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COMMENT ON THE RENORMALIZED NUMEROV METHOD FOR SOLVING DIFFERENTIAL EIGENVALUE EQUATIONS

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We report here that the Renormalized Numerov (RN) method, commonly used to solve a system of coupled differential eigenvalue equations (CDEE), has an unexpected convergence behaviour as the step size is decreased. Furthermore, incorporation of the appropriate asymptotic behaviour of the wave function, in place of a sharp cut off, enhances the binding energy by about 10%. As an illustration we solve for the deuteron ground state with Reid soft core potential, and obtain the covergence behaviour as a function of step size.

1. Introduction

In problems of physics, one often encounters coupled differential eigenvalue equation (CDEE), which must be solved subject to appropriate boundary conditions, for the eigenvalue as well as the eigenfunction. A commonly used method is the so called renormalized Numerov (RN) method[1]. In the Numerov method, a three term recursion relation is used to integrate the wave function, knowing its value at two given consecutive mesh points (or alternatively, knowing the value of the wave function and its first derivative at a given point). The Renormalized Numerov (RN) method consists of setting up recurrence relations for the ratio of wave functions at successive mesh points, thus simplifying the calculation as well as imposition of the boundary conditions. We find that this method has an unexpected convergence behaviour as a function of step size (p). While one commonly experiences that the binding energy (BE) increases, as p is decreased for most other

methods of solving CDEE (which conforms with the Rayleigh-Ritz principle), in the RN method, *BE decreases* as p is decreased. All these methods reach smooth convergence as $p \to 0$.

In this communication we investigate convergence behaviour for the numerical integration of coupled differential eigenvalue equations (CDEE) by the Renormalized Numerov (RN) method[1], as a function of the step size. In addition we also investigate the effect of incorporating an exponential asymptotic tail of the wave function in contrast to the sharp cut off tail which is commonly employed. The latter is seen to give about 10% less *BE*.

A set of coupled differential eigenvalue equations is frequently encountered in the few body problem. A multidimensional Schrödinger equation can be reduced to a set of coupled differential equations in one variable by removing the angular part (or hyperangular part in the case of a many body problem) by projection on an angular eigenfunction. The coupling terms are obtained by integrating the total interaction potential multiplied by angular eigenfunctions[2,3].

A set of M coupled differential eigenvalue equations for the partial waves $\Phi_1, \Phi_2, \ldots, \Phi_M$ can be written as

$$-\frac{\hbar^2}{m}\frac{\mathrm{d}^2\Phi_i(r)}{\mathrm{d}r^2} + \sum_{j=1}^{M} V_{ij}(r)\,\Phi_j(r) = E\Phi_i(r), \qquad i = 1, 2, \ldots, M \tag{1}$$

where m is a suitable mass parameter, $V_{ij}(r)$ is the interaction potential giving rise to coupling and E is the energy eigenvalue.

For a state with $l \neq 0$ the centrifugal potential (which is diagonal) can be included in $V_{ij}(r)$.

For solving Eq. (1) we have the usual boundary conditions

$$\Phi_i(0) = 0, \qquad \Phi_i(r) \underset{r\to\infty}{\to} e^{-\beta r} \tag{2}$$

where $\beta = \left(-\frac{mE}{\hbar^2}\right)^{1/2}$, $E > 0$.

However, if $V_{ij}(r)$ has a strong r dependence for $r \to 0$, then the simple boundary condition (2) at $r = 0$ is to be replaced by its appropriate analytic behaviour for $r \to 0$.

2. *Renormalized Numerov method of integration*

In the RN method Eq. (1) is rewritten in a matrix form[1]

$$\left([I]\frac{\mathrm{d}^2}{\mathrm{d}r^2} + [Q(r)]\right)[\Phi(r)] = [0] \tag{3}$$

where

$$[Q(r)] = \frac{m}{\hbar^2}(E[I] - [V(r)]) \tag{4}$$

each quantity within square brackets is a $M \times M$ matrix and $[I]$ represents the unit matrix.

