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1987 J. Phys. A: Math. Gen. 20 4153

(http://iopscience.iop.org/0305-4470/20/13/022)

J. Phys. A: Math. Gen. **20** (1987) 4153–4160. Printed in the UK

(Extended) Numerov method for computing eigenvalues of specific Schrödinger equations

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Received 27 January 1987

Abstract. Numerov's method and an extended version of it are introduced for computing eigenvalues of Schrödinger equations with potentials $V(x)$ which are even functions with respect to x. Furthermore it is assumed that the wavefunctions tend to zero for $x \to \pm\infty$. The derived results are compared with previously derived numerical data and with available exact values.

1. Introduction

The last decade has seen a great deal of interest in the analytical as well as the numerical study of one-dimensional Schrödinger equations of the type

$$[D^2+(E-V(x))]y(x)=\mathrm{d}^2y(x)/\mathrm{d}x^2+(E-V(x))y(x)=0 \qquad (1.1)$$

with $V(x)$ an even function and $y(x)\to 0$ for $x\to\pm\infty$. The following typical examples of potentials have been considered:

the one-dimensional anharmonic oscillator potential

$$V_1(x)=x^2+\lambda x^2/(1+gx^2) \qquad \lambda, g \text{ parameters} \qquad (1.2)$$

the symmetric double-well potential

$$V_2(x)=x^6-bx^2 \qquad b \text{ parameter} \qquad (1.3)$$

the Razavy potential

$$V_3(x)=1/8m^2(\cosh(4x)-1)-m(n+1)\cosh(2x) \qquad n, m \text{ parameters} \qquad (1.4)$$

the doubly anharmonic oscillator of the type

$$V_4(x)=\lambda x^2+\mu x^4+\eta x^6 \qquad \eta>0, \lambda, \mu, \eta \text{ parameters.} \qquad (1.5)$$

Each of these potentials plays a role in several areas of physics.

Among the methods followed in the determination of the eigenvalues of the differential equation (1.1), let us mention the variational Rayleigh–Ritz formalism (Mitra 1978), perturbation algorithms (Kaushal 1979, Bessis and Bessis 1980, Killingbeck 1979), schemes based upon Padé approximants (Lai and Lin 1982), direct numerical integration techniques (Fack and Vanden Berghe 1985, 1986, Fack *et al* 1987) and an operator method based upon the SO(2, 1) dynamic group (Fack *et al* 1986). Exact solutions to the Schrödinger equation (1.1) have been constructed with $V(x)$ given by (1.2) (Flessas 1981, 1982, Varma 1981, Whitehead *et al* 1982) and by (1.4) (Razavy 1980).

In previous papers (Fack and Vanden Berghe 1985, 1986, Fack *et al* 1987) the authors have introduced the so-called classical second-, fourth- and sixth-order numerical methods whereby (1.1) is in each case discretised in the form

$$(J+h^2V)y=h^2Ey+t(h) \tag{1.6}$$

in which J is a suitable band matrix, $V=(v_{ij})$ is a diagonal matrix with $v_{ii}=V(x_i)$, $y=(y_0,\ldots,y_{N-1})^{\mathrm{T}}$ and $t(h)$ is the error matrix. Although the solutions of (1.1) are explicitly defined in $[-\infty,+\infty]$, it should be noted that these solutions are either of even or odd parity, i.e. $y(x)=\pm y(-x)$, so that the determination of $y(x)$ can be restricted to the region $[0,+\infty]$. Furthermore it has been supposed that the wavefunctions are approximately restricted to obey the Dirichlet boundary condition $y(x)=0$ at some x value R, for which an acceptable value is guessed numerically. The interval $[0,R]$ is subdivided into equal parts of length h, such that $y_0=y(0)$, $y_1=y(h),\ldots,y_N=y(Nh)=y(R)$. Depending on the order of the method J is either of a tri-, penta- or hepta-diagonal form.

In the present paper we shall treat the Schrödinger equation (1.1) first of all with the fourth-order method of Numerov (Fröberg 1979). Afterwards an extended Numerov method of sixth order will be developed and applied. Sections 2 and 3 explain the mathematics which form the basis of the proposed methods. The appropriate discretised formulae are presented. In § 4 we compare some numerical results with those of previous numerical calculations and exact solutions.

