

# Analysis of the Spectral Singularities of Schrödinger Operator with Complex Potential by Means of the SPSS Method

V Barrera Figueroa

Sección de Estudios de Posgrado e Investigación de UPIITA-IPN. Av. Inst. Politécnico Nal. 2580, Col. Barrio la Laguna Ticomán, México D.F., C.P. 07340 MÉXICO

E-mail: vbarreraf@ipn.mx

**Abstract.** In this work we present an effective way of finding the spectral singularities of the one-dimensional Schrödinger operator with a complex-valued potential defined in the half-axis  $[0, \infty)$ . The spectral singularities are certain poles in the kernel of the resolvent, which are not eigenvalues of the operator. In this work, the spectral singularities are calculated from the real zeros of  $\varkappa(\varrho) = 0$ , where  $\varkappa(\varrho)$  is an analytic function of the complex variable  $\varrho$ , which is obtained by means of the Spectral Parameter Power Series Method. This representation is convenient from a numerical point of view since its numerical implementation implies truncating the series up to a  $M$ -th term. Hence, finding the approximate spectral singularities is equivalent to finding the real roots of a certain polynomial of degree  $2M$ . In addition, we provide explicit formulas for calculating the eigenvalues of the operator, as well as the eigenfunctions and generalized eigenfunctions associated to both the continuous spectrum and the spectral singularities.

## 1. Introduction

Let us consider the differential expression  $\ell(y) := -y'' + q(x)y$ , in the half-axis  $x \in (0, \infty)$ , with the boundary condition at the origin  $y(0) = 0$ , where

$$q(x) := \begin{cases} V(x), & 0 \leq x \leq a, \\ 0, & a < x < \infty \end{cases} \quad (1)$$

is a complex-valued function called the potential function, and  $V$  satisfies certain regularity conditions. By  $L$  we denote a differential operator defined by the formula  $Ly := \ell(y)$ , with the domain  $D_L = \{y \in H^2(0, a) \cup H^2(a, \infty) : y(0) = 0, \ell(y) \in \mathcal{L}^2(0, \infty)\}$ , where  $H^2(\alpha, \beta)$  is the Sobolev space [1, Suppl. 2]. Since we are not assuming that  $\text{Im}V(x) \equiv 0$  in  $[0, a]$ , the operator  $L$  is non-self-adjoint in  $D_L$ . In the work [2] it was addressed a similar differential expression on the whole real axis by considering a real-valued potential function, which leads to a self-adjoint operator without spectral singularities.

In the classical theory of the Sturm-Liouville equation, the spectrum of  $L$  is analysed on the basis of certain Volterra integral equations of the second kind representing the solutions of the equation  $\ell(y) = \varrho^2 y$ , being  $\varrho \in \mathbb{C}$  the spectral parameter (see, e.g., [3]). However, in the present work we analyse the spectrum of  $L$  from the properties of the solutions of the equation



$\ell(y) = \varrho^2 y$ , which are given explicitly in the form of power series of the spectral parameter [4], without using the theory of the integral equations. In addition, we are interested in investigating the spectral singularities of the operator  $L$ . The spectral singularities were first discovered by Naimark [5], though the term *spectral singularity* was introduced by Schwartz [6], who defined the spectral singularities for a non-self-adjoint operator in terms of the spectral family of the operator. Comprehensive investigation on the spectral singularities for differential operators has been done by Pavlov [7–9], Lyantse [10], Krein [11] and Langer [12]. The latter investigated the spectral singularities for abstract operators. Nagy [13–15] gave a general notion of the spectral singularities for closed linear operators on a Banach space.

In quantum mechanics, the spectral singularities typically appear in non-Hermitian Hamiltonians having a continuous part of the spectrum [16]. Non-Hermitian Hamiltonians have raised special interest in the literature as complex extensions of quantum mechanics [17]. It is well-known that non-Hermitian Hamiltonians operators with potentials that fulfil the property of  $\mathcal{PT}$ -symmetry [18] have real spectra, where  $\mathcal{P}$  and  $\mathcal{T}$  denote the operations of space reflection and time reversal, respectively. Such symmetry does not by itself guarantee reality of the spectrum, but it does imply that the eigenvalues are either real, or appear as complex-conjugate pairs [19]. Physically, the spectral singularities for some complex potentials have been identified with some resonance phenomena (see, *e.g.*, [20, 21]). Hence, identifying the spectral singularities may lead to define their precise physical meaning.

