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Extension of the Renormalized Numerov Method for Second-Order Differential Eigenvalue Equations

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The Renormalized Numerov Method [Johnson, *J. Chem. Phys.* **67**, 4086 (1977)] is extended to include equations possessing an explicit first-order derivative term. The variety of boundary conditions which can be employed is enlarged. Comparison with other numerical methods is made. © 1986 Academic Press, Inc.

1. INTRODUCTION

This paper is concerned with the numerical solution of second-order differential eigenvalue equations which can be written in the form

$$\Psi''(x) = p(x)\,\Psi'(x) + q_{\lambda s}(x)\,\Psi(x), \quad a \leqslant x \leqslant b, \tag{1.1}$$

where $p(x)$ and $q_{\lambda s}$ are continuously differentiable functions which may present some singularity at the bounds;

$$q_{\lambda s} = k(x)[V_s(x) - \lambda], \tag{1.2}$$

λ denotes the eigenvalue, s is some parameter, $V_s(x)$ is analytic or may be expressed in the form of some polynomial expansion. Such boundary value equations occur frequently in the solution of Schroedinger equations encountered in molecular physics [2]. The paper presents an extension of the well-known renormalized Numerov method (RNM) as developed by Johnson [1] in the form of a two term recurrence algorithm.

Two particular cases of Eq. (1.1) are relevant to our purpose.

(a) That in which the first derivative term is absent, yielding the simpler equation

$$\Psi''(x) = q_{\lambda s}(x)\,\Psi(x), \qquad a \leqslant x \leqslant b. \tag{1.3}$$

(b) That in which the first derivative term may be expressed as a function $g(x)$, Eq. (1.1) taking the form of an inhomogeneous equation

$$\Psi''(x) = q_{\lambda s}(x)\,\Psi(x) + g(x). \tag{1.4}$$

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While Eq. (1.1) may in principle always be transformed by a suitable change of the dependent variable into the form (1.3), the resulting equation may not satisfy the conditions required to determine the solutions, e.g., if the function q is anywhere negative on the interval $[a, b]$, hence an approach such as that outlined above is appropriate.

The Johnson algorithm has been applied to equations of the form (1.3) with boundary conditions such that $\Psi(x)=0$ at both bounds. The technique has not been extended to include other boundary conditions or to equations explicitly possessing a first derivative term in instances other than those with trivially simple potentials.

We shall explore the solutions of Eq. (1.1) by means of two term recurrence algorithms associated with one of the following statements regarding boundary conditions:

$$\Psi(a)=\alpha, \qquad \Psi(b)=\beta, \tag{1.5a}$$

$$\Psi(a)=\alpha, \qquad \Psi'(b)=\beta \qquad \text{or} \qquad \Psi'(a)=\alpha, \qquad \Psi(b)=\beta, \tag{1.5b}$$

$$\Psi'(a)=\alpha, \qquad \Psi'(b)=\beta. \tag{1.5c}$$

Each of these boundary conditions is translated into a condition governing the quantities R and S of the Numerov algorithm by the means of (1.5) after which iteration may be performed [1, 2].

As a separate problem related to boundary conditions we shall have reason to consider equations for which the initial values of R and S at the bounds are not determinable a priori. A technique will be presented which permits an estimate of the starting value of R and S to be made.

The above considerations were determined by the requirements of certain equations encountered in the field of molecular physics, notably radial and angular Schrodinger equations describing large amplitude nuclear motion in molecules. Algorithms developed and the techniques of evaluation of boundary conditions have been tested on specific equations and the results compared with those of some other approaches.

2. Algorithms

The following difficulties stand in the way of exploiting the useful characteristics of the RNM approach:

(i) The explicit presence of the first derivative term precludes direct application of RNM since the Numerov algorithm applies only to equations in which the first derivative term is absent.

(ii) The presence of singularities at $x=a$ and/or $x=b$ requires some alternate procedure in the vicinity of the bounds.

(iii) The boundary values α and β are not necessarily known explicitly. In some cases a certain amount of information is available from the form of the function $V_s(x)$ and a procedure to determine α and β may be implemented.

(iv) The function $q_{\lambda,s}$ is not necessarily positive over the entire interval $[a, b]$ in which case the operator L is not of "monotone" kind [3, 4].

Difficulty (i) may be overcome in one of several ways discussed below. Difficulties (ii) and (iii) have been overcome elsewhere [2] by the implementation of a graphical procedure. We here present an alternate which has the advantage of removing the singularities at the bound while also preventing the operator L becoming nonmonotone at the bounds. This procedure therefore solves difficulty (iv) in addition to (ii) and (iii).

