kappa_0,ib]$ for some positive b. We must prove that $\mathcal{H}$ is a finite set. If it were not a finite set, being bounded, $\mathcal{H}$ would have to have an accumulation point in $[i\kappa_0, ib]$. However, the analyticity of $\det J(k)$ in $\mathbf{C}^+$ would then require $\det J(k)\equiv 0$ in $\mathbf{C}^+$, contradicting (7.17). ■

Let us assume that the N distinct zeros of $\det J(k)$ on the positive imaginary axis occur at $k=i\kappa_j$ with $j=1,\ldots,N$. If there are no bound states, then we have $N=0$. If there any bound states, as stated in Theorem 8.6, the positive integer N is finite. Let us use m_{κ_j} to denote the multiplicity of the bound state at $k=i\kappa_j$. As in (8.10), we have

$$m_{\kappa_j}=\dim\operatorname{Ker}[J(i\kappa_j)],$$

and hence m_{κ_j} is a positive integer not exceeding n. From Theorems 8.1 and 8.6 we conclude that, the number of bound states including the multiplicities, $\mathcal{N}$, is a finite number and given by

$$\mathcal{N} := \sum_{j=1}^{N} m_{\kappa_j}. \tag{8.47}$$

From Theorem 8.5 it follows that the multiplicity of the zero of $\det J(k)$ at $k = i\kappa_j$ is the same as the multiplicity m_{κ_j} of the bound state at $k = i\kappa_j$. Thus, from (8.47) we have the following result.

Corollary 8.7: Consider the Schrödinger operator corresponding to (1.1) with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Let $J(k)$ be the corresponding Jost matrix given in (3.1), and let $\mathcal{N}$ be the corresponding number of bound states (including multiplicities), as indicated in (8.47). Then, $\mathcal{N}$ is also equal to the number of zeros (including multiplicities) of $\det J(k)$ *in* $\mathbf{C}^+$.

In Sec. IX we will relate $\mathcal{N}$ to the change in the argument of the determinant of the scattering matrix $S(k)$ along the positive real axis.

IX. LEVINSON's THEOREM

In this section we establish Levinson's theorem for the selfadjoint matrix Schrödinger operator with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). We do this by relating the argument of the determinant of the scattering matrix $S(k)$ defined in (3.8) to the number (including multiplicities) of bound states $\mathcal{N}$ given in (8.47). We achieve our goal by applying the argument principle to the determinant of the Jost function $J(k)$ given in (3.1).

Let us define $h(k)$ as

$$h(k) := \det J(k). \tag{9.1}$$

The region we will use in the argument principle is the region whose boundary is $\mathcal{C}_{\epsilon,R}$, which consists of four pieces as given by

$$\mathcal{C}_{\epsilon,R} := (-R, -\epsilon) \cup \mathcal{C}_\epsilon \cup (\epsilon, R) \cup \mathcal{C}_R. \tag{9.2}$$

The first piece $(-R, -\epsilon)$ is the directed line segment on the real axis for some small positive ϵ and for a large positive R, with the direction of the path from $-R + i0$ to $-\epsilon + i0$. The second piece $\mathcal{C}_\epsilon$ consists of the upper semicircle centered at the origin with radius ϵ and traversed from the point $-\epsilon + i0$ to the point $\epsilon + i0$. The third piece (ϵ, R) is the directed line segment of the positive real axis from $\epsilon + i0$ to $R + i0$. The fourth piece $\mathcal{C}_R$ is the upper semicircle centered at the origin with radius R and traversed from the point $R + i0$ to the point $-R + i0$. The analyticity of $h(k)$ in our region and its continuity in the closure of our region follows from Theorem 3.1(a). By choosing R large enough and by choosing ϵ small enough, from Theorem 8.6 we know that the only zeros of $h(k)$ in our region can occur on the positive imaginary axis at N distinct points $k = i\kappa_j$ for some nonnegative integer N and that $h(k)$ does not vanish on the boundary of our region.

Let us use $\arg[h(k)]\big|_{\mathcal{C}}$ for the change in the argument of $h(k)$ along a path $\mathcal{C}$, and let us recall that an overdot indicates the k-derivative.