The outline of this work is as follows: in Section 2 we construct some solutions of the equation  $\ell(y) = \varrho^2 y$  in  $(0, a)$  and in  $(0, \infty)$ , by means of the SPPS method. Next, in Section 3 we investigate the spectrum of  $L$  consisting of the point spectrum and the continuous spectrum, and we identify the spectral singularities. We obtain explicit expressions for calculating the eigenvalues, the spectral singularities and the generalized eigenfunction associated to them. Finally, in Section 4 we provide some concluding remarks.

## 2. Construction of some solutions of equation $\ell(y) = \varrho^2 y$

Let us introduce the parameter  $\lambda \in \mathbb{C}$  admitting the polar representation

$$\lambda := |\lambda| e^{i\theta}, \quad 0 \leq \theta < 2\pi, \quad (2)$$

and let  $\varrho \in \mathbb{C}$  be a complex number such that  $\lambda = \varrho^2$ . Thus,  $\varrho$  is defined as a branch of  $\lambda^{1/2}$  according to the expression

$$\varrho := \sqrt{|\lambda|} e^{i\theta/2}, \quad 0 \leq \theta/2 < \pi. \quad (3)$$

Definition (2) specifies a Riemann sheet in the complex  $\lambda$ -plane with a branch cut on the half-axis  $[0, \infty)$ . Formula (3) implies that the condition  $\text{Im} \varrho \geq 0$  holds in each point of this sheet, which is called the proper Riemann sheet [22, 23]. Once the condition  $\text{Im} \varrho \geq 0$  is invoked, any result with  $\text{Im} \lambda^{1/2} < 0$  will violate the requirement of being in the proper Riemann sheet.

Expression (1) leads us to the differential equations

$$-y'' + V(x)y = \varrho^2 y, \quad 0 < x < a, \quad (4a)$$

$$-y'' = \varrho^2 y, \quad a < x < \infty. \quad (4b)$$

If  $y$  satisfies equations (4) simultaneously and if the matching conditions  $y(a-0) = y(a+0)$ ,  $y'(a-0) = y'(a+0)$  hold, then  $y$  satisfies the equation  $\ell(y) = \varrho^2 y$  in  $(0, \infty)$ . Here we have used the notation  $y(a \pm 0) = \lim_{x \rightarrow a \pm 0} y(x)$  for the one-sided limits. If  $V$  were a real-valued function, then equation (4) would be a stationary Schrödinger equation in the proper units, being (4a) the equation describing the bound states, and (4b) the equation describing the scattering states. Thus  $\varrho^2$  would represent the real *eigen*-energies of the bound states and the continuous energy spectrum of the scattering states, respectively. Should  $V$  were a complex-valued potential

yielding a real spectrum, the physical meaning of  $\varrho^2$  would still be that of energy. However, a complex *eigen*-energy resulting from a complex potential  $\varrho^2$  carries information regarding the lifetime of a decaying *eigen*-state in resonant systems (see, *e.g.*, [24, 25] and references therein).

### 2.1. A general solution of $\ell(y) = \varrho^2 y$ in the interval $(0, a)$

By  $y_1$  and  $y_2$  we denote two linearly independent solutions of equation (4a) in  $(0, a)$ , then  $y(x) = c_1 y_1(x) + c_2 y_2(x)$  is a general solution of (4a) in  $(0, a)$ , where  $c_1, c_2$  are arbitrary numbers. Let  $y_0$  be a non-vanishing particular solution of the equation  $\ell(y) = 0$  satisfying the regularity conditions  $y_0^2, 1/y_0^2 \in \mathcal{C}[0, a]$ . According to [4], the series

$$y_1(x) = y_0(x) \sum_{k=0}^{\infty} (-1)^k \varrho^{2k} \tilde{X}^{(2k)}(x), \quad y_2(x) = y_0(x) \sum_{k=0}^{\infty} (-1)^k \varrho^{2k} X^{(2k+1)}(x)$$

