Eigenvalue problems, spectral parameter power series, and modern applications

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In the present review, we deal with the recently introduced method of spectral parameter power series (SPPS) and show how its application leads to an explicit form of the characteristic equation for different eigenvalue problems involving Sturm–Liouville equations with variable coefficients. We consider Sturm–Liouville problems on finite intervals; problems with periodic potentials involving the construction of Hill’s discriminant and Floquet–Bloch solutions; quantum-mechanical spectral and transmission problems as well as the eigenvalue problems for the Zakharov–Shabat system. In all these cases, we obtain a characteristic equation of the problem, which in fact reduces to finding zeros of an analytic function given by its Taylor series. We illustrate the application of the method with several numerical examples, which show that at present, the SPPS method is the easiest in the implementation, the most accurate, and efficient. We emphasize that the SPPS method is not a purely numerical technique. It gives an analytical representation both for the solution and for the characteristic equation of the problem. This representation can be approximated by different numerical techniques and leads to a powerful numerical method, but most important, it offers a different insight into the spectral and transmission problems. Copyright © 2014 John Wiley & Sons, Ltd.

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1. Introduction

Solution of second-order linear DEs belongs to a classical field of mathematics in which as an overwhelming majority of its users from students to active researchers believe that everything that was possible to do theoretically is essentially carried out, and whatever the analysts invent, in the domain of practical solution of equations and related models, the numerical discrete schemes more and more refined due to the massive efforts of experts in numerical analysis and computer sciences will be more accurate and efficient. However, analysts and advanced users of mathematical methods in physics are aware of many strong limitations in applicability of available numerical schemes. For example, if the discrete spectrum of a problem is not necessarily real, practically the whole machinery of advanced numerical techniques does not apply bringing to the surface very few options such as, for example, finite differences. The importance of this technique lies in its universality. Nevertheless, it usually gives way to many other approaches whenever they become applicable. The main difficulty in finding complex eigenvalues is due to the fact that the universally used shooting method works if only there is a clear criterion for choosing every next shot. Meanwhile, the real number is an ordered set, and zero is located always between a negative and a positive outcomes of the corresponding shots; the complex plane does not admit such a simple rule. There are many other situations (even when the eigenvalues are real) when the shooting procedure finds considerable difficulties and at the same time the method of finite differences is not applicable at all. For example, when the spectral parameter participates in the boundary conditions. Such situation in fact is more common in applications than otherwise.

In the present review, we discuss an approach developed in the last few years and called the spectral parameter power series (SPPS) method. It is important to notice that the SPPS method is not merely another numerical technique. On the contrary, it is an analytical approach giving new analytical results and at the same time lending itself to numerical calculation. The SPPS method allows one...
to obtain two linearly independent solutions of the Sturm–Liouville equation (in Section 2, we specify the conditions imposed on the coefficients)

\[(pu')' + qu = \lambda ru\]  \hspace{2cm} (1)

in the form

\[u_1(x) = \sum_{k=0}^{\infty} a_k(x) \lambda^k \quad \text{and} \quad u_2(x) = \sum_{k=0}^{\infty} b_k(x) \lambda^k\]  \hspace{2cm} (2)

where \(\lambda\) is a spectral parameter, and the series are uniformly convergent. Moreover, in the recent works [1], [2], such representation for solutions was obtained for a considerably more general equation of the form

\[(p(x)u')' + q(x)u = \sum_{k=1}^{N} \lambda^k R_k[u], \quad x \in (a, b)\]  \hspace{2cm} (3)

where \(R_k[u] := r_k(x)u + s_k(x)u', k = 1, \ldots, N\), \(p, q, r_k, s_k\) are continuous on the finite segment \([a, b]\). Representations of the form (2) from time to time appear in mathematical literature in different contexts. We mention here [3, Section 10] and [4]. The main difference is the form in which the coefficients \(a_k\) and \(b_k\), \(k = 0, 1, \ldots\) are represented. In previous works, the calculation of the coefficients was proposed in terms of successive integrals with the kernels in the form of iterated Green functions [3, Section 10]. This makes any computation based on such representation difficult and less practical. Moreover, theoretical study of the corresponding series and their properties becomes considerably more complicated. We show that (i) for solving initial value and BVPs, the SPPS method performs better or equal in comparison to purely numerical methods; (ii) it is highly advantageous when the solution is required for many different values of the spectral parameter; and (iii) the SPPS method allows us to write down an explicit form of the characteristic equations for many different spectral problems, which in practice reduces the spectral problem to finding zeros of a corresponding analytic function given by its Taylor series. We emphasize that the method is applicable in different situations when some other approaches are unavailable (complex eigenvalues, \(\lambda\)-dependent boundary conditions, etc.) The method is simple and can be introduced in mathematical courses for physicists.

In Section 2, we review the main results in [6] and [7] concerning the SPPS representation of the solutions of (1) and show that even in solving initial and BVPs, this technique converted into a simple numerical algorithm is clearly competitive when compared to standard routines for numerical integration of linear ordinary DEs. In Section 3, we apply the SPPS method to Sturm–Liouville spectral problems with or without the spectral parameter in the boundary conditions. Here, together with some results from [7], we present new results concerning the problems admitting complex eigenvalues. Section 4 is dedicated to the spectral problems for periodic potentials. We give an SPPS representation for Hill’s discriminant [8] and show how the SPPS method allows one to construct the Bloch solutions of the problem. In Section 5, we consider two classical problems of mathematical physics, the quantum-mechanical spectral problem and the transmission problem. Following [9], we present a characteristic (dispersion) equation equivalent to the eigenvalue problem for the Schrödinger operator with a potential, which is an arbitrary continuous function on a finite interval outside of which it is constant. We discuss some numerical tests as well. The transmission problem is presented in the context of electromagnetic wave propagation as the problem of calculation of the reflection and transmission coefficients for a plane wave, which is incident on an inhomogeneous layer under an arbitrary angle of incidence. Following [10], we discuss application of the SPPS method to this problem. Section 6 is dedicated to the eigenvalue problem for the Zakharov–Shabat system. We present the dispersion equation [11] for the problem for a real-valued, finitely supported potential and discuss its practical application. Finally, in Section 7, we make some concluding remarks.

This review is for the colleagues interested in all kinds of problems involving the solution of Sturm–Liouville type equations. We hope to attract more attention to the SPPS approach, which combines the possibility to work with analytical representations of solutions and of characteristic equations of the problems with simplicity, rapid convergence, and accuracy when used for numerical computation.

### 2. Spectral parameter power series representation for solutions of the Sturm–Liouville equation

Let us consider the Sturm–Liouville equation

\[(pu')' + qu = \lambda ru,\]  \hspace{2cm} (4)
where \( p, q, \) and \( r \) are complex-valued functions and \( \lambda \) is a complex parameter. The following result (first obtained in [6], here, we follow [7]) gives us a convenient form for a general solution of (4) as an SPPS.

**Theorem 1**

[7] Assume that on a finite interval \([a, b]\), equation

\[
(pv')' + qv = 0,
\]

possesses a particular solution \( u_0 \) such that the functions \( u_0^2r \) and \( 1/(u_0^2p) \) are continuous on \([a, b]\). Then the general solution of (4) on \((a, b)\) has the form

\[
u = c_1u_1 + c_2u_2,
\]

where \( c_1 \) and \( c_2 \) are arbitrary complex constants,

\[
u_1 = u_0\sum_{k=0}^{\infty} \lambda^k X^{(2k)} \quad \text{and} \quad \nu_2 = u_0\sum_{k=0}^{\infty} \lambda^k X^{(2k+1)}
\]

with \( X^{(n)} \) and \( X^{(n)} \) being defined by the recursive relations

\[
X^{(0)} = 1, \quad X^{(1)} = 1,
\]

\[
X^{(n)}(x) = \begin{cases} 
\int_{x_0}^{x} X^{(n-1)}(s)u_0^2(s)r(s) \, ds, & n \text{ odd}, \\
\int_{x_0}^{x} X^{(n-1)}(s)\frac{1}{u_0^2(s)p(s)} \, ds, & n \text{ even},
\end{cases}
\]

\[
X^{(n)}(x) = \begin{cases} 
\int_{x_0}^{x} X^{(n-1)}(s)\frac{1}{u_0^2(s)p(s)} \, ds, & n \text{ odd}, \\
\int_{x_0}^{x} X^{(n-1)}(s)u_0^2(s)r(s) \, ds, & n \text{ even},
\end{cases}
\]

where \( x_0 \) is an arbitrary point in \([a, b] \) such that \( p \) is continuous at \( x_0 \) and \( p(x_0) \neq 0 \). Further, both series in (7) converge uniformly on \([a, b]\).

For a detailed proof, we refer to [7]. It is based on some simple observations. First of all, the knowledge of a particular solution of (5) allows one to factorize the Sturm–Liouville operator \( L = \frac{d}{dx}p\frac{d}{dx} + q \) in the form \( L = \frac{1}{u_0^2} \frac{d}{dx}p \frac{d}{dx} \frac{1}{u_0^2} + q \), also known as the Polya factorization [5] as mentioned before. This form is well suited for establishing how the operator \( \frac{1}{u_0^2}L \) acts on each member of the series (7). For example,

\[
\frac{1}{u_0^2}L(u_0X^{(2k)}) = u_0X^{(2k-2)}, \quad k \in \mathbb{N}.
\]

Analogously, \( \frac{1}{u_0^2}L(u_0X^{(2k+1)}) = u_0X^{(2k-1)} \).

Considering the system of functions \( \{\psi_n\}_{n=0}^{\infty} \) defined as follows \( \psi_0 = u_0^2 \):

\[
\psi_n(x) = \begin{cases} 
\psi_0(x)X^{(n)}(x), & n \text{ odd}, \\
\psi_0(x)X^{(n)}(x), & n \text{ even},
\end{cases}
\]

we find that \( \frac{1}{u_0^2}L\psi_{n+1} = 0 \) and \( \frac{1}{u_0^2}L\psi_n = \psi_{n-2}, \quad n = 2, 3, \ldots \) These properties are characteristic for the so-called \( L \)-bases (introduced in [12], unfortunately this important book has not been translated into English), and hence, formulas (8)–(10) represent a practical way to calculate an \( L \)-basis. In [13], it was established that the system of functions \( \{\psi_n\}_{n=0}^{\infty} \) is complete in \( L_2(a, b) \). For further related properties, we refer to [14].

To establish the uniform convergence of the series in (7) as well as to obtain a rough but useful estimate for the velocity of their convergence, it is sufficient to observe that

\[
|X^{(2k)}| \leq (\max |ru_0^2|)^k \left( \max |\frac{1}{pu_0^2}| \right)^k |b - a|^{2k}/(2k)!
\]

(a similar inequality is available for \( |X^{(2k+1)}| \) as well). Thus, the series \( \sum_{k=0}^{\infty} \lambda^k X^{(2k)} \) is majorized by a convergent numerical series \( \sum_{k=0}^{\infty} \frac{c^k}{(2k)!} \) with \( c = |\lambda| (\max |ru_0^2|) (\max |\frac{1}{pu_0^2}|) |b - a|^2 \).

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It is worth noticing that from (7), it is easy to obtain that \( u_1 \) and \( u_2 \) satisfy the following initial conditions

\[
\begin{align*}
  u_1(x_0) &= u_0(x_0), & u_1'(x_0) &= u_0'(x_0), \\
  u_2(x_0) &= 0, & u_2'(x_0) &= \frac{1}{u_0(x_0)p(x_0)}.
\end{align*}
\]

Remark 1

The possibility mentioned in Section 1 to represent solutions of the Sturm–Liouville equation in the form of SPPS is by no means a novelty, although it is not a widely used tool. In fact, besides the work reviewed in the succeeding text, we are able to mention only [3, Section 10], [4] and the recent paper [15], and to the best of our knowledge, it was applied for the first time for solving spectral problems in [7]. The reason of this underuse of the SPPS lies in the form in which the expansion coefficients were sought. Indeed, in previous works, the calculation of coefficients was proposed in terms of successive integrals with the kernels in the form of iterated Green functions [3, Section 10]. However, this makes any computation based on such representation difficult, less practical, and even proofs of the most basic results like, for example, the uniform convergence of the SPPS for any value of \( \lambda \in \mathbb{C} \) (established in Theorem 1) are not an easy task. For example, in [3, p. 16], the parameter \( \lambda \) is assumed to be small, and no proof of convergence is given. Moreover, in [16], a discrete analog of Theorem 1 together with some further applications to Jacobi operators were established, and it was pointed out that as well as in the continuous case the SPPS representation for solutions of the Jacobi operators was considered as a perturbation technique; however, even the situation with the convergence of such series was not satisfactorily understood. We refer to the book [17] where the possibility of divergence of such series is assumed. Because of the representation of the expansion coefficients similar to (9), (10), it was shown in [16] that the series are not only convergent but in the discrete case they are actually finite sums.