2. Numerov's fourth-order method

Numerov's method applies to second-order differential equations of the form

$$y''=f(x,y) \tag{2.1}$$

where terms depending on y' are not present. An easy way to derive that method is given by Fröberg (1979). One starts from the operator relation

$$\frac{\delta^2}{U^2}=1+\frac{\delta^2}{12}-\frac{\delta^4}{240}+\frac{31\delta^6}{60\,480}-\ldots \tag{2.2}$$

between the second power of $U=hD$ and the even powers of the central difference operator δ which applies on a function $y(x)$ as follows:

$$\delta y(x)=y(x+\tfrac{1}{2}h)-y(x-\tfrac{1}{2}h) \tag{2.3}$$

with h the considered step length. After introduction of (2.2) into (2.1) one obtains

$$\delta^2y(x)=h^2\left(1+\frac{\delta^2}{12}-\frac{\delta^4}{240}+\frac{31\delta^6}{60\,480}-\ldots\right)f(x,y). \tag{2.4}$$

Taking into account only two terms in the series expansion, and denoting $x=kh$ $(k=0,(1),N-1;\ Nh=R)$, $y(x)=y(kh)=y_k$, (2.4) can be written in the following discretised form:

$$y_{k+1}-2y_k+y_{k-1}=h^2[f_k+\tfrac{1}{12}(f_{k+1}-2f_k+f_{k-1})]+t_k(h) \tag{2.5}$$

where $f_k\equiv f(kh,y(kh))$ and

$$t_k(h)=-\tfrac{1}{240}\delta^6y_k=-\tfrac{1}{240}h^6D^6y_k. \tag{2.6}$$

Applying (2.5) to (1.1) results in

$$y_{k+1}-2y_k+y_{k-1}=\tfrac{1}{12}h^2[(V_{k+1}-E)y_{k+1}+10(V_k-E)y_k+(V_{k-1}-E)y_{k-1}]+t_k(h)$$

or

$$y_{k+1}(12-h^2V_{k+1})+y_k(-24-10h^2V_k)+y_{k-1}(12-h^2V_{k-1}) = -h^2E(y_{k+1}+10y_k+y_{k-1})+t_k(h) \tag{2.7}$$

with $V_k=V(kh)$.

It has been shown by Chawla and Katti (1980) and Andrew (1986) that the approximations for E provided by Numerov's method are $O(h^4)$ convergent, i.e.

$$|E^{\text{appr}}-E|=O(h^4). \tag{2.8}$$

It is worth mentioning that this result is closely related to the fact that the error term $t_k(h)$ (see (2.6)) is proportional to h^6. Considering $y_{-k}=\pm y_k$, depending on the parity of the considered eigenfunctions, one obtains a discretisation of (1.1) in the form

$$AY=-h^2E^{\text{appr}}BY \tag{2.9}$$

with

$$\begin{aligned}(a_{0,0}, a_{0,1}; b_{0,0}, b_{0,1}) &= (-24-10h^2V_0, 2(12-h^2V_1); 10, 2) \qquad \text{for even-parity solutions}\\ &= (-24-10h^2V_0, 0; 10, 0) \qquad \text{for odd-parity solutions}\end{aligned}$$

$$\begin{aligned}(a_{k,k-1}, a_{k,k}, a_{k,k+1}; b_{k,k-1}, b_{k,k}, b_{k,k+1}) &= (12-h^2V_{k-1}, -24-10h^2V_k, 12-h^2V_{k+1}; 1, 10, 1) \quad \text{for } k=2, (1), N-2\end{aligned}$$

and

$$(a_{N-1,N-2}, a_{N-1,N-1}; b_{N-1,N-2}, b_{N-1,N-1})=(12-h^2V_{N-2}, -24-10h^2V_{N-1}; 1, 10)$$

all other matrix elements of A and B equal to zero and with $Y=(y_0, y_1, \ldots, y_{N-1})^{\mathrm{T}}$.

Equation (2.9) is a so-called generalised eigenvalue problem. For the non-singular matrix B, this problem is equivalent to the classical eigenvalue problem

$$B^{-1}AY=-h^2E^{\text{appr}}Y. \tag{2.10}$$

One has to realise that the matrices A, B and $B^{-1}A$ are non-symmetric. After transforming $B^{-1}A$ to a Hessenberg form, its eigenvalues can be obtained, for example, by the well known QR method. Typical FORTRAN and PASCAL computer codes solving (2.10) along the above-mentioned lines can be found in Press *et al* (1986).