are two linearly independent solutions of equation (4a) that converge uniformly in  $[0, a]$ , where the formal powers  $\tilde{X}^{(n)}$  and  $X^{(n)}$  are defined by the recursive integration procedure

$$\tilde{X}^{(n)}(x) := \int_{x_0}^x \tilde{X}^{(n-1)}(s) (y_0^2(s))^{(-1)^{n-1}} ds, \quad X^{(n)}(x) := \int_{x_0}^x X^{(n-1)}(s) (y_0^2(s))^{(-1)^n} ds,$$

with the seeds  $\tilde{X}^{(0)} \equiv 1$  and  $X^{(0)} \equiv 1$ , being  $x_0$  an arbitrary point in  $[0, a]$ . By choosing  $x_0 = a$ , the solutions  $y_1$  and  $y_2$  satisfy the initial conditions  $y_1(a) = y_0(a)$ ,  $y_1'(a) = y_0'(a)$ , and  $y_2(a) = 0$ ,  $y_2'(a) = 1/y_0(a)$ .

*Remark 1.* The previous recursive integration procedure yields the estimate  $|\tilde{X}^{(2k)}| \leq c_\varrho^k / (2k)!$ , where  $c_\varrho := |\varrho^2| |x - a|^2 (\max |y_0^2|) (\max |1/y_0^2|)$ . Hence, there exist a majorant series such that

$$|y_1(x)| \leq |y_0(x)| \sum_{k=0}^{\infty} \frac{c_\varrho^k}{(2k)!}, \quad 0 \leq x \leq a.$$

Since the right-hand series converges, then  $y_1$  converges uniformly on  $[0, a]$ . The uniform convergence of  $y_2$  on  $[0, a]$  is proven similarly.

### 2.2. Solutions of $\ell(y) = \varrho^2 y$ in the half-axis $(0, \infty)$ asymptotically equal to $\exp(\pm i\varrho x)$

The function  $d_1 e^{i\varrho x} + d_2 e^{-i\varrho x}$  satisfies equation (4b) in the interval  $(a, \infty)$ , where  $d_1, d_2$  are arbitrary complex numbers. If the particular solution  $y_0$  is chosen so that  $y_0(a) = 1$  and  $y_0'(a) = i$ , the matching conditions lead to the piecewise continuous function

$$y(x) = \begin{cases} c_1 y_1(x) + c_2 y_2(x), & 0 \leq x \leq a, \\ d_1 e^{i\varrho x} + d_2 e^{-i\varrho x}, & a \leq x < \infty, \end{cases} \quad (5)$$

satisfying  $\ell(y) = \varrho^2 y$  in  $(0, \infty)$ , where  $d_1 = \frac{e^{-i\varrho a}}{2i\varrho} [c_1 i(\varrho + 1) + c_2]$ ,  $d_2 = \frac{e^{i\varrho a}}{2i\varrho} [c_1 i(\varrho - 1) - c_2]$ .

A solution of the equation  $\ell(\varphi) = \varrho^2 \varphi$  in  $(0, \infty)$  with the asymptotic behaviour  $\varphi(x, \varrho) \sim e^{i\varrho x}$  as  $x \rightarrow \infty$  is obtained by taking  $d_2 = 0$  in expression (5), which implies that  $c_2 = c_1 i(\varrho - 1)$ . In this case, the sought solution is given by

$$\varphi(x, \varrho) := c_1 \begin{cases} y_1(x) + i(\varrho - 1) y_2(x), & 0 \leq x \leq a, \\ e^{i\varrho(x-a)}, & a \leq x < \infty. \end{cases} \quad (6)$$

On the other hand, a solution of the equation  $\ell(\psi) = \varrho^2 \psi$  in  $(0, \infty)$  with the asymptotic behaviour  $\psi(x, \varrho) \sim e^{-i\varrho x}$  as  $x \rightarrow \infty$  is obtained by taking  $d_1 = 0$  in (5). This implies that  $c_2 = -c_1 i(\varrho + 1)$ , which in turn leads us to the solution

$$\psi(x, \varrho) := c_1 \begin{cases} y_1(x) - i(\varrho + 1)y_2(x), & 0 \leq x \leq a, \\ e^{-i\varrho(x-a)}, & a \leq x < \infty. \end{cases} \quad (7)$$

