

## Note

### The Numerov Method and Singular Potentials\*

One of the most efficient and simple methods to determine numerically the eigenvalues of the radial Schrodinger equation  $y'' + (V - E)y = 0$  is the Numerov method. It consists in a three-point integration rule

$$\left\{1 - \frac{h^2}{12}(V_{n-1} - E)\right\} y_{n-1} - 2 \left\{1 - \frac{h^2}{12}(V_n - E)\right\} y_n + \left\{1 - \frac{h^2}{12}(V_{n+1} - E)\right\} y_{n+1} = h^2(V_n - E) y_n \tag{1}$$

which allows the determination of the eigenvalues  $E$  by means of the following algorithm. Assume a trial value  $E$  and the values  $y_N = 0$  and  $y_{N-1} = c$ , some arbitrary constant. Then repeatedly use Eq. (1) up to  $n = 1$ . At  $n = 1$  Eq. (1) determines  $y_0$ , the radial function at  $r = 0$ , and the trial value  $E$  will be the correct one if the last value  $y_0$  is null. The precise value of  $E$  is obtained starting from two trial values  $E_1$  (whose corresponding  $y_0$  is positive) and  $E_2$  (whose corresponding  $y_0$  is negative) and interpolating repeatedly. In the above algorithm we must also input a given value  $R = Nh$ , a maximum distance from which the radial function may be considered negligibly small. The parameter  $h$  is the step size of the mesh used for the integration.

The above algorithm corresponds to an *inwards* integration, going from far away to the origin. Other strategies for the application of Eq. (1) may also be used (*outwards* integration, mixed forms, and matrix methods).

It has been shown [1, 2] that in most cases Eq. (1) determines the eigenvalue with an error proportional to  $h^4$ , so that a subsequent application of the Richardson extrapolation technique produces very precise results [2, 3]. It is also worth mentioning a simple modification of the Numerov method due to Killingbeck [4] which gives an energy error of order  $h^6$  for smooth nonsingular potentials. However, when Numerov's algorithm is applied to the Coulomb [2] potential, the resulting eigenvalues have an error proportional to  $h^2$ , as in the case of the simple central differences method where the second derivative is approximated by the operator  $\delta^2/h^2$ .

Johnson [5] recognized the need of introducing some special corrections to the above algorithm in the case of singular potentials, particularly in the  $s$ -wave states of potentials which behave at short distances like  $1/r$  and the  $p$ -wave states of any

\* Work supported by CAICYT under Contract 0837.

potential. In these cases to correctly apply Eq. (1) we need to know the limit  $V(r)y(r)$  at  $r=0$ , and this is just the quantity we are interested in to determine  $E$ . In the case of the Coulomb potential Johnson [5] describes a simple technique to overcome this problem which consists in determining analytically the above limit, using that result to carry out the integration outwards. However, this approach cannot be applied in cases where the potential is not known analytically, as happens in the successive iterations of a Hartree-Fock calculation.

We have found a simple method which solves this trouble numerically, and which produces impressively good results in some well-known problems. Equation (1) is used in the inwards direction to determine the radial function at the points  $y_N, y_{N-1}, \dots, y_3, y_2$ , and  $y_1$ . Then the prediction for  $y_0$  is obtained as follows. Taking into account the points  $y_0, y_1$ , and  $y_2$  the relation

$$\delta^2 y_1 = h^2 y_1'' + h^4 y_1^{iv} / 12 + O(h^6) \quad (2)$$

is easily obtained. Then  $y_1^{iv}$  is written in terms of the second derivatives of the radial function at  $y_1, y_2$ , and  $y_3$ ,

$$h^2 y_1^{iv} = \delta^2 y_2'' + O(h^3)$$

arriving finally at the relation

$$\delta^2 y_1 = h^2 y_1'' + h^2 \delta^2 y_2'' / 12 + O(h^5) \quad (3)$$

to be compared with the standard Numerov method

$$\delta^2 y_1 = h^2 y_1'' + h^2 \delta^2 y_1'' / 12 + O(h^6). \quad (4)$$

Equation (3) permits the determination of  $y_0$  in a form which does not involve the value of  $y_0''$ , the unknown quantity when dealing with singular potentials. In practical applications, all second derivatives appearing in Eqs. (3) and (4) are computed with the help of the differential equation  $y'' = (V - E)y$ .