The way of how the expansion coefficients in (7) are calculated according to (9) and (10) is relatively simple and straightforward. This is why the estimation of the rate of convergence of the series (7) presents no difficulty, see (12). Another crucial feature of the introduced representation of the expansion coefficients in (7) consists in the fact that as we repeatedly observe in subsequent pages not only the expansion coefficients themselves also denoted by \( \psi_\ell \) in (11) are necessary in solving different spectral problems related to the Sturm–Liouville equation but also the formal powers apparently obtained as a by-product of the recursive integration procedure (9) and (10), namely the functions \( X^{(2\ell+1)} \) and \( X^{(2\ell)} \), \( \ell = 0, 1, 2, \ldots \), which do not participate explicitly in the representation of solutions (7), naturally appear in dispersion equations corresponding to the spectral problems. See (24) and (25) for the dispersion equations equivalent to the classical Sturm–Liouville eigenvalue problem, (42) for the SPPS representation of the Hill discriminant, (64) for the dispersion equation equivalent to the quantum-mechanical eigenvalue problem on the whole axis, or (91) for the dispersion equation equivalent to the Zakharov–Shabat eigenvalue problem.

The consideration of formal powers (9) and (10) as infinite families of functions intimately related to the corresponding Sturm–Liouville operator led in [18], [19] and [20] to a deeper understanding of the transmutation operators [21], [22] also known as transformation operators [23], [24]. Indeed, the functions \( \psi_n(x) \) resulted to be the images of the powers \( x^n \) under the action of a corresponding transmutation operator [19]. This makes it possible to apply the transmutation operator even when the operator itself is not a differential operator (and this is the usual situation – there are very few explicitly constructed examples available) due to the fact that its action on any polynomial is known. This result was used in [18] and [19] to prove the completeness (Runge-type approximation theorems) for families of solutions of two-dimensional Schrödinger and Dirac equations with variable complex-valued coefficients and to develop new representations for the transmutation operators [25], [26].

Remark 2

One of the functions \( ru_0^2 \) or \( 1/(pu_0^2) \) may not be continuous on \([a, b]\) and yet \( u_1 \) or \( u_2 \) may make sense. For example, in the case of the Bessel equation \( (xu')' + \frac{1}{x}u = -\lambda xu \), we can choose \( u_0(x) = x/2 \). Then \( 1/(pu_0^2) \not\in C[0, 1] \). Nevertheless, all integrals (9) exist and \( u_1 \) coincides with the nonsingular \( \left( \frac{1}{\sqrt{\lambda}} \right) J_1 \left( \frac{\sqrt{\lambda}}{x} \right) \), while \( u_2 \) is a singular solution of the Bessel equation. More on the SPPS representations for perturbed Bessel equations can be found in [27].

Remark 3

When \( p \) and \( q \) are real-valued, \( p(x) \neq 0 \) for all \( x \in [a, b] \) and \( p, p', q \) are continuous functions on \([a, b]\), the equation

\[
Lv = 0
\]

is a regular Sturm–Liouville equation and possesses two linearly independent real-valued solutions \( v_1 \) and \( v_2 \). Because of Sturm’s separation theorem (see, e.g., [28, p. 10]), their zeros occur alternately and hence \( u_0 = v_1 + iv_2 \) can be chosen as the particular solution required in Theorem 1. If \( r \) is continuous on \([a, b]\) (in general, complex-valued) function, then the conditions of Theorem 1 are fulfilled.

The solutions \( v_1 \) and \( v_2 \) from Remark 4 can be in fact calculated using the same procedure from Theorem 1. Indeed, consider equation (15), which can be written in the form

\[
(pv')' = -qv.
\]

It has the form (4) with \( r := -q, \lambda = 1 \) and with a convenient solution \( v_0 \equiv 1 \) of the (homogeneous) equation \((pv_0')' = 0\). Application of Theorem 1 gives us the following two linearly independent solutions of (15),

\[
v_1 = \sum_{k=0}^{\infty} v^{(2k)} \quad \text{and} \quad v_2 = \sum_{k=0}^{\infty} v^{(2k+1)}
\]
\[
\tilde{y}^{(0)} = 1, \quad v^{(0)} = 1,
\]
\[
\tilde{y}^{(n)}(x) = \begin{cases} 
- \int_{x_0}^{x} \tilde{y}^{(n-1)}(s)q(s) \, ds, & n \text{ odd}, \\
\int_{x_0}^{x} \tilde{y}^{(n-1)}(s) \frac{1}{p(s)} \, ds, & n \text{ even},
\end{cases}
\]
\[
y^{(n)}(x) = \begin{cases} 
\int_{x_0}^{x} y^{(n-1)}(s) \frac{1}{p(s)} \, ds, & n \text{ odd}, \\
- \int_{x_0}^{x} y^{(n-1)}(s)q(s) \, ds, & n \text{ even},
\end{cases}
\]

and the series in the equalities for \(v_1\) and \(v_2\) converge uniformly on \([a, b]\).

Note that
\[v_1(x_0) = 1, \quad v_1'(x_0) = 0, \quad v_2(x_0) = 0, \quad v_2'(x_0) = 1/p(x_0).\]

Solutions of (15) in the form (16) is a long-known result (see, e.g., [29]).

Before we proceed to discuss eigenvalue and scattering problems, it is worth noticing that the representation of a general solution of the Sturm–Liouville equation in the form of an SPPS given by Theorem 1 represents a natural and highly competitive method for numerical solution of initial and BVPs. Compared to the best standard routines, it performs better or equal and with minimal programmer’s efforts. Moreover, the advantages of using SPPS become even more transparent when the solution of the problem is required for many different values of the spectral parameter. In such case, the auxiliary functions \(X^{(n)}\) and \(\tilde{X}^{(n)}\), \(n = 0, 1, 2, \ldots\) should be computed only once, and then substitution of values of \(\lambda\) into the expressions (7) gives us a solution of Equation (4) for as many different values of the spectral parameter as needed at no additional computational cost. Nevertheless, first, let us show how SPPS performs at the terrain of numerical ODE solvers for solution of IVPs. In [10], we made use of Matlab 7 and as a first step compared our results with standard Matlab ODE solvers [30, 31], especially with ode45, which in the considered examples gave always better results than other similar programs. Here, we give two examples from [10].

For numerical approximations, we consider partial sums of the infinite series (7) and (16), for example, \(u_1 = u_0 \sum_{k=0}^{N} \lambda^k \tilde{X}^{(2k)}\) and \(u_2 = u_0 \sum_{k=0}^{N} \lambda^k X^{(2k+1)}\). The algorithm was implemented in MATLAB. For the recursive integration, we have chosen the following strategy. On each step, the integrand is represented through a cubic spline using the spapi routine, and the integration is performed using the fnint routine (both from the spline toolbox of MATLAB). This is the simplest alternative because it implies the usage of the standard routine and gives sufficiently good results. Nevertheless, if one is interested in faster and more accurate calculations, other options explored, for example, in [1] are preferable.

Consider the following IVP for (15); \(p = 1, q = c^2, v(0) = 1, v'(0) = -1\) on the interval \((0, 1)\). For \(c = 1\), the absolute error of the result calculated by ode45 (with an optimal tolerance chosen) was of order \(10^{-9}\), and the relative error was of order \(10^{-6}\) whereas the absolute error of the result calculated with the aid of the SPPS representation with \(N\) from 55 to 58 was of order \(10^{-16}\) and the relative error was of order \(10^{-14}\). Taking \(c = 10\) under the same conditions, the absolute and the relative errors of ode45 were of order \(10^{-6}\) and \(10^{-5}\), respectively; meanwhile, our algorithm gave values of order \(10^{-12}\) in both cases. For the IVP: \(p = -1, q = c^2, v(0) = 1, v'(0) = -1\) on the interval \((0, 1)\) in the case \(c = 1\) the absolute and the relative errors of ode45 were of order \(10^{-8}\) whereas in our method this value was of order \(10^{-15}\) already for \(N = 50\). For \(c = 10\), the absolute and the relative errors of ode45 were of order \(10^{-3}\) and \(10^{-7}\), respectively, and in the case of our method, these values were of order \(10^{-11}\) and \(10^{-14}\) for \(N = 50\).

Consider yet another example. Let \(p = -1, q(x) = c^2 x^2 + c\) in (15). In this case, the general solution has the form
\[
v(x) = e^{c x^2/2} \left( c_1 + c_2 \int_0^x e^{-c t^2} \, dt \right).
\]

Take the same initial conditions as before, \(v(0) = 1, v'(0) = -1\). Then, while for \(c = 1\) the absolute and the relative errors of ode45 were both of order \(10^{-11}\) and for \(c = 30\) the absolute error was 0.28 and the relative error was of order \(10^{-6}\), our algorithm \((N = 58)\) gave the absolute and relative errors of order \(10^{-15}\) for \(c = 1\) and the absolute and relative errors of order \(10^{-9}\) and \(10^{-15}\), respectively, for \(c = 30\). All calculations were performed on a common PC with the aid of Matlab 7.

The results of our numerical experiments show that in fact the SPPS representations offer a powerful method for numerical solution of initial value and BVPs for linear ordinary differential second-order equations. The numerical calculation of the involved integrals does not represent any considerable difficulty and can be performed with a remarkable accuracy.
Another observation that can be of use in many different situations is that if for some purposes a derivative of the solution of (4) is required, there is no need to apply to the obtained solution an algorithm for numerical differentiation. Instead, it is easy to see that

\[ u_1' = \frac{u_1'}{u_0} u_1 + \frac{1}{u_0 p} \sum_{k=1}^{\infty} \lambda^k \tilde{X}^{(2k-1)} \quad \text{and} \quad u_2' = \frac{u_2'}{u_0} u_2 + \frac{1}{u_0 p} \sum_{k=0}^{\infty} \lambda^k \tilde{X}^{(2k)}. \]  

Thus, the calculated auxiliary functions \( \tilde{X}^{(n)} \) and \( \tilde{X}^{(n)} \), \( n = 0, 1, 2, \ldots \) are used once more, this time for obtaining the derivative of the solution.

3. Solution of Sturm–Liouville problems

In this section, we outline the main ideas behind the application of the SPPS method to the solution of Sturm–Liouville eigenvalue problems referring the interested reader to [7] for additional details and numerical examples as well as to a more recent [1]. The SPPS method allows one to reduce the Sturm–Liouville problem to the problem of finding zeros of an analytic function of the complex variable \( \lambda \). Numerically, the problem is reduced to finding roots of a polynomial in \( \lambda \). To find the precise expressions for Taylor coefficients of that analytic function, let us consider the general Sturm–Liouville problem with unmixed boundary conditions. Thus, we look for the eigenvalues and eigenfunctions of the problem

\begin{align*}
(p u')' + qu &= \lambda u, \quad (21) \\
u(a) \cos \alpha + u'(a) \sin \alpha &= 0, \quad (22) \\
u(b) \cos \beta + u'(b) \sin \beta &= 0, \quad (23)
\end{align*}

where \([a, b]\) is a finite segment of the x-axis and \( \alpha \) and \( \beta \) are arbitrary real numbers.

