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On the numerical integration of the Schrödinger equation for symmetrical potentials: a highly stable shooting method with the Numerov integrator

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Abstract. The problem of the stability of the numerical solution of the one-dimensional Schrödinger equation with symmetrical potential $V(x)$ is considered. This problem is illustrated by the example $y''+(E-x^2)y=0$ with $y(0)=1$ and $y(x)\to 0$ when $x\to\infty$, for which the conventional shooting method using the Numerov integrator fails for $E=-1$, to find $y(x)$ beyond $x=5$. It is shown that these values are reached by using a different procedure for shooting with the same Numerov integrator. This procedure starts the integration at any 'large' value L of x, and steps backward towards $x=0$. The method is applied to another value of E for which an exact value of $y(x)$ is available. This test shows that the accuracy of the computed values of $y(x)$ is independent of the choice of L. Thus the present method does not improve the eigenvalue computation, but it allows the determination of the solution $y(x)$ for large x when such values are needed.

1. Introduction

In seeking the numerical solution of the equation

$$-D^2y+x^2y=Ey \tag{1}$$

with $y(0)=1$ and $y(x)\to 0$ when $x\to\infty$, many authors noticed a problem with the stability of $y(x)$ for 'large' x. Among these we mention Holt (1964), Osborne (1969), Roberts and Shipman (1971) and Gupta and Agarwal (1985), who used simple shooting methods with $E=-1$ and pointed out that these methods become unstable beyond $x\sim 3.5$. In a recent work, Killingbeck 1987 devised a new shooting method starting at $x=0$ and reaching $x\sim 5$. In a more recent work, Kobeissi *et al* 1989 showed that the 'canonical functions method' allowed another slight improvement. Other authors considered related problems and tried to improve the stability of the solution $y(x)$ at large x by replacing the conventional Numerov integrator, largely used in shooting methods, by higher-order difference equations (e.g. Hajj *et al* 1974, Cash and Raptis 1984, Fack and Vanden Berghe 1985, 1986 and Killingbeck 1986).

This particular problem may be inscribed in a more general one, that of the radial Schrödinger equation

$$-D^2y+V(x)y=Ey \tag{2}$$

where V is an even function of x ($V(-x)=V(x)$), and the solution $y(x)$ obeys the boundary conditions

$$y(\pm\infty)=0. \tag{3}$$

For this general problem, two needs may arise: (i) the 'parameter' E is given and the solution $y(x)$ obeying the boundary condition (3) is to be found, (ii) E is not given, and the eigenvalues E_n for $V(x)$ are to be found. For these two needs the stability of the numerical solution $y(x)$ at large x plays an important role in the accuracy of the results. For this specific problem of stability, the example given in (1) is a good illustration.

According to the canonical functions scheme (Kobeissi *et al* 1989), the eigenvalue problem may be reduced to that of the computation, for an arbitrary E, of the logarithmic derivative $G(E) = y'(E; x)/y(E; x)|_{x=0}$. When E varies, the function $G(E)$ for $V = x^2$ (for example) has a shape similar to that of the function $f(E) = \tan(aE + b)$ (a and b are given constants) with successive zeros and asymptotes. A zero of $G(E)$ corresponds to $y'(E; 0) = 0$, i.e. to an even eigenvalue $E_{n'}$; an asymptote of $G(E)$ corresponds to $y(E; 0) = 0$, i.e. to an odd eigenvalue $E_{n''}$. In all cases, the whole problem is reduced to a single simple one: for a given E, find the solution $y(E; x)$ of equation (2) which obeys the boundary condition (3) and at $x = 0$ has a given value of $y(E; 0)$ (so $y'(E; 0)$ is to be found), or a given value of $y'(E; 0)$ (and $y(E; 0)$ is to be found). The problem illustrated in (1) is a conventional example of each of these two alternatives.

The present work aims to show that conventional and simple numerical techniques are suitable to solve equation (1) with a high stability. This new procedure is outlined in section 2 and tested in section 3.

2. The theory

We formulate the basic problem as follows: find the solution $y(x)$ of equation (2) (where V is an even function, E is given) obeying the boundary conditions

$$y(0) = a \qquad y(L) = 0 \tag{4}$$

a is given, L must be as large as possible.

