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Efficient Computation of the Prüfer Phase Function for Determining Eigenvalues of Sturm–Liouville Systems

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It is shown that a combination of phase integral approximation and numerical integration of the Prüfer phase function yields a computationally effective technique for numerical solution of Sturm–Liouville eigenvalues. The technique is tested with sample Sturm–Liouville systems and compared with other methods. © 1986 Academic Press, Inc.

1. INTRODUCTION

Many methods suggested for solving Sturm–Liouville eigenvalue problems

$$\begin{aligned} \Psi''(x) + \{\lambda - p(x)\}\,\Psi(x) &= 0 \qquad \text{on } (a, b) \\ A_1\,\Psi(a) + A_2\,\Psi'(a) &= 0 \\ B_1\,\Psi(b) + B_2\,\Psi'(b) &= 0 \end{aligned} \tag{1}$$

utilize the logarithmic derivative defined by

$$y(x) = \frac{\Psi'(x)}{\Psi(x)}. \tag{2}$$

Differentiating Eq. (2) and using Eq. (1) to eliminate the second derivative term yields the first-order Ricatti equation

$$y'(x) + \{\lambda - p(x)\} + y^2(x) = 0 \tag{3}$$

from which the eigenvalues λ may be determined. However, Eq. (3) cannot be integrated by the usual numerical techniques for solving differential equations

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because $y(x)$ has singular points at the zeros of $\Psi(x)$ and it is impossible to integrate across these points. Among many special methods of solution of Eq. (3) [1–9], there are several [10–22] which employ either the standard Prüfer transformation

$$\frac{\Psi'(x)}{\Psi(x)} = \tan \theta(x) \tag{4}$$

or the modified Prüfer transformation

$$\frac{\Psi'(x)}{\Psi(x)} = \{\lambda - p(x)\}^{1/2} \tan \varphi(x) \tag{5}$$

to associate the singular points of $y(x)$ with $\pi/2 + n\pi$ of the $\theta(x)$- or $\varphi(x)$-function. Using Eqs. (4) or (5), the equations corresponding to Eq. (3)

$$\theta'(x) = -\sin^2 \theta(x) - \{\lambda - p(x)\} \cos^2 \theta(x) \tag{6}$$

for $\theta(x)$ and

$$\varphi'(x) = \{\lambda - p(x)\}^{1/2} - \frac{1}{4} \frac{\{\lambda - p(x)\}'}{\{\lambda - p(x)\}} \sin 2\varphi(x) \tag{7}$$

for $\varphi(x)$ have no singularities at the zeros of $\Psi(x)$ and may be integrated along the real axis by any general purpose integrator. The eigenvalues may now be obtained from one first-order differential equation and the approach is convenient because the number of zeros of the desired solution is present explicitly thus making this procedure safe from missing eigenvalues. The Prüfer methods have been used for determining sample Sturm–Liouville eigenvalues by Bailey [11, 15] and Hargrave [17], who used standard numerical integrators, and by Fix [20], who, for $\{\lambda - p(x)\} > 0$, solved Eq. (7), the modified Prüfer phase, by successive iterations thus obtaining asymptotic eigenvalues for a number of cases. A general purpose code SLEIGN for automatic solution of the Sturm–Liouville problem was created by Bailey, Gordon, and Shampine [16].

The purpose of the present article is twofold. On one hand, it will be shown that, in many cases, application of higher-order phase integral methods provides a computationally efficient way to compute the Prüfer phase and Sturm–Liouville eigenvalues. Numerical integration of Eqs. (6) or (7) may then be replaced by a set of 3- to 30-point quadratures to yield eigenvalues of high accuracy. On the other hand, it is well known that the phase integral approximation which is not an exact method is plagued by its divergence for certain cases. It is shown how the numerical integration of the Prüfer equations may be used within the phase integral method. Some of those cases, classical turning points, can often be handled by so-called connection formulae while for some other, more complicated cases there are correction functions to account for the divergence of the phase integral method. However, such functions are known only for a very few cases. In this work, numerical integration of the Prüfer phase function is used to connect phase integral

approximations across regions in which they are too inaccurate or perhaps not valid at all.

In the following, Section 2 presents the higher-order phase integral approximations to the Prüfer phase and Section 3 reviews the connection formulae required for determination of Sturm–Liouville eigenvalues. The use and usefulness of the phase integral methods are then tested by computing sample Sturm–Liouville eigenvalues in Section 4. Section 5 gives practical recommendations for using the phase integral methods and discusses their relation to the Prüfer equations.

