Spectral analysis of non-selfadjoint matrix Schrödinger equation on the half-line with general boundary condition at the origin

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Abstract

We examine the spectral properties of the non-selfadjoint matrix Schrödinger equation on the half-line

$$-y'' + Q(x)y = k^2 y, \quad x \in \mathbb{R}_+,$$

where $n \times n$ matrix potential is symmetric but not Hermitian for each $x \in \mathbb{R}_+$, each entry of the matrix Q is a complex-valued, Lebesgue measurable function on $\mathbb{R}_+$ with a finite first moment. We impose the most general boundary condition at the origin

$$Ay(0) + By'(0) = 0,$$

such that the constant $n \times n$ matrices A and B satisfy

$$AB^T - BA^T = 0, \quad Rank[A|B] = n.$$

We obtain the resolvent operator, the point spectrum, continuous spectrum and the set of spectral singularities of the resulting non-selfadjoint matrix Schrdinger operator.

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1 Introduction

Physical observables in quantum mechanics are represented by selfadjoint operators on a Hilbert space. Therefore, one-dimensional Schrödinger equation

$$-y'' + q(x)y = k^2 y, \quad x \in \mathbb{R}_+ := (0, \infty), \tag{1.1}$$

has been studied in detail when the potential q is a real-valued function and the most general selfadjoint boundary condition at $x = 0$ is given

$$(cos\gamma)y(0) + (sin\gamma)y'(0) = 0, \tag{1.2}$$

where $\gamma \in (0, \pi]$ (see [22]). Equation (1.1) and the boundary condition (1.2) generate the selfadjoint Schrödinger operator on the half-line. On the other hand, in some physical systems that proceed without conservation of energy, non-selfadjoint Hamiltonians are present. For example; in problems with friction, in the theory of open resonators, in problems of inelastic scattering, and many others one has to deal with non-selfadjoint Hamiltonians. Certain self-adjoint problems, in which by

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separation of variables an operator-valued function appears that depends non-linearly on a spectral parameter, also lead to a study of non-selfadjoint operators.

The non-selfadjoint one-dimensional Schrödinger operator is generated by Equation (1.1) with a complex-valued potential q and with the most general boundary condition at $x = 0$

$$y'(0) - hy(0) = 0,$$

where $h \in \mathbb{C}$. This non-selfadjoint operator may have complex eigenvalues and has spectral singularities which are special points in the spectrum [27]. Explicitly, spectral singularities are the points in the continuous spectrum which are the poles of the resolvent's kernel and are not eigenvalues. Recently, spectral singularities are identified for some concrete complex scattering potentials and some physical interpretations are suggested [23].

Matrix Schrödinger equation on the half-line is given

$$-y'' + Q(x)y = k^2 y, \quad x \in \mathbb{R}_+, \tag{1.3}$$

where the potential Q is an $n \times n$ matrix-valued function and k^2 is a spectral parameter. Equation (1.3) has many applications in quantum mechanics. For example, it can describe the scattering in quantum mechanics involving particles of internal structures such as spins, scattering on quantum graphs [7, 8, 9, 11, 17, 18, 19, 20, 21] and in quantum wires [14, 15]. More explicitly, the matrix Schrödinger equation on the half-line corresponds to the system which consists of n very thin quantum wires with open ends connected at a central vertex and thus it is equivalent in terms of spectral analysis to a quantum star graph with n leads (edges of infinite length). This physical model can be useful to design elementary gates in quantum computing and nanotubes for microscopic electronic devices in which strings of atoms may form a star graph. In this model, the behavior at each wire is described by Schrödinger operator on the edges and the boundary conditions at the central vertex which are called vertex conditions impose certain restrictions. For problems related to quantum graphs, consideration of general boundary condition at origin rather than the Dirichlet boundary condition is more useful and relevant. Recently, the research on quantum graphs has grown extensively since quantum graphs are used to model systems in mathematics, physics, chemistry and engineering. Moreover, quantum graphs are also used for modeling quantum chaos [16].

