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An Iterative Solution to the Second Order Eigenvalue Equation with Periodic Boundary Conditions

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A procedure for determining the ground state eigenvalue and eigenfunction of the Sturm–Liouville equation with periodic boundary conditions has been developed. This procedure is based on Picard's method, which, through the use of Chebyshev polynomials, provides for an efficient computational scheme.

I. INTRODUCTION

The problem considered here is that of determining the ground state eigenvalue, E, and the eigenfunction, $y(x)$, which is a solution to the Sturm–Liouville equation,

$$y'' + (E - V(x))\, y = 0, \tag{1}$$

subject to periodic boundary conditions. An appropriate change of the independent variable allows these conditions always to be written as

$$y(1) = y(-1) \tag{2a}$$

and

$$y'(1) = y'(-1). \tag{2b}$$

V is a known periodic and piecewise continuous function of the independent variable.

The proposed procedure can be viewed as a modification of the iteration method of Picard. For computer applications, this approach is superior to those in which approximations are taken to certain orders, since once the mathematical technique is developed, the final accuracy depends on the number of iterations. No modification of the expressions need be made in order to improve the accuracy. A further advantage is that the initial approximation may in all cases be $y =$ constant. Thus, in order to proceed, no previous operations are required.

II. Mathematical Formulation

In order to integrate Eq. (1) it is convenient to express y and V as series in x. For the range $-1 \leqslant x \leqslant 1$, the Chebyshev polynomials may be chosen [1]. These polynomials are defined by

$$T_n = \cos(n \arccos x), \tag{3}$$

which gives $T_0 = 1$ and $T_1 = x$. A trigonometric identity applied to Eq. (3) produces the general recursion relation

$$2T_n T_m = T_{m+n} + T_{m-n} . \tag{4}$$

The orthogonality relations are

$$\int_{-1}^{1} T_m T_n (1 - x^2)^{-1/2}\, dx = \begin{cases} \pi/2 & m = n \neq 0 \\ \pi & m = n = 0 \\ 0 & m \neq n. \end{cases} \tag{5}$$

In the procedure, y is represented by a Chebyshev series

$$y = \sum a_n T_n , \tag{6}$$

where the sum is from $n = 0$ (unless otherwise noted by a constant which appears under the summation sign) to M, the largest Chebyshev term specified. As previously noted, the iteration procedure begins with $y = a_0$; all later expressions for y will contain the complete series. The product Vy can be expressed as

$$Vy = \sum b_n T_n , \tag{7}$$

and Eq. (1) can now be written as

$$y'' = -E \sum a_n T_n + \sum b_n T_n . \tag{8}$$

This equation is formally integrated using the following properties of the Chebyshev polynomials

$$2 \int T_n\, dx = \frac{T_{n+1}}{n+1} - \frac{T_{n-1}}{n-1} , \tag{9a}$$

$$\int T_1\, dx = \tfrac{1}{4}(T_2 - T_0), \tag{9b}$$

$$\int T_0\, dx = T_1 .$$

The constant that results from integrating T_1 is combined with the constant of integration into one constant, c. The result is a new Chebyshev series

$$y' = c - E \sum_1 f_n T_n + \sum_1 g_n T_n . \tag{10}$$

At this point, all coefficients on the right side of Eq. (10) are known with the exceptions of c and E. The value of E is obtained from the periodic boundary conditions on y'. Equating $y'(1)$ with $y'(-1)$ in Eq. (10) eliminates c and all even polynomials, giving

$$E = \sum_1{}' g_n \Big/ \sum_1{}' f_n , \tag{11}$$

where $\sum'$ indicates a sum over odd n only. Here use has been made of the fact that

$$T_n(1) = T_n(-1) \qquad n \text{ even}, \tag{12}$$

and

$$T_n(1) = -T_n(-1) \qquad n \text{ odd}. \tag{13}$$

With E thus determined, it is possible to combine the coefficients $-Ef_n$ and g_n into one coefficient, h_n. Equation (10) is then written

$$y' = c + \sum_1 h_n T_n \tag{14}$$

with c undetermined. The integration of Eq. (14) yields

$$y = a_0 + a_1 x + \sum_2 H_n T_n , \tag{15}$$

where H_n is directly constructed from h_n by means of Eqs. (9). The constant of integration and the T_0 term from the integration of the T_1 have been combined into a_0. Also, the constant a_1 includes c and a contribution from the integration of the h_2 term in Eq. (14). At this point the values of a_0 and a_1 are not known. Once they are determined, however, a new expression for y is ready for the next iteration cycle, with the identification

$$(\text{new})\, a_n = H_n \qquad n = 2, 3, \ldots \tag{16}$$

This notation will now be employed.