Let us choose the point \( x_0 \) from Theorem 1 being equal to \( a \) and consider the solutions \( u_1 \) and \( u_2 \) of (21) defined by (7). Then from (13) and (14), we obtain that a linear combination \( u = c_1 u_1 + c_2 u_2 \) satisfies the following conditions at \( a \):

\[ u(a) = c_1 u_0(a) \quad \text{and} \quad u'(a) = c_1 u_0'(a) + c_2/(u_0(a)p(a)). \]

Thus, in order that \( u \) satisfy (22), the constants \( c_1 \) and \( c_2 \) must satisfy the equation

\[ c_1 (u_0(a) \cos \alpha + u_0'(a) \sin \alpha) + c_2 \left( \frac{\sin \alpha}{u_0(a)p(a)} \right) = 0, \]

which gives \( c_2 = \gamma c_1 \) when \( \alpha \neq \pi n \), with \( \gamma = -u_0(a)p(a)(u_0(a) \cot \alpha + u_0'(a)) \), whereas \( c_1 = 0 \) when \( \alpha = \pi n \). In the latter case, we have that if an eigenfunction of the problem for a given \( \lambda \) exists up to a multiplicative constant, it must have a form \( u = u_2 \). The second boundary condition (23) together with (20) leads to the following characteristic equation for the eigenvalues

\[ \cos \beta u_0(b) \sum_{k=0}^{\infty} \lambda^k X^{(2k+1)}(b) + \sin \beta \left( u_0'(b) \sum_{k=0}^{\infty} \lambda^k X^{(2k+1)}(b) + \frac{1}{u_0(b)p(b)} \sum_{k=0}^{\infty} \lambda^k X^{(2k)}(b) \right) = 0, \]

which is the same to

\[ \sum_{k=0}^{\infty} \lambda^k \left( X^{(2k+1)}(b) \cos \beta u_0(b) + \sin \beta u_0'(b) + \frac{\sin \beta}{u_0(b)p(b)} X^{(2k)}(b) \right) = 0. \]  

(24)

Thus, the Sturm–Liouville problem (21)–(23) in the case \( \alpha = \pi n \) reduces to find zeros of the analytic function \( \sum_{k=0}^{\infty} a_k \lambda^k \) where the Taylor coefficients \( a_k \) have the form \( a_k = X^{(2k+1)}(b) \cos \beta u_0(b) + \sin \beta u_0'(b) + \frac{\sin \beta}{u_0(b)p(b)} X^{(2k)}(b) \).

Now let us suppose \( \alpha \neq \pi n \). Then the boundary condition (23) implies that

\begin{align*}
(u_0(b) \cos \beta + u_0'(b) \sin \beta) \left( \sum_{k=0}^{\infty} \lambda^k \tilde{X}^{(2k)}(b) + \gamma \sum_{k=0}^{\infty} \lambda^k X^{(2k+1)}(b) \right) ^{\gamma} \sum_{k=0}^{\infty} \lambda^k \tilde{X}^{(2k-1)}(b) + \gamma \sum_{k=0}^{\infty} \lambda^k X^{(2k)}(b) = 0.
\end{align*}

(25)

Thus, the spectral problem (4), (22), and (23) reduces to the problem of calculating zeros of the analytic function \( \kappa(\lambda) = \sum_{m=0}^{\infty} a_m \lambda^m \)

where

\[ a_0 = (u_0(b) \cos \beta + u_0'(b) \sin \beta)(1 + \gamma X^{(1)}(b)) + \frac{\gamma \sin \beta}{u_0(b)p(b)}. \]
function exists, it necessarily coincides with spectral parameter dependent boundary conditions. In any case, the knowledge of an explicit characteristic Equation (27) for the additional (or on the contrary less) zeros whenever

\[ \beta_1 u(b) - \beta_2 u'(b) = \psi(\lambda) \left( \beta_1 u(b) - \beta_2 u'(b) \right), \tag{26} \]

where \( \psi \) is a complex-valued function of the variable \( \lambda \) and \( \beta_1, \beta_2, \beta_1', \beta_2' \) are complex numbers. For some special forms of the function \( \psi \) such as \( \psi(\lambda) = \lambda \) or \( \psi(\lambda) = \lambda^2 + c_1 \lambda + c_2 \), results were obtained [35], [38] concerning the regularity of the problem (21), (22), and (26); we will not dwell upon the details. In general, the presence of the spectral parameter in boundary conditions introduces additional considerable difficulties both in theoretical and numerical analysis of the problems. Nevertheless, the SPPS approach gives a simple and natural insight into the problem, and its practical application for numerical calculations is not in fact more difficult than in the previously considered situation of \( \lambda \)-independent boundary conditions.

For simplicity, let us suppose that \( a = 0 \) and hence the condition (22) becomes \( u(a) = 0 \). Then, as was shown earlier, if an eigenfunction exists, it necessarily coincides with \( u_2 \) up to a multiplicative constant. In this case, condition (26) becomes equivalent to the equality [7]

\[ (u_0(b)\psi_1(\lambda) - u_0'(b)\psi_2(\lambda)) \sum_{k=0}^{\infty} \lambda^{2k} X^{(2k+1)}(b) - \frac{\psi_2(\lambda)}{u_0(b)p(b)} \sum_{k=0}^{\infty} \lambda^{2k} X^{(2k)}(b) = 0, \tag{27} \]

where \( \psi_{1,2}(\lambda) = \beta_{1,2} - \beta_{1,2}' \psi(\lambda) \). Calculation of eigenvalues given by (27) is especially simple in the case of \( \psi \) being a polynomial of \( \lambda \). Precisely, this particular situation was considered in all of the aforementioned references concerning Sturm–Liouville problems with spectral parameter dependent boundary conditions. In any case, the knowledge of an explicit characteristic Equation (27) for the spectral problem (21), (22), and (26) makes possible its accurate and efficient solution.

The papers [7], [27], [1] contain several numerical tests corresponding to a variety of computationally difficult problems. All they reveal is an excellent performance of the SPPS method. We do not review them here. Instead, we consider an interesting example from [1], a Sturm–Liouville problem admitting complex eigenvalues.

**Example 3.1**

[1]

\[
\begin{align*}
\psi' + \lambda^2 \psi - i \lambda x \psi &= 0, \\
\psi(0) &= 0, \quad \psi'(1) + i \lambda \psi(1) - \lambda^2 \psi(1) = 0.
\end{align*}
\tag{28}
\]

With the aid of **MATHEMATICA** (Wolfram) software, the exact characteristic equation of the problem was found

\[
\beta \left( i \lambda \right)^{k/3} \left( i \lambda + 1 \right) \left( i \lambda + 1 \sqrt{i \lambda} \right) - \lambda \left( i \lambda + 1 \sqrt{i \lambda} \right) + \beta \left( i \lambda \right)^{k/3} \left( i \lambda + 1 \right) \left( i \lambda + 1 \sqrt{i \lambda} \right) - \lambda \left( i \lambda + 1 \sqrt{i \lambda} \right) = 0,
\tag{29}
\]

where \( \beta \) are the Airy functions. In Table 1, we present the approximate eigenvalues produced by the SPPS method [1] with \( N = 100 \) and with the use of the spectral shift technique (introduced in [7]), the exact eigenvalues obtained from the characteristic equation (29) with the help of Mathematica’s function `FindRoot` and the absolute errors of the approximate eigenvalues compared.
to the exact ones. The eigenvalues are symmetric with respect to the imaginary axis, so we included only the eigenvalues with the positive real part. Note that our method allows one to obtain more eigenvalues; however, Mathematica was unable to find more zeros of the characteristic equation.

4. Periodic potentials: Floquet–Bloch solutions and Hill’s discriminant

Toward the end of the 19th century, Hill [39] and Floquet [40] initiated the rigorous study of the spectral properties of Sturm–Liouville operators with real periodic coefficients. In 1883, Floquet established Floquet’s theorem asserting that every solution is a linear superposition of independent solutions, both of the form of exponential factors multiplied by periodic functions, while Hill’s work published in 1877 in Cambridge, Massachusetts, and reprinted in Europe in 1886, deals with a special component of the motion of the lunar perigee. Other fundamental results concerning the sequence of eigenvalues have been obtained by Lyapunov in 1902 [41]. The paper of Hill made this class of equations of interest for many authors, and the term Hill equations has been commonly used since about a century for second-order linear DEs with periodic coefficients, in particular for $y'' + f(t)y = 0$ with $f(t)$ a periodic function.

In this section, we consider the Sturm–Liouville equation

$$ -(p(x)f''(x, \lambda))' + q(x)f(x, \lambda) = \lambda f(x, \lambda). \tag{30} $$

assuming that $p(x) > 0$, $p'(x)$ and $q(x)$ are real-valued continuous bounded periodic functions of period $T$, $x \in \mathbb{R}$.

For each $\lambda$, there exists a fundamental system of solutions, that is, two linearly independent solutions of (30) $f_1(x, \lambda)$ and $f_2(x, \lambda)$, which satisfy the initial conditions

$$ f_1(0, \lambda) = 1, \quad f'_1(0, \lambda) = 0, \quad f_2(0, \lambda) = 0, \quad f'_2(0, \lambda) = 1. \tag{31} $$

The following expression is known as Hill’s discriminant

$$ D(\lambda) = f_1(T, \lambda) + f'_2(T, \lambda). $$

The values of $\lambda$ for which $|D(\lambda)| \leq 2$ form the allowed bands or stability intervals; meanwhile, the values of $\lambda$ such that $|D(\lambda)| > 2$ belong to forbidden bands or instability intervals (see, e.g., [42]). The band edges (values of $\lambda$ such that $|D(\lambda)| = 2$) correspond to such values of the spectral parameter $\lambda$ for which there exist regular nontrivial solutions of (30) satisfying either the periodic boundary conditions ($D(\lambda) = 2$)

$$ f(0, \lambda) = f(T, \lambda), \quad f'(0, \lambda) = f'(T, \lambda), \tag{32} $$

or the antiperiodic (semi-periodic) boundary conditions ($D(\lambda) = -2$)

$$ f(0, \lambda) = -f(T, \lambda), \quad f'(0, \lambda) = -f'(T, \lambda). $$

They are called eigenvalues and form an infinite sequence $\lambda_0 < \lambda_1 \leq \lambda_2 < \lambda_3...$ An important property of the minimal eigenvalue $\lambda_0$ is the existence of a corresponding periodic nodeless (nonvanishing) solution $f_0(x, \lambda_0)$ [42].

For $|D(\lambda)| \leq 2$, besides the computation of the eigenvalues and corresponding eigenfunctions, one of the important tasks is the construction of Bloch (sometimes called quasiperiodic) solutions (see, e.g., [42, 43]). They are solutions of (30) such that

$$ f(x + T, \lambda) = \beta f(x, \lambda), \quad x \in \mathbb{R}, $$

where $\beta$ are complex numbers, known as Floquet multipliers, satisfying the quadratic equation

$$ \beta^2 - D(\lambda) \beta + 1 = 0. $$

| $n$ | $\lambda_n$ (Our method) | $\lambda_n$ (Exact) | Absolute error |
|---|---|---|---|
| 1 | 0.724600759561354 + 0.4655129753730082i | 0.724600759561355 + 0.465512975730082i | 1.1 · 10^-15 |
| 2 | 3.41348175703277 + 0.260973728680318i | 3.41348175703277 + 0.260973728680321i | 2.1 · 10^-15 |
| 3 | 6.43085017426924 + 0.255763443512501i | 6.43085017426926 + 0.255763443512497i | 2.4 · 10^-14 |
| 4 | 9.52497224975746 + 0.252665874553727i | 9.52497224975755 + 0.252666587455373i | 3.8 · 10^-14 |
| 5 | 12.6419970813013 + 0.251521276777511i | 12.6419970813014 + 0.251521276777512i | 4.8 · 10^-14 |
| 7 | 18.9002072286181 + 0.250683194824278i | 18.9002072286181 + 0.250683194824283i | 2.5 · 10^-14 |
| 10 | 28.3081715202515 + 0.250305064462683i | 28.3081715202511 + 0.250305060446279i | 3.4 · 10^-13 |
| 15 | 44.0040711901387 + 0.250126347925522i | 44.0040711901389 + 0.250126347925564i | 2.4 · 10^-13 |
| 20 | 59.7063095058408 + 0.250068647436092i | 59.7063095058413 + 0.250068647435942i | 5.8 · 10^-13 |

Table I. The eigenvalues of the problem (28) (Example 3.1).
In this paper, we use the matching procedure from [44] for which the main ingredient is the pair of solutions \( f_1(x, \lambda) \) and \( f_2(x, \lambda) \) of (30) satisfying conditions (31). Namely, using \( f_1(x, \lambda) \) and \( f_2(x, \lambda) \), one obtains the quasiperiodic solutions \( f_\pm(x + T) = \beta_\pm f_\pm(x) \) as follows:

\[
f_\pm(x, \lambda) = \beta_\pm^{n_0} F_\pm(x - nT, \lambda), \quad \begin{cases} nT \leq x < (n + 1)T \\ n = 0, \pm1, \pm2, \ldots \end{cases}
\]

(33)

where \( F_\pm(x, \lambda) \) are the so-called self-matching solutions, which are the following linear combinations of the algebraic equation \( f_\pm(T, \lambda) \alpha^2 + (f_2(T, \lambda) \lambda - f_1(T, \lambda)) \alpha - f_1(T, \lambda) = 0 \). The Floquet multipliers \( \beta_\pm \) are a measure of the rate of increase (or decrease) in magnitude of the self-matching solutions \( F_\pm(x, \lambda) \) when one goes from the left end of the cell to the right end, that is, \( \beta_\pm(\lambda) = \frac{F_\pm(T, \lambda)}{F_\pm(0, \lambda)} \). The values of \( \beta_\pm \) are directly related to the Hill discriminant, \( \beta_\pm(\lambda) = \frac{1}{2} (D(\lambda) \pm \sqrt{D^2(\lambda) - 4}) \), and obviously at the band edges \( \beta_+ = \beta_- = \pm 1 \) for \( D(\lambda) = \pm 2 \), correspondingly.

