JOURNAL OF COMPUTATIONAL PHYSICS 72, 270–274 (1987)

Note

The Numerov Method and Singular Potentials

In a recent homonym paper [1], Buendia and Guardiola examined the accuracy of the Numerov method for the solution of the radial Schrödinger equation (SE) $y'' = (V(x) - E)\, y$ in the case when the potential is singular at the origin. They considered potentials of the form

$$V(x) = l(l+1)/x^2 + \alpha(x)/x + \beta(x), \tag{1}$$

where $\alpha(x)$ and $\beta(x)$ are well-behaved functions and l is some nonnegative integer. We are interested in the eigenvalue problem as solved in a shooting process with backwards integration at each trial value of the energy.

Briefly, a step size h is introduced and the points $x_n = nh$, $n = 0, 1, 2, \ldots, N$, are used in the numerical procedure. The Numerov algorithm

$$y_{n+1} - 2y_n + y_{n-1} = \tfrac{1}{12}h^2(y''_{n+1} + 10y''_n + y''_{n-1}) \tag{2}$$

in which $y''_i = (V_i - E)\, y_i$, $i = n-1$, n, $n+1$, yields y_{n-1} in terms of V_{n-1}, V_n, V_{n+1}, y_n, y_{n+1}, and E. On imposing some suitable values for y_N and y_{N-1} in terms of the known asymptotic behavior of the solution, algorithm (2) is applied successively at $n = N-1$, $N-2, \ldots, 1$, and the calculation of the eigenenergy means finding that value of E at which y is regular at the origin or, equivalently, $y_0 = 0$.

The difficulty is that, when the potential is singular at the origin, the application of Eq. (2) at $n = 1$ is impossible because y''_0 involves $V(0)$ which is infinite. The authors of [1] derived an approximation to y_0 which avoids the appearance of y''_0. They arrived at the representation $y_0 \simeq D$, where

$$D = -2y_1 + y_2 - \tfrac{1}{12}h^2(13y''_1 - 2y''_2 + y''_3) \tag{3}$$

is an easily computable expression which permits the localization of the eigenenergy as the value of E at which $D = 0$. The standard finite differences technique was used in [1] to derive Eq. (3) but an alternative, more systematic procedure exists and this is as follows.

We introduce the three-point functional

$$\mathscr{F}[y] = a_1\, y(h) + a_2\, y(2h) + a_3\, y(3h) - h^2(b_1\, y''(h) + b_2\, y''(2h) + b_3\, y''(3h)) \tag{4}$$

0021-9991/87 $3.00

and search for the weights a_i and b_i such as $\mathscr{F}[y]=0$ for some preset forms of y. If we take $y=x^m$ we have $\mathscr{F}[y]=h^m F_m$ with

$$F_m=a_1+2^m a_2+3^m a_3-m(m-1)(b_1+2^{m-2}b_2+3^{m-2}b_3). \tag{5}$$

Now, if we set $F_m=0$ for five different values for m we get a system of five equations for six unknowns which, because each equation is homogeneous, admits a unique solution provided one unknown is taken as a free parameter. This is, however, the maximal possibility; we can fix ab initio some more weights $1<p<6$ and determine the remaining $6-p$ weights from the equal number of equations. In particular, if we choose $p=2$, $a_1=-2$, $a_3=0$, and take $m=1$, 2, 3, and 4, we get $a_2=1$, $b_1=\frac{13}{12}$, $b_2=-\frac{1}{6}$ and $b_3=\frac{1}{12}$, i.e., exactly the weights of D. Likewise, if we set $p=3$, $a_1=-2$, $a_3=b_3=0$, and $m=1$, 2, and 3, the resultant three weights are $a_2=b_1=1$ and $b_2=0$, so that the expression

$$S=-2y_1+y_2-h^2y_1'' \tag{6}$$

is another possible candidate for being used in the search for eigenenergies.

This way of generating the weights raises the question of finding the most suitable values of m to describe the regular solution of *SE*. We start from the known fact that in the vicinity of the origin the regular solution is $y(x)=x^{l+1}Y(x)$, where $Y(x)$ is a function which can be represented by the power series $Y(x)=Y_0+Y_1x+Y_2x^2+\cdots$. It follows that the maximal achievement of Eq. (4) is reached if $p=1$ and

$$m=l+1,\ l+2,\ l+3,\ l+4,\ \text{and}\ l+5. \tag{7}$$

The resultant system of equations admits, if we take $a_1=1$ as an ab initio determination, the solution

$$a_i=A_i/Q,\ i=2,3, \qquad b_i=B_i/Q,\ i=1,2,3 \tag{8}$$

with

$$\begin{aligned} A_2&=2^{-(l+1)}(4l^4+28l^3-l^2-217l+240), & B_1&=2l^2+15l-5,\\ A_3&=3^{-(l+2)}(2l^4+41l^3+232l^2+301l-540), & B_2&=2^{1-l}(4l^2+24l-25), \\ Q&=2l^4+5l^3-68l^2+85l-60, & B_3&=3^{-(l+1)}(6l^2+9l-15). \end{aligned} \tag{9}$$

We thus conclude that the expression

$$P=y_1+a_2y_2+a_3y_3-h^2(b_1y_1''+b_2y_2''+b_3y_3'') \tag{10}$$

with the l-dependent weights just determined represents the optimal three-point formula for checking whether the solution is regular and, in particular, for calculating the eigenenergies.