Equation (1.3) with a selfadjoint $n \times n$ matrix potential Q in $L_1^1(\mathbb{R}_+)$ together with the most general selfadjoint boundary condition at $x = 0$ is investigated [2, 3, 4, 5, 29]. A matrix-valued function Q lies in the class $L_1^1(\mathbb{R}_+)$ if each entry of the matrix Q is Lebesgue measurable on $\mathbb{R}_+$ and

$$\int_0^\infty (1 + x)\|Q(x)\|dx < \infty,$$

holds where "$\|,\|$" denotes any of the equivalent matrix norms. The most general selfadjoint boundary condition at $x = 0$ has been formulated in several equivalent forms [2, 5, 12, 14, 15]. One of these formulations may be given

$$A_1 y(0) + B_1 y'(0) = 0, \tag{1.4}$$

such that the constant $n \times n$ matrices A_1 and B_1 satisfy

$$A_1 B_1^* = B_1 A_1^*, \tag{1.5}$$

$$Rank[A_1|B_1] = n, \tag{1.6}$$

where "$*$" denotes the adjoint of a matrix [2]. The dependence of the Jost solution, Jost matrix, regular solution and the scattering matrix to the parameters A_1 and B_1 used in the conditions (1.4)-(1.6) is examined [4]. The small-energy [2] and high-energy [4] asymptotics of scattering solutions, the Jost matrix, the inverse of the Jost matrix and the scattering matrix are derived for (1.3) with a selfadjoint potential $Q \in L_1^1(\mathbb{R}_+)$. Further, the continuity of the scattering matrix $S(k)$ at $k = 0$ is proven [2] and the Levinson's theorem is derived [4]. Spectral properties of the non-selfadjoint matrix Schrödinger operator on the half-line have been also investigated [13, 25]. Equation (1.3) with $Q \neq Q^*$ and the Dirichlet boundary condition at the origin is examined [25]. Eigenvalues and spectral singularities are identified with the zeros of the determinant of the Jost matrix [25].

If the matrix potential Q in Equation (1.3) is not necessarily a finite dimensional operator we obtain Schrödinger's operator equation on the half-line, namely, Equation (1.3) with $Q(x)$ is an operator in a separable Hilbert space H $(dimH \leq \infty)$ for each $x \in \mathbb{R}_+$. Spectral properties of Schrödinger's operator equation where $Q(x)$ is a selfadjoint, completely continuous operator in a separable Hilbert space H $(dimH \leq \infty)$ for each $x \in \mathbb{R}_+$ have been studied [10]. Recently, spectral properties of Schrödinger's operator equation with non-selfadjoint, completely continuous operator coefficient $Q(x)$ on the half-line with Dirichlet boundary condition at origin [6] and on the real line [24] have been investigated. These studies extended the results in finite dimensional case [13, 25] to the infinite dimension by considering Q in Equation (1.3) as an operator in an infinite dimensional Hilbert space. This transition to infinite dimensional case requires a new approach since in this case eigenvalues and spectral singularities correspond to the singular points of an operator-valued function (see [6, 24]).

In this paper, we consider Equation (1.3) where $n \times n$ matrix potential Q is in $L_1^1(\mathbb{R}_+)$ and Q is symmetric but not Hermitian i.e. $Q^*(x) \neq Q(x)$ but $Q^T(x) = Q(x)$ for each $x \in \mathbb{R}_+$ together with the most general boundary condition at $x = 0$

$$Ay(0) + By'(0) = 0, \tag{1.7}$$

such that the constant $n \times n$ matrices A and B satisfy

$$AB^T - BA^T = 0, \tag{1.8}$$

$$Rank[A|B] = n, \tag{1.9}$$

where "A^T" denotes the transpose of A. Note that the condition (1.9) is required to ensure that there are correct number of independent boundary conditions and the condition (1.8) is required for the construction of the resolvent operator. Note also that the wavefunction $y(k, x)$ in (1.3) can be regarded both as a vector-valued function in $\mathbb{C}^n$ or as an $n \times n$ matrix-valued function. Let us denote this non-selfadjoint matrix Schrödinger operator with the most general boundary condition at the origin by L hereafter. This paper is aimed at extending the studies [2, 3, 4, 5, 28, 29] on the selfadjoint matrix Schrödinger equation on the half-line with general boundary condition at the origin to the non-selfadjoint case by considering the non-Hermitian but symmetric potential Q. Furthermore, by considering the most general boundary condition at the origin, this study complements the study [25] in which the non-selfadjoint matrix Schrödinger equation on the half-line is considered with the Dirichlet boundary condition at $x = 0$. Note that the consideration of the general boundary condition (1.7) completely changes the structure of the Jost matrix and hence the problem itself.

This paper is organized as follows. In Section 2 we present some preliminary results related to the spectral properties of L. In Section 3 we introduce the Jost matrix and derive the resolvent of L. Then, we obtain the continuous spectrum, the point spectrum and the set of spectral singularities of L. Finally, in Section 4 we present some concluding remarks.