The general procedure is as follows.

In the problem as stated in (1.1), any derivatives are replaced by some finite difference approximation. The resulting linearized difference equations may be written very generally as follows:

$$A\Psi_{n-1} + B\Psi_n + C\Psi_{n+1} = 0 \qquad (1 \leqslant n < N+1) \tag{2.1}$$

associated with one of the boundary conditions (1.5) and where A, B, and C are some expressions depending upon the values of $p(x)$ and $q_{\lambda,s}(x)$ at various grid points.

The above three term recurrence relation may be transformed to a two term relation provided certain convergence criteria are met [6]:

$$R_n = -(B/C) - (A/C)\, R_{n-1}^{-1} \qquad \text{(forward iteration)}, \tag{2.2}$$

$$S_n = -(B/A) - (C/A)\, S_{n+1}^{-1} \qquad \text{(backward iteration)}, \tag{2.3}$$

where

$$R_n = \Psi_{n+1}/\Psi_n, \tag{2.4}$$

$$S_n = \Psi_{n-1}/\Psi_n. \tag{2.5}$$

Given an arbitrary value of the parameter λ, the backward iteration is perfomed using (2.5) and starting from the value S_{n+1}. When the condition $S_n < 1$ first occurs, the iteration is stopped at that point which is by definition the matching point x_M. This is approximately the position where the first derivative of the solution is zero. The forward iteration is then carried out using as starting value R_1 and employing (2.4). During the calculations the nodes are counted (a node is located between x_n and x_{n+1} when $R_n < 0$). The function $D(\lambda)$ [8] is computed from

$$D(\lambda) = [A_{M+1}(S_{M+1}^{-1} - R_M) - A_{M-1}(S_M - R_{M-1}^{-1})][1 - T_\lambda], \tag{2.6}$$

where the functions A and T at grid point x_n are defined by

$$T_n = (h^2/12)\, q_n, \tag{2.6a}$$

$$A_n = (0{,}5 - T_n)/(1 - T_n). \tag{2.6b}$$

If λ is an eigenvalue, $D(\lambda)$ is zero. The iterations may be implemented once the initial values R_1 and S_{N+1} are defined, in other words once $\Psi(x)$ is known (or may be estimated) at grid points 1, 2, N, $N+1$.

Dependent upon which alternate for solving the first difficulty (i) is adopted, three distinct approaches present themselves.

a. *Method* (1)

Substituting the usual three term algorithm [3]

$$(h/2)\, L_h(u_j) = -b_j u_{j-1} + a_j u_{j-1} + a_j u_j - c_j u_{j+1} = 0,$$

where

$$a_j = 1 + (h^2/2)\, q_j,$$

$$b_j = \tfrac{1}{2}[1 + hp_j/2],$$

$$c_j = \tfrac{1}{2}[1 - hp_j/2],$$

into (2.1) we obtain

$$A = 1 + hp_n/2, \qquad B = -(2 + 12T_n), \qquad C = (1 - hp_n/2), \tag{2.7}$$

where

$$T_n = (h^2/12)\, q_n, \qquad U_n = (2 + 10T_n)/(1 - T_n). \tag{2.8}$$

Thus

$$R_n = U_n/(1 - hp_n/2) - [(1 + hp_n/2)/(1 - hp_n/2)]\, R_{n-1}^{-1}, \tag{2.9}$$

$$S_n = U_n/(1 + hp_n/2) - [(1 - hp_n/2)/(1 + hp_n/2)]\, S_{n+1}^{-1}. \tag{2.10}$$

R_n and S_n can be iterated once R_1 and S_{N+1} (i.e., the ratios Ψ_2/Ψ_1 and Ψ_N/Ψ_{N+1}) are specified.

To keep the degree of accuracy similar to that of the Numerov algorithm, hence to be able to compare the different methods, the computations must be carried out for two values of h (h and $h/2$) and the results introduced in the Richardson extrapolation leading to a theoretical result in $O(h^4)$. Then at each step of the computation, R_n and S_n are evaluated for h and $h/2$ and extrapolated.