3. An extended Numerov method

For the considered eigenvalue problems there is no reason to restrict the number of terms taken into account in the right-hand side of (2.4). As an extension of the classical Numerov method, we construct the discretised formulae when three terms in the series expansion are included, i.e.

$$y_{k+1}-2y_k+y_{k-1}=h^2[f_k+\tfrac{1}{12}(f_{k+1}-2f_k+f_{k-1}) -\tfrac{1}{240}(f_{k+2}-4f_{k+1}+6f_k-4f_{k-1}+f_{k-2})]+t_k^*(h). \tag{3.1}$$

One can easily show that

$$t_k^*(h) = \tfrac{31}{60\,480}\delta^8 y_k = \tfrac{31}{60\,480} h^8 D^8 y_k. \tag{3.2}$$

It is quite clear that the accuracy of these solutions with respect to Numerov's method increases roughly by a factor h^2. Applied to the class of Schrödinger equations considered one obtains again a discretisation of (1.1) in the form (2.9). The matrices A and B have now a pentadiagonal form instead of the tridiagonal one in § 2, i.e.

$$\begin{aligned}
&(a_{0,0}, a_{0,1}, a_{0,2}; b_{0,0}, b_{0,1}, b_{0,2}) \\
&\qquad = (-480 - 194h^2 V_0, 2(240 - 24h^2 V_1), \\
&\qquad\quad 2h^2 V_2; 194, 48, -2) \qquad \text{for even-parity solutions} \\
&\qquad = (-480 - 194h^2 V_0, 0, 0; 194, 0, 0) \qquad \text{for odd-parity solutions}
\end{aligned}$$

$$\begin{aligned}
&(a_{1,0}, a_{1,1}, a_{1,2}, a_{1,3}; b_{1,0}, b_{1,1}, b_{1,2}, b_{1,3}) \\
&\qquad = (240 - 24h^2 V_0, -480 - 194h^2 V_1 \pm h^2 V_1, \\
&\qquad\quad 240 - 24h^2 V_2, h^2 V_3; 24, 194 \pm 1, 24, -1)
\end{aligned}$$

with the plus sign for even-parity solutions and the minus sign for the odd-parity ones,

$$\begin{aligned}
&(a_{k,k-2}, a_{k,k-1}, a_{k,k}, a_{k,k+1}, a_{k,k+2}; b_{k,k-2}, b_{k,k-1}, b_{k,k}, b_{k,k+1}, b_{k,k+2}) \\
&\qquad = (h^2 V_{k-2}, 240 - 24h^2 V_{k-1}, -480 - 194h^2 V_k, 240 - 24h^2 V_{k+1}, h^2 V_{k+2}; \\
&\qquad\quad -1, 24, 194, 24, -1) \qquad \text{for } k = 3, (1), N-3
\end{aligned}$$

$$\begin{aligned}
&(a_{N-2,N-4}, a_{N-2,N-3}, a_{N-2,N-2}, a_{N-2,N-1}; b_{N-2,N-4}, b_{N-2,N-3}, b_{N-2,N-2}, b_{N-2,N-1}) \\
&\qquad = (h^2 V_{N-4}, 240 - 24h^2 V_{N-3}, -480 - 194h^2 V_{N-2}, \\
&\qquad\quad 240 - 24h^2 V_{N-1}; -1, 24, 194, 24)
\end{aligned}$$

and

$$\begin{aligned}
&(a_{N-1,N-3}, a_{N-1,N-2}, a_{N-1,N-1}; b_{N-1,N-3}, b_{N-1,N-2}, b_{N-1,N-1}) \\
&\qquad = (h^2 V_{N-3}, 240 - 24h^2 V_{N-2}, -480 - 194h^2 V_{N-1}; -1, 24, 194).
\end{aligned}$$

Numerically the extended Numerov method can be tackled in a completely analogous way to Numerov's method itself.

4. Numerical results

To study the accuracy of the two proposed methods we have applied them using some of the potentials (1.2)–(1.5) for specific choices of the occurring parameters. For each potential, an appropriate value of R is guessed as described in Fack and Vanden Berghe (1985). The R values used are mentioned in the tables. In each considered case we have chosen an N value equal to 200.