In the rest of this section, we briefly describe our recent result [8] of expressing the Hill discriminant in terms of SPPS.

4.1. The spectral parameter power series representation of Hill’s discriminant

The SPPS construction method of the solutions \( f_1(x, \lambda) \) and \( f_2(x, \lambda) \) satisfying the initial conditions (31) is based on the knowledge of one non-vanishing particular solution \( f_0(x, \lambda) \) bounded on \([0, T]\) together with \( f_0(T, \lambda) = f_0(0, \lambda) \). In the case of Hill’s equation, the first eigenvalue \( \lambda_0 \) generates a nodeless periodic eigenfunction \( f_0(x, \lambda_0) \). In what follows, we initially suppose that the value of \( \lambda_0 \) is known. Note that it can be obtained by different methods including the same SPPS method [7] as we explain in Section 4.5.

Given \( \lambda_0 \), we proceed in three steps in order to obtain the representation of Hill’s discriminant:

- The first one is the construction of a particular nodeless solution \( f_0(x, \lambda_0) \), which is periodic, that is, \( f_0(x + T, \lambda_0) = f_0(x, \lambda_0) \).
- The second one is the construction of the fundamental system of solutions \( f_1(x, \lambda) \) and \( f_2(x, \lambda) \) for all values of the parameter \( \lambda \).
- The final step is obtaining the representation of Hill’s discriminant.

We detail each of the steps in the following subsections.

4.2. The nodeless periodic solution

We want to obtain the nodeless periodic solution \( f_0(x, \lambda_0) \) for \( \lambda = \lambda_0 \) of the equation

\[
- \left( \frac{p(x)f_0(x)}{f_0(x)} \right)' + q(x)f_0(x) = \lambda_0 f_0(x).
\]

(34)

To achieve this goal, we first have to construct in SPPS form the fundamental system of solutions of (34). These solutions are not necessarily periodic. However, one can follow the old procedure of James [44] allowing to obtain from \( f_{0,1}(x, \lambda_0) \) and \( f_{0,2}(x, \lambda_0) \) the Floquet type solutions, which degenerate to a single periodic solution \( f_0(x, \lambda_0) \) because \( \lambda_0 \) represents a band edge.

The functions \( f_{0,1}(x, \lambda_0) \) and \( f_{0,2}(x, \lambda_0) \) can be calculated according to iteration formulas of the type (17)–(19)

\[
f_{0,1}(x, \lambda_0) = \sum_{n=0}^{\infty} X_0^{(n)}(x) \quad \text{and} \quad f_{0,2}(x, \lambda_0) = p(0) \sum_{n=1}^{\infty} X_0^{(n)}(x),
\]

(35)

where

\[
X_0^{(0)}(x) = 1, \quad X_0^{(0)} = 1,
\]

\[
X_0^{(n)}(x) = \begin{cases} \frac{f_0(x)}{f_0(0)} X_0^{(n-1)}(x) q(x) - \lambda_0 X_0^{(n-1)} d^2_{\xi} & \text{for an odd } n \\ \frac{f_0(x)}{f_0(0)} X_0^{(n-1)}(x) \frac{1}{p(\xi)} d^2_{\xi} & \text{for an even } n \end{cases}
\]

\[
X_0^{(n)}(x) = \begin{cases} \frac{f_0(x)}{f_0(0)} X_0^{(n-1)}(x) q(x) - \lambda_0 X_0^{(n-1)} d^2_{\xi} & \text{for an odd } n \\ \frac{f_0(x)}{f_0(0)} X_0^{(n-1)}(x) \frac{1}{p(\xi)} d^2_{\xi} & \text{for an even } n \end{cases}
\]

The periodic nodeless solution of (34) is constructed as a particular case of a quasi-periodic solution (33), essentially as a self-matching solution, that is,

\[
f_0(x, \lambda_0) = f_{0,1}(x - nT, \lambda_0) + \alpha f_{0,2}(x - nT, \lambda_0),
\]

(36)

\[
\begin{cases} nT \leq x < (n + 1)T \\ n = 0, 1, 2, \ldots \end{cases}
\]

because the Floquet phase multiplier is \( \beta = 1 \) in the periodic case and \( \alpha = \frac{f_{0,1}(T, \lambda_0) - f_{0,2}(T, \lambda_0)}{d_{0,2}(T, \lambda_0)} \), see [44].
4.3 \ Fundamental system of solutions

Once having the function \( f_0(x, \lambda_0) \), the solutions \( f_1(x, \lambda) \) and \( f_2(x, \lambda) \) for all values of the parameter \( \lambda \) can be given using the SPPS method once again

\[
\begin{align*}
 f_1(x, \lambda) &= \frac{f_0(x)}{f_0(0)} \Sigma_0(x, \lambda, \lambda_0) + p(0)f_0'(0)f_0(x)\Sigma_1(x, \lambda, \lambda_0), \\
 f_2(x, \lambda) &= -p(0)f_0(0)f_0(x)\Sigma_1(x, \lambda, \lambda_0).
\end{align*}
\] (37)

The SPPS summations \( \Sigma_0 \) and \( \Sigma_1 \) have the following expressions:

\[
\begin{align*}
 \Sigma_0(x, \lambda, \lambda_0) &= \sum_{n=0}^{\infty} \hat{X}^{(2n)}(\lambda - \lambda_0)^n, \\
 \Sigma_1(x, \lambda, \lambda_0) &= \sum_{n=1}^{\infty} X^{(2n-1)}(\lambda - \lambda_0)^{n-1},
\end{align*}
\] (38)

where the coefficients \( \hat{X}^{(n)}(x) \), \( X^{(n)}(x) \) are given by the recursive relations

\[
\begin{align*}
 \hat{X}^{(0)} &= 1, \quad X^{(0)} = 1, \\
 \hat{X}^{(n)}(x) &= \left\{ \begin{array}{ll}
 f_0^2(x) & \text{for odd } n \\
 \int_0^x \hat{X}^{(n-1)}(\xi)f_0'(\xi)d\xi & \text{for even } n
\end{array} \right., \\
 X^{(n)}(x) &= \left\{ \begin{array}{ll}
 -f_0^2(x) & \text{for odd } n \\
 \int_0^x X^{(n-1)}(\xi)f_0'(\xi)d\xi & \text{for even } n,
\end{array} \right.
\end{align*}
\] (39) (40)

which are identical to Equations (8)–(10) unless for obvious sign changes.

One can check by a straightforward calculation that the solutions \( f_1 \) and \( f_2 \) fulfill the initial conditions (31). Having obtained the fundamental system of solutions for any value of \( \lambda \), one can apply the construction (33) in order to obtain the Bloch solutions, which become eigenfunctions for \( \lambda \) being eigenvalues.

4.4 \ Hill's discriminant in spectral parameter power series form

We are ready now to write the Hill discriminant \( D(\lambda) = f_1(T, \lambda) + f_2'(T, \lambda) \) in a simple explicit form using the SPPS expressions of \( f_1(T, \lambda) \) and \( f_2'(T, \lambda) \) in (37)

\[
\begin{align*}
 D(\lambda) &= \frac{f_0(T)}{\hat{f}_0(0)} \Sigma_0(T, \lambda, \lambda_0) + \frac{f_0(0)}{\hat{f}_0(T)} \Sigma_0(T, \lambda, \lambda_0) \\
 &\quad + \left( f_0'(0)f_0(T) - f_0(0)f_0'(T) \right)p(0)\Sigma_1(T, \lambda, \lambda_0)
\end{align*}
\] (41)

where \( \Sigma_0 \) and \( \Sigma_1 \) are defined by (38) and \( \Sigma_0(x, \lambda, \lambda_0) = \sum_{n=0}^{\infty} \hat{X}^{(2n)}(x)(\lambda - \lambda_0)^n \).

Finally, taking into account that \( f_0 \) is a \( T \)-periodic function and writing the explicit expressions for \( \Sigma_0(T, \lambda, \lambda_0) \) and \( \Sigma_0(T, \lambda, \lambda_0) \), we obtain a representation for Hill's discriminant associated with (30)

\[
D(\lambda) = \sum_{n=0}^{\infty} \left( \hat{X}^{(2n)}(T) + X^{(2n)}(T) \right)(\lambda - \lambda_0)^n.
\] (42)

Thus, only one particular nodeless and periodic solution \( f_0(x, \lambda_0) \) of (30) is needed for constructing the associated Hill discriminant. We formulate the result (42) as the following theorem.

Theorem 2

Let \( \lambda_0 \) be the lowest eigenvalue of the periodic Sturm–Liouville problem (30), (32) and \( f_0(x, \lambda_0) \) be the corresponding eigenfunction. Then the Hill discriminant for (30) has the form (42) where \( \hat{X}^{(2n)} \) and \( X^{(2n)} \) are calculated according to (39) and (40), and the series converges uniformly on any compact set of values of \( \lambda \).

To illustrate the formula (42), we consider a simple example. Let \( q(x) = 0, p(x) = 1 \) in Equation (30). It is easy to see that the associated discriminant is \( D(\lambda) = 2 \cos \sqrt{T} \lambda \), from where we obtain \( \lambda_0 = 0 \) and a corresponding non-trivial periodic solution is
Now making use of this solution, we construct the discriminant by means of the formula (42). The coefficients \(\tilde{\chi}^{(2n)}(T)\) and \(\chi^{(2n)}(T)\) given by (39) and (40) take the form

\[
\tilde{\chi}^{(2n)}(T) = \chi^{(2n)}(T) = (-1)^n \frac{T^{2n}}{(2n)!}, \quad n = 0, 1, 2, \ldots
\]

The substitution in (42) gives \(D(\lambda) = 2 \cos \sqrt{\lambda} T\).

### 4.5 Construction of the first eigenvalue \(\lambda_0\) by the spectral parameter power series method

Notice that in the expression (41) for \(D(\lambda)\) and in all reasonings previous to it, we do not use the periodicity of the solution \(f_0(x, \lambda_0)\), therefore (41), and the whole procedure for obtaining it are valid for any \(\lambda_+\) such that there exists a corresponding solution \(f_s(x, \lambda_+)\), which is bounded on \([0, T]\) together with \(1/(pf_s')\). Such a solution \(f_s(x, \lambda_+)\) can be obtained in the following way:

\[
f_s(x, \lambda_+) = f_{s,1}(x, \lambda_+) + if_{s,2}(x, \lambda_+)
\]

where \(f_{s,1}(x, \lambda_+)\) and \(f_{s,2}(x, \lambda_+)\) are given by (35) with \(\lambda_+\) instead of \(\lambda_0\). For more details, see [6]. The pair of the independent solutions \(f_1(x, \lambda)\) and \(f_2(x, \lambda)\) of (30) given by (37) of course is independent of the choice of the solution \(f_0(x, \lambda_0)\); hence, instead of \(f_0(x, \lambda_0)\) in (41), one can take \(f_s(x, \lambda_+)\) given by (43). Thus, in terms of \(f_s(x, \lambda_+)\) where \(\lambda_+\) is essentially arbitrary, \(D(\lambda)\) can be represented as a series in powers of \((\lambda - \lambda_+)\)

\[
D(\lambda) = \sum_{n=0}^{\infty} \left( \frac{f_s(T)}{f_s(0)} \tilde{\chi}^{(2n)}(T) + \frac{f_s(0)}{f_s(T)} \chi^{(2n)}(T) + \left( f_s'(0)f_s(T) - f_s(0)f_s'(T) \right) p(0)\chi^{(2n+1)}(T) \right) (\lambda - \lambda_+)^n.
\]

Now the band edge \(\lambda_0\) required for the formula (42) can be calculated as a first zero of the expression \(D(\lambda) - 2\) where \(D(\lambda)\) is given by (44). For the numerical purpose, it can be useful to know the interval containing \(\lambda_0\). Because \(q\) is a bounded periodic function, there is a number \(\Lambda\) that satisfies the inequality \(q(x) > \Lambda, \forall x \in \mathbb{R}\). It is known [43] that \(D(\lambda) > 2\) for all \(\lambda \leq \Lambda\); therefore, the lower estimate for \(\lambda_0\) is the following:

\[
\lambda_0 \geq \min q(x).
\]

The upper bound can be obtained considering the Rayleigh quotient for periodic problems [45]

\[
\lambda_0 \leq \frac{\int_0^T (p(x)(u'(x))^2 + q(x)(u(x))^2) \, dx}{\int_0^T (u(x))^2 \, dx},
\]

where \(u \in C^2[0, T]\) is periodic with period \(T\). The equality occurs if and only if \(u\) is an eigenfunction corresponding to \(\lambda_0\).