In expressions (6) and (7) the number  $c_1$  plays the role of a free parameter depending on no boundary condition, so we fix  $c_1 = 1$  for simplicity. It follows that the Wronskian  $W[\varphi, \psi]$  of the solutions  $\varphi$  and  $\psi$  in the whole half-axis  $x \in [0, \infty)$  is

$$W[\varphi, \psi](x) := \begin{vmatrix} \varphi(x, \varrho) & \psi(x, \varrho) \\ \varphi'_x(x, \varrho) & \psi'_x(x, \varrho) \end{vmatrix} = -2i\varrho.$$

This implies that  $\varphi$  and  $\psi$  are linearly independent in the region  $\text{Im}\varrho \geq 0$ ,  $\varrho \neq 0$ .

*Remark 2.* Let us write  $\varrho = \alpha + i\beta$ . The solutions  $\varphi$  and  $\psi$  have the asymptotics  $\varphi(x, \varrho) = \mathcal{O}(e^{-\beta x})$ ,  $\psi(x, \varrho) = \mathcal{O}(e^{\beta x})$  as  $x \rightarrow \infty$ . Therefore, in the region  $\text{Im}\varrho > 0$  of the complex  $\varrho$ -plane, the solutions satisfy  $\varphi(x, \cdot) \in \mathcal{L}^2(0, \infty)$ ,  $\psi(x, \cdot) \notin \mathcal{L}^2(0, \infty)$ .

### 3. The spectrum of the operator $L$

Let us consider the initial value problem

$$\ell(y) = \varrho^2 y, \quad 0 < x < \infty, \quad (8a)$$

$$y(0) = 0, \quad y'(0) = 1. \quad (8b)$$

If  $y \in D_L$  fulfils this problem, then  $y$  also satisfies the equation  $Ly = \lambda y$ . Since  $\varphi$  and  $\psi$  are linearly independent solutions of (8a) for  $\varrho \neq 0$ , then the function

$$s(x, \varrho) := \frac{\psi(\varrho)\varphi(x, \varrho) - \varphi(\varrho)\psi(x, \varrho)}{2i\varrho} \quad (9)$$

is a solution of problem (8) in the region  $\text{Im}\varrho \geq 0$ ,  $\varrho \neq 0$ , where  $\varphi(\varrho) := \varphi(0, \varrho) = y_1(0) + i(\varrho - 1)y_2(0)$ , and  $\psi(\varrho) := \psi(0, \varrho) = y_1(0) - i(\varrho + 1)y_2(0)$ . Moreover, the function

$$s(x, 0) = \begin{cases} \vartheta_1(0)\vartheta_2(x) - \vartheta_2(0)\vartheta_1(x), & 0 \leq x \leq a, \\ \vartheta_1(0)(x - a) - \vartheta_2(0), & a \leq x < \infty \end{cases} \quad (10)$$

satisfies problem (8) for  $\varrho = 0$ , where  $\vartheta_1$  and  $\vartheta_2$  are two linearly independent solutions of  $\ell(y) = 0$ , which can also be constructed with the SPPS method. On the basis of the solutions  $s(x, \varrho)$  and  $s(x, 0)$  we will investigate the spectrum of the operator  $L$ .

#### 3.1. The point spectrum of the operator $L$

**Theorem 3.** *The operator  $L$  has no positive eigenvalues, moreover,  $\lambda = 0$  is not an eigenvalue.*

*Proof.* Let  $\lambda \geq 0$  so that  $\varrho = \pm\sqrt{\lambda}$  lies in the proper Riemann sheet. The asymptotics of  $s$  is

$$s(x, \sqrt{\lambda}) \sim \begin{cases} \frac{y_1(0) - iy_2(0)}{\sqrt{\lambda}} \sin \sqrt{\lambda}(x - a) - y_2(0) \cos \sqrt{\lambda}(x - a), & \lambda > 0, \\ \vartheta_1(0)(x - a) - \vartheta_2(0), & \lambda = 0, \end{cases}$$

as  $x \rightarrow \infty$ . Hence  $s(x, \sqrt{\lambda}) \notin \mathcal{L}^2(0, \infty)$  for  $\lambda \geq 0$ . □

**Theorem 4.** In order for  $\lambda$  to be an eigenvalue of  $L$  it is necessary and sufficient that  $\lambda = \varrho^2$ ,  $\text{Im} \varrho > 0$ ,  $\varphi(\varrho) = 0$ .