The value of a_1 is obtained from the periodic boundary conditions on y. Setting $y(1) = y(-1)$ in Eq. (15) will eliminate a_0 and all the even Chebyshev polynomials, yielding

$$a_1 = -\sum_3{}' a_n . \tag{17}$$

Finally, a_0 is obtained by working with Eq. (1). Equation (15) is differentiated twice to give

$$y'' = \sum_2 a_n T_n'' . \tag{18}$$

The direct use of Eq. (15) gives

$$Ey = Ea_0 + E \sum_1 a_n T_n \tag{19}$$

and

$$-Vy = -\sum \sum v_m T_m a_n T_n , \tag{20}$$

where the Chebyshev expansion coefficients of V are designated as v_m . Equation (1) is now obtained by the direct addition of Eqs. (18)–(20) in the form

$$\sum_2 a_n T_n'' + Ea_0 + E \sum_1 a_n T_n - \sum \sum v_m T_m a_n T_n = 0. \tag{21}$$

This is solved for a_0 by multiplying Eq. (21) by $(1 - x^2)^{-1/2}$ and integrating from -1 to 1. The use of the orthogonality relation, Eq. (5), and the fact that

$$\int_{-1}^{1} (1 - x^2)^{-1/2} T_n'' \, dx = \begin{cases} (\pi/2) \, n^3 & n \text{ even} \\ 0 & n \text{ odd}, \end{cases} \tag{22}$$

yields

$$\frac{\pi}{2} \sum{}'' n^3 a_n + \pi E a_0 - \pi v_0 a_0 - \frac{\pi}{2} \sum_1 a_n v_n = 0, \tag{23}$$

where $\sum''$ implies a sum over even n. The only unknown in Eq. (23) is a_0 which is now evaluated. In the special case, however, where $V(x)$ is an antisymmetric function, both E and v_0 along with both sums in Eq. (23) are zero in the initial cycle which leaves a_0 undetermined. In this particular situation, a_0 may be set equal to the sum of the absolute values of the Chebyshev coefficients. This choice of the constant guarantees that the next approximation will have no nodes, a characteristic of the ground state solution.

At this point, all coefficients a_n in Eq. (6) have been determined and the cycle may be reinitiated. The process is repeated until convergence to within the desired limits occurs. Normalization is not necessary, but it can be easily included in the procedure.

III. Numerical Analysis Aspects

In the procedure outlined previously, it is necessary to expand one function, V, in Chebyshev polynomials. The coefficients in this expansion,

$$V = v_0 + v_1 T_1 + v_2 T_2 + \cdots + v_m T_m , \tag{24}$$

are given by

$$v_n = A \int_{-1}^{1} (1 - x^2)^{-1/2} T_n V \, dx, \tag{25}$$

where A is the normalization factor (see Eqs. (5)).

The numerical evaluation is accomplished by Gauss–Chebyshev integration [2]; that is, use is made of the quadrature formula

$$\int_{-1}^{1} (1 - x^2)^{-1/2} F \, dx = \frac{\pi}{N} \sum_{k=1}^{N} F(x_k), \tag{26}$$

where the points x_k are given by

$$x_k = \cos Q_k \tag{27}$$

with

$$Q_k = \frac{2k - 1}{2N} \pi. \tag{28}$$

The advantages of employing a Chebyshev representation now become readily apparent. First, the quadrature points are easily calculated by Eqs. (27) and (28), and all have the same weighing factor of π/N. Consequently, no input tables are required. Secondly, the polynomials themselves are directly evaluated at the summation points, x_k, by

$$T_n(x_k) = \cos(nQ_k), \tag{29}$$

which follows from Eqs. (3) and (27). The accuracy inherent in Gaussian quadrature is always a distinct advantage. The error term associated with Eq. (26) is $2\pi F^{(2N)} 2^{-2N} (2N!)^{-1}$ where $F^{(2N)}$ is the $2N$th derivative of F evaluated at some point within the range. The error in the integration itself can be eliminated from consideration by taking N sufficiently large, say $N = 2M$. To increase the overall accuracy, it is only necessary to increase the number of terms kept.