This procedure is somewhat lengthy since we use two iterations at every step.

b. *Method* (2)

Let us consider the problem as stated in (1.4) and expand $\Psi(x)$ in the following power series:

$$\Psi_{n+1}+\Psi_{n-1}=\sum_k [2h^{(2k)}/(2k)!]\,\Psi_n^{(k)}, \tag{2.11}$$

$$\Psi_{n+1}-\Psi_{n-1}=\sum_k [2h^{(2k+1)}/(2k+1)!]\,\Psi_n^{(k+1)}. \tag{2.12}$$

To the fourth order, we get the well-known results [7]:

$$\Psi_{n+1}[1-T_{n+1}]-\Psi_n[2+10T_n]+\Psi_{n-1}[1-T_{n-1}] = (h^2/12)[g_{n+1}+10g_n+g_{n-1}], \tag{2.13}$$

$$\Psi_{n+1}[0,5-T_{n+1}]-\Psi_{n-1}[0,5-T_{n-1}] = (h^2/12)[g_{n+1}-g_{n-1}+(12/h)\,\Psi'_n]. \tag{2.14}$$

Equation (2.13) is the usual Numerov algorithm. Considering the function $p(x)\,\Psi'(x)$ as $g(x)$ in (1.4) and setting

$$A_n=(0,5-T_n)/(1-T_n), \tag{2.15}$$

$$y_n=\Psi_n(1-T_n), \tag{2.16}$$

we obtain

$$y_{n+1}-[(2+10T_n)/(1-T_n)]\,y_n+y_{n+1} = (h^2/12)[p_{n+1}\Psi'_{n+1}+10p_n\Psi_n+p_{n-1}\Psi'_{n-1}], \tag{2.17}$$

$$A_{n+1}y_{n+1}-A_{n-1}y_{n-1} = (h^2/12)[p_{n+1}\Psi'_{n+1}+(12/h)\,\Psi'_n-p_{n-1}\Psi'_{n-1}]. \tag{2.18}$$

Since

$$[p_n\Psi'_n]'=\Psi'_n(p'_n+p_n^2)+p_nq_n\Psi_n, \tag{2.19}$$

$$[p_n\Psi'_n]''=\Psi'_n(3p_np'_n+p_n^3+p''_n+q_n)+\Psi_n(2q_np'_n+p_n^2q_n+p_nq_n). \tag{2.20}$$

We finally get, after dropping the terms in $O(h^4)$,

$$y_{n+1}-y_n[2+10T_n+h^2(2T_np'_n+p_n^2T_n+p_nT_n)]/(1-T_n)+y_{n-1} = (h^2/12)[12p_n+h^2\alpha_n)\,\Psi'_n, \tag{2.21}$$

$$A_{n+1}y_{n+1}-[2hp_nT_n/(1-T_n)]\,y_n-A_{n-1}y_{n-1} = h\Psi'_n[1+(h^2/6)(p'_n+p_n^2)], \tag{2.22}$$

where

$$\alpha_n=3p_np'_n+p_n^3+p''_n+q_np_n. \tag{2.23}$$

We now eliminate Ψ'_n between (2.21) and (2.22), obtaining, after rearranging the terms

$$a_n y_{n-1} + b_n y_n + c_n y_{n+1} = 0, \tag{2.24}$$

where

$$a_n = 6 + 6hp_n A_{n-1} + h^2(p'_n + p_n^2), \tag{2.25}$$

$$b_n = -(1 - T_n)^{-1}\,[12 + 60T_n + 2h^2(p'_n + p_2^2 + 5p'_n T_n - p_n^2 T_n)], \tag{2.26}$$

$$c_n = 6 - 6hp_n A_{n+1} + h^2(p'_n + p_n^2). \tag{2.27}$$

Finally, the two-term recurrence relations can be written as follows:

$$R_n = (U_n/Y_n) - (Z_n/Y_n)\,R_{n-1}^{-1}, \tag{2.28}$$

$$S_n = (U_n/Z_n) - (Y_n/Z_n)\,S_{n+1}^{-1}, \tag{2.29}$$

where

$$Y_n = [\alpha_n - hp_n A_{n+1}][1 - T_{n+1}], \tag{2.30}$$

$$Z_n = [\alpha_n + hp_n A_{n-1}][1 - T_{n-1}], \tag{2.31}$$

$$U_n = [(2 + 10T_n\alpha_n - 2h^2 p_n^2 T_n], \tag{2.32}$$

and

$$\alpha_n = 1 + (h^2/6)(p'_n + p_n^2). \tag{2.33}$$

Note that R_n and S_n are defined here by:

$$R_n = y_{n+1}/y_n \qquad \text{and} \qquad S_n = y_{n-1}/y_n. \tag{2.34}$$

Clearly this algorithm reduces to the Numerov algorithm when $p(x) = 0$ and furthermore to the algorithm of method 1 if terms of degree higher than h^2 are dropped.