*Proof.* According to Remark 2,  $\varphi(x, \cdot) \in \mathcal{L}^2(0, \infty)$ ,  $\psi(x, \cdot) \notin \mathcal{L}^2(0, \infty)$  in the region  $\text{Im} \varrho > 0$ . The solution  $s$  defined in (9) will satisfy  $s(x, \cdot) \in \mathcal{L}^2(0, \infty)$  in the same region iff  $\varphi(\varrho) = 0$ .  $\square$

**Corollary 5.** Let  $\varrho_n$  be a zero of the equation  $\varkappa(\varrho) = 0$  lying in the region  $\text{Im} \varrho > 0$ , where  $\varkappa$  is an analytic function of the complex variable  $\varrho$  defined by its Taylor series

$$\varkappa(\varrho) := \sum_{k=0}^{\infty} (-1)^k \tilde{X}^{(2k)}(0) \varrho^{2k} + i(\varrho - 1) \sum_{k=0}^{\infty} (-1)^k X^{(2k+1)}(0) \varrho^{2k}. \quad (11)$$

Then  $\lambda_n = \varrho_n^2$  is an eigenvalue of the operator  $L$ .

*Proof.* The condition  $\varphi(\varrho) = 0$  is equivalent to  $y_1(0) + i(\varrho - 1)y_2(0) = 0$ . The result comes of substituting  $y_1$  and  $y_2$  by their SPPS representations.  $\square$

The equation  $\varkappa(\varrho) = 0$  is often referred to as the characteristic equation or dispersion relation of the operator  $L$ .

**Corollary 6.** Let  $\lambda_n$  be an eigenvalue of the operator  $L$ , then the function

$$y_n(x, \lambda_n) := k_n \frac{\psi(\lambda_n^{1/2})}{2i\lambda_n^{1/2}} \varphi(x, \lambda_n^{1/2}), \quad x \geq 0,$$

is its corresponding eigenfunction, up to a multiplicative constant  $k_n$ .

*Proof.* The result comes by putting  $\varphi(\varrho) = 0$  in expression (9).  $\square$

### 3.2. The continuous spectrum of the operator $L$

**Theorem 7** ([26]). The resolvent  $R_\lambda$  of the operator  $L$  is defined by the integral operator

$$R_\lambda f(x) := \int_0^\infty G(x, \xi; \lambda) f(\xi) d\xi, \quad f \in \mathcal{L}^2(0, \infty),$$

where the kernel is specified by the expression

$$G(x, \xi; \varrho^2) := \frac{1}{\varphi(\varrho)} \begin{cases} \varphi(x, \varrho) s(\xi, \varrho), & 0 < \xi < x, \\ s(x, \varrho) \varphi(\xi, \varrho), & x < \xi < \infty. \end{cases}$$

Every number of the form  $\lambda = \varrho^2$ ,  $\text{Im} \varrho > 0$ ,  $\varphi(\varrho) \neq 0$ , belongs to the resolvent set  $\rho_L$  of  $L$ .

**Theorem 8.** Every number  $\lambda \geq 0$  belongs to the continuous spectrum  $\sigma_c$  of the operator  $L$ .

*Proof.* Let us prove that for  $\lambda \geq 0$  the range  $\mathcal{R}(L - \lambda I)$  of the operator  $L - \lambda I$  is dense in  $\mathcal{L}^2(0, \infty)$ . It means that the orthogonal complement of  $\mathcal{R}(L - \lambda I)$  consists only on the zero element. Indeed, the orthogonal complement of the set  $\mathcal{R}(L - \lambda I)$  is the space of solutions  $u$  of the equation  $L^*u = \lambda u$ , where  $L^*$  is the adjoint operator of  $L$ , which is defined by the differential expression  $\ell^*u = -u'' + \overline{q(x)}u$  and the boundary condition  $u(0) = 0$ . But according to Theorem 3,  $\lambda \geq 0$  is not an eigenvalue of the operator  $L^*$ , which yields the trivial solution.  $\square$

