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CONVERGENCE BEHAVIOUR FOR NUMERICAL INTEGRATION OF DIFFERENTIAL EQUATIONS BY RUNGE-KUTTA AND RENORMALIZED NUMEROV METHODS

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Convergence behaviours of Runge-Kutta (RK) and Renormalized Numerov (RN) methods of integrating differential eigenvalue equation have been investigated. $^3s_1$ state of deuteron has been solved with Afnan Tang S3 potential. Although RN method is much faster than RK method, the former has a peculiar convergence behaviour, viz, binding energy (*BE*) decreases as step size decreases. Choice of asymptotically exponential wave function improves *BE* over the usually adopted sharp cut off form.

1. Introduction

In problems of physics, one frequently encounters a differential eigenvalue equation, which must be solved subject to specified boundary conditions, for the eigenvalue as well as the eigenfunction. In this communication, we investigate convergence behaviours for the numerical integration of an uncoupled differential eigenvalue equation by two different methods, namely, the Runge-Kutta (RK) method[1] and the Renormalized Numerov (RN) method[2].

We consider a differential eigenvalue equation of the form

$$\left[-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2}+V(r)\right]u(r)=Eu(r) \tag{1}$$

which is the form of the Schrödinger equation in one variable. For a multidimensional Schrödinger equation a coupled version of Eq. (1) is obtained by removing the angular part (or hyperangular part in the case of many body problem) and coupling interaction terms are obtained by integrating the total interaction multiplied by angular eigenfunctions over all the angle variables[3]. A coupled set of differential eigenvalue equation can be approximately decoupled to the form (1), by the uncoupled adiabatic approximation procedure[4]. For a state with $l \neq 0$, the centrifugal potential can be included in $V(r)$. Eq. (1) is to be solved subject to the usual boundary conditions

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

where

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

Note that for all practical problems

$$V(r) \underset{r\to\infty}{\to} 0. \tag{3}$$

If $V(r)$ has a strong r dependence for $r \to 0$, then the simple boundary condition at $r = 0$ is to be replaced by its appropriate analytic behaviour for $r \to 0$.

2. *Runge-Kutta method of integration*

In the Runge-Kutta integration procedure, the second order equation (1) is rewritten as a set of two first order coupled differential equations

$$\frac{du(r)}{dr} = p(r)$$

$$\frac{dp(r)}{dr} = \frac{2m}{\hbar^2}(V(r) - E)\,u(r). \tag{4}$$

Choosing a guess value of $E = E_0$, these equations are then integrated point by point by Runge-Kutta integration procedure[1] outwards from $r = 0$ to a chosen matching point r_m, starting from

$$u_{out}(r \to 0) = 0$$

$$p_{out}(r \to 0) = C_1 \tag{5}$$

and inwards from an asymptotically large value of r (for which $V(r)$ is practically zero) to r_m, starting from the asymptotic boundary conditions

$$u_{in}(r \to \infty) = C_2\, e^{-\beta r}$$

$$p_{in}(r \to \infty) = -\beta C_2\, e^{-\beta r} \tag{6}$$

where C_1 and C_2 are two arbitrary constants.

The energy eigenvalue is obtained by imposing the condition of continuity of log-derivatives of the outward and inward solutions at $r = r_m$

$$f(E) \equiv \frac{p_{in}(r_m)}{u_{in}(r_m)} - \frac{p_{out}(r_m)}{u_{out}(r_m)} = 0. \tag{7}$$

Note that the difference of log-derivatives is a function of energy (E). Then Eq. (4) can be solved by a simple linearization procedure (Newton-Kantorovic method[5]) or by more sophisticated numerical techniques. In the Newton-Kantorovic method $f(E)$ is expanded in a Taylor series about E_0 and only linear terms are retained:

$$f(E) = 0 = f(E_0) + \left(\frac{df}{dE}\right)_{E=E_0} (\Delta E) + \ldots \tag{8}$$

From Eq. (8) the correction to energy ΔE is calculated and the initial guess is improved by $E = E_0 + \Delta E$. The process is repeated until convergence in energy eigenvalue is achieved. For a proper bound state, this process can be shown to converge. However the rate of convergence is not fast and one usually uses more sophisticated numerical methods for a faster convergence of Eq. (7).

3. *Renormalized Numerov method of integration*

In the renormalized Numerov method[2], Eq. (1) is rewritten in the form

$$\left[\frac{d^2}{dr^2} + Q(r)\right] u(r) = 0 \tag{9}$$

where

$$Q(r) = \frac{2m}{\hbar^2}(E - V(r)).$$

Then a three term recurrence relation can be written[6]

$$(1 - T_{n+1})\, u_{n+1} - (2 + 10T_n)\, u_n + (1 - T_{n-1})\, u_{n-1} = 0 \tag{10}$$

where

$$u_n = u(r_n)$$

$$T_n = -\left(\frac{h^2}{12}\right) Q(r_n). \tag{11}$$

Here u_n is the wave function at the n-th grid point (equispaced) with spacing h.