Equation (3) is a four-point relation, but this creates no troubles as far as the integration is carried out inwards. Actually, all step-by-step integration is done using either Eq. (4) or Eq. (1), which are the same, and only at the last step is Eq. (3) to be used.

To show the dramatic effect of this correction to the standard Numerov method we have plotted the values of the error as a function of the step size in several cases. Figure 1 refers to the  $s$ -wave ground state of two singular potentials, Coulomb and Yukawa potentials. Figure 2 refers to two cases where the dominant singularity comes from the centrifugal barrier. In both cases we have plotted the base 10 logarithm of the absolute value of the error versus the base 10 logarithm of the step size. Note that the values of the error corresponding to the dashed lines of Fig. 2

change their sign at a particular value of the step size  $h$ , and the cusps correspond to a null error. Precise details of the calculations are presented in Table I.

Both figures show an impressive gain of precision of several orders of magnitude due to our simple modification.

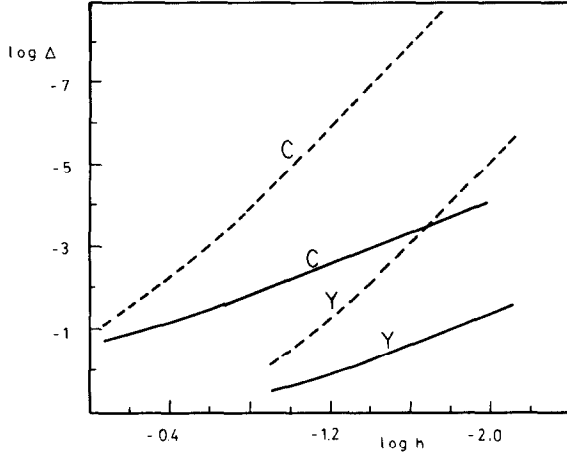


FIG. 1. Plot of the logarithm of the absolute error of the eigenvalue as a function of the logarithm of the step size. The continuous lines correspond to the calculation using the standard Numerov method, and the dashed lines the calculations with our modification. The letters C and Y refer to Coulomb and Yukawa  $s$ -wave potentials, respectively. Details of the calculations are presented in Table I.

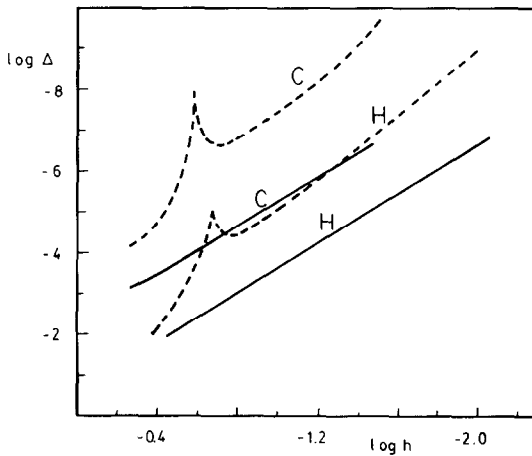


FIG. 2. Same as Fig. 1 but corresponding to the  $p$ -wave harmonic oscillator potential (H) and  $p$ -wave Coulomb potential (Y).

TABLE I  
Effective Potentials Used in the Calculations Shown in Figs. 1 and 2<sup>a</sup>

Potential		R	Exact value	Figure
Coulomb	$-2/r$	16	-1	1
Yukawa	$-10 \exp(-r)/r$	8	-16.3404255695 <sup>b</sup>	1
Coulomb <i>p</i> -wave	$-2/r + 2/r^2$	32	-0.25	2
H oscillator <i>p</i> -wave	$r^2 + 2/r^2$	8	5	2

<sup>a</sup> The value of *R*, the exact value, and the corresponding figure are included in the table.

<sup>b</sup> Value from Ref. [6].

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RECEIVED July 25, 1984

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