2 Preliminaries

In this section, we outline some results regarding certain $n \times n$ matrix solutions of (1.3) required for our study. We give the results without proofs and refer the interested reader to [1]. Let us denote the upper-half complex plane by $\mathbb{C}_+$, its closure by $\overline{\mathbb{C}_+} = \mathbb{C}_+ \cup \mathbb{R}$ and $n \times n$ unit matrix by I_n. Let $L_2(\mathbb{R}_+, \mathbb{C}^n)$ denote the Hilbert space of complex-valued vector functions

$$f(x) = (f_1(x), f_2(x), \dots, f_n(x)) \quad (0 < x < \infty),$$

such that each component of f lies in $L_2(0, \infty)$.

The domain of L consists of vector functions f from $L_2(\mathbb{R}_+, \mathbb{C}^n)$ such that

- f has an absolutely continuous derivative f' on every interval $[0, a]$, $0 < a < \infty$,
- $Lf := -f'' + Qf \in L_2(\mathbb{R}_+, \mathbb{C}^n)$,
- f satisfies the boundary condition (1.7).

The Jost solution $f(x, k)$ is the $n \times n$ matrix solution of Equation (1.3) which satisfies the asymptotic relations [1]

$$f(x, k) = e^{ikx}[I_n + o(1)], \quad f_x(x, k) = ike^{ikx}[I_n + o(1)], \quad x \to \infty,$$

for $k \in \overline{\mathbb{C}_+} \setminus \{0\}$. The Jost solution can be represented

$$f(x, k) = e^{ikx} I_n + \int_x^\infty e^{ikt} K(x, t) dx, \quad k \in \overline{\mathbb{C}_+} \setminus \{0\},$$

where

$$\|K(x, t)\| \leq c \int_{\frac{x+t}{2}}^\infty \|Q(s)\| ds,$$

for some positive constant c [1].

Equation (1.3) has an $n \times n$ matrix solution $g(x, k)$ satisfying the asymptotic relations [1]

$$g(x, k) = e^{-ikx}[I_n + o(1)], \quad g_x(x, k) = -ike^{-ikx}[I_n + o(1)], \quad x \to \infty,$$

for $k \in \overline{\mathbb{C}_+} \setminus \{0\}$.

It is well known that $f(x, k)$, $f_x(x, k)$, $g(x, k)$, $g_x(x, k)$ are analytic in $k \in \mathbb{C}_+$ and continuous in $k \in \overline{\mathbb{C}_+}$ for each fixed x [1]. It is also known that every vector solution $u(x, k)$ to (1.3) for $k \in \overline{\mathbb{C}_+} \setminus \{0\}$ can be expressed

$$u(x, k) = f(x, k)\alpha + g(x, k)\beta,$$

for some constant vectors $\alpha, \beta \in \mathbb{C}^n$ [4].

It is well known that we can find various $n\times n$ matrix solutions to (1.3) determined by specifying some constant initial conditions at a finite x. These solutions are entire functions in k for each fixed x [4]. In particular, it can be shown that Equation (1.3) has an $n\times n$ matrix solution $\varphi(x,k)$ called the regular solution satisfying the initial conditions

$$\varphi(0,k)=B^T,\quad \varphi'(0,k)=-A^T. \tag{2.1}$$

3 Spectral properties of L

In this section we introduce the Jost matrix related to (1.3) with symmetric but not Hermitian matrix potential $Q\in L_1^1(\mathbb{R}_+)$ together with the boundary condition (1.7). Then, we construct the resolvent operator of L and then introduce the continuous spectrum, point spectrum and the set of spectral singularities.

Let us denote the Wronskian

$$[F,G]:=FG'-F'G$$

of two $n\times n$ matrix solutions $F(x,k)$ and $G(x,k)$ of (1.3). Let $u(x,k)$ and $v(x,k)$ be two $n\times n$ matrix solutions of (1.3). It follows $v(x,k)^T$ is a solution of

$$-z''+zQ(x)=k^2z,\quad x\in\mathbb{R}_+. \tag{3.1}$$

It easily follows by a direct computation that the Wronskian $\left[v(x,k)^T,u(x,k)\right]$ is independent of x for each k. As a result, we can obtain various equalities by evaluating the Wronskian at different values of x. For example evaluating the Wronskian at $x=0$ and $x\to\infty$ yields