For this method the basic formula is the three term recurrence relation which is obtained by the generalization of the derivation of the ordinary Numerov algorithm[4] to matrix quantities as

$$([I] - [T_{n+1}])[\Phi_{n+1}] - (2[I] + 10[T_n])[\Phi_n] + \\ + ([I] - [T_{n-1}])[\Phi_{n-1}] = [0] \tag{5}$$

where

$$[\Phi_n] \equiv [\Phi(r_n)] \text{ and } [T_n] = -\left(\frac{p^2}{12}\right)[Q(r_n)]. \tag{6}$$

Here $[\Phi_n]$ is the matrix of wave functions at the n^{th} grid point and p is the spacing between $n+1$ equally spaced grid points $r_0, r_1, r_2, \ldots, r_n$ and the square matrix $[Q(r)]$ is defined by Eq. (4).

The Renormalized Numerov algorithm is obtained by defining

$$[F_n] = ([I] - [T_n])[\Phi_n]. \tag{7}$$

Substitution of this in Eq. (5) gives

$$[F_{n+1}] - [U_n][F_n] + [F_{n-1}] = [0] \tag{8}$$

where

$$[U_n] = ([I] - [T_n])^{-1}(2[I] + 10[T_n]). \tag{9}$$

Now a two term recurrence relation is obtained by defining the ratio matrix

$$[R_n] = [F_{n+1}][F_n]^{-1}. \tag{10}$$

Then from (8) one obtains the two term recurrence relation

$$[R_n] = [U_n] - [R_{n-1}^{-1}]. \tag{11}$$

This is the basic equation of the RN method. It can be solved once the value of $[R_0]$ is specified. The initial values of wave functions are

$$[\Phi_0] = [0] \text{ and } [\Phi_1] \neq [0].$$

Hence

$$[R_0^{-1}] = [0].$$

For computational convenience one defines

$$[W_n] = [I] - [T_n]. \tag{12}$$

Then from (9)

$$[U_n] = 12\,[W_n^{-1}] - 10\,[I]. \tag{13}$$

Eq. (11) can be iterated outwards starting from a given grid point (n) to obtain $[R_j]$, $(j = n, n+1, \ldots)$.

For the inward integration, one defines

$$[\hat{R}_n] = [F_{n-1}]\,[F_n^{-1}]. \tag{14}$$

Substituting this into (8) one obtains a two-term inward recurrence formula

$$[\hat{R}_n] = [U_n] - [\hat{R}_{n+1}^{-1}]. \tag{15}$$

As before knowing the value of $[\hat{R}_n]$ at a given grid point n, one can iterate Eq. (15) inward to obtain $[\hat{R}_j]$, $(j = n, n-1, n-2, \ldots)$.

The boundary condition for $r \to \infty$ can be taken as

$$[\hat{R}_n^{-1}] = [F_N]\,[F_{N-1}] \approx e^{-\beta\rho}\,[I] \tag{16}$$

where N is the final mesh point. It is to be noted that the final mesh point is expected to be well outside the range of the potential, so that

$$[T_N] \approx [T_{N-1}] \approx -\left(\frac{p^2}{12}\right)\left(\frac{m}{\hbar^2}\right) E\,[I]. \tag{17}$$

It is a common practice in literature[1] that $[\Phi_N]$ is taken as zero and $[\Phi_{N-1}] \neq 0$ which gives $[\hat{R}_n^{-1}] = 0$. Eq. (16) represents a more correct asymptotic behaviour.

One can calculate the log-derivatives of the outward and inward integrated wave functions and match them at a suitably chosen match point (r_m)[1]. Alternative requirement is that the inward and outward solutions are equal at the two adjacent grid points r_m and r_{m+1}, and one then has

$$([R_m] - [\hat{R}_{m+1}^{-1}])\,f(r_m) = 0 \tag{18}$$

where

$$f(r_n) = ([I] - [T_n])\,\Phi(r_n). \tag{19}$$

Eq. (18) will have a nontrivial solution only if the determinant

$$D(E) = |[R_m] - [\hat{R}_{m+1}^{-1}]| = 0. \tag{20}$$

Thus, the determinant $D(E)$, which is a function of the trial energy E, will vanish at each of the eigenvalues. The search for the zeros of $D(E)$ can be carried out by any standard one-dimensional search method. Hence to obtain correct eigenenergy we have to solve Eq. (20).