**Corollary 9.** *Let  $\lambda > 0$  belong to the continuous spectrum  $\sigma_c$  of the operator  $L$ . Then the bounded, piecewise continuous function*

$$s(x, \sqrt{\lambda}) = k \begin{cases} y_1(0) y_2(x) - y_2(0) y_1(x), & 0 \leq x \leq a, \\ \frac{1}{\sqrt{\lambda}} [y_1(0) - i y_2(0)] \sin \sqrt{\lambda}(x-a) - y_2(0) \cos \sqrt{\lambda}(x-a), & a \leq x < \infty, \end{cases}$$

*is its associated generalized eigenfunction. The generalized eigenfunction associated to  $\lambda = 0$  is given by the function (10), up to a multiplicative constant  $k$ .*

*Proof.* The assertion follows by substituting  $\varphi$  and  $\psi$  in their SPPS form into  $s(x, \varrho)$ . □

### 3.3. Spectral singularities

The previous results establish that the complex  $\lambda$ -plane is decomposed as  $\mathbb{C} = \rho_L \cup \sigma_p \cup \sigma_c$ , i.e., the operator  $L$  has no residual spectrum. The continuous spectrum consists of points  $\lambda = \varrho^2 \geq 0$  lying in the axis  $\text{Im} \varrho = 0$ , such that  $\varphi(\varrho) \neq 0$ . In turn, the eigenvalues are points  $\lambda = \varrho^2$  lying in the region  $\text{Im} \varrho > 0$ , such that  $\varphi(\varrho) = 0$ . This condition is equivalent to the equation  $\varkappa(\varrho) = 0$ . A natural question arises regarding the role of the zeros of the equation  $\varkappa(\varrho) = 0$  lying in the continuous part of the spectrum of  $L$ .

Let us define a singular value of the operator  $L$  by a zero of the equation  $\varphi(\varrho) = 0$  lying in the region  $\text{Im} \varrho \geq 0$ ,  $\varrho \neq 0$ . Let  $\varrho_n$  be a zero of the equation  $\varphi(\varrho) = 0$  lying in the region  $\text{Im} \varrho \geq 0$ ,  $\varrho \neq 0$ . The non-real singular values indeed correspond to the eigenvalues of  $L$ , while the real singular values are the spectral singularities of the operator  $L$ . In other words, the point  $\lambda_0$  is a spectral singularity of the operator  $L$  if it is not an eigenvalue of  $L$ , and for each  $\lambda$  in the resolvent set  $\rho_L$  the kernel  $G(x, \xi; \lambda)$  of the resolvent operator  $(L - \lambda I)^{-1}$  satisfies  $G(x, \xi; \lambda) \rightarrow \infty$  as  $\lambda \rightarrow \lambda_0$  (see, e.g., [27]). The set of the spectral singularities can be identified in the complex  $\lambda$ -plane according to the following result.

**Theorem 10.** *Let  $\alpha_n \in \mathbb{R}$  be a zero of the equation  $\varkappa(\alpha) = 0$ , where  $\varkappa$  is an analytic function defined in (11). Then  $\lambda_n = \alpha_n^2$  is a spectral singularity of the operator  $L$ .*

**Corollary 11.** *Let  $\alpha_n \neq 0$  be a spectral singularity of the operator  $L$ , then its corresponding generalized eigenfunction  $u_n$  is a bounded function given by the formula*

$$u_n(x, \alpha_n) := c_n \frac{\psi(\alpha_n)}{2i\alpha_n} \varphi(x, \alpha_n), \quad x \geq 0,$$

*up to a multiplicative constant  $c_n$ . If  $\alpha_n = 0$  is a spectral singularity, its corresponding eigenfunction is an unbounded function given by expression (10).*

*Proof.* The result comes of applying the condition  $\varphi(\alpha) = 0$  in expression (9). □

**Theorem 12.** *If the potential  $V$  is a real-valued function, then the operator  $L$  has no spectral singularities.*

*Proof.* In that case the operator  $L$  is self-adjoint in the domain  $D_L$ . It is well known that the spectrum of a self-adjoint operator is real, and its residual spectrum is empty [28, p. 182]. Furthermore, all its singular values (eigenvalues) are negative (see, e.g., [1, §2.5], cf. [29, §20]) and none of them lie in the continuous part of the spectrum located on  $\lambda \geq 0$ . □