$$\left[f(x,\pm k)^T,f(x,\pm k)\right]=\pm 2ikI_n,\quad k\in\mathbb{R}, \tag{3.2}$$

$$\left[f(x,k)^T,f(x,k)\right]=0,\quad k\in\overline{\mathbb{C}_+}. \tag{3.3}$$

The Jost matrix $J(k)$ of L is defined for $k\in\overline{\mathbb{C}_+}$ as

$$J(k):=\left[f(x,k)^T,\varphi(x,k)\right], \tag{3.4}$$

where $f(x,k)$ is the Jost solution and $\varphi(x,k)$ is the regular solution defined by (2.1). Since the Wronskian (3.4) is independent of x, evaluating at $x=0$ and (2.1) yields

$$J(k)=-f(0,k)^TA^T-f'(0,k)^TB^T. \tag{3.5}$$

Note that since $f(0,k)$ and $f'(0,k)$ are analytic in $k\in\overline{\mathbb{C}_+}$ and continuous in $k\in\overline{\mathbb{C}_+}$, $J(k)$ is also analytic in $k\in\overline{\mathbb{C}_+}$ and continuous in $k\in\overline{\mathbb{C}_+}$.

Theorem 3.1. The resolvent set $\rho(L)$ of L is

$$\rho(L)=\left\{k^2:k\in\mathbb{C}_+,\ \det J(k)\neq 0\right\},$$

and the resolvent operator $R_k(L):=(L-k^2I)^{-1}$ is defined by

$$R_k(L)g(x)=\int_0^\infty R(x,t;k)g(t)dt,$$

where $g\in L_2(\mathbb{R}_+,\mathbb{C}^n)$ and

$$R(x,t;k)=\begin{cases}f(x,k)(J(k)^T)^{-1}\varphi(t,k)^T, & 0\le t\le x,\\ \varphi(x,k)J(k)^{-1}f(t,k)^T, & x<t<\infty.\end{cases}$$

Proof. We must find the general solution of the equation

$$-y'' + Q(x)y - k^2 y = g(x), \quad x \in (0, \infty), \tag{3.6}$$

where $y, g \in L_2(\mathbb{R}_+, \mathbb{C}^n)$ and the vector function $y(x,k)$ satisfies the boundary condition (1.7). Recall that a vector solution of the homogeneous part of (3.6) can be written

$$y(x,k) = f(x,k)\alpha + \varphi(x,k)\beta,$$

for some constant vectors $\alpha, \beta \in \mathbb{C}^n$ and $k \in \mathbb{C}_+$ (see Section 2). Suppose that $\det J(k) \neq 0$. We use the variation of parameters method and try to find the general solution of (3.6) in the form

$$y(x,k) = f(x,k)a(x) + \varphi(x,k)b(x), \tag{3.7}$$

where $a(x)$ and $b(x)$ are vector functions in $\mathbb{C}^n$. Suppose that

$$f(x,k)a'(x) + \varphi(x,k)b'(x) = 0. \tag{3.8}$$

Differentiating (3.7) with respect to x and plugging in (3.6) we have

$$f'(x,k)a'(x) + \varphi'(x,k)b'(x) = -g(x). \tag{3.9}$$

Multiplying (3.8) with $\varphi'(x,k)^T$ and (3.9) with $\varphi(x,k)^T$ from left and subtracting two equalities we obtain

$$\left[\varphi(x,k)^T, f(x,k)\right] a'(x) + \left[\varphi(x,k)^T, \varphi(x,k)\right] b'(x) = -\varphi(x,k)^T g(x). \tag{3.10}$$

Since the Wronskian $\left[\varphi(x,k)^T, \varphi(x,k)\right]$ is independent of x evaluating at $x = 0$ and using (1.8) we have

$$\left[\varphi(x,k)^T, \varphi(x,k)\right] = 0.$$

Furthermore, the Wronskian $\left[\varphi(x,k)^T, f(x,k)\right]$ is independent of x and evaluating at $x = 0$ and using (3.4) we get

$$\left[\varphi(x,k)^T, f(x,k)\right] = -(J(k))^T.$$

Since $J(k)$ is invertible, $J(k)^T$ is also invertible and from (3.10) we have

$$a(x) = \int_0^x (J(k)^T)^{-1} \varphi(t,k)^T g(t)dt + \alpha, \tag{3.11}$$

for some constant vector α.