In order to solve this problem we replace equation (2) by a convenient difference equation, and we use the initial values $y(0) = a = 1$ and $y'(0) = b$, b is a trial parameter to be adjusted in order to satisfy the condition $y(L) = 0$. As we mentioned in the introduction, such a simple shooting method is unable to give an accurate solution for a 'large' value of L. The reason of this failure is known: the slightest mismatch of the initial conditions would introduce into $y(x)$ a growing exponential component which would become dominant at large x (Killingbeck 1987).

This last remark used by Killingbeck to devise his new technique is what inspired our present work. We simply eliminate the 'spurious' component by starting the integration at $x = L$, instead of $x = 0$, and by shooting backwards towards $x = 0$, with the initial conditions $y(L) = 0$, $y'(L) = b \neq 0$, b being an arbitrary (small) constant.

When one wishes to use the Numerov integrator, the distance L is divided into equally spaced points x_i, with a constant step-length h. The initial conditions for $y(L)$ and $y'(L)$ are replaced here by $y(L) = 0$ and $y(L - h) = b$; the arbitrary constant b corresponds to an unnormalized solution $y(x)$.

We give in table 1 the solution $y(x)$ of (1) with $E = -1$, computed by the present method and compared with the solution found by Killingbeck (1987). We used the same Numerov integrator used by Killingbeck, with the same step-length $h = 0.05$. We give in column 3 the function $y(x)$ computed with $L = 10$, and normalized to 1 at $x = 0$. We give in the last column $y(x)$ for $L = 15$. All the computations are done on the computer HP 9000/220 to 15 figures.

Table 1. Computed values of the solution $y(x)$ of (1) with $E=-1$ at several values of x. The values obtained by the present method for $L=10$ and $L=15$ are compared with those obtained by Killingbeck (1987). In all cases the Numerov integrator is used with a step-length $h=0.05$. (Numbers between parentheses are exponents.)

		Present work	
x	Killingbeck	$L=10$	$L=15$
15			0‡
14			1.088 249 (−44)
13			8.592 491 (−39)
12			2.505 953 (−33)
11			2.703 355 (−28)
10		0‡	1.080 744 (−23)
9		1.603 927 (−19)	1.603 927 (−19)
8		8.858 874 (−16)	8.858 874 (−16)
7		1.826 847 (−12)	1.826 847 (−12)
6		1.412 885 (−9)	1.412 885 (−9)
5	0†	4.125 496 (−7)	4.125 496 (−7)
4	4.6 (−5)	4.595 804 (−5)	4.595 804 (−5)
3	1.988 5 (−3)	1.988 523 (−3)	1.988 523 (−3)
2	3.456 41 (−2)	3.456 405 (−2)	3.456 405 (−2)
1	2.593 426 (−1)	2.593 425 (−1)	2.593 425 (−1)
0	1	1§	1§

† Rendered formally 0 by choice of weighting factors.
‡ Rendered 0 by imposing boundary conditions.
§ Rendered 1 by normalization.

Table 2. Computed values of the solution $y(x)$ of (2) with $V(x)=x^2+x^2/(1+x^2)$ and $E=1.232\,351$ at several values of x and for several values of L. The Numerov integrator is used with a step-length $h=0.05$. (Numbers between parentheses are exponents.)

x	$L=7$	$L=10$	$L=15$
15			0†
14			1.098 488 9 (−43)
13			8.286 186 9 (−38)
12			2.300 422 7 (−32)
11			2.352 477 8 (−27)
10		0†	8.869 018 5 (−23)
9		1.233 799 8 (−18)	1.233 799 8 (−18)
8		6.339 734 3 (−15)	6.339 734 3 (−15)
7	0†	1.204 726 6 (−11)	1.204 726 6 (−11)
6	8.479 944 6 (−9)	8.479 954 6 (−9)	8.479 954 6 (−9)
5	2.215 899 6 (−6)	2.215 892 6 (−6)	2.215 892 6 (−6)
4	2.156 525 0 (−4)	2.156 525 0 (−4)	2.156 525 0 (−4)
3	7.853 347 5 (−3)	7.853 347 5 (−3)	7.853 347 5 (−3)
2	1.076 653 1 (−1)	1.076 653 1 (−1)	1.076 653 1 (−1)
1	5.549 501 1 (−1)	5.549 501 1 (−1)	5.549 501 1 (−1)
0	1‡	1‡	1‡

† Rendered formally 0 by imposing boundary conditions.
‡ Rendered 1 by normalization.