2. The Phase Integral Approximations to the Prüfer Phase

The phase integral approximations are a solution of the Ricatti equation, Eq. (3), in the complex plane by successive approximations yielding in the symmetric phase integral approximation [23, 24]

$$\Psi(z) = (q(z))^{-1/2} \exp(\pm i\, w(z)) \tag{8}$$

where

$$w(z) = \int^z q(z)\, dz \tag{9}$$

and

$$q(z) = q^{(1)}(z) + q^{(3)}(z) + q^{(5)}(z) + \cdots \tag{10}$$

with the first few functions $q^{(i)}(z)$ defined by [26]

$$q^{(1)}(z) = \{\lambda - p(z)\}^{1/2}, \tag{11}$$

$$q^{(3)}(z) = \left(\frac{1}{8}\right)(p''(z)/\{\lambda - p(z)\}^{3/2} + \left(\frac{5}{4}\right)(p'(z))^2/\{\lambda - p(z)\}^{5/2}), \tag{12}$$

$$q^{(5)}(z) = -\left(\frac{1}{32}\right)(p''''(z)/\{\lambda - p(z)\}^{5/2} + \left(\left(\frac{19}{4}\right)(p''(z))^2 + 7p'(z)\, p'''(z)\right)\Big/\{\lambda - p(z)\}^{7/2} + \left(\frac{221}{8}\right)(p'(z))^2\, p''(z)/\{\lambda - p(z)\}^{9/2} + \left(\frac{1105}{64}\right)(p'(z))^4/\{\lambda - p(z)\}^{11/2}) \tag{13}$$

where primes denote differentiation with respect to z.

From the phase integral approximations to the solution $\Psi(z)$, the corresponding approximations to the Prüfer phase on the real axis may be obtained. For $\{\lambda - p(z)\} < 0$, the functions $q(x)$ are purely imaginary and the two linearly independent solutions, Eq. (8), are real, exponentially increasing and decreasing solutions. For Sturm–Liouville eigenvalue problems in which the boundary point is in the region where $\{\lambda - p(x)\}$ is large and negative, only the negative exponential is acceptable and for those cases

$$\theta(x) = \arctan\left(-\frac{1}{2}\frac{q'(x)}{q(x)} - iq(x)\right). \tag{14}$$

In a region where $\{\lambda - p(x)\} > 0$, the function $q(x)$ is real on the real axis and the two linearly independent phase integral solutions are complex. A suitable linear combination which is real on the real axis is

$$\Psi(x) = 2(q(x))^{-1/2}\cos(w(x)) \tag{15}$$

and the corresponding Prüfer phase is

$$\theta(x) = \arctan\left(-\frac{1}{2}\frac{q'(x)}{q(x)} + q(x)\tan(w(x))\right). \tag{16}$$

The validity and accuracy of the phase integral approximations are discussed in [23] and numerical tests on the real axis may be found in [27]. For numerical purposes it is important to realize that phase integral approximations are asymptotic. Their accuracy cannot be increased arbitrarily but it can be estimated by computing the various-order contributions to $q(z)$ and $w(z)$, Eqs. (10) and (9), respectively, and investigating their behaviour. The lower limit of integration in $w(z)$, Eq. (9), is often chosen to be a zero of $\{\lambda - p(z)\}$. Definitions of the integration paths and evaluation of the various-order contributions to $w(z)$ in that case are described in [23, 28, 29]. If $\{\lambda - p(z)\} > 0$, the lower limit of integration may be chosen such that the integrands of $w(z)$ are well behaved and in that case virtually any standard quadrature will do.

3. The Connection Formulae

In a region where $|\lambda - p(x)|$ is very small, neither one of the approximations, Eqs. (14) and (15), is valid; the whole phase integral expansion is divergent. However, for determining eigenvalues, accurate solutions are required only at the boundary points and, provided the boundary point is not too close to such a region, the situation may be handled by so-called connection formulae. For isolated simple zero of $\{\lambda - p(x)\}$, there is a well known connection formula [30] which

connects a solution in the region where $\{\lambda - p(x)\} < 0$ to a solution of Eq. (15) in the region where $\{\lambda - p(x)\} > 0$. In terms of the Prüfer phase, the connection is

$$\arctan\left(-\frac{1}{2}\frac{q'(x)}{q(x)} - iq(x)\right) \to \arctan\left(-\frac{1}{2}\frac{q'(x)}{q(x)} + q(x)\tan\left(w(x) - \frac{\pi}{4}\right)\right). \tag{17}$$

Of the other, more complicated, connection formulae, only the case of two adjacent zeros of $\{\lambda - p(z)\}$ with $\{\lambda - p(z)\} > 0$ between them has been solved in higher-order approximations. In [31], by means of comparison equation methods, a connection formula for phase integral solutions on opposite sides of a region of two adjacent zeros of $\{\lambda - p(z)\}$ with a parabolic shape in that region was obtained. The connection formula involves comparison equation correction functions in terms of phase integrals between the two zeros in question.