In table 1 the obtained energy values (E_n, $n = 1, 4$) for the potential (1.2) with $(\lambda, g) = (0, 0)$ are compared with the exact values and with the results derived in classical fourth- and sixth-order methods (Fack and Vanden Berghe 1985). From this it becomes clear that the results of the classical method of the form (1.6) with J pentadiagonal and Numerov's method are comparable. Both methods are of fourth order in the step length. Even so the heptadiagonal approximation and the extended Numerov method, which are both sixth-order methods, reproduce similar results, although the extended Numerov method seems to have a little more accuracy.

Table 1. Comparison of the results for the potential (1.2) with $(\lambda, g) = (0, 0)$ derived with the classical fourth- and sixth-order method (formula (1.6)) with the Numerov method, the extended Numerov method and exact values, respectively. For the numerical values differences between exact and computed results are listed in absolute values. The considered value R is equal to 10 and the step length $h = 0.05$ ([a] refers to Fack and Vanden Berghe (1985)).

	E_1	E_2	E_3	E_4
Exact	1	3	5	7
Absolute differences between exact value and computed value:				
[a] pentadiagonal	0.000 000 1	0.000 000 9	0.000 003	0.000 008
[a] heptadiagonal	0.000 000 000 2	0.000 000 002	0.000 000 007	0.000 000 02
Numerov	0.000 000 05	0.000 000 3	0.000 001	0.000 003
Extended Numerov	0.000 000 000 06	0.000 000 000 5	0.000 000 002	0.000 000 007

In table 2 the present results for potential (1.2) with $(\lambda, g) = (0.1, 0.1)$ and (10.0, 10.0), respectively, are listed together with previously derived results obtained within the classical finite difference approach of the present authors (Fack and Vanden Berghe 1985) and with the dynamic group techniques of Fack *et al* (1986). Again the high degree of precision obtained with the extended Numerov method is obvious.

Several authors have studied a class of exact solutions of the Schrödinger equation (1.1) with potential (1.2). These solutions all correspond to negative λ values. They yield interesting material for testing the validity and accuracy of our numerical methods. The formulae describing these exact eigenvalues have been discussed in Fack and Vanden Berghe (1985). In table 3 we compare for $g = 0.1$ these exact values with the

Table 2. Comparison of the results for the potential (1.2) for two sets of (λ, g) derived with the classical sixth-order method (heptadiagonal case) ([a] Fack and Vanden Berghe (1985)), dynamic group techniques ([b] Fack *et al* (1986)) and the present methods, respectively. Again $R = 10$, $h = 0.05$.

	$\lambda = 0.1$ $g = 0.1$	$\lambda = 10.0$ $g = 10.0$
E_1 [a] heptadiagonal	1.043 173 713	1.580 022 326
[b] dynamic group	1.043 173 713	1.580 022 327
Numerov	1.043 173 657	1.580 022 204
Extended Numerov	1.043 173 713	1.580 022 327
E_2 [a] heptadiagonal	3.120 081 862	3.879 036 829
[b] dynamic group	3.120 081 864	3.879 036 830
Numerov	3.120 081 484	3.879 036 435
Extended Numerov	3.120 081 863	3.879 036 830
E_3 [a] heptadiagonal	5.181 094 777	5.832 767 522
[b] dynamic group	5.181 094 786	—
Numerov	5.181 093 448	5.832 766 134
Extended Numerov	5.181 094 783	5.832 767 530
E_4 [a] heptadiagonal	7.231 009 954	7.903 154 133
[b] dynamic group	7.231 009 981	—
Numerov	7.231 006 646	7.903 150 884
Extended Numerov	7.231 009 973	7.903 154 152

Table 3. Comparison of some exact eigenvalues (derived in [a] Fack and Vanden Berghe (1985)) for the potential (1.2) with $g = 0.1$ and a special selection of negative λ values with the heptadiagonal case [a] and the present results. By $(i+)$, respectively $(i-)$, we indicate the ith even, respectively odd, eigenvalue. Again $R = 10$, $h = 0.05$.

λ $(i\pm)$	Exact value [a]	Absolute differences between exact value and computed value: [a] heptadiagonal	Numerov	extended Numerov
-0.42 (1+)	0.8	0.000 000 000 08	0.000 000 03	0.000 000 000 03
$-0.67+0.1\sqrt{3.05}$ $\approx -0.495\,357\,51$ (2+)	$2.3+\sqrt{3.05}$ $\approx 4.046\,424\,920$	0.000 000 004	0.000 000 7	0.000 000 01
-0.46 (1−)	2.4	0.000 000 000 8	0.000 000 2	0.000 000 000 2
$-0.73+0.1\sqrt{4.09}$ $\approx -0.527\,762\,52$ (2−)	$3.7+\sqrt{4.09}$ $\approx 5.722\,374\,842$	0.000 000 01	0.000 002	0.000 000 03

present and previous numerical results. Again for the lowest-lying states the supremacy of the extended Numerov method is evident.