By comparing our results with those of Killingbeck, we notice the excellent agreement between them for $0<x<5$; $x=5$ is the limit obtained by Killingbeck. Yet, for our results, we have apparently no such limit since the 'limit' L is chosen as large as one likes. In table 1 two examples are given for $L=10$ and $L=15$, but we obtained similar results for $L=20$ and $L=25$.

This excellent stability of $y(x)$ at large x is not altered by any 'side-effect'. To verify this we considered the logarithmic derivative $G=y'(0)/y(0)$ and we studied the variation of G with L. We noticed that $G(L)$ takes, successively, the following values: $G(3)=1.128\,403$, $G(3.5)=1.128\,379$, $G(4)=1.128\,3784$, and $G(L)=1.128\,3783$ for $L\geqslant 4.5$. This result proves that the stability 'imposed' at $x=L$ does not generate any instability at the other boundary $x=0$.

This procedure gives similar results when applied to other potentials. We give in table 2 another example for the potential $V(x)=x^2+x^2/(1+x^2)$.

3. Discussion

In order to verify the accuracy of the present method we consider the application used by Killingbeck (1987) for $E=1$, where the exact solution of (1) is given by $y(x)=\exp(-x^2/2)$. Here again we make use of the same Numerov integrator used by Killingbeck, with the same step-length $h=0.05$; and we normalize the computed solution $y(x)$ to 1 at $x=0$.

We give in table 3 our results for $L=10$ and $L=15$ (similar results were obtained for $L>15$), along with those of Killingbeck (1987) (limited at $L=10$) on one side, and with the exact values of the other side. For $0\leqslant x\leqslant 10$, we notice an agreement between our results and those of Killingbeck with a slight advantage for our results compared with the exact value of $y(x)$ (last column). Yet the main advantage of the present method is, here too, its high stability.

In order to determine the source of the discrepancy $\delta y(x)=|y^{\mathrm{c}}(x)-y^{\mathrm{e}}(x)|$ between computed and exact values, we give in table 4 the values of $\delta y(x)/y^{\mathrm{e}}(x)$ for several values of h ($h=0.1$, 0.05, 0.025 and 0.01). We notice that the discrepancy decreases with h. When we add to this remark the fact that the choice of L has no effect on the computed $y(x)$ (see tables 1 and 2), we may deduce that the accuracy of the present method is mainly related to that of the integrator itself; this is most probably the unique source of error; when other difference equations are used, as in table 5, the results are quite different.

As we mentioned before, the numerical integration of the Schrödinger equation may be used to determine the solution $y(x)$ for a given E, or to find the eigenvalues E_n. For this last problem, we cause E to vary, and we look for the values E_n for which $y(0)=0$ (odd eigenvalues) or $y'(0)=0$ (even eigenvalues). In all cases one operation is repeated, i.e. the determination of $y(x)$ for trial values of E.

We computed the eigenvalues E_n of the potential $V=x^2+\lambda x^2/(1+gx^2)$ by following the procedure already suggested by Kobeissi *et al* (1989), i.e. by looking for the values of E verifying the equations $G(E)=0$ and $G(E)=\infty$. In this application $y(x)$ is obtained by the present shooting method (with the Numerov integrator), $y'(x)$ is calculated just at $x=0$ by using the simple formula given in the work of Blatt (1967) by the expression

$$y'(0)=(c_1y(h)-c_2y(-h))/2h$$

with $c_1=1-h^2(V(h)-E)/6$ and $c_2=1-h^2(V(-h)-E)/6$.