This algorithm presents the advantage of having theoretical local truncation errors similar to those of the Numerov algorithm and is usable in any general problem as stated in (1.1).

c. *Method* (3)

The first derivative term $p(x)\,\Psi'(x)$ in (1.1) can be removed mathematically by a change of the function $\Psi(x)$:

$$\Psi(x) = \chi(x)\,A(x). \tag{2.35}$$

This leads to an equation for which the Numerov algorithm may be applied directly. However, the transformation may be difficult and, considered

mathematically, the transformed function may be badly behaved (particularly at the bounds) as shown in the Sect. 4 (Legendre equation). This kind of transformation has been successfully used in solving the radial equation for the hydrogen atom [8].

Let us substitute (2.35) into (1.1),

$$\chi''(x) = [(p(x)\,A(x) - 2A'(x))/A(x)] \times \chi'(x) + [(q_s(x)\,A(x) + p(x)\,A'(x) - A''(x))/A(x)]\,\chi(x). \tag{2.36}$$

It is easy to see that by choosing

$$A(x) = \exp\left[\int (1/2)\,p(x)\,dx\right] \tag{2.37}$$

the system (1.1) becomes

$$\chi''(x) = [q_s(x) + \tfrac{1}{4}p^2(x) - \tfrac{1}{2}p'(x)]\,\chi(x) \tag{2.38}$$

while the boundary conditions are:

$$\chi(a) = \alpha/A(a), \qquad \chi(b) = \beta/A(b). \tag{2.39}$$

Introduce

$$Q_s(x) = q_s(x) + \tfrac{1}{4}p^2(x) - \tfrac{1}{2}p'(x), \tag{2.40}$$

$$\tau_n = (h^2/12)\,Q_{s,n} = T_n + (h^2/24)(p_n^2/2 - p_n'). \tag{2.41}$$

The Numerov algorithm can now be written in the form

$$\chi_{n-1}(1 - \tau_{n-1}) - (2 + 10\tau_n)\,\chi_n + \chi_{n+1}(1 - \tau_{n+1}) = 0. \tag{2.42}$$

Finally, by performing the usual substitution

$$\chi_n(1 - \tau_n) = F_n, \tag{2.43}$$

we obtain in setting $R_n = F_{n+1}/F_n$ and $S_n = F_{n-1}/F_n$,

$$R_n = U_n - 1/R_{n-1}, \tag{2.44}$$

$$S_n = U_n - 1/S_{n+1}, \tag{2.45}$$

where

$$U_n = (2 + 10\tau_n)/(1 - \tau_n). \tag{2.46}$$

For the evaluation of the eigenfunctions this method requires a supplementary step consisting in multiplying the function $\chi(x)$ by $A(x)$ and care must be taken especially at the bounds where some indeterminacy may result. For example, in

TABLE I

Functions involved in the Various Algorithms

Method	U_n	Y_n	Z_n
(1):(Ψ)	$2+12T_n$	$1-.5hp_n$	$1+.5hp_n$
(2):(Ψ)	$(2+10T_n)\alpha_n-2h^2p_n^2T_n$	$\alpha_n^-(1-T_n)$	$\alpha_n^+(1-T_{n-1})$
(3):(χ)	$2+10\tau_n$	$1-\tau_{n+1}$	$1-\tau_{n-1}$
(3):(F)	$(2+10\tau_n)(1-\tau_n)^{-1}$	1	1

Note. $\alpha^+=\alpha_n+hp_nA_{n-1}$, $\alpha^-=\alpha_n-hp_nA_{n+1}$.

Legendre-type equations, $A(x)=(1-x^2)^{-1/2}$ and $A(-1)=A(1)=$ infinity. Care must be taken in the evaluation of the boundary conditions in (2.39). The change of function may also present problems concerning the volume element which must be verified for the transformation and it is necessary to make sure by examining the behaviour of $\chi(x)$ at the bounds that $\Psi(x)$ is actually an acceptable solution of the equation in all of the space including the bounds and that this solution is normalizable [9]. In spite of these difficulties, they present no major problems in the applications discussed below.