The integration by Gaussian quadrature is rather slow, but it is required only once to obtain the coefficients in Eq. (24). Since the expansion coefficients of y are known from the previous cycle, the coefficients of the expansion of the product required by Eq. (7) is readily constructed by means of Eq. (4). The computational scheme gains efficiency from the fact that the Chebyshev series representation of either the integration of a Chebyshev series or the product of two Chebyshev series is easily obtained. After the initial expansion, therefore, each cycle is a sequence of operations with the known coefficients.

IV. Examples

Two examples are presented below. The first, the Mathieu equation, is an important differential equation in physics and engineering. The second example illustrates the technique for transforming an equation containing a first derivative term into the standard form of Eq. (1). In both cases, the calculations were performed using double precision on an IBM 360, Model 40 until the change in the eigenvalue was less than 1×10^{-8}. Twenty-four terms in the Chebyshev expansion were retained ($M = 24$) and the number of integration points used was forty-eight ($N = 48$). The computer required 0.7 seconds for an iteration.

A. *Mathieu Equation*

The Mathieu equation [3],

$$y'' + (a - 2q \cos 2z)\, y = 0, \tag{30}$$

has period π in z. The change of the independent variable,

$$\pi x = 2z, \tag{31}$$

transforms the boundary conditions into the form of Eqs. (2) and produces the identification

$$E = \tfrac{1}{4}\pi^2 a. \tag{32}$$

In the test case, the particular choice

$$q = 2/\pi^2 \tag{33}$$

was taken, and now Eq. (30) reads

$$y'' + (E - \cos \pi x)\, y = 0. \tag{34}$$

The ground state eigenvalue of Eq. (30) can be calculated by a series expansion [3], and, for this choice of q, Eq. (34) corresponds to a value of E given by

$$E = -0.050435182. \tag{35}$$

The routine converged in 14 cycles to the above value. Of the twenty-four Chebyshev terms used, the last ten had values less than 1×10^{-8}. The odd terms are theoretically zero in the case of a symmetric V; they were computed to be less than 1×10^{-12}.

B. *An Equation Containing the First Derivative*

Consider the equation,

$$z'' + P(x)\, z' + (E - Q(x))\, z = 0, \tag{36}$$

subject to the periodic boundary conditions $z(1) = z(-1)$ and $z'(1) = z'(-1)$ and where P and Q are periodic. The transformations,

$$y = \exp\left[\frac{1}{2}\int P\, dx\right] z \tag{37}$$

and

$$V = \frac{1}{2}\frac{dP}{dx} + \frac{1}{4}P^2 + Q, \tag{38}$$

permit Eq. (36) to be immediately written in the standard form given by Eq. (1). The boundary conditions are again given by Eq. (2). Note that the eigenvalue is unaffected by the transformation.

The particular case taken is

$$z'' + (\cos \pi x)\, z' + (E + \pi \sin \pi x)\, z = 0. \tag{39}$$

The ground state solution of Eq. (39) can be written as

$$z = 1 + A \sin \pi x \tag{40}$$

with

$$A = -\tfrac{1}{2}\pi + \tfrac{1}{2}(\pi^2 + 4)^{1/2}, \tag{41}$$

and the corresponding eigenvalue is

$$E = -\pi A = -0.91514456. \tag{42}$$

The above transformation of Eq. (39) produces

$$y'' + (E + 3/2\, \pi \sin \pi x - \tfrac{1}{4}\cos^2 \pi x)\, y = 0. \tag{43}$$

The computed result converged to the above value after 65 cycles. In this example, the last five of the twenty-four Chebyshev terms were less than 1×10^{-8}.

V. Conclusion

The method presented here gives a straightforward way of obtaining the solutions and ground state eigenvalue of a Sturm–Liouville equation with periodic boundary conditions. It is not necessary to have any prior knowledge of the solution in order to initiate the iteration process. The degree of accuracy obtained is determined by the number of iterations performed and the number of terms kept in the Chebyshev expansions. A program based on this method would allow both to be specified as input data. Accuracy, therefore, becomes a matter of computer time since no modification of the general procedure is required.

References

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