Table 3. Computed values of the solution $y(x)$ of (1) with $E = 1$ at several values of x. The values obtained by the present method for $L = 10$ and $L = 15$ are compared with those obtained by Killingbeck (1987) and to the exact values. In all cases the Numerov integrator is used with a step-length $h = 0.05$. (Numbers between parentheses are exponents.)

		Present work		
x	Killingbeck	$L = 10$	$L = 15$	Exact value
15			0‡	
14			2.708 873 (−43)	2.748 785 (−43)
13			1.986 565 (−37)	2.005 009 (−37)
12			5.350 091 (−32)	5.380 186 (−32)
11			5.293 887 (−27)	5.311 092 (−27)
10	0†	0‡	1.925 340 (−22)	1.928 750 (−22)
9	2.5793 (−18)	2.574 450 (−18)	2.574 450 (−18)	2.576 757 (−18)
8	1.2671 (−14)	1.265 895 (−14)	1.265 895 (−14)	1.266 417 (−14)
7	2.2903 (−11)	2.289 356 (−11)	2.289 356 (−11)	2.289 735 (−11)
6	1.5232 (−8)	1.522 915 (−8)	1.522 915 (−8)	1.522 998 (−8)
5	3.7268 (−6)	3.726 606 (−6)	3.726 606 (−6)	3.726 653 (−6)
4	3.3547 (−4)	3.354 622 (−4)	3.354 622 (−4)	3.354 626 (−4)
3	1.1109 (−2)	1.110 900 (−2)	1.110 900 (−2)	1.110 900 (−2)
2	1.3534 (−1)	1.353 353 (−1)	1.353 353 (−1)	1.353 353 (−1)
1	6.0653 (−1)	6.065 306 (−1)	6.065 306 (−1)	6.065 307 (−1)
0	1	1§	1§	1

† Rendered formally 0 by choice of weighting factors.
‡ Rendered 0 by imposing boundary conditions.
§ Rendered 1 by normalization.

Table 4. Relative error $\delta y(x)/y^{e}(x)$ in the computed value of the solution $y(x)$ of (1) with $E = 1$ at several values of x, where $\delta y(x) = |y^{c}(x) - y^{e}(x)|$, y^{c} and y^{e} are the computed and the exact values, respectively. Values are obtained by using the Numerov integrator, and given for several values of the step-length h. (Numbers between parentheses are exponents.)

$x\backslash h$	0.1	0.05	0.025	0.01
10	1.6 (−1)	1.8 (−3)	1.1 (−4)	3.3 (−6)
9	1.4 (−2)	8.9 (−4)	5.6 (−5)	1.4 (−6)
8	6.5 (−3)	4.1 (−4)	2.6 (−5)	6.6 (−7)
7	2.6 (−3)	1.7 (−4)	1.0 (−5)	2.7 (−7)
6	8.7 (−4)	5.4 (−5)	3.4 (−6)	8.7 (−8)
5	2.0 (−4)	1.3 (−5)	7.9 (−7)	2.0 (−8)
4	1.8 (−5)	1.1 (−6)	7.2 (−8)	1.8 (−9)
3	3.6 (−6)	2.3 (−7)	1.4 (−8)	3.6 (−10)
2	2.1 (−6)	1.3 (−7)	8.1 (−9)	2.1 (−10)
1	1.7 (−6)	1.0 (−7)	6.5 (−9)	1.7 (−10)
0	—	—	—	—

By using the same step-length $h = 0.05$ used by Fack and Vanden Berghe (1987) for this same application, we found numerical values of E_n ($n = 0, 1, 2, 3$) similar to those found by Fack and Vanden Berghe (1987), with the same integrator and the same step-length (see table 6).