For the symmetric double-well potential (1.3) eigenvalues can be obtained by using an extended version of the method of continued fractions as introduced by Morse and Stückelberg (1931). For $b = 4i + 1$ ($b = 4i + 3$), $i \in N$, the continued fraction corresponding to odd- (even-) parity states is terminated and the first i eigenvalues can be obtained with a very high degree of accuracy. Table 4 lists for some b values the exact eigenvalues and the differences between the computed and exact values. Also here, the extended

Table 4. Comparison of some exact eigenvalues ([a] Morse and Stückelberg (1931)) with the heptadiagonal case ([b] Fack and Vanden Berghe (1985)) and the present methods for the potential (1.3). The value used for R is 4 and the step length h is 0.02.

b	Parity	Exact value [a]	Absolute differences between exact value and computed value: [b] heptadiagonal	Numerov	extended Numerov
11	even	−8	0.000 000 001	0.000 000 3	0.000 000 000 4
		0	0.000 000 002	0.000 000 5	0.000 000 000 8
		8	0.000 000 01	0.000 003	0.000 000 004
13	odd	−11.313 708 500	0.000 000 001	0.000 000 5	0.000 000 000 4
		0	0.000 000 009	0.000 002	0.000 000 003
		11.313 708 500	0.000 000 04	0.000 007	0.000 000 01
15	even	−15.077 508 510	0.000 000 004	0.000 000 5	0.000 000 002
		−3.559 316 943	0.000 000 005	0.000 001	0.000 000 001
		3.559 316 943	0.000 000 02	0.000 003	0.000 000 009
		15.077 508 510	0.000 000 09	0.000 01	0.000 000 03
17	odd	−19.158 416 010	0.000 000 007	0.000 000 6	0.000 000 004
		−5.740 652 916	0.000 000 01	0.000 003	0.000 000 001
		5.740 652 916	0.000 000 06	0.000 007	0.000 000 02
		19.158 416 010	0.000 000 2	0.000 03	0.000 000 06

Numerov method delivers similar results to the heptadiagonal sixth-order classical method.

For the Razavy potential (1.4) an analytical solution exists for the first $(n+1)$ levels (Razavy 1980). In table 5 we compare these exact solutions with our results for some values of n and m. For these examples the extended Numerov method reproduces the most accurate results.

Table 5. Comparison of some exact eigenvalues ([a] Razavy (1980)) with the classical sixth-order method ([b] Fack and Vanden Berghe (1985)) and the present Numerov methods for the potential (1.4). The R and h values used are also listed.

				Absolute differences between exact value and computed value		
n	m	$R(h)$	Exact value [a]	[b] heptadiagonal	Numerov	extended Numerov
1	1	2.48	-2	0.000 000 000 03	0.000 000 004	0.000 000 000 04
		(0.0124)	0	0.000 000 000 07	0.000 000 02	0.000 000 000 03
2	1	2.48	$-2(1+\sqrt{2})$	0.000 000 000 6	0.000 000 02	0.000 000 000 003
		(0.0124)	-4	0.000 000 001	0.000 000 03	0.000 000 000 03
			$2(\sqrt{2}-1)$	0.000 000 003	0.000 000 07	0.000 000 000 05
1	10	1.32	-11	0.000 000 000 3	0.000 000 01	0.000 000 000 08
		(0.0066)	9	0.000 000 005	0.000 000 14	0.000 000 001
2	10	1.32	$-2(1+\sqrt{101})$	0.000 000 001	0.000 000 01	0.000 000 000 3
		(0.0066)	-4	0.000 000 02	0.000 000 1	0.000 000 004
			$2(\sqrt{101}-1)$	0.000 000 1	0.000 000 5	0.000 000 03

5. Summary

In this paper we have presented a fourth- and a sixth-order numerical method for the determination of the solutions of some specific Schrödinger equations. We have introduced an extended version of the well known Numerov method. The obtained numerical results for a variety of potentials considered confirm the high degree of precision obtainable with this new method. It is however clear that still more terms in the series expansion on the right-hand side of (2.4) can be included and that still higher accuracy can be obtained in this way.

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