#### 4. Concluding remarks

Throughout this work we have investigated the spectrum of the operator  $L$  by means of the properties of the solutions of the equation  $\ell(y) = \varrho^2 y$  in  $(0, \infty)$ , on the assumption that the potential has compact support on  $[0, a]$ . In the classical theory of the Sturm-Liouville equation the solutions of the equation  $\ell(y) = \varrho^2 y$  in  $(0, \infty)$  are represented in the form of Volterra integral equations of the second kind [5, 10, 30–33]. Certain constraints derived from  $V \in \mathcal{L}^1(0, \infty)$  are imposed to the potential  $V$  in order for the solutions of the integral equations to exist and to be analytic in the domain  $\text{Im} \varrho \geq 0$  and  $|\varrho| \geq \delta > 0$ . If the particular solution  $y_0$  were constructed by means of the SPPS method itself, the only condition imposed to the potential would be  $V \in \mathcal{C}[0, a]$ . Hence, the present analysis allows the applicability of the theory here presented to a larger class of complex potentials.

Though the theory of the Sturm-Liouville equation  $\ell(y) = \varrho^2 y$  is well-known, in the present work we obtained explicit formulas for calculating the eigenvalues, the spectral singularities, and the associated eigenfunctions. Such formulas are given in a SPPS form. From a numerical point of view, the series can be truncated up to a  $M$ -th term. In this way, the eigenvalues  $\lambda_n = \varrho_n^2$ ,  $\text{Im} \varrho_n > 0$ , of the operator  $L$  can be calculated approximately from the polynomial roots of the equation  $\varkappa_M(\varrho) = 0$ , where  $\varkappa_M$  is the polynomial of order  $2M$  defined by

$$\varkappa_M(\varrho) := \sum_{k=0}^M (-1)^k \tilde{X}^{(2k)}(0) \varrho^{2k} + i(\varrho - 1) \sum_{k=0}^M (-1)^k X^{(2k+1)}(0) \varrho^{2k}.$$

Similarly, the spectral singularities  $\lambda_n = \alpha_n^2 \geq 0$  can be calculated approximately from the polynomial roots of the equation  $\varkappa_M(\alpha) = 0$ . The number of approximate eigenvalues (spectral singularities) that can be calculated from the roots of the equation  $\varkappa_M(\varrho) = 0$  ( $\varkappa_M(\alpha) = 0$ ) is, in general, lower than  $M$ . The remaining spurious roots are due to the truncation of the series  $\varkappa(\varrho)$  ( $\varkappa(\alpha)$ ). One would expect that the number of approximate eigenvalues would increase by increasing the number  $M$ . However, the upper roots of  $\varkappa_M(\varrho) = 0$  ( $\varkappa_M(\alpha) = 0$ ) are numerically more unstable than the lower roots due to small errors in the calculation of the polynomial coefficients. Nonetheless, it is always possible to calculate increasingly higher approximate eigenvalues (spectral singularities) for a fixed  $M$  by means of the shifting of the spectral parameter, as is described in [4]. The results presented here show the advantages of the present analysis and the necessity of its further study and numerical deployment, which will be included in a subsequent paper.

#### References

- [1] Berezin F A and Shubin M A 1991 *The Schrödinger Equation* (Dordrecht: Kluwer Academic Publ.)
- [2] Castillo-Pérez R, Kravchenko V V, Oviedo-Galdeano H and Rabinovich V S 2011 *J. Math. Phys.* **52**, 043522
- [3] Marchenko V A 1986 *Sturm-Liouville Operators and Applications* (Operator Theory: Advances and Applications vol 22) ed I. Gohberg (Basel: Birkhuser-Verlag)
- [4] Kravchenko V V and Porter R M 2010 *Math. Method Appl. Sci.* **33**, 459
- [5] Naimark M A 1954 *Trudy Moskov. Mat. Obshch.* **3**, 181 (In Russian.)
- [6] Schwartz J 1960 *Comm. Pure Appl. Math.* **13**, 609
- [7] Pavlov B S 1962 *Dokl. Akad. Nauk SSSR* **146**, 1267 (In Russian.) (English Transl. 1962 *Soviet Math. Dokl.* **3**, 1483)
- [8] Pavlov B S 1966 On a non-selfadjoint Schrödinger operator I. In: *Probl. Math. Phys. No. 1, Spectral Theory and Wave Processes* ed M S Birman (Leningrad: Izdat. Leningrad Univ.) pp 102–132 (In Russian.) (English Transl. 1967 *Topics in Mathematical Physics* (New York: Consultants Bureau) pp 87–113)
- [9] Pavlov B S 1967 On a non-selfadjoint Schrödinger operator II. In: *Probl. Math. Phys. No. 2, Spectral Theory, Diffraction Problems* ed M S Birman (Leningrad: Izdat. Leningrad Univ.) pp 133–157 (In Russian.) (English Transl. 1968 *Topics in Mathematical Physics* (New York: Consultants Bureau) pp 111–134)
- [10] Lyantse V È 1964 *Mat. Sb. (N. S.)*, I: **64(106)**, 521; II: **65(107)**, 47 (In Russian.) (English transl.: 1967 *Amer. Math. Soc. Transl.* **2** **60**, 185)