In Table I the various expressions for the discrete functions U_n, Y_n, and Z_n involved in the algorithm of general form are summarized:

$$R_n=[U_n/Y_n]-[Z_n/Y_n]\,R_{n-1}^{-1}, \tag{2.47}$$

$$S_n=[U_n/Z_n]-[Y_n/Z_n]\,S_{n+1}^{-1}. \tag{2.48}$$

Note that in this method, the iterations may be performed in terms of either χ_n (method 3a) or F_n (method 3b), the latter being faster since one calculation per step is saved.

Before presenting the results obtained from each of the algorithms we must discuss how the boundary conditions translate in terms of the starting values R_1 and S_{n+1}.

3. Numerical Examples: Simple Cases

The methods described above are first illustrated by solving two eigenvalue problems of the form (1.3) associated with non standard boundary conditions.

The determination of the starting values R_1 and S_{N+1} has been treated in a previous publication [2]. Let us recall briefly how the boundary conditions (1.5) translate in terms of the two-term recurrence algorithms:

$$\Psi(a)=0 \quad \rightarrow R_1 = \text{infinity},$$

$$\Psi(b)=0 \quad \rightarrow S_{N+1} = \text{infinity},$$

$$\Psi'(a)=0 \quad \rightarrow R_1 = U_1/2,$$

$$\Psi'(b)=0 \qquad \to S_{N+1}=U_{N+1}/2,$$
$$\Psi'(a)=\alpha\Psi(a)\to R_1 \quad =U_1/2+h\alpha/(2-2T_1),$$
$$\Psi'(b)=\beta\Psi(b)\to S_{N+1}=U_{N+1}/2-h\beta/(2-2T_{N+1}).$$

EXAMPLE 1. Consider the eigenvalue problem presented by the Mathieu equation

$$y''_{ns}(x)=[2s\cos x-a_n(s)]\,y_{ns}(x) \qquad (0\leqslant x\leqslant\pi), \tag{3.1}$$

where s is an integer and a_n the eigenvalues. The solutions to this equation are known to be periodic (period π or 2π). There exists a set of eigenvalues a_n corresponding to even solutions and a set b_n corresponding to odd solutions [10]. The odd solutions are related to boundary conditions

$$y_{ns}(0)=y_{ns}(\pi)=0 \tag{3.2}$$

while the even solutions are related to boundary conditions:

$$y'_{ns}(0)=y'_{ns}(\pi)=0. \tag{3.3}$$

Method 2 (with the term $p(x)=0$, i.e., the usual RNM) has been employed for this problem (even solutions, i.e., with boundary conditions $\Psi'(0)=\Psi'(\pi)=0$). Approximate eigenvalues λ_n have been computed corresponding to different values of step-size h. The results are presented in Table II for a selection of values of the parameter s. The relative errors are also presented using as exact eigenvalues a_n of reference [10]. We observe that $1-\lambda/E$ behaves as $O(h^4)$ as expected.

EXAMPLE 2. The eigenvalue problem

$$y''(x)+a(1+x^2)^{-2}\,y(x)=0, \qquad 0\leqslant x\leqslant 1 \tag{3.4}$$

TABLE II

$y''\times(2s\cos x-a)y=0$, $0\leqslant x\leqslant\pi$, $y'(0)=y'(\pi)=0$, Method 2

h	λ^a	e	λ^b	e	λ^c	e
$\frac{1}{4}$	−6.662567	1.29(−1)	2.970220	3.74(−1)		
$\frac{1}{8}$	−5.815025	2.58(−3)	1.782272	4.26(−2)	−40.643858	9.52(−3)
$\frac{1}{16}$	−5.800894	1.46(−4)	1.853593	2.48(−3)	−40.267857	2.75(−4)
$\frac{1}{32}$	−5.800099	9.14(−6)	1.857876	1.67(−4)	−40.257444	1.65(−5)
$\frac{1}{64}$	−5.800049	5.20(−7)	1.858164	1.24(−5)	−40.256821	1.24(−5)
$\frac{1}{128}$	−5.800046	2.01(−8)	1.858186	5.40(−7)	−40.256782	7.02(−8)

Note. λ is the computed eigenvalue

[a] Corresponds to $s=10$, the exact eigenvalue is $a=-5.800046$ $(n=0)$.

[b] Corrresponds to $s=10$, the exact eigenvalue is $a=1.858187$ $(n=1)$.

[c] Corresponds to $s=50$, the exact eigenvalue is $a=-40.256779$ $(n=0)$, $e=1-a/\lambda$.