### 4.6 Hill’s discriminant of the supersymmetric (SUSY)-related equation

In this subsection, we consider the supersymmetric (SUSY) partner equation of Equation (30) and write down the SPPS form of its solutions. The latter allow us to prove the equality between the Hill discriminants of Equation (30) and its SUSY-related Equation (47). For various aspects of SUSY periodic problems, see [46–48].

The left-hand side of Equation (30) can be factorized in the following way [49]:

\[
\left(-d_x p^{\frac{1}{2}}(x) + \Phi(x)\right) \left(p^{\frac{1}{2}}(x) d_x + \Phi(x)\right) f(x),
\]

where \(d_x\) means the \(x\)-derivative, the superpotential \(\Phi(x)\) is defined as follows \(\Phi(x) = -p^{\frac{1}{2}}(x) \frac{\partial (q(x, \lambda_0))}{\partial (q, \lambda_0)}\). Using this factorization, the coefficient \(q(x)\) can be expressed as

\[
q(x) = \Phi'(x) - \left(p^{\frac{1}{2}}(x) \Phi(x)\right)' + \lambda_0.
\]

Introducing the following Darboux transformation,

\[
\left(p^{\frac{1}{2}}(x) d_x + \Phi(x)\right) f(x, \lambda) = \tilde{f}(x, \lambda),
\]

one obtains the equation supersymmetrically related to Equation (30)

\[
\left(p^{\frac{1}{2}}(x) d_x + \Phi(x)\right) \left(-d_x p^{\frac{1}{2}}(x) + \Phi(x)\right) \tilde{f}(x, \lambda) = \lambda \tilde{f}(x, \lambda),
\]

which can be written as follows:

\[
-d_x(p(x)d_x \tilde{f}(x, \lambda)) + \tilde{q}(x) \tilde{f}(x, \lambda) = \lambda \tilde{f}(x, \lambda),
\]

\[\text{Math. Meth. Appl. Sci. 2015, 38 1945–1969}\]
where \( \tilde{q}(x) \) is the SUSY partner of the coefficient \( q(x) \) given by

\[
\tilde{q}(x) = q(x) + 2p^\frac{1}{2}(x)\Phi'(x) - p^\frac{3}{2}(x) \left( p^\frac{1}{2}(x) \right)''.
\]

(48)

It is worth noting that as \( \Phi(x) \) is a \( T \)-periodic function, the Darboux transformation assures the \( T \)-periodicity of \( \tilde{q}(x) \). In addition, when \( p(x) \) is a constant, the SL coefficient \( q \) is a quantum-mechanical potential, while \( \tilde{q}(x) \) is its Darboux counterpart also termed as a SUSY partner in quantum mechanics.

The pair of linearly independent solutions \( \tilde{f}_1(x, \lambda) \) and \( \tilde{f}_2(x, \lambda) \) of (47) can be obtained directly from the solutions (37) by means of the Darboux transformation (46). We additionally take the linear combinations in order that the solutions \( \tilde{f}_1(0, \lambda) = \tilde{f}_2(0, \lambda) = 1 \) and \( \tilde{f}_1(0, \lambda) = \tilde{f}_2(0, \lambda) = 0 \)

\[
\tilde{f}_1(x, \lambda) = \frac{p^\frac{1}{2}(0)f_0(0)}{\lambda - \lambda_0} \Sigma_0(x, \lambda) \left( \frac{\left[ p^\frac{1}{2}(x) \right]'_{|x=0} - \Phi(0)}{(\lambda - \lambda_0)f_0(0)p^\frac{1}{2}(x)f_0(x)} \right) \Sigma_1(x, \lambda),
\]

(49)

\[
\tilde{f}_2(x, \lambda) = \frac{p^\frac{1}{2}(0)/(\lambda - \lambda_0)f_0(0)p^\frac{1}{2}(x)f_0(x)}{\Sigma_1(x, \lambda)}.
\]

(50)

These two solutions allow us to write the expression for Hill's discriminant associated to Equation (47), which is

\[
\tilde{D}(\lambda) = \tilde{f}_1(T, \lambda) + \tilde{f}_2(T, \lambda).
\]

This requires the expression of the derivative of \( f_j(x, \lambda_0) \) and evaluating it for \( x = T \). In addition, one should notice that as the functions \( f_0(x, \lambda_0) \) and \( p(x) \) are \( T \)-periodic, that is, \( f_0(T, \lambda_0) = f_0(0, \lambda_0) \) and \( p(0) = p(T) \), then obviously, the functions \( f_0'^{\frac{1}{2}}(x, \lambda_0), p^\frac{1}{2}(x) \) and \( [p^\frac{1}{2}(x)]' \) possess the same properties. The result is [8]

\[
\tilde{D}(\lambda) = \Sigma_0(T, \lambda) + \Sigma_0(T, \lambda) + \left( \frac{\left[ p^\frac{1}{2}(x) \right]'_{|x=0} - \Phi(0)}{(\lambda - \lambda_0)f_0(0, \lambda_0)p^\frac{1}{2}(T)f_0(0, \lambda_0)} \right) \tilde{\Sigma}_1(T, \lambda).
\]

(51)

The substitution \( \Phi(0) = -p^\frac{1}{2}(0)f_0'^{\frac{1}{2}}(0, \lambda_0) \) clearly shows that the expression in brackets vanishes leading to the simple formula

\[
\tilde{D}(\lambda) = \Sigma_0(T, \lambda) + \tilde{\Sigma}_0(T, \lambda) = \sum_{n=0}^{\infty} \left( \tilde{q}^{(2n)}(T) + q^{(2n)}(T) \right) (\lambda - \lambda_0)^n,
\]

which is identical to (42) and therefore

\[
D(\lambda) \equiv \tilde{D}(\lambda).
\]

(51)

Thus, we can make the following statement.

**Theorem 3**

Let \( \lambda_0 \) be the first eigenvalue of the problem (30), (32) and \( f_0(x, \lambda_0) \) the corresponding \( T \)-periodic nodeless eigenfunction. Then the Darboux transformation (46) with \( \Phi(x) = -p^\frac{1}{2}(x)f_0'^{\frac{1}{2}}(0, \lambda_0) \) leads to a SUSY-related Equation (47) with the preservation of the Hill discriminant, that is, Equation (51) holds.

From the identity of discriminants (51), it is clear that \( \lambda_0 \) gives rise to a nodeless periodic solution \( \tilde{f}_0(x, \lambda_0) \) of Equation (47). Taking \( \lambda = \lambda_0 \) in (49) and (50), we obtain this eigenfunction in the form

\[
\tilde{f}_0(x, \lambda_0) = \frac{1}{p^\frac{1}{2}(x)f_0(0, \lambda_0)}.
\]

Notice that the factorization method can be applied to Equation (47) with the superpotential \( \Phi_1(x) = -p^\frac{1}{2}(x)f_0'^{\frac{1}{2}}(0, \lambda_0) \), in which case, we obtain the representation

\[
\tilde{q} = \Phi_1^\frac{1}{2}(x) - \left( p^\frac{1}{2}(x)\Phi_1(x) \right)' + \lambda_0,
\]

which reduces to the equality (48) if one notices the relationship \( \Phi_1(x) = \left( p^\frac{1}{2}(x) \right)' - \Phi(x) \). It can be also shown that \( \tilde{q} = \tilde{q}(x) + 2p^\frac{1}{2}(x)\Phi'(x) - p^\frac{3}{2}(x) \left( p^\frac{1}{2}(x) \right)'' \) is the superpartner of \( q(x) \). Thus, the Darboux transformation (46) with the superpotential \( \Phi_1(x) \) applied to Equation (47) does not produce a different potential.

### 4.7. Numerical calculation of the eigenvalues based on Hill's discriminant in spectral parameter power series form

As was mentioned in the beginning of this section, the zeros of the functions \( D(\lambda) \pm 2 \) represent eigenvalues of the corresponding periodic and antiperiodic Sturm–Liouville problems. In this section, we show that besides other possible applications, the representation (42) gives us an efficient tool for their calculation.
The first step of the numerical realization of the method consists in the calculation of the minimal eigenvalue $\lambda_0$ by means of the procedure given in Section 4.5 and subsequently in construction of the corresponding nodeless periodic solution $f_0(x, \lambda_0)$ using formula (36). The next step of the algorithm is to compute the functions $\tilde{X}^{(n)}$ and $X^{(n)}$ given by (39) and (40), respectively. This construction is based on the eigenfunction $f_0(x, \lambda_0)$. Finally, by truncating the infinite series for $D(\lambda)$ in (42), we obtain a polynomial in $\lambda - \lambda_0$

$$D_N(\lambda) = \sum_{n=0}^{N} \left( \tilde{X}^{(2n)}(T) + X^{(2n)}(T) \right) (\lambda - \lambda_0)^n = 2 + \sum_{n=1}^{N} \left( \tilde{X}^{(2n)}(T) + X^{(2n)}(T) \right) (\lambda - \lambda_0)^n. \quad \text{(52)}$$

The roots of the polynomials $D_N(\lambda) \pm 2$ give us eigenvalues corresponding to Equation (30) with periodic and antiperiodic boundary conditions.

As an example, we consider the Mathieu equation with the following coefficients:

$$\rho(x) = 1, \quad q(x) = 2r \cos 2x.$$ 

The algorithm was implemented in Matlab 2006. The recursive integration required for the construction of $\tilde{X}^{(n)}$, $X^{(n)}$, and $\tilde{X}^{(n)}$ was performed by representing the integrand through a cubic spline using the spapi routine with a division of the interval $[0, T]$ into 7000 subintervals and integrating using the finint routine. Next, the zeros of $D_N(\lambda) \pm 2$ were calculated by means of the fnzeros routine.

In Table II, the Mathieu eigenvalues were calculated employing the SPPS representation (42) for two values of the parameter $r$. For comparison, the same eigenvalues from the National Bureau of Standards tables are also displayed [50].

Figures 1 and 2 display the plots of the calculated Hill discriminants for two values of the Mathieu parameter. A SUSY Mathieu potential can be written in terms of the even Mathieu cosine function as follows [51]:

$$V_2 = 2 \left( \frac{d_x C_e(\lambda_0, r, x)}{C_e(\lambda_0, r, x)} \right)^2 + 2\lambda_0 - 2r \cos(2x), \quad \text{(53)}$$

and has the same Hill discriminants for identical values of the parameter $r$.