- [11] Krein M G and Langer H (= Langer G K) 1963 *Dokl. Akad. Nauk SSSR* **152**, 39 (In Russian.)
- [12] Langer H 1982 Spectral functions of definitizable operators in Krein spaces. In: *Functional Analysis* (Lecture Notes in Mathematics vol 948) ed D Butković, H Kraljević and S Kurepa (Berlin: Springer), pp 1–46
- [13] Nagy B 1986 *J. Oper. Theo.* **15**, 307
- [14] Nagy B 1987 *Acta Math. Hung.* **49**, 51
- [15] Nagy B 1988 *Acta Math. Hung.* **51**, 225
- [16] Samsonov B F 2005 *J. Phys. A: Math. Gen.* **38** L571
- [17] Mostafazadeh A 2010 *Int. J. Geom. Meth. Mod. Phys.* **7**, 1191
- [18] Bender C M and Boettcher S 1998 *Phys. Rev. Lett.* **80**, 5243
- [19] Dorey P, Dunning C and Tateo R 2002 The ODE/IM correspondence and  $\mathcal{PT}$ -symmetric quantum mechanics. In: *Statistical Field Theories* (NATO Science Series vol 73) ed A Cappelli and G Mussardo (Netherlands: Springer) pp 13–23
- [20] Mehri-Dehnavi H and Mostafazadeh A 2008 *J. Math. Phys.* **49**, 082105
- [21] Mostafazadeh A 2009 *Phys. Rev. Lett.* **102**, 220402
- [22] Dudley D G 1994 *Mathematical Foundations for Electromagnetic Theory* (New York: IEEE Press)
- [23] Hanson G W and Yakovlev A B 2002 *Operator Theory for Electromagnetics. An Introduction* (New York: Springer)
- [24] Rosas-Ortiz O, Fernández-García N, and Cruz y Cruz S 2008 *AIP Conference Proceedings* **1077**, 31
- [25] Sudarshan E C G, Chiu C B, and Gorini V 1978 *Phys. Rev. D* **18**, 2914
- [26] Lyantse V È 1968 The non-self-adjoint differential operator of the second order on the half-axis. In: *Linear Differential Operators Part II. Linear Differential Operators in Hilbert Space* ed M A Naimark (London: George G. Harrap & Co., Ltd.), Appendix II
- [27] Guseinov G S 2009 *Pramana J. Phys.* **73**, 587
- [28] Stakgold I 2000 *Boundary Value Problems of Mathematical Physics. Volume I* (Philadelphia: SIAM)
- [29] Vladimirov V S 1971 *Equations of Mathematical Physics* (New York: Marcel Dekker, Inc.)
- [30] Levin B Y 1950 *Zap. Nauch. Issled. Inst. Khar. Gos. Univ.* **20**, 83 (In Russian.)
- [31] Agranovich Z S and Marchenko V A 1963 *The Inverse Problem in Scattering Theory* (New York: Gordon-Breach)
- [32] Levin B Y 1956 *Doklad. Akad. Nauk SSSR* **106**, 187 (In Russian.)
- [33] Naimark M A 1968 *Linear Differential Operators Part II. Linear Differential Operators in Hilbert Space* (London: George G. Harrap & Co., Ltd.)