It is obvious that, apart from a simple isolated zero which essentially only requires the inclusion of the constant $\pi/4$ to the basic Eq. (16), use of the connection formulae may become rather complex. In the present work therefore, direct numerical integration of Eq. (6) is suggested as an alternative for connecting the phase integral solutions across regions in which the phase integral approximation cannot be used.

4. Tests

The approximations and expressions above were tested by computing Sturm–Liouville eigenvalues for sample problems and comparing the accuracy and efficiency of the present technique with previous calculations by other authors. The first test case was Mathieu's equation [15, 17]

$$\psi''(x) + \{\lambda - 2h\cos(2x)\}\,\psi(x) = 0 \tag{18}$$

which is a regular Sturm–Liouville system on the interval $[0, \pi/2]$. For this problem, the phase integral calculation is presented for the first few, $\lambda \ll 2h$, and for the high, $\lambda \gg 2h$, eigenvalues and compared with the values computed by Hargrave [17], who computed the two lowest eigenvalues of even eigenfunctions

$$\psi'(0) = \psi'(\pi/2) = 0 \tag{19}$$

for several h-values by 50- and 100-step numerical integration of Eqs. (6) or (7).

The phase integral eigenvalue condition for this case [32] is obtained by using the connection formula at the zero of $\{\lambda - 2h\cos(2x)\}$ to connect the exponentially decreasing solution near $\pi/2$ to the solution of Eq. (15) valid near 0, yielding

$$\frac{1}{\pi}\int_\Gamma q(z)\,dz = \left(m + \frac{1}{2}\right), \qquad m = 0, 1, 2, \ldots. \tag{20}$$

TABLE I

Lowest Eigenvalues of Mathieu's Equation Corresponding to Even Eigenfunctions: (a) 50-Step Numerical Integration, (b) 100-Step Numerical Integration, (c) 5th-Order Phase Integral, and (d) 6 Decimal Exact

h	(a)	(b)	(c)	(d)
5	−5.800046	−5.800046	−5.790010	−5.800046
10	−13.936980	−13.936980	−13.936536	−13.936980
15	−22.513037	−22.513038	−22.512997	−22.513038
20	−31.313419	−31.313391	−31.313383	−31.313390
25	−40.256785	−40.256783	−40.256777	−40.256780

The integration path Γ and details of the evaluation of the integrals are described in [28, 29]. A rapid second-order iteration to find λ_m may be established because the partial derivative of $(m+\frac{1}{2})$ with respect to λ [33]

$$\frac{\partial(m+\frac{1}{2})}{\partial\lambda}=\frac{1}{\pi}\int_{\Gamma}\frac{\partial q(z)}{\partial\lambda}\,dz \tag{21}$$

obtained from Eqs. (11)–(13), consists of a set of integrals very similar to those of Eq. (20) and may therefore be evaluated at each trial value of λ_m for very little extra computational cost. In Table I, the fifth-order phase integral eigenvalues are compared with the exact ones and those computed in [17]. It is seen that the general trends in accuracy with the numerical integration and the phase integral integration are complementary. The former is more efficient for small h-values whilst the latter improves with increasing h.

The same behaviour may be seen for high eigenvalues. Table II presents some higher eigenvalues of odd Mathieu eigenfunctions calculated with the boundary conditions

$$\psi(0)=\psi(\pi/2)=0 \tag{22}$$

TABLE II

Higher Eigenvalues of Mathieu's Equation Corresponding to Odd Eigenfunctions $h=1$: a) Numerical Integration, (b) 1st-Order Phase Integral, (c) 3rd-Order Phase Integral, (d) 5th-Order Phase Integral, and (e) Two-Term Asymptotic Series