TABLE III

$y'' + \beta(1+x)^{-2} y = 0,\ 0 \leqslant x \leqslant 1,\ y(0) = y'(1) = 0$, Method 2

h	λ	(a)	(b)	(c)
$\frac{1}{4}$	6.782418742	7.51(−3)	6.61(−3)	2.96(−4)
$\frac{1}{8}$	6.743273383	1.69(−3)	1.84(−3)	1.26(−5)
$\frac{1}{16}$	6.734640928	4.12(−4)	4.70(−4)	1.89(−7)
$\frac{1}{32}$	6.732552927	1.02(−4)	1.18(−4)	6.09(−8)
$\frac{1}{64}$	6.732037890	2.56(−5)	2.96(−5)	1.27(−8)
$\frac{1}{128}$	6.731909184	6.50(−6)	7.39(−6)	1.69(−9)

Note. The exact value is $\beta_1 = 6.731865405$, λ is the computed eigenvalue. (a), (b) and (c) are the absolute values of $1 - \beta_1/\lambda_1$ using, respectively, method 2, method (2.3) and method (2.9) from Usmani [11].

with boundary conditions

$$y(0) = y'(1) = 0 \tag{3.5}$$

represents an other example where a direct application of the RNM may be used with boundary conditions other that the standard $\Psi(x) = 0$ at bounds. This problem has recently been studied by Usmani [11]. Comparison of the present method of solution with his results is presented in Table III. The rate of convergenge is equivalent to that of method (2.3) described in Ref. [11].

4. Application to Legendre-Type Equations

Let us consider the following equation:

$$\Psi''(x) = [(2x/(1-x^2)]\ \Psi'(x) + [1/(1-x^2)][s^2/(1-x^2) + V(x) - \lambda]\ \Psi(x) \qquad (-1 \leqslant x \leqslant 1) \tag{4.1}$$

with boundary conditions:

$$\Psi(-1) = \alpha, \qquad \Psi(1) = \beta. \tag{4.2}$$

With $V(x) = 0$ and $\alpha = \pm 1, 0$; $\beta = 1$ this is the Legendre equation. The addition of the term $V(x)$ gives rise to the Legendre equation with an added potential, an equation which is of importance in molecular quantum theory and in molecular scattering [2].

$V(x)$ is commonly expressed in the form of an expansion around $x = \pm 1$,

$$V(x) = \sum_i A_i (x - x_{eq})^i \qquad (i = 1, 2, \ldots), \tag{4.3}$$

where x_{eq} is that value of x at which the potential is a minimum.

Since $x=-1$ is a regular singular point, Eq. (4.1) has a Frobenius-type series solution around the singularity:

$$\Psi=(x-a)^c\left(\sum_j a_j(x-a)^j\right). \tag{4.4}$$

Proceeding as usual, the coefficients are given for methods (1) and (2) by

$$c=s/2, \tag{4.5}$$

$$a_0=1, \tag{4.6}$$

$$a_1=(s^2-s-2\lambda)/4(s+1), \tag{4.7}$$

$$a_2=[s^4+5s^3-4s^2(\lambda-2)-4s(2\lambda-2A_1-1)+4(\lambda^2-2\lambda+2A_1)]/[32(s+1)(s+2)]. \tag{4.8}$$

Near $x=-1$, the solution may therefore be expressed as

$$\Psi(x)=(x+1)^{s/2}+a_1(x+1)^{s/2+1}+a_2(x+1)^{s/2+2}. \tag{4.9}$$

Replacing x by -1 and by $-1+h$, we may evaluate the ratio $R_1=\Psi(-1+h)/\Psi(-1)$. For instance $R_1=\Psi(-1+h)$ for $s=0$ and $R_1=$ infinity for $s>0$.

The same procedure can be used at the upper bound $x=1$. This result is in agreement with analytic values calculated from the Legendre polynomials and associated functions.

For method (3.a), the Frobenius coefficients for χ evaluated at $x=-1$ are:

$$c=(s+1)/2, \tag{4.10}$$

$$a_0=1, \tag{4.11}$$

$$a_1=(s^2-2\lambda-1)/4(s+1), \tag{4.12}$$

$$a_2=[2c^2(2c^2-c-\lambda-1)+2c(2A_1+\lambda)+\lambda^2]/[16c(2c+1)], \tag{4.13}$$

and around $x=-1$, the solution is given by

$$\chi(x)=(1+x)^{(s+1)/2}[1+a_1(1+x)+a_2(1+x)^2]. \tag{4.14}$$

Here, in both cases ($s=0$, $s>0$), $R_1=$ infinity. Analytic evaluation of $\chi(x)$ from the Legendre polynomials and $A(x)=(1-x^2)^{-1/2}$ gives the same result, for instance $\chi(\pm 1)=0$, irrespective of the value of s.