Proposition 9.1: Consider the Schrödinger operator corresponding to (1.1) with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Let $J(k)$ and $S(k)$ be the corresponding Jost and scattering matrices defined in (3.1) and (3.8), respectively. Then, the change in the argument of $\det S(k)$ *along the directed path* (ϵ, R) *and the change in the argument of* $\det J(k)$ *along the directed paths* $(-R, -\epsilon)$ *and* (ϵ, R) *are related to each other as*

$$\arg[\det S(k)]\big|_{(\epsilon,R)} = -\arg[\det J(k)]\big|_{(\epsilon,R)} - \arg[\det J(k)]\big|_{(-R,-\epsilon)}. \tag{9.3}$$

Proof: From (3.8) we have

$$\det S(k) = (-1)^n \frac{\det J(-k)}{\det J(k)}, \qquad k \in \mathbf{R} \setminus \{0\}. \tag{9.4}$$

From (3.11) we get $|\det S(k)| = 1$ and hence

$$\det S(k) = e^{i \arg[\det S(k)]}, \qquad k \in (\epsilon, R), \tag{9.5}$$

$$|\det J(-k)| = |\det J(k)|, \qquad k \in \mathbf{R} \setminus \{0\}, \tag{9.6}$$

where we have also used (9.4) to obtain (9.6). By Theorem 3.1(c) we have $|\det J(k)| \neq 0$ for $k \in \mathbf{R}\setminus\{0\}$, and hence with the help of (9.6) we get

$$\det J(k) = |\det J(k)|\, e^{i \arg[\det J(k)]}, \qquad k \in (\epsilon, R), \tag{9.7}$$

$$\det J(-k) = |\det J(k)|\, e^{i \arg[\det J(-k)]}, \qquad k \in (\epsilon, R). \tag{9.8}$$

Using (9.5), (9.7), and (9.8) in (9.4) we get

$$e^{i \arg[\det S(k)]} = (-1)^n e^{i \arg[\det J(-k)]} e^{-i \arg[\det J(k)]}, \qquad k \in (\epsilon, R),$$

from which we obtain (9.3). ■

In the following proposition, we provide the change in the argument of $h(k)$ along the pieces of paths appearing in (9.2).

Proposition 9.2: Consider the Schrödinger operator corresponding to (1.1) with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). Then, the function $h(k)$ defined in (9.1) satisfies

$$\lim_{\epsilon\to 0^+} \lim_{R\to+\infty} \int_{\mathcal{C}_{\epsilon,R}} dk\, \frac{\dot h(k)}{h(k)} = 2\pi i \mathcal{N}, \tag{9.9}$$

$$\lim_{R\to+\infty} \int_{\mathcal{C}_R} dk\, \frac{\dot h(k)}{h(k)} = \pi i (n_{\mathrm{M}} + n_{\mathrm{N}}), \tag{9.10}$$

$$\lim_{\epsilon\to 0^+} \int_{\mathcal{C}_\epsilon} dk\, \frac{\dot h(k)}{h(k)} = -\pi i \mu, \tag{9.11}$$

$$\int_{(-R,-\epsilon)\cup(\epsilon,R)} dk\, \frac{\dot h(k)}{h(k)} = i \left(\arg[h(k)]\Big|_{(\epsilon,R)} + \arg[h(k)]\Big|_{(-R,-\epsilon)} \right), \tag{9.12}$$

where $\mathcal{N}$ is the nonnegative integer appearing in (8.47), the paths $\mathcal{C}_{\epsilon,R}$, $\mathcal{C}_\epsilon$, and $\mathcal{C}_R$ are those in (9.2), n_{M} and n_{N} are the nonnegative integers defined after (4.2), and μ is the (algebraic and geometric) multiplicity of the eigenvalue $+1$ of the zero-energy scattering matrix $S(0)$, with $S(k)$ being the scattering matrix defined in (3.8).

Proof: Because of Corollary 8.7, the number of bound states $\mathcal{N}$ (including multiplicities) is equal to the number of zeros of $\det J(k)$ (including multiplicities) in $\mathbf{C}^+$. We get (9.9) by applying the argument principle to $h(k)$ along the closed path $\mathcal{C}_{\epsilon,R}$ and by using the fact that $\mathcal{N}$ is the number of zeros (including multiplicities) of $h(k)$ inside $\mathcal{C}_{\epsilon,R}$. We note that (9.10) directly follows from (7.17), and (9.11) directly follows from (6.5). Finally, (9.12) is obtained with the help of (9.6). ■

We next state Levinson's theorem.