Multiplying (3.8) with $f'(x,k)^T$ and (3.9) with $f(x,k)^T$ from left and subtracting two equalities we obtain

$$\left[f(x,k)^T, f(x,k)\right] a'(x) + \left[f(x,k)^T, \varphi(x,k)\right] b'(x) = -f(x,k)^T g(x).$$

From (3.3) and (3.4) it follows

$$b(x) = \beta + \int_x^\infty J(k)^{-1} f(t,k)^T g(t)dt, \tag{3.12}$$

for some constant vector β.

Plugging (3.11) and (3.12) in (3.7) we obtain

$$\begin{aligned} y(x,k) =& f(x,k)\alpha + \int_0^x f(x,k)(J(k)^T)^{-1}\varphi(t,k)^T g(t)dt \\ &+ \varphi(x,k)\beta + \int_x^\infty \varphi(x,k)J(k)^{-1}f(t,k)^T g(t)dt. \end{aligned}$$

Since the vector function $y(x,k)$ should lie in $L_2(\mathbb{R}_+,\mathbb{C}^n)$ it follows $\beta = 0$. We have

$$y'(x,k) = f'(x,k)a(x) + \varphi'(x,k)b(x). \tag{3.13}$$

Evaluating (3.13) at $x = 0$ and imposing the boundary condition (1.7) yield

$$J(k)^T\alpha = 0.$$

Since $J(k)^T$ is invertible the last equality implies $\alpha = 0$. Finally we find

$$\begin{aligned} y(x,k) = & \int_0^x f(x,k)(J(k)^T)^{-1}\varphi(t,k)^T g(t)dt \\ &+ \int_x^\infty \varphi(x,k)J(k)^{-1}f(t,k)^T g(t)dt. \end{aligned}$$

Q.E.D.

Corollary 3.2. Let us denote the continuous spectrum, the set of eigenvalues and the set of spectral singularities of L by $\sigma_c(L)$, $\sigma_d(L)$ and $\sigma_{ss}(L)$ respectively. It follows

$$\begin{aligned} &\sigma_c(L) = [0,\infty)\,, \\ &\sigma_d(L) = \{k^2 :\ k \in \mathbb{C}_+,\ \det(J(k)) = 0\}, \\ &\sigma_{ss}(L) = \{k^2 :\ k \in \mathbb{R}\setminus\{0\},\ \det(J(k)) = 0\}. \end{aligned}$$

Proof. It easily follows from Theorem 3.1 that k^2 is an eigenvalue of L iff $\det(J(k)) = 0$ for $k \in \mathbb{C}_+$. It can be shown similarly to the scalar case [26] that $\sigma_c(L) = [0,\infty)$. Spectral singularities are the poles of the kernel of the resolvent and are also in the continuous spectrum. Therefore, it follows from Theorem 3.1 that

$$\sigma_{ss}(L) = \{k^2 :\ k \in \mathbb{R}\setminus\{0\},\ \det(J(k)) = 0\}$$

. Q.E.D.

4 Conclusions

In this study we aim to complement the results [25] on the non-selfadjoint matrix Schrödinger operator on the half-line with Dirichlet boundary condition at $x = 0$ by considering the most general boundary condition at $x = 0$. We also aim to extend the studies [2, 3, 4, 5, 28, 29] on the selfadjoint matrix Schrödinger equation on the half-line with general boundary condition at origin to the non-selfadjoint case by considering the non-Hermitian but symmetric potential Q.

The particular case $B = 0$ in (1.7) implies that A is invertible from (1.9) and thus yielding the Dirichlet boundary condition at origin. Let us denote the matrix Schrödinger equation on the half-line together with the Dirichlet boundary condition at the origin such that the $n \times n$ non-selfadjoint matrix potential Q is in $L_1^1(\mathbb{R}_+)$ by L_0. It is well known that the set of eigenvalues of L_0 is bounded, countable and the limit points can only occur in a bounded subinterval of the real line (see Theorem 1 in [25]). This result follows from the asymptotic relation

$$f(x,k) = e^{ikx}\left[I_n + o(1)\right], \quad |k| \to \infty, \quad k \in \overline{\mathbb{C}_+},$$

of the Jost solution. Note that considering the most general boundary condition at the origin i.e. $A \neq 0, B \neq 0$ in (1.7), the Jost matrix depends on A and B and thus the boundedness of eigenvalues of L depends on the matrices A and B. Moreover, it has been proven that the set of spectral singularities of L_0 is bounded and has zero Lebesgue measure (see Theorem 1 in [25]). Similarly, if the most general boundary condition at the origin assumed, then the boundedness of spectral singularities of L depends on the matrices A and B.

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