m	(a)	(b)	(c)	(d)	(e)
5	100.005050675	100.0050002	100.00505017	100.005050670	100.005
10	400.001253135	400.0012500	400.001253128	100.001253135	400.00125
15	900.00055617	900.00055556	900.000556173	900.000556174	900.0005556
100	40000.0000	40000.0000125	40000.0000125	40000.0000125	40000.0000125
1000	4000000.000000	4000000.000000	400000.000000	4000000.000000	400000.000000

by numerical integration [17], by phase integral method, and by analytic asymptotic series. The phase integral eigenvalue condition for this problem is obtained directly from Eq. (16) which is valid on the whole interval $[0, \pi/2]$, yielding

$$\frac{1}{\pi}\int_0^{\pi/2} q(x)\,dx = m \tag{23}$$

and a formula analogous to Eq. (21) for rapid convergence to the desired eigenvalue.

It is seen in Table II that in the numerical integration of column (a), for a given number of integration steps, the accuracy is very good for the lower eigenvalues and then levels out for higher eigenvalues while the accuracy of the phase integral calculation improves with increasing m. Comparing with the asymptotic analytic methods, it should be noted that the asymptotic series may actually be obtained by expanding the integrals in Eq. (23). For moderate values of λ, however, many terms may be required for high accuracy and the direct integration of Eq. (23) is more efficient. Finally, to demonstrate the efficiency of the phase integral calculation, Table III lists the number of function evaluations per trial energy needed in standard numerical integration and in slightly modified numerical integration (see [15] for those definitions) compared with phase integral calculations. Note that for levels $m \geqslant 100$, the first-order phase integral calculation is sufficiently accurate and therefore, for those levels, the function to be evaluated is the same in all three columns of Table III.

The second test case is the Lamé equation

$$\psi''(x) + \{\lambda - n(n+1)\,k^2 sn^2 x\}\,\psi(x) = 0 \tag{24}$$

TABLE III

Number of Function Evaluations N per Integration Required
by (a) Standard Numerical Integration,
(b) Improved Numerical Integration [15], and
(c) Phase Integral Calculation at the Eigenlevels of Table II

	$\langle N \rangle$		
m	(a)	(b)	(c)
5	1084	128	15
10	2812	146	15
100	48719	128	7
1000			3

where *snx* is the Jacobian elliptic function of modulus k, and the solutions of Eq. (24) are the Lamé polynomials if n is an integer. Four possible types of boundary conditions are considered,

$$\psi(0)=\psi(K)=0, \tag{25}$$

$$\psi(0)=\psi'(K)=0, \tag{26}$$

$$\psi'(0)=\psi(K)=0, \tag{27}$$

$$\psi'(0)=\psi'(K)=0, \tag{28}$$

where K is complete elliptic integral of the first kind. The phase integral eigenvalue condition for this problem covering all the four cases is very similar to that of Mathieu's equation [32, 34]

$$m\pi=\alpha+\sigma\pm\arctan(\exp(\beta)) \tag{29}$$

where α and β are the sums of various-order contributions to the phase integrals on the $\{\lambda-p(x)\}>0$ and $\{\lambda-p(x)\}<0$ range, respectively, and σ is the sum of various-order comparison equation correction functions [31]. Equation (29) yields Eqs. (20) and (23) considered with the Mathieu's equation as limiting cases for low and high eigenvalues but in order to compute all eigenvalues for a given n, Eq. (29) in needed. Note, however, that the eigenvalues $\lambda>n(n+1)$ may be obtained from the symmetry relation for the eigenvalues [35]

$$\lambda_m(k^2)=(n(n+1))-\lambda_{N-m}(k'^2), \tag{30}$$

where $N=2n+1$ and k' is the complementary modulus defined as

$$k'=(1-k^2)^{1/2}. \tag{31}$$

The computation of the phase integrals requires values of elliptic functions *snx* and its derivatives on the range $[0, K]$. To avoid extensive calculations of various elliptic functions, an array of sn^2x-values was first created and its values and derivatives required in the phase integral calculations were computed by local polynomial interpolation by using the computer program of [36], which was also used for evaluating the phase integrals from this numerical data.

For large values of n, Hargrave [17] reports that the eigenvalues obtained by 100-step numerical integration are accurate to ten significant figures. The phase integral calculations of the present work yield for $k^2\approx 0.5$ results which are accurate to six significant figures at $n=10$, to seven significant figures at $n=20$, and so on for much less computational work than with numerical integration. For low n-values, on the other hand, the phase integral method is less accurate and numerical integration is to be preferred.