As another example, consider the potential

$$V_1 = \frac{\xi^2}{8} (1 - \cos 4x) - 3\xi \cos 2x, \quad \text{(54)}$$

which belongs to the quasi-exactly solvable family of the so-called trigonometric Razavy potentials [52]. The parameter $\xi$ is a positive real number. In Table III, the Razavy eigenvalues were calculated employing the SPPS representation (42) for two different values of the parameter $\xi$. For comparison, we use the eigenvalues given by Razavy analytically in terms of the parameter $\xi$ as follows [52]:

$$\lambda_0 = 2 \left(1 - \sqrt{1 + \xi^2}\right), \quad \lambda_3 = 4, \quad \lambda_4 = 2 \left(1 + \sqrt{1 + \xi^2}\right).$$

### Table II. $\lambda_n$ for the Mathieu Hamiltonian.

| $n$ | $\lambda_n$ (SPPS) | $\lambda_n$ (NBS) | $n$ | $\lambda_n$ (SPPS) | $\lambda_n$ (NBS) |
|-----|---------------------|---------------------|-----|---------------------|---------------------|
| 0   | -0.455139055973837 | -0.45513860         | 0   | -5.800045777242780  | -5.80004602         |
| 1   | -0.110248420387377 | -0.11024882         | 1   | -5.790080596840196  | -5.79008060         |
| 2   | 1.85910170521687   | 1.85910807          | 2   | 1.8581904384309548  | 1.8581754           |
| 3   | 3.917024962694820  | 3.91702477          | 3   | 2.099460384254221   | 2.09946045          |
| 4   | 4.371299312651704  | 4.37130098          | 4   | 7.449142541577460   | 7.44910974          |
| 5   | 9.047736927007582  | 9.04773926          | 5   | 9.236272731534002   | 9.236272731534002  |
| 6   | 9.078369587941564  | 9.07836885          | 6   | 11.548906947651728  | 11.548906947651728 |
| 7   | 16.03301884895410  | 16.03297008         | 7   | 16.648219815375526  | 16.648219815375526 |
| 8   | 16.0375039658117   | 16.03383234         | 8   | 17.096668282587867  | 17.096668282587867 |
| 9   | 25.020598536509114  | 25.02084082         | 9   | 25.510753265631860  | 25.510753265631860 |
| 10  | 25.021087773181282  | 25.02085434         | 10  | 25.55167735720167   | 25.55167735720167  |

SPPS, spectral parameter power series; NBS, National Bureau of Standards.
Figure 1. The polynomial $D_N(\lambda)$ for the Mathieu equation with the parameter $r = 1$ calculated by means of formula (52) for $N = 100$.

Figure 2. Same as in the previous figure but for $r = 5$. The first minimum goes down to $-292.0066$.

Table III. $\lambda_n$ for the Razavy Hamiltonian.

| $\xi$ | $\lambda_n$ (SPPS) | $\lambda_n$ (Reference [52]) | $\lambda_n$ (Reference [52]) |
|-------|---------------------|-----------------------------|-----------------------------|
| 0     | $-0.828430172936322$ | $-0.828427124746190$ | $0$ | $-2.472136690058546$ | $-2.472135954999580$ |
| 1     | $-0.627099642286704$ | $-2.428288532265432$ | $1$ | $3.19355954313260$ |
| 2     | $2.315154289053194$ | $2$ | $2.472170127477180$ | $6.472135954999580$ |
| 3     | $3.99994825296118$ | $4$ | $4.000042398350143$ | $4$ |
| 4     | $4.834668005757639$ | $4$ | $6.472170127477180$ | $6.472135954999580$ |
| 5     | $9.246360795065604$ | $5$ | $9.864070609921770$ |
| 6     | $9.30595768676312$ | $6$ | $10.253303565368553$ |

SPPS, spectral parameter power series.

In Figures 3 and 4, we display the plots of the Hill discriminants for the values of the Razavy parameter $\xi = 1$ and $\xi = 2$, respectively. According to our results in Section 4.6, the Hill discriminant is the same in the case of the SUSY partner potential

$$V_2 = V_1 + 4 \cos 2x \left( \frac{\xi}{2} - \frac{2A(\xi)}{\xi - A(\xi) \cos 2x} \right) + \frac{8A(\xi) \sin^2 2x}{(\xi - A(\xi) \cos 2x)^2}$$

(55)
Figure 3. The polynomial $D_N(\lambda)$ for the Razavy equation with the parameter $\xi = 1$ calculated by means of formula (52) for $N = 100$.

Figure 4. Same as in the previous figure but for $\xi = 2$. The first minimum of Hill's discriminant goes down to $-55.01$.

for the same values of the parameter $\xi$. In the latter equation, $A(\xi) = \left( 1 - \sqrt{1 + \xi^2} \right)$.

As final comments to this subsection, we believe that the calculation of the Hill discriminant through (52) offers clear numerical advantages with respect to other more complicated formulas for this important quantity provided in the literature, such as Jagerman's so-called cardinal series representation [53], the infinite determinant representation involving the Fourier coefficients of the potential as well as the spectral parameter in the book of Magnus and Winkler [42], a matrix representation whose entries are complicated phase integrals obtained by the phase-integral method used by Fröman [54], and Boumenir's representation in terms of integrals derived from the inverse spectral theory [55].

5. Spectral and transmission problems on the whole line

In this section, we consider the one-dimensional Schrödinger equation

$$Hu(x) = -u''(x) + Q(x)u(x) = \lambda u(x), \quad x \in \mathbb{R},$$

(56)

where

$$Q(x) = \begin{cases} \alpha_1, & x < 0, \\ q(x), & 0 \leq x \leq h, \\ \alpha_2, & x > h, \end{cases}$$

(57)

$\alpha_1$ and $\alpha_2$ are complex constants and $q$ is a continuous complex-valued function defined on the segment $[0, h]$. Thus, outside a finite segment, the potential $Q$ admits constant values, and at the end points of the segment, the potential may have discontinuities. We are interested in two classical problems. The first is the quantum-mechanical spectral problem; we are looking for such values of the spectral parameter $\lambda \in \mathbb{C}$ for which the Schrödinger equation possesses a solution $u$ belonging to the Sobolev space $H^2(\mathbb{R})$, which in the case of the potential of the form (57) means that we are looking for solutions exponentially decreasing at $\pm \infty$. 

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The second consists in finding the reflectance and transmittance of the inhomogeneous layer described by \( q \). We will formulate this problem in the form in which it arises in electromagnetic theory although both problems come not from one but from many different branches of physics and engineering.

5.1. Quantum-mechanical spectral problem

The eigenvalue problem (56) is one of the central in quantum mechanics for which \( H \) is a self-adjoint operator in \( L^2(\mathbb{R}) \) with the domain \( H^0(\mathbb{R}) \). It implies that \( Q \) is a real-valued function. In this case, the operator \( H \) has a continuous spectrum \( \{ \min \{ \alpha_1, \alpha_2 \}, +\infty \} \) and a discrete spectrum located on the set

\[
\left\{ \min_{x \in [0,h]} q(x), \min \{ \alpha_1, \alpha_2 \} \right\},
\]

(58)

Computation of energy levels of a quantum well described by the potential \( Q \) is a problem of physics of semiconductor nanostructures (see, e.g., [65]). Other important models that reduce to the spectral problem (56) arise in studying the electromagnetic and acoustic wave propagation in inhomogeneous waveguides (see for instance [57–63]).

Hence, in the applied problems, it is important to have effective and rapid numerical methods for the solution of the problem (56). The most frequently applied is the shooting method (see, e.g., [56]). It has well known limitations due to the intrinsic difficulties of the shooting procedure, especially when the spectral parameter as in the problem under consideration participates in the boundary conditions (see equalities (60) and (63) in the succeeding text). It is much more convenient to have an available analytical form of a solution of the problem in the form in which it arises in electromagnetic theory although both problems come not from one but from many different branches of physics and engineering.

From these relations, we obtain that the solution of (59) satisfying the initial conditions (60) has the form

\[
u(0) = 1 \quad \text{and} \quad u'(0) = \mu.
\]

(60)

This gives us the initial conditions for the solution on the interval \((0, h)\), which we will construct following Theorem 1. For that we need first a nonvanishing particular solution of the equation

\[- u''(x) + q(x)u(x) = \lambda u(x), \quad x \in (0, h),
\]

(59)

with three boundary conditions at the end points of the interval \((0, h)\) (see in the succeeding text); meanwhile, the application of the SPPS method suffers no essential changes. Our analysis follows that from [9].

For \( x < 0 \), we have to consider the equation \(- u'' + (\alpha_1 - \lambda)u = 0 \). Its solutions decreasing at \(-\infty \) exist if only \( \alpha_1 - \lambda > 0 \). Denote \( \mu = +\sqrt{\alpha_1 - \lambda} \). Then the required solution for \( x < 0 \) has the form \( u(x) = c_1 e^{\mu x} \) and the multiplicative constant can always be chosen equal to one. Thus, \( u(x) = e^{\mu x}, \quad x < 0, \) from where

\[
u(0) = 1 \quad \text{and} \quad u'(0) = \mu.
\]

(60)

which as was explained in Section 2 can be constructed by means of the same SPPS method. Indeed, formulas (16)–(19) where \( p \) should be chosen equal to \(-1 \) and \( x_0 = 0 \) give us a couple of linearly independent real-valued particular solutions \( v_1 \) and \( v_2 \) of (61). Hence (Remark 3), the required nonvanishing solution of (61) can be chosen as \( u_0 = v_1 + iv_2 \). Let us notice that as \( u_0(0) = 1 \) and \( u_0'(0) = i \), the initial conditions satisfied by the solutions of (59) \( u_1 \) and \( u_2 \) constructed according to (7) have the form

\[
u_1(0) = u_0(0) = 1, \quad u_1'(0) = u_0'(0) = i,
\]

\[
u_2(0) = 0, \quad u_2'(0) = -\frac{1}{u_0(0)} = -1.
\]

From these relations, we obtain that the solution of (59) satisfying the initial conditions (60) has the form

\[
u(x) = u_1(x) + (i - \mu)u_2(x) \quad 0 \leq x \leq h.
\]

(62)

In the region \( x > h \), the solution of Equation (56) has the form

\[
u(x) = C_1 e^{-\sqrt{\alpha_1 - \lambda} (x-h)} + C_2 e^{\sqrt{\alpha_1 - \lambda} (x-h)},
\]
from which we obtain that the existence of an eigenfunction is possible if only \( \sqrt{\alpha_2 - \lambda} \in \mathbb{R} \). Hence, \( \alpha_2 > \lambda \), and we denote \( \nu = +\sqrt{\alpha_2 - \lambda} \). Consequently, \( u(x) = Ce^{-\nu(x-h)} \) and \( u(h) = C, u'(h) = -\nu C \) where \( C \) is an arbitrary constant. Thus, the eigenvalues of the problem are such values of \( \lambda \) for which the solution (62) satisfies the condition

\[
 u'(h) + \nu u(h) = 0
\]

(63)

where, as in the preceding text, \( \nu = +\sqrt{\alpha_2 - \lambda} \) and \( \alpha_2 > \lambda \).

In order to write down the explicit form of the dispersion equation (63) in terms of the SPPS, we calculate the derivatives of the solutions of (59),

\[
u' = \frac{\nu_0}{u_0} u_1 - \frac{\lambda}{u_0} \sum_{i=0}^{\infty} \lambda^{n} \hat{x}^{(2n+1)}(1)
\]

and

\[
u' = \frac{\nu_0}{u_0} u_2 - \frac{1}{u_0} \sum_{i=0}^{\infty} \lambda^{n} \hat{x}^{(2n)}(2).
\]

Thus, the derivative of the solution (62) has the form

\[
u' = \frac{\nu_0}{u_0} u_1 - \frac{1}{u_0} \left( \sum_{i=0}^{\infty} \lambda^{n+1} \hat{x}^{(2n+1)} + (i-\mu) \sum_{i=0}^{\infty} \lambda^{n} \hat{x}^{(2n)} \right).
\]

Substituting this expression into (63), we arrive at the following result obtained in [9] and formulated here in the form of a theorem.