Theorem 9.3: *Consider the Schrödinger operator corresponding to (1.1) with the selfadjoint boundary condition (1.6)–(1.8) and with the potential V satisfying (1.3) and (1.5). The number*

$\mathcal{N}$ of bound states (including multiplicities) appearing in (8.47) is related to the argument of the determinant of the scattering matrix $S(k)$ defined in (3.8) as

$$\arg[\det S(0^+)] - \arg[\det S(+\infty)] = \pi\,(2\mathcal{N} + \mu - n_{\mathrm{M}} - n_{\mathrm{N}})\,, \tag{9.13}$$

where μ is the (algebraic and geometric) multiplicity of the eigenvalue $+1$ of the zero-energy scattering matrix $S(0)$ and n_{M} and n_{N} are the nonnegative integers defined after (4.2).

Proof: By Proposition 3.3, the determinant of $S(k)$ is continuous on $\mathbf{R}$ and hence the left-hand side in (9.3) is given by

$$\lim_{\epsilon\to 0^+}\lim_{R\to+\infty}\left(\arg[\det S(k)]\Big|_{(\epsilon,R)}\right) = -\arg[\det S(0^+)] + \arg[\det S(+\infty)], \tag{9.14}$$

By combining the results in (9.10)–(9.12) and by using the relationships among (9.3), (9.12), and (9.14), we evaluate the sum of the integrals in (9.10)–(9.12) in the limit as $\epsilon \to 0^+$ and $R \to +\infty$. That sum then must be equal to the value of the integral given in (9.9), resulting in (9.13). ■

Let us comment on (9.13) and how it is related to Levinson's theorem appearing in the literature elsewhere. In our analysis of the selfadjoint Schrödinger operator with the general selfadjoint boundary condition (1.6)–(1.8), the unperturbed Hamiltonian is chosen to satisfy the Neumann boundary condition. Such a choice is compatible with the time-dependent derivation of the scattering matrix and is motivated[16] by applications in quantum wires. One consequence of that choice is apparent in the large-k limits of $S(k)$. As seen from (5.7), (5.10), and (7.20), we have $S(k) = S(\infty) + O(1/k)$ as $k \to \pm\infty$, with

$$S(\infty) = M\,\mathrm{diag}\{I_{n_{\mathrm{M}}}, -I_{n_{\mathrm{D}}}, I_{n_{\mathrm{N}}}\}\,M^{\dagger}, \tag{9.15}$$

where M is the unitary matrix appearing in (4.11). As a result of (9.15), the argument of the determinant of $S(k)$ as $k \to +\infty$ is given by

$$\lim_{k\to+\infty}\arg[\det S(k)] = \arg[\det S(\infty)] = (-1)^{n_{\mathrm{D}}}\pi + 2\pi j, \qquad j = 0, \pm 1, \pm 2, \ldots.$$

One can choose a branch with $\arg[\det S(\infty)] = 0$ if n_{D} is even and a branch with $\arg[\det S(\infty)] = \pi$ if n_{D} is odd. So, in the purely Dirichlet case, i.e., when $n_{\mathrm{M}} = n_{\mathrm{N}} = 0$ and $n_{\mathrm{D}} = n$, from (9.15) we get $S(k) = -I_n + O(1/k)$ as $k \to \pm\infty$. On the other hand, in the literature[1,24,25] dealing solely with the Dirichlet case, it is customary to choose the unperturbed Hamiltonian to satisfy the Dirichlet boundary condition, yielding $S(k) = I_n + O(1/k)$ as $k \to \pm\infty$. Hence, in the literature dealing solely with the Dirichlet case, it is also customary to use the particular branch of the argument function for $\det S(k)$ in such a way that that argument takes the zero value at $k = +\infty$. In fact, in such a case, it is customary to let

$$\det S(k) = e^{2i\delta_S(k)}, \qquad k \in (0, +\infty),$$

with $\delta_S(+\infty) = 0$. Then, Levinson's theorem in such a case is given by

$$\delta_S(0^+) = \pi\left(\mathcal{N} + \frac{\mu}{2}\right). \tag{9.16}$$

In particular, in the scalar case, we have (9.16) with $\mu = 1$ in the exceptional case and $\mu = 0$ in the generic case.[24]