In some exceptional cases, Eq. (29) may be numerically unstable. For $k^2\approx 0.5$,

there is one level almost at $\lambda = n(n+1)$, which in Eq. (29) implies that β is very small but α and σ extremely large, which leads to numerical difficulties. This situation may be remedied by a combination of numerical integration and the phase integral method. Using Eq. (16) with lower limit of integration at K and direct numerical integration of the equation from 0 with fitting in the middle yields stable eigenvalues also for this case.

The final test case is the eigenvalues of the singular Sturm–Liouville problem

$$\psi''(x) + \{\lambda - x^4\}\,\psi(x) = 0 \tag{32}$$

with the boundary conditions

$$\psi(-\infty) = \psi(\infty) = 0. \tag{33}$$

For this problem, there is a region where $\{\lambda - x^4\}$ is positive and two regions in which $\{\lambda - x^4\}$ is negative. For $\{\lambda - x^4\} < 0$, Eq. (14) is valid, provided x is not too close to a turning point, but for $\{\lambda - x^4\} > 0$ inspection of various-order contributions to $w(z)$ shows that Eq. (16) yields accurate results only for higher eigenlevels. For the lowest levels, $m = 0$–3, therefore, a transition to numerical integration is required in the $\{\lambda - x^4\} < 0$ regions at $x = \pm 3 \cdot \lambda^{1/4}$, say, while for higher levels application of the connection formula, Eq. (17), at the two turning points yields the eigenvalue condition

$$\frac{1}{2\pi}\int_\Gamma q(z)\,dz = \left(m + \frac{1}{2}\right), \qquad m = 4, 5, 6, \ldots, \tag{34}$$

TABLE IV

The Six-Figure Eigenvalues λ_m of the Problem Eq. (35) for $m = 0$–10, 20, 30, 50, 100

m	λ_m
0	1.06036
1	3.79967
2	7.45570
3	11.6447
4	16.2618
5	21.2384
6	26.5285
7	32.0986
8	37.9230
9	43.9812
10	50.2563
20	122.605
30	208.232
50	407.874
100	1020.99

which by symmetry is the same as Eq. (20) and employs the same rapid iteration for determining the eigenvalues. Table IV presents a selection of eigenvalues for this problem computed for $m = 0$–3 by a combination of phase integral method and numerical integration and by Eq. (34) for $m \geqslant 4$. As before in the phase integral calculations, the accuracy of the eigenvalues increases with increasing m while the computational cost per eigenvalue decreases.

5. Conclusions

It has been shown by numerical examples that a combination of phase integral approximations and numerical integration of the Prüfer phase function equation yields a computationally effective technique for numerical solution of Sturm–Liouville eigenvalues. The two methods are complementary in the sense that in the situations for which the phase integral method is very well applicable, high eigenlevels in particular, numerical integration becomes expensive and for cases in which the phase integral method is less accurate or cannot be used at all, numerical integration is typically very efficient. If the phase integral approximation is valid and accurate enough, it is computationally less expensive than numerical integration, but it is an asymptotic technique which implies that its accuracy is largely determined by the problem and cannot be arbitrarily increased by adding higher-order terms in the approximation. Therefore, for very high accuracy, numerical integration may be required to obtain the desired accuracy. However, experience has shown that in most physical problems, while the traditional first-order JWKB-method usually is too inaccurate, application of third- or fifth-order phase integral approximation yields the best compromise between accuracy and the computational cost.

In some cases the phase integral method fails to yield accurate eigenvalues. However, this breakdown of the approximation is very often local; it takes place only for some eigenvalues and on a narrow region of the argument and does not affect the accuracy of the approximation elsewhere. In the phase integral description, correction functions have been introduced but they are known only for a few cases. It has been shown in the present work that a flexible transition between the phase integral approximation and numerical integration yields a general way of treating these cases.

In the region for which the phase integral method is recommended in this work, modified Prüfer substitution has been used in numerical integration. These two methods are very closely related and the phase integral method corresponds to solving the modified Prüfer phase function equation by the method of successive approximations.

For many problems, analytic asymptotic formulae for the eigenvalues may be derived from the phase integral eigenvalue conditions. However, those formulae are specific to the problem considered while the phase integral eigenvalue conditions are more general. For numerical purposes, asymptotic formulae offer no real benefit

because the phase integral calculations for high levels are extremely fast, and for moderate eigenvalues for which the asymptotic series may require many terms for sufficient accuracy, phase integral methods typically yield high accuracy for low computational cost.

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