**Theorem 4**

Let \( \alpha_1, \alpha_2 \) be real numbers, \( q \) be a real-valued continuous function defined on \([0,h]\), and \( Q \) be defined by (57). Then \( \lambda \in \min_{x \in [0,h]} q(x), \min \{\alpha_1, \alpha_2\} \) is an eigenvalue of the problem (56) if and only if the following dispersion equation

\[
u_0(p, h) \left( \sum_{n=0}^{\infty} \lambda^{n} \hat{x}^{(2n)}(1) + (i-\mu) \sum_{n=0}^{\infty} \lambda^{n} \hat{x}^{(2n+1)}(2) \right)
\]

\[
u_0(p, h) \left( \sum_{n=0}^{\infty} \lambda^{n+1} \hat{x}^{(2n+1)}(1) + (i-\mu) \sum_{n=0}^{\infty} \lambda^{n} \hat{x}^{(2n)}(2) \right)
\]

\[
u_0(p, h) \left( \sum_{n=0}^{\infty} \lambda^{n} \hat{x}^{(2n)}(1) + (i-\mu) \sum_{n=0}^{\infty} \lambda^{n} \hat{x}^{(2n+1)}(2) \right) = 0,
\]

is satisfied and the corresponding (unique up to a multiplicative constant) eigenfunction has the form

\[
u = \begin{cases} \exp(i \lambda x), & x < 0, \\ u_1(h) + (i-\mu) u_2(h) e^{-\nu h}, & x > h, \\ \end{cases} u_1(x) + (i-\mu) u_2(x), & 0 \leq x \leq h,
\]

where \( \mu = +\sqrt{\alpha_1 - \lambda}, \nu = +\sqrt{\alpha_2 - \lambda} \) and \( u_1, u_2 \) are defined by (7) where \( u_0 \) is the nonvanishing solution of (61) on \((0,h)\) satisfying the initial conditions \( u_0(0) = 1 \) and \( u_0'(0) = i, p = -1, r = 1 \) and \( x_0 = 0 \).

All the coefficients in Equation (64): \( u_0(h), u_0'(h), X^{(1)}(h) \) and \( X^{(2)}(h) \) are easily and (as our numerical tests show) accurately obtained from the definitions introduced in the preceding text, and the roots of the dispersion equation coincide with the eigenvalues of the problem and can be found using many available methods.

In what follows, let us consider a relatively simple situation: \( \alpha_1 = \alpha_2 \). Rearranging the terms in Equation (56), this case always can be reduced to the case \( \alpha_1 = \alpha_2 = 0 \). Then \( \nu = \mu = \sqrt{-\lambda}, \mu^2 = -\lambda \) and \( \lambda^n = (-1)^n \mu^{2n} \). The dispersion equation takes the form (here, we correct some easily detectable misprints in [9])

\[
u_0(h) \left( 1 + \nu^{(1)} \right) - \frac{i}{u_0(h)}
\]

\[
+ \sum_{n=1}^{\infty} (-1)^n \mu^{2n} (u_0(h) \hat{x}^{(2n)}(1)) - \frac{1}{u_0(h)} \hat{x}^{(2n-1)}(1) + u_0(h) \hat{x}^{(2n+1)}(2)
\]

\[
- \frac{i}{u_0(h)} \hat{x}^{(2n)}(1) + u_0(h) \hat{x}^{(2n-1)}(1)
\]

\[
+ \sum_{n=0}^{\infty} (-1)^n \mu^{2n+1} (-u_0(h) \hat{x}^{(2n+1)}(1)) + \frac{1}{u_0(h)} \hat{x}^{(2n)}(2)
\]

\[
i u_0(h) \hat{x}^{(2n+1)}(1) + u_0(h) \hat{x}^{(2n)}(2) = 0.
\]
Thus, the dispersion equation has the form

$$\sum_{k=0}^{\infty} a_k \mu^k = 0,$$

where

$$a_0 = u_0'(h) \left( 1 + i x^{(1)}(h) \right) - \frac{i}{u_0(h)},$$

$$a_{2n} = (-1)^n u_0''(h) x^{(2n)}(h) - \frac{1}{u_0(h)} x^{(2n-1)}(h) + i u_0'(h) x^{(2n+1)}(h)$$

$$- \frac{i}{u_0(h)} x^{(2n)}(h) + u_0(h) x^{(2n-1)}(h), \quad n \in \mathbb{N},$$

$$a_{2n+1} = (-1)^n (-u_0''(h) x^{(2n+1)}(h) + \frac{1}{u_0(h)} x^{(2n)}(h))$$

$$+ i u_0'(h) x^{(2n+1)}(h) + u_0(h) x^{(2n)}(h), \quad n = 0, 1, 2, \ldots$$

The problem is reduced to the problem of finding zeros of an analytic function given by its Taylor series with the coefficients \(a_k, k = 0, 1, 2, \ldots\).

The usual approach to the numerical solution of the considered eigenvalue problem consists in applying the shooting method (see, e.g., [56]), which is known to be unstable, relatively slow, and with no explicit equation for the difference of our approach does not offer any explicit equation for the potential. In [65], another method based on approximation of the potential by square wells was proposed. It is limited to the case of symmetric potentials. The approach based on the SPPS is completely different and does not require any shooting procedure, approximation of the potential or numerical differentiation. Derived from the exact dispersion equation (65), we consider its approximation \(\sum_{k=0}^{N} a_k \mu^k = 0\) and in fact look for zeros of the polynomial \(\sum_{k=0}^{N} a_k \mu^k\) in the interval \([\min q(x), 0]\). Here, we give only one example of numerical computation of eigenvalues referring to [9] for more examples and discussion.

We consider the potential \(Q\) defined by the expression \(Q(x) = -\nu \text{sech}^2 x, x \in (-\infty, \infty)\). It is not of a finite support; nevertheless, its absolute value decreases rapidly when \(x \to \pm \infty\). We approximate the original problem by a problem with a finite support potential \(\overline{Q}\) defined by the equality

$$\overline{Q}(x) = \begin{cases} 0, & x < -a \\ -\nu \text{sech}^2 x, & -a \leq x \leq a \\ 0, & x > a. \end{cases}$$

An attractive feature of the potential \(Q\) is that its eigenvalues can be calculated explicitly (see, e.g., [64]). In particular, for \(\nu = m(m + 1)\), the eigenvalue \(\lambda_n\) is given by the formula \(\lambda_n = -(m - n)^2, n = 0, 1, \ldots\).

The results of application of the SPPS method for \(\nu = 12\) are given in Table IV in comparison with the exact values and the results from [65].

5.2. Transmission problem for inhomogeneous layers

In this subsection, we apply the SPPS method to the problem of finding the reflectance and transmittance of a finite inhomogeneous layer. This is a classical problem that still attracts a lot of attention because of its numerous applications in modern engineering, optical physics, solution of nonlinear problems, and many other fields. Different methods for numerical solution of the problem have been proposed, mainly based on well known canonical techniques for approximate solution of ordinary DEs such as the finite differences or expansion in power series (see, e.g., [66–69]). One of the most used methods involves the approximation of the inhomogeneous layer by a structure consisting of many homogeneous layers (see, e.g., [70–73]). Asymptotic methods such as the perturbation method or the WKB method are also applied to this problem (see, e.g., [67, 74–76]), although in the case of a finite inhomogeneous layer the WKB technique does not seem advantageous. Meanwhile, the mentioned numerical approaches can give satisfactory results for certain fixed parameters of the problem; their applicability is questionable when the solution of the problem is required, for example, for many different angles of incidence. The treatment of the oblique incidence case is not only interesting because of the many applications in which that incidence is needed – in optical filters, light couplers – but also because sometimes the interfaces are rough – their effects and analysis depending on their size – and/or are not parallel (see, e.g., [76]). This is due to imperfect deposition conditions. Such problems in the generation of the inhomogeneous layer (or multilayer) have generated systems in which the feedback of

| Table IV. Approximations of \(\lambda_n\) of the Hamiltonian \(H = -D^2 - 12\text{sech}^2 x\). |
|---|---|---|
| \(n\) | Exact values | Numerical results from [65] | Numerical results using SPPS (\(N = 180\)) |
| 0  | 9  | -9.094 | -8.999628656 |
| 1  | 4  | -4.295 | -3.999998053 |
| 2  | 1  | -0.885 | -0.999927816 |

SPPS, spectral parameter power series.
a reflectance, transmittance, or scattered light measurement is used to characterize the layer as it is created and to correct any discrepancies with the pre-established values. Such application must be able to recalculate the required correction profile and requires a real-time computation of transmittance and reflectance.

The mathematical statement of the problem involves a Helmholtz equation with a coefficient that is an arbitrary continuous function on a finite segment and constant outside. More precisely, the scalar function $u$ that represents a component of a linearly polarized electromagnetic wave in the case of an $s$-polarization satisfies the Helmholtz equation

$$u''(x) + \left[k^2n^2(x) - \beta^2\right]u(x) = 0,$$  \hspace{1cm} (69)

where $u$ stands for the transverse component of the electric field, and in the case of a $p$-polarization satisfies the following Sturm–Liouville equation (see, e.g., [77], [78])

$$n^2(x) \left(\frac{1}{n^2(x)} v'(x)\right)' + \left[k^2n^2(x) - \beta^2\right]v(x) = 0$$  \hspace{1cm} (70)

in which $v$ represents the transverse component of the magnetic field. Here, $k$ is the free-space circular wave number. The refractive index $n$ preserves constant values $n_1$ and $n_2$ in the regions $x < 0$ and $x > d$, respectively, and is an arbitrary continuous function in the interval $0 \leq x \leq d$ (Figure 5). For simplicity, we assume $n$ to be real valued although the method is equally applicable to the case of a complex refractive index.

The propagation constant $\beta$ is related to the angle of incidence of the wave in the following way $\beta = k \sin \theta$ (see, e.g., [77]), and $\beta$ vanishes in the case of normal incidence.

In spite of the fact that equations (69) and (70) describe the behavior of different components of an electromagnetic wave, corresponding to an electric and a magnetic field, respectively, there exists a simple transformation from (70) to (69) and vice versa (see, e.g., [77]). Namely, if $v$ is a solution of (69), then $U = v / n$ is a solution of the equation

$$U''(x) + \left[k^2N^2(x) - \beta^2\right]U(x) = 0,$$

where $k^2N^2 = k^2n^2 + n'' / n - 2 (n' / n)^2$. Thus, in both cases, the problem reduces to an equation of the form (69).

We denote $k_1 = \sqrt{k^2n_1^2 - \beta^2}$ and $k_2 = \sqrt{k^2n_2^2 - \beta^2}$. The solution $u$ of (69) or $v$ of (70), respectively, together with their first derivatives must be continuous at all $x$ including the points $x = 0$ and $x = d$. The incident wave in the region I (Figure 6) is assumed to have the form $e^{-ik_1x}$, and together with the reflected wave, the whole solution for $x < 0$ is the combination

$$u(x) = e^{-ik_1x} + Re^{ik_1x}, \hspace{1cm} x < 0,$$

![Figure 5. An inhomogeneous layer.](image)

![Figure 6. Incident, reflected, and transmitted waves.](image)
where the constant $R$ is the reflection coefficient whose absolute value is less than 1. The solution corresponding to the transmitted wave in the region II has the form

$$ u(x) = Te^{-ikx}, \quad x > d, $$

where $T$ is the transmission coefficient. In the case of unabsorptive media for the normally incident waves, the following energy conservation relation holds

$$ |R|^2 + n_2 |T|^2 / n_1 = 1. \quad (71) $$

Let us suppose that the two linearly independent solutions $y_1$ and $y_2$ of (69) in the interval of inhomogeneity $0 \leq x \leq d$ are known such that the following initial conditions are satisfied:

$$ y_1(0) = 1, \quad y'_1(0) = 0, \quad (72) $$

and

$$ y_2(0) = 0, \quad y'_2(0) = 1. \quad (73) $$

Then we are able to obtain analytic expressions for $R$ and $T$ in terms of $u_1$ and $u_2$ [10]. We have

$$ R = \frac{-k_1k_2y_1(d) - y'_1(d) - ik_2y_1(d) + ik'_2(d)}{[y'_1(d) - k_1k_2y_1(d)] + ik_1y_1(d) + k_1y'_2(d)}, \quad (74) $$

and

$$ T = \frac{2ik_1[y_1(d)y'_2(d) - y'_1(d)y_2(d)]e^{ik_1d}}{[y'_1(d) - k_1k_2y_1(d)] + ik_1y_1(d) + k_1y'_2(d)}. \quad (75) $$

These formulas remain valid for Equation (70) when one substitutes $y_1$ and $y_2$ with the solutions $v_1$ and $v_2$ of (70) satisfying the initial conditions (72) and (73), respectively.

Thus, the transmission problem for an inhomogeneous layer consists in computing a couple of solutions of (69) (or (70)) in the interval of inhomogeneity $0 \leq x \leq d$, satisfying the initial conditions (72) and (73), and then the reflection and transmission coefficients are found from (74) and (75). For computation of these solutions, we use Theorem 1 and take into account (13) and (14) where it is convenient to choose $x_0 = 0$.