The case $l=0$ requires some special attention. Here the weights are $a_1=a_3=1$, $a_2=-2$, $b_1=b_3=\frac{1}{12}$ and $b_2=\frac{5}{6}$, i.e., just the weights of the Numerov method and then P becomes senseless. Technically the reason is that in this case it happens that $F_m=0$ also when $m=0$, a value which does not belong to the set (7). A way to overcome this difficulty consists of taking two weights as fixed and evaluating the other four weights from the system with $m=1, 2, 3, 4$, which is exactly the way Eq. (3) was derived. In other words, D remains the optimal expression when $l=0$ but P is better for $l>0$.

The error in the eigenvalues localized by the expressions S, D, and P behaves as h^{l+4} for $l=1, 2, 3$ and h^{2l+1} for $l>3$, as h^{l+5} for $l=1, 2, 3, 4$ and h^{2l+1} for $l>4$, and as h^{2l+6} for all $l\geqslant 1$, respectively. Since the systematic proof of this statement is rather long we give only a check in the case of S and for $l=1$ and $l=4$.

In general, the solution of SE is a linear combination of the regular and irregular solutions,

$$y^{\text{gen}}(x)=y(x)+C(E)\,z(x),$$

and the localization of the eigenenergy essentially means finding the value E^* of E at which $C(E^*)=0$. The irregular solution is of the form $z(x)=x^{-l}Z(x)$, where $Z(x)$ admits a power series representation $Z(x)=Z_0+Z_1x+Z_2x^2+\cdots$ and then

$$\begin{aligned} y^{\text{gen}}(x)=C(E)&(Z_0x^{-l}+Z_1x^{-l+1}+\cdots+Z_{2l}x^l)\\ &+(C(E)\,Z_{2l+1}+Y_0)\,x^{l+1}+(C(E)\,Z_{2l+2}+Y_1)\,x^{l+2}+\cdots. \end{aligned}$$

Accounting for that for S we have $F_1=F_2=F_3=0$ and taking $l=1$, functional (4) reads

$$\mathscr{F}[y^{\text{gen}}]=h^{-1}[C(E)(Z_0F_{-1}+Z_1F_0h+Z_5F_4h^5)+Y_3F_4h^5+O(h^6)].$$

This vanishes at $\bar{E}$ such that

$$C(\bar{E})=-F_4Y_3h^5/(Z_0F_{-1}+Z_1F_0h+Z_5F_4h^5)+O(h^6)\sim O(h^5)$$

and, if Δ is the deviation of the computed $\bar{E}$ from the exact E^*, $\Delta=E^*-\bar{E}$, we may write $C(E^*)-C(\bar{E})\simeq\Delta\cdot C'(E^*)$ and thus $\Delta\simeq -C(\bar{E})/C'(E^*)\sim O(h^5)$. Likewise, when $l=4$ it results that

$$C(\bar{E})=-F_5Y_0h^9/(Z_0F_{-4}+Z_1F_{-3}h+\cdots+Z_4F_0h^4+Z_8F_4h^8+Z_9F_5h^9)+O(h^{10})$$

and thus $\Delta\simeq O(h^9)$. The check is completed.

The afore-mentioned behavior of the error in eigenvalues implies that real differences should appear in practice only if the numerical method used to generate y_1, y_2, and y_3 is of sufficiently high order.

If, for instance, this is the fourth-order method of Numerov, y_1, y_2, and y_3 are falsified by contributions proportional to h^4 and this swallows the difference between the accuracies of S, D, and P for any $l=1, 2, 3,\ldots$. It follows that the plot $\log|\Delta|$ vs. $\log h$ has, in the limit of small h, the form of one and the same straight