The evaluation of R_1 expressed in terms of the function $F_n=(1-T_n)\,\chi_n$ (method 3.b) where T_n is defined by Eq. (2.8) is obtained in the following way.

Let the equation be written as:

$$\chi_n''=Q_n\chi_n. \tag{4.15}$$

Multiplying both sides by $h^2/12$ and substituting in the expression for F_n we obtain

$$F_n = \chi_n - (h^2/12)\,\chi_n''. \tag{4.16}$$

The second derivative of $\chi(x)$ at grid point x_n is determined from (4.14):

$$\chi''(x) = A(1+x)^{(s-3)/2} + B(1+x)^{(s-1)/2} + C(1+x)^{(s+1)/2}, \tag{4.17}$$

where

$$A = (s^2-1)/4, \tag{4.18}$$

$$B = a_1(s+3)(s+1)/4, \tag{4.19}$$

$$C = a_2(s+3)(s+5)/4. \tag{4.20}$$

Substituting in (4.16) we obtain the values of F_n at $x=-1$ and $x=-1+h$ and therefore the value of R_1.

Note that a boundary condition such that $\chi(-1)=0$ does not imply necessarily $F(-1)=0$; this situation occurs only if $\chi''(-1)=0$. Therefore the starting values R_1 will differ if method (3) is used in terms of Ψ_n or in terms of F_n.

Both procedures have been tested on the Legendre equation itself. The Eq. (4.1) is considered as an eigenvalue equation. The analytic eigenvalues are given by $\lambda_L = L(L+1)$ and the corresponding eigenfunctions are the Legendre polynomials ($s=0$) and the associated Legendre functions ($s>0$) $P_L^s(x)$. The numerical solutions are carried out with the three methods and the results presented in Table IV.

As shown, for $s=0$, the better results were obtained from method (2) (convergence is as $O(h^4)$. For $s>3$, methods (2) and (3) are also in $O(h^4)$. For $0<s<3$, both (2) and (3) are in $O(h^2)$. We mention nevertheless that (3) is more stable for higher eigenvalues.

The RNM has been shown by Johnson [8] to be extremely sensitive to the initial values of R_1 and S_{N+1}. For small values of s, methods (3) fail to give expected fourth order convergent results even though the values of $\chi(x)$ at the bounds evaluated from the series expansion agree with the corresponding analytic values. In spite of that, successful results were obtained by using R_2 and S_N as initial values for the iterations, i.e., starting the iterations one grid point removed from the bounds and fixing $\chi(\pm 1)=0$.

The success attained for the Legendre equation suggests a similar scheme to solve the analogous equation with a potential $V(x)$.

To test the method described above, a previously employed potential was adopted since eigenvalues and vectors obtained by a more customary numerical (complete set expansion) method of solution were available. [12]. It must be recalled that this equation has no analytic solution.

The potential function is zero at $x=-1$ and tends to infinity as x tends to 1 and is expressible by the following expansion:

$$V(x) = \sum_i A_1(x+1)^i \qquad (i=1, 2,\ldots), \tag{4.21}$$

TABLE IV

Legendre Equation

h	Method (1)	Method (2)	Method (3)	Method (3b)
$s=0, n=1$				
$\frac{1}{4}$	1.63(−1)	3.62(−1)	4.96(−1)	1.69(−2)
$\frac{1}{8}$	2.49(−2)	1.05(−2)	4.44(−1)	1.24(−2)
$\frac{1}{16}$	4.66(−3)	8.81(−4)	4.04(−1)	1.13(−2)
$\frac{1}{32}$	7.85(−4)	6.65(−5)	3.70(−1)	1.09(−2)
$\frac{1}{64}$	2.27(−4)	4.28(−6)	3.42(−1)	1.07(−2)
$\frac{1}{128}$	8.78(−5)	2.61(−7)	3.17(−1)	9.97(−3)
$s=1, n=1$				
$\frac{1}{4}$	1.74(−1)	6.32(−2)	5.26(−2)	
$\frac{1}{8}$	9.39(−2)	2.35(−2)	1.41(−2)	9.65(−2)
$\frac{1}{16}$	4.71(−2)	5.41(−3)	3.69(−3)	8.14(−3)
$\frac{1}{32}$	2.35(−2)	1.08(−3)	9.48(−4)	5.02(−4)
$\frac{1}{64}$	1.17(−2)	3.98(−4)	2.40(−4)	3.17(−5)
$\frac{1}{128}$	5.87(−3)	8.71(−5)	6.06(−5)	2.01(−6)
$s=4, n=1$				
$\frac{1}{4}$	1.16(−2)	1.67(−1)	1.81(−2)	*n/a*
$\frac{1}{8}$	2.46(−3)	2.57(−2)	1.36(−3)	*n/a*
$\frac{1}{16}$	5.93(−4)	2.43(−3)	9.48(−5)	*n/a*
$\frac{1}{32}$	1.48(−4)	1.04(−4)	6.54(−6)	*n/a*
$\frac{1}{64}$	3.65(−5)	1.85(−5)	4.47(−7)	*n/a*
$\frac{1}{128}$	9.00(−6)	3.00(−6)	3.10(−8)	*n/a*

Note. Absolute values of $1-\lambda_L/\lambda_c$, λ_c is the computed value, λ_L the analytic value.

where the A_i are the following constants:

$$A_1 = 865.596, \qquad A_2 = 1065.19, \qquad A_3 = 118.02,$$
$$A_4 = 138.8, \qquad A_5 = -41, \qquad A_6 = 53.447.$$

The various methods were tested for different values of h. Equation (4.1) becomes here

$$\Psi''(x) = p(x)\,\Psi'(x) + q_{K,J}(x)\,\Psi(x), \tag{4.22}$$

where

$$q_{K,J}(x) = (1-x^2)^{-1}\,[J^2/(1-x^2) + V(x) - E_{K,J}]. \tag{4.23}$$

The $J=0$ case corresponds once more to boundary conditions such that the eigenfunction is not zero at the lower bound but is zero at the upper bound. The first derivative is nonzero at the lower bound and is zero at the upper bound. The $J>0$ case corresponds to boundary conditions such that the eigenfunction is zero at both bounds, its first derivative being non zero at the lower bound but zero at the upper

TABLE V

Angle Bending Equation

h	Method (1)	Method (2)	Method (3)	Method (3b)
$J=0, K=1$				
$\frac{1}{4}$	5.23(−2)	1.84(−1)	—	—
$\frac{1}{8}$	1.14(−2)	3.51(−2)	—	—
$\frac{1}{16}$	2.61(−3)	6.29(−4)	6.18(−1)	4.31(−2)
$\frac{1}{32}$	5.18(−4)	1.29(−4)	3.70(−1)	3.89(−2)
$\frac{1}{64}$	1.03(−4)	2.66(−5)	5.01(−1)	3.47(−2)
$\frac{1}{128}$	3.61(−5)	4.19(−6)	4.64(−1)	3.21(−2)
$J=1, K=1$				
$\frac{1}{4}$	4.81(−1)	9.66(−2)	7.25(−2)	3.16(−1)
$\frac{1}{8}$	1.62(−2)	3.06(−2)	1.01(−2)	2.04(−2)
$\frac{1}{16}$	6.44(−2)	8.60(−3)	2.45(−3)	8.04(−4)
$\frac{1}{32}$	2.05(−2)	1.84(−3)	4.61(−4)	6.20(−5)
$\frac{1}{64}$	7.00(−3)	7.11(−4)	6.80(−5)	3.27(−6)
$\frac{1}{128}$	3.21(−3)	2.04(−4)	9.91(−6)	8.64(−7)

Note. Absolute values of $1-\lambda_L/\lambda_c$, λ_c is the computed value, λ_L is the value obtained by method (2) with 2001 grid points and is assumed to be the exact value.

one. Therefore the initial value R_1 has to be extrapolated either graphically or from the series expansion in the case $J=0$. In both cases S_{n+1} is infinity (since $\Psi(x)$ tends to zero very quickly) or as $U_{N+1}/2$ (since the first derivative of $\Psi(x)$ is zero at the upper bound). The results are given in table 5 for $J=0$ and $J=1$ $(K=1)$.

The numerical methods presented here do have the great advantage of speed of computation when compared to the complete set method together with the fact that the functional form of the eigenfunctions is immediately obtained rather than the usual set of eigenvector coefficients which accompany the complete set expansion.

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