There are several examples of explicitly solvable inhomogeneous profiles [79], [67]. These were used in [10] for testing the results obtained by means of SPPS. In all numerical simulations, the achieved accuracy was remarkable.

6. Zakharov–Shabat eigenvalue problem

In this section, we study the Zakharov–Shabat system with a real-valued potential. It arises in the solution via the inverse scattering method of several nonlinear evolution equations such as the nonlinear Schrödinger equation, the sine-Gordon equation, and the modified Korteweg-de Vries equation. For example, in the case of the nonlinear Schrödinger equation, eigenvalues of the Zakharov–Shabat system correspond to soliton solutions implemented in fiber optics (see, e.g., [80]). The assumption that the potential is real valued is natural and common in the engineering literature – it includes the conventional profiles such as the rectangular, the Gaussian, and the hyperbolic secant. The SPPS representation for solutions of the Zakharov–Shabat system with a complex potential was studied recently in [2].

In [11], a general solution of the Zakharov–Shabat system with a real potential in terms of SPPS was obtained and used for deriving a dispersion equation corresponding to the eigenvalue problem with a compactly supported potential. Once again, the problem is reduced to a problem of localizing zeros of an analytic function given by its Taylor series. For numerical approximation of eigenvalues, one can consider a truncated series, and thus for practical computation, the eigenvalue problem reduces to finding roots of a polynomial.

The Zakharov–Shabat system with a real potential has the form [81,82]

$$ \partial n_1(x) - \lambda n_1(x) = U(x)n_2(x), \quad (76) $$

$$ \partial n_2(x) + \lambda n_2(x) = -U(x)n_1(x), \quad (77) $$

where $\partial := \frac{d}{dx}, U : \mathbb{R} \rightarrow \mathbb{R}$ is the potential and $U \in L_1(-\infty, \infty)$; the solutions $n_1$ and $n_2$ in general are complex valued and the spectral parameter $\lambda$ is a complex constant. It is convenient to rewrite the Zakharov–Shabat system using the following notations

$$ u = n_1 + in_2, \quad v = n_1 - in_2, \quad q = iU. $$
Then (76) and (77) take the form of a Dirac system with a scalar potential (see, e.g., [83–86])

\[
(\partial - q(x))u = \lambda u, \quad (\partial - q(x))v = \lambda v.
\]

(78)

(79)

From these equalities, it is easy to see that \(u\) and \(v\) are solutions of the following second-order DEs

\[
(\partial - q(x))(\partial + q(x))u(x) = \lambda^2 u(x),
\]

(80)

and

\[
(\partial + q(x))(\partial - q(x))v(x) = \lambda^2 v(x).
\]

(81)

The differential operators on the left-hand side can be written in the form of stationary Schrödinger operators describing SUSY partners

\[
(\partial - q)(\partial + q) = \partial^2 + (\partial q - q^2) \quad \text{and} \quad (\partial + q)(\partial - q) = \partial^2 - (\partial q + q^2).
\]

Nevertheless, precisely, the factorized form (80) and (81) present certain advantage for applying the SPPS method because of the possibility to write down closed-form solutions of (80) and (81) for \(\lambda = 0\). Namely, let \(Q(x) = \int q(x)dx\). Then \(u_0(x) = e^{-Q(x)}\) and \(v_0(x) = e^{Q(x)}\) are solutions of the equations \((\partial - q)(\partial + q)u_0 = 0\) and \((\partial + q)(\partial - q)v_0 = 0\), respectively. Note that for a continuous function \(q\) defined on a closed finite interval, both \(u_0\) and \(v_0\) are devoid of zeros.

The systems of auxiliary functions \(\{X^{(n)}\}_{n=0}^{\infty}\) and \(\{\bar{X}^{(n)}\}_{n=0}^{\infty}\) in this case are defined as follows:

\[
X^{(n)}(x) = \bar{X}^{(n)}(x) = 1,
\]

(82)

\[
X^{(n)}(x) = \int_{x_0}^{x} X^{(n-1)}(s)e^{(-1)^nQ(s)}ds,
\]

(83)

\[
\bar{X}^{(n)}(x) = \int_{x_0}^{x} \bar{X}^{(n-1)}(s)e^{(-1)^{n+1}Q(s)}ds.
\]

(84)

We obtain the following SPPS form of a general solution of the Zakharov–Shabat system.

**Theorem 5**

[11] Let \(U\) be a continuous real-valued function defined on a finite segment \([a, b] \subset \mathbb{R}\). Then the general solution of the Zakharov–Shabat system (76) and (77) has the form

\[
n_1(x) = \frac{c_1}{2} \sum_{n=0}^{\infty} (-1)^n e^{(-1)^{n+1}Q(x)} \lambda^n X^{(n)}(x) + \frac{c_2}{2} \sum_{n=0}^{\infty} (-1)^n e^{(-1)^nQ(x)} \lambda^n \bar{X}^{(n)}(x),
\]

(85)

\[
n_2(x) = \frac{i c_1}{2} \sum_{n=0}^{\infty} (-1)^n e^{(-1)^nQ(x)} \lambda^n X^{(n)}(x) + \frac{i c_2}{2} \sum_{n=0}^{\infty} (-1)^n e^{(-1)^{n+1}Q(x)} \lambda^n \bar{X}^{(n)}(x),
\]

(86)

where \(c_1\) and \(c_2\) are arbitrary complex constants, \(Q\) is an antiderivative of \(q = iU\), \(x_0 \in [a, b]\) and the series converge uniformly in \([a, b]\).

Solutions of the Zakharov–Shabat system (76) and (77) satisfying the following asymptotic relations

\[
\tilde{\sigma}(x, \lambda) \cong \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} e^{\lambda x}, \quad x \to -\infty,
\]

(87)

\[
\tilde{\xi}(x, \lambda) \cong \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} e^{-\lambda x}, \quad x \to \infty,
\]

(88)

are called the Jost solutions [87]. The eigenvalue problem for the Zakharov–Shabat system with a real-valued potential consists in finding such values of the spectral parameter \(\lambda\) for which \(\text{Re} \lambda > 0\) and there exists a nontrivial solution \(n\) satisfying the Jost conditions (87) and (88).

If the real-valued potential \(U\) has a compact support on the segment \([-a, a]\), it is easy to see that the eigenvalue problem reduces to find such values of \(\lambda\) (\(\text{Re} \lambda > 0\)) for which there exists a solution of (76) and (77) satisfying the following boundary conditions:

\[
n_1(-a) = 1, \quad n_2(-a) = 0,
\]

(89)
We refer here to [88] and [89] for estimates of the number of real eigenvalues of a compactly supported potential. The next statement gives us a dispersion equation equivalent to the Zakharov–Shabat eigenvalue problem for the real, compactly supported potentials.

**Theorem 6**

Let \( U \) be a continuous real-valued function with a compact support on the segment \([-\alpha, \alpha]\). Then \( \lambda \) (\( \text{Re} \lambda > 0 \)) is an eigenvalue of the Zakharov–Shabat system if and only if the following equation is satisfied:

\[
\sum_{n=0}^{\infty} \lambda^n \left( e^{(1-n)e^{\alpha}} \tilde{x}^{(n)}(\alpha) + e^{(1-n+1)e^{\alpha}} \tilde{x}^{(n)}(\alpha) \right) = 0, \quad (91)
\]

where \( Q(x) = i \int_{-\alpha}^{x} U(t) \, dt \) and \( x_0 = -\alpha \) in (89)–(90).

If \( \lambda \) is an eigenvalue, then the corresponding eigenvector is given by

\[
\mathbf{n} = \tilde{\psi} + \tilde{\varphi},
\]

with

\[
\tilde{\psi}(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix} = \begin{pmatrix} \frac{1}{\pi} \sum_{n=0}^{\infty} e^{(1-n)e^{\alpha}} \lambda^n \tilde{x}^{(n)}(x) \\ \frac{1}{\pi} \sum_{n=0}^{\infty} (-1)^n e^{(1-n)e^{\alpha}} \lambda^n \tilde{x}^{(n)}(x) \end{pmatrix},
\]

\[
\tilde{\varphi}(x) = \begin{pmatrix} \varphi_1(x) \\ \varphi_2(x) \end{pmatrix} = \begin{pmatrix} \frac{1}{\pi} \sum_{n=0}^{\infty} e^{(1-n+1)e^{\alpha}} \lambda^n \varphi^{(n)}(x) \\ \frac{1}{\pi} \sum_{n=0}^{\infty} (-1)^n e^{(1-n+1)e^{\alpha}} \lambda^n \varphi^{(n)}(x) \end{pmatrix}.
\]

The theorem reduces the Zakharov–Shabat eigenvalue problem with a compactly supported potential to the problem of localizing zeros (in the right half-plane) of an analytic function \( \kappa(\lambda) = \sum_{n=0}^{\infty} a_n \lambda^n \) of the complex variable \( \lambda \) with the Taylor coefficients \( a_n \) given by the expressions

\[
a_n = e^{(1-n)e^{\alpha}} \tilde{x}^{(n)}(\alpha) + e^{(1-n+1)e^{\alpha}} \tilde{x}^{(n)}(\alpha).
\]

Equation (91) represents a dispersion equation of the eigenvalue problem. The coefficients \( a_n \) can be easily and accurately calculated following the definitions introduced in the preceding text. For the numerical solution of the eigenvalue problem, one can consider a polynomial

\[
\kappa_N(\lambda) = \sum_{n=0}^{N} a_n \lambda^n,
\]

approximating the function \( \kappa \). For a reasonably large \( N \), its roots give an accurate approximation of the eigenvalues of the problem.

As a numerical example, we consider the rectangular box referring the reader to [11] for further numerical tests and details. For the rectangular box, the exact solution satisfying the boundary conditions (89) is known. Such system can be applied to describe the problem of the diffraction of a wave by a screen with a slit [90]. Discrete eigenvalues of the spectral parameter can also be approximated using a variational principle approach [91]. The potential is defined by the equality

\[
U(x) = \begin{cases} A, & |x| < \alpha, \\ 0, & \text{elsewhere}. \end{cases}
\]

A dispersion equation in this case can be obtained explicitly and written as follows:

\[
\gamma \cos 2\gamma + \lambda \sin 2\gamma = 0,
\]

where \( \gamma = \sqrt{A^2 - \lambda^2} \).

For solving the dispersion Equation (96), the routine `NSolve` of Wolfram Mathematica 7 was used. We considered \( \alpha = 1 \). In the case \( A = 1 \), the routine `NSolve` delivers one solution of (96) \( \lambda_{NSolve} = 0.31902252414261895 \). Application of the SPPS method with
m = 2000 and N = 120 gives us the value \( \lambda_0 = 0.31902252414254 \). The agreement is up to the 12th digit. Taking \( m = 4000 \) and \( N = 180 \), we obtain still a better approximation \( \lambda_0 = 0.319022524142619 \). The agreement is up to the 14th digit.

In the case \( A = 4 \), there are three eigenvalues. \( N_{\text{Soln}} \) delivers the following values \( \lambda_{0,1}^{N_{\text{Soln}}} = 0.41262411401896715, \lambda_{0,2}^{N_{\text{Soln}}} = 2.8945478628203027, \) and \( \lambda_{0,3}^{N_{\text{Soln}}} = 3.749624961605374 \). Application of the SPPS method with \( m = 2000 \) and \( N = 100 \) gives us the values \( \lambda_1 = 0.41262441002, \lambda_1 = 2.8945478628329, \) and \( \lambda_2 = 3.7496249616095 \), and with \( m = 4000 \) and \( N = 180 \): \( \lambda_0 = 0.4126241140179, \lambda_1 = 2.89454786283226, \) and \( \lambda_2 = 3.7496249616045 \).

7. Conclusions

We presented a review of recent research and applications of spectral parameter powers series (SPPS) representations for solving initial and BVPs as well as spectral and related problems for Sturm–Liouville equations. Application of the SPPS approach allows one to obtain explicit analytic forms of characteristic equations for a variety of problems. Approximation of these equations represents a powerful, universal, and accurate numerical method highly competitive with the best purely computational techniques. The SPPS method is algorithmically simple and can be easily implemented using available routines of such environments for scientific computing as Matlab.

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