Table 5. Relative error $\delta y(x)/y^e(x)$ in the computed value of the solution $y(x)$ of (1) with $E = 1$ at several values of x, where $\delta y(x) = |y^c(x) - y^e(x)|$, y^c and y^e are the computed and the exact values, respectively. δy is displayed for the following difference equations: Numerov (1933), Cash and Raptis (1984) and Kobeissi (1982). The value of the step-length in each case is displayed in the last line. (Numbers between parentheses are exponents.)

x	Numerov (1933)	Cash and Raptis (1984)	Kobeissi (1982)
10	1.8 (−3)	4.1 (−6)	4.3 (−8)
9	8.9 (−4)	1.7 (−6)	2.1 (−9)
8	4.1 (−4)	8.3 (−7)	1.2 (−10)
7	1.7 (−4)	3.6 (−7)	3.3 (−12)
6	5.4 (−5)	1.3 (−7)	1.6 (−13)
5	1.3 (−5)	3.7 (−8)	1.4 (−14)
4	1.1 (−6)	6.1 (−9)	1.1 (−15)
3	2.3 (−7)	2.2 (−10)	3.1 (−16)
2	1.3 (−7)	2.3 (−10)	2.1 (−16)
1	1.0 (−7)	5.6 (−11)	1.8 (−16)
0	—	—	—
h	0.05	0.05	0.5

Table 6. Comparison of the eigenvalue E^c computed for the potential $V = x^2 + \lambda x^2/(1 + gx^2)$ for three sets of (λ, g) by the present method and by Fack and Vanden Berghe (1987) both using the Numerov integrator with the same step-length $h = 0.05$. For each entry the exact eigenvalue E^e is given in first line, $\Delta E = E^e - E^c$ in absolute value is given in second line for the present method and in third line for that of Fack and Vanden Berghe (1987).

E	$\lambda = 0, g = 0$	$\lambda = 0.1, g = 0.1$	$\lambda = 10, g = 10$
E_1	1	1.043 173 713†	1.580 022 326†
	5 (−8)‡	6 (−8)	1 (−7)
	5 (−8)	6 (−8)	1 (−7)
E_2	3	3.120 081 862	3.879 036 829
	3 (−7)	4 (−7)	4 (−7)
	3 (−7)	4 (−7)	4 (−7)
E_3	5	5.181 094 777	5.832 767 522
	1 (−6)	1 (−6)	1 (−6)
	1 (−6)	1 (−6)	1 (−6)
E_4	7	7.231 009 954	7.903 154 133
	3 (−6)	3 (−6)	3 (−6)
	3 (−6)	3 (−6)	3 (−6)

† Highly accurate values by Fack and Vanden Berghe (1985) considered here as exact.
‡ Figures between parentheses are exponents.

4. Conclusion

It is commonly believed that the numerical solution of the radial Schrödinger equation (equation (1)) with given E and given initial values at an 'origin' x_0 becomes unstable for 'large' x when the Numerov integrator is used.

We showed in the present work that the values of the solution $y(x)$ can be obtained for large values of x, by just imposing the desired boundary condition and by shooting backwards towards the origin. This goal is reached even when the Numerov integrator is used.

We verified that the two procedures give the same accuracy for $y(x)$ when the same step-length is used, and that the eigenvalues obtained by both methods are practically identical. The present method is recommended when values of the solution $y(x)$ for large x are needed.

References

Blatt J M 1967 *J. Comput. Phys.* **1** 382
Cash J R and Raptis A D 1984 *Comput. Phys. Commun.* **33** 299
Fack V and Vanden Berghe G 1985 *J. Phys. A: Math. Gen.* **18** 3355
—— 1986 *Comput. Phys. Commun.* **39** 187
—— 1987 *J. Phys. A: Math. Gen.* **20** 4153
Gupta R C and Agarwal R P 1985 *J. Math. Anal. Appl.* **112** 210
Hajj F Y, Kobeissi H and Nassif N 1974 *J. Comput. Phys.* **16** 150
Holt J F 1964 *Commun. ACM* **7** 366
Killingbeck J 1986 *Phys. Lett.* **115A** 301
—— 1987 *J. Phys. A: Math. Gen.* **20** 1411
Kobeissi H 1982 *J. Phys. B: At. Mol. Phys.* **15** 693
Kobeissi H, Kobeissi M and El-Hajj A 1989 *J. Phys. A: Math. Gen.* **22** 287
Numerov B 1933 *Publ. Obs. Central Astrophys. Russ.* **2** 188
Osborne M R 1969 *J. Math. Anal. Appl.* **27** 417
Roberts S M and Shipman J S 1971 *J. Opt. Theor. Appl.* **7** 301