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[1] Z. S. Agranovich and V. A. Marchenko, *The Inverse Problem of Scattering Theory* (Gordon and Breach, New York, 1963).
[2] T. Aktosun, M. Klaus, and R. Weder, "Small-energy analysis for the self-adjoint matrix Schrödinger equation on the half line," J. Math. Phys. **52**, 102101 (2011).
[3] T. Aktosun and R. Weder, "Inverse spectral-scattering problem with two sets of discrete spectra for the radial Schrödinger equation," Inverse Probl. **22**, 89–114 (2006).
[4] J. Behrndt and A. Luger, "On the number of negative eigenvalues of the Laplacian on a metric graph," J. Phys. A **43**, 474006 (2010).
[5] J. Behrndt, M. M. Malamud, and H. Neidhardt, "Scattering matrices and Weyl functions," Proc. London Math. Soc. **97**, 568–598 (2008).
[6] *Quantum Graphs and Their Applications*, Contemporary Mathematics Vol. 415, edited by G. Berkolaiko, R. Carlson, S. A. Fulling, and P. Kuchment (American Mathematical Society, Providence, RI, 2006).
[7] J. Boman and P. Kurasov, "Symmetries of quantum graphs and the inverse scattering problem," Adv. Appl. Math. **35**, 58–70 (2005).
[8] *Analysis on Graphs and its Applications*, Proceedings of Symposia in Pure Mathematics Vol. 77, edited by P. Exner, J. P. Keating, P. Kuchment, T. Sunada, and A. Teplyaev (American Mathematical Society, Providence, RI, 2008).
[9] N. I. Gerasimenko, "The inverse scattering problem on a noncompact graph," Theor. Math. Phys. **75**, 460–470 (1988).
[10] N. I. Gerasimenko and B. S. Pavlov, "A scattering problem on noncompact graphs," Theor. Math. Phys. **74**, 230–240 (1988).
[11] B. Gutkin and U. Smilansky, "Can one hear the shape of a graph?," J. Phys. A **34**, 6061–6068 (2001).
[12] M. S. Harmer, "Inverse scattering for the matrix Schrödinger operator and Schrödinger operator on graphs with general self-adjoint boundary conditions," ANZIAM J. **44**, 161–168 (2002).
[13] M. S. Harmer, "The matrix Schrödinger operator and Schrödinger operator on graphs," Ph.D. dissertation (University of Auckland, New Zealand, 2004).
[14] M. Harmer, "Inverse scattering on matrices with boundary conditions," J. Phys. A **38**, 4875–4885 (2005).
[15] V. Kostrykin and R. Schrader, "Kirchhoff's rule for quantum wires," J. Phys. A **32**, 595–630 (1999).
[16] V. Kostrykin and R. Schrader, "Kirchhoff's rule for quantum wires. II: The inverse problem with possible applications to quantum computers," Fortschr. Phys. **48**, 703–716 (2000).
[17] P. Kuchment, "Quantum graphs. I. Some basic structures," Waves Random Media **14**, S107–S128 (2004).
[18] P. Kuchment, "Quantum graphs. II. Some spectral properties of quantum and combinatorial graphs," J. Phys. A **38**, 4887–4900 (2005).
[19] P. Kurasov and M. Nowaczyk, "Inverse spectral problem for quantum graphs," J. Phys. A **38**, 4901–4915 (2005).
[20] P. Kurasov and M. Nowaczyk, "Geometric properties of quantum graphs and vertex scattering matrices," Opusc. Math. **30**, 295–309 (2010).
[21] P. Kurasov and F. Stenberg, "On the inverse scattering problem on branching graphs," J. Phys. A **35**, 101–121 (2002).
[22] B. M. Levitan, *Inverse Sturm-Liouville Problems* (VNU Science Press, Utrecht, 1987).
[23] V. A. Marchenko, *Sturm-Liouville Operators and Applications* (Birkhäuser, Basel, 1986).
[24] R. G. Newton, *Scattering Theory of Waves and Particles*, 2nd ed. (Springer, New York, 1982).
[25] R. G. Newton and R. Jost, "The construction of potentials from the *S*-matrix for systems of differential equations," Nuovo Cimento **1**, 590–622 (1955).