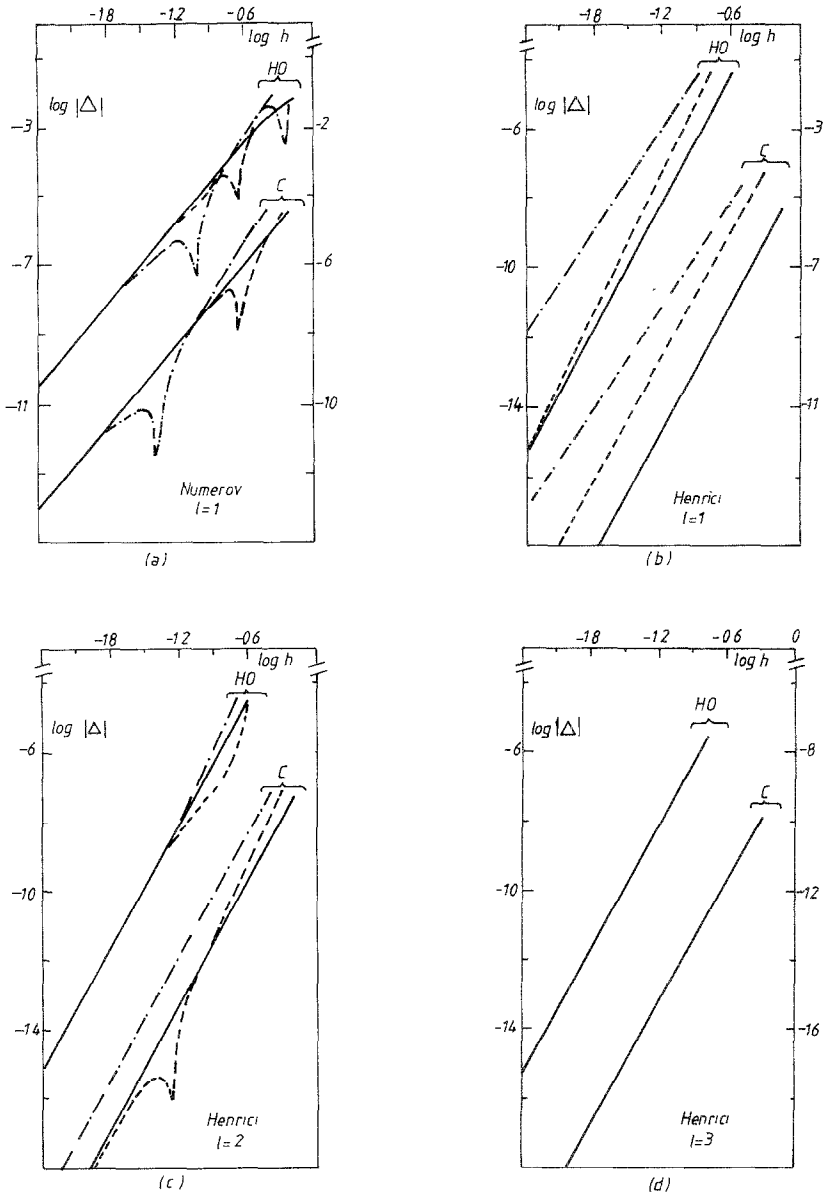

FIG. 1. Plot of the logarithm of the absolute error of the eigenvalue as a function of the logarithm of the step size for the harmonic oscillator (HO) and for the Coulomb (C) potential. The dot-and-dash, dashed, and solid lines correspond respectively to the expressions S, D, and P for the localization of the eigenenergy. When the vertical scales are different that on the left (right) refers to HO (C).

line of slope four for all three expressions. If the intergration method is of higher order, say, six, the slope is expected to be five for S and six for D and for P when $l=1$, and six for all S, D, and P when $l \geqslant 2$. Some shift between the lines of the same slope may also occur when the order of one expression equals that of the integration method as is the case when we compare S and P for a sixth-order method and $l=2$.

All these predictions are fairly well confirmed experimentally and for illustration we have chosen the harmonic oscillator (HO) $V(x)=x^2+l(l+1)/x^2$ and the Coulomb (C) potential $V(x)=-2/x+l(l+1)/x^2$, also considered in [1]. The exact eigenenergies are $E^*=2l+3$ for HO and $E^*=-1/(l+1)^2$ for C. Figure 1 shows $\log|\Delta|$ vs. $\log h$ when the integration method is Numerov and Henrici. The latter is a four step method of the sixth order with the algorithm

$$y_{n+2}-y_{n+1}-y_{n-1}+y_{n-2}=h^2\left[\tfrac{17}{240}\left(y''_{n+2}+y''_{n-2}\right)+\tfrac{29}{30}\left(y''_{n+1}+y''_{n-1}\right)+\tfrac{37}{40}y''_n\right],$$

see [2, Eq. (6–76)]. To start the intergration we have used $x_N=10$ for HO and $x_N=150$ for C, and WKB estimates as starting values. The cusps indicate the sign changes in Δ. We see that only the P curves are free of cusps and this is indeed a significant advantage in current applications.

REFERENCES

1. E. BUENDIA AND R. GUARDIOLA, *J. Comput. Phys.* **60**, 561 (1985).
2. P. HENRICI, *Discrete Variable Methods in Ordinary Differential Equations* (Wiley, New York, 1964).

RECEIVED. August 13, 1986

L. GR. IXARU
Institute of Physics and Nuclear Engineering
Division of Fundamental Physics
P.O. Box MG-6, Bucharest, Romania