At first one has to guess an energy value and iterate in the forward and backward direction up to match point (r_m) using Eqs. (11) and (15) and the whole process is repeated until condition (20) is satisfied to within the desired accuracy.

After obtaining correct eigenenergy, the eigenvectors $f(r_n)$ for $n > m$ and for $n < m$ are obtained by the relations

$$f(r_n) = [R_n^{-1}] f(r_{n+1}), \qquad n = m-1, m-2, \ldots, 0 \tag{21}$$

and

$$f(r_n) = [\hat{R}_n^{-1}] f(r_{n-1}), \qquad n = m+1, m+2, \ldots, N \tag{22}$$

which are obtained from (10) and (14), respectively. The wave function $\Phi(r_n)$ is then calculated at each grid point using Eq. (19).

3. *Results*

As a typical application of the above method, we have calculated binding energy (BE) and wave function of deuteron with the Reid soft core potential[5] as the nucleon-nucleon interaction. Calculated binding energy (in double precision on HP1000/A700 computer) for various choices of stepsize (p) by this method has been presented in Table 1. The convergence behaviour for RN method as a function of p is shown in Fig. 1. The dotted curve corresponds to the wave function with sharp cut off tail (for large r) which is usually employed[1] while the continuous curve represents the calculation with the correct exponential asymptotic tail. (Note the different scales used for these two curves as indicated in Fig. 1). One immediately notices from Table 1 and Fig. 1 that the correct exponential tail

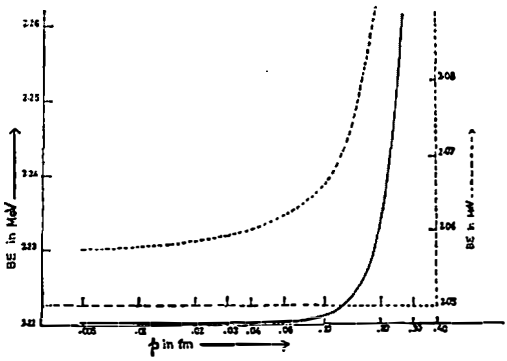

Fig. 1. Convergence of BE by RN method (dotted curve for sharp cut off tail (right side scale) and continuous curve for exponential tail (left side scale)).

TABLE 1.

p (f_m)	BE (MeV) With sharp cut off tail	BE (MeV) With exponential tail
0.30	2.20962	2.32845
0.25	2.11298	2.25404
0.20	2.08703	2.23347
0.10	2.06613	2.22126
0.08	2.06403	2.22078
0.06	2.06379	2.22055
0.04	2.06050	2.22047
0.03	2.06050	2.22046
0.02	2.05885	2.22046
0.01	2.05803	2.22046

Calculation of deuteron binding energy.

for the RN method gives a much better result than the conventional[1] sharp cut off tail. Furthermore, as p is decreased, *BE decreases* gradually and attains convergence. This feature is unusual as compared to other numerical methods and indicates that the RN method does not satisfy Rayleigh-Ritz criterion.

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PRIMJEDBE NA RENORMALIZIRANU NUMEROVU METODU PRI RJEŠAVANJU VEZANIH DIFERENCIJALNIH JEDNADŽBI ZA VLASTITA STANJA

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Ovdje iznosimo zapažanje da renormalizirana Numerova metoda (RN), koja se obično koristi pri rješavanju sistema vezanih diferencijalnih jednadžbi (CDEE) za vlastite vrijednosti, ima neočekivano konvergentno ponašanje kada se dužina koraka smanji. Daljnja ugradnja odgovarajućeg asimptotskog ponašanja valne funkcije, umjesto oštrog rezanja, poveća energiju vezanja za oko 10%. Kao ilustraciju rješavamo problem osnovnog stanja deuterona s Reidovim potencijalom mekane sredice i dobivamo konvergentno ponašanje kao funkciju dužine koraka.