The renormalized Numerov algorithm is obtained by defining

$$F_n = (1 - T_n)\, u_n. \tag{12}$$

Substitution of this in Eq. (10) gives

$$F_{n+1} - W_n F_n + F_{n-1} = 0 \tag{13}$$

where

$$W_n = (2 + 10T_n)(1 - T_n)^{-1}.$$

Next a two point recurrence relation is obtained by introducing

$$R_n = F_{n+1}/F_n. \tag{14}$$

Then from (13) one obtains

$$R_n = W_n - R_{n-1}^{-1}. \tag{15}$$

This equation can now be iterated outwards starting from a given grid point (n) to obtain R_j, ($j = n, n+1, n+2, \ldots$).

The boundary condition (5) is easily seen to give

$$R_0 = \infty \tag{16}$$

at the initial grid point ($r \to 0$). Knowing R_n at each grid point, the wave function u_n can be calculated from Eqs. (12) and (14)

$$\begin{aligned} u_{n+1} &= C(1 - T_{n+1})^{-1} R_n \\ u_n &= C(1 - T_n)^{-1} \\ u_{n-1} &= C(1 - T_{n-1})^{-1} R_{n-1}^{-1} \end{aligned} \tag{17}$$

where C is an arbitrary normalization constant, obtained in terms of u_r, ($C = (1 - T_n) u_n$) for each step. One thus renormalizes the wave function at each step, which is why this method is called renormalized Numerov method.

For the inward integration, one defines

$$\hat{R}_n = F_{n-1}/F_n. \tag{18}$$

Substitution on Eq. (13) once again gives a two term recurrence relation (similar to Eq. (15))

$$\hat{R}_n = W_n - \hat{R}_{n+1}^{-1}. \tag{19}$$

As before knowing the value of $\hat{R}_n$ at a given grid point n, one can iterate Eq. (19) inwards to obtain $\hat{R}_j$, ($j = n, n-1, n-2, \ldots$).

The boundary condition for $r \to \infty$ can be seen from Eq. (6) to be

$$\hat{R}_N^{-1} = \frac{F_N}{F_{N-1}} \approx \frac{U_N}{U_{N-1}} = e^{-\beta h} \tag{20}$$

where N is the final mesh point. Note that the final mesh point is expected to be well outside the range of the potential $V(r)$, so that

$$T_N \approx T_{N-1} = -\left(\frac{h^2}{12}\right)\left(\frac{2m}{\hbar^2}\right) E. \tag{21}$$

It is a common practice in literature[2] that U_N is taken as zero and $U_{N-1} \neq 0$ which gives $\hat{R}_N^{-1} = 0$. Eq. (20) 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 conveniently chosen matching point[2]. However, the same condition can be achieved by the continuity of R_n and $\hat{R}_n$ across the matching point, since the wave functions are actually obtained in terms of R_n and $\hat{R}_n$ (cf. Eq. (17)). Thus if M be the matching grid point, the condition

$$\hat{R}_M = \hat{R}_{M+1}^{-1} \tag{22}$$

must be satisfied for the correct eigenenergy. Eq. (22) is obtained directly from Eqs. (14) and (18). Thus we have to solve the equation

$$D(E) = \hat{R}_{M+1}^{-1} - \hat{R}_M = 0 \tag{23}$$

to obtain the correct eigenenergy.

The usual procedure is to start inward integration at $r = r_N$ and continue iteration of Eq. (19) until $\hat{R}_n < 1$ first occurs; then the iteration is stopped and this point is chosen as the matching point r_M. Next Eq. (15) is iterated outwards from $r = 0$ using the condition (16) (or a more appropriate value calculated analytically from the form of $V(r \to 0)$) up to the matching point r_M. The guess energy is then changed and the whole process repeated until condition (23) is satisfied to within the desired accuracy.

Two values of energy (E_L and E_H) are guessed between which the correct eigenenergy is expected to lie, such that $D(E_L)$ and $D(E_H)$ have opposite signs. Then $D(E_L)$, $D(E_H)$ and $D(E_M)$ where $E_M = \frac{1}{2}(E_L + E_H)$ are calculated. If sign of $D(E_M)$ is same as $D(E_L)$, then E_L is set equal to E_M; otherwise E_H is set equal to E_M and the bisection procedure repeated until $|E_H - E_L|$ is smaller than the desired accuracy ε. On the other hand if $|D(E_M)| < \varepsilon_1$, where ε_1 is the prescribed upper limit in the value of $|D|$, we get the desired energy E_M. The linearization method discussed in Section 2 can also be used after a few bisections.

4. Results

For a comparison of the two methods, we have calculated the binding energy (*BE*) and wave function for the $^3s_1$ state of the deuteron with the *S*3 potential of Afnan and Tang[7]. Table 1 presents the calculated binding energy for the above mentioned potential for various choices of the step size (h) by both the methods. Table 1 also displays the CPU time necessary for each calculation (calculations were done in double precision on HP 1000/A 700 computer). It is seen that the RN method is much faster than the RK method for the same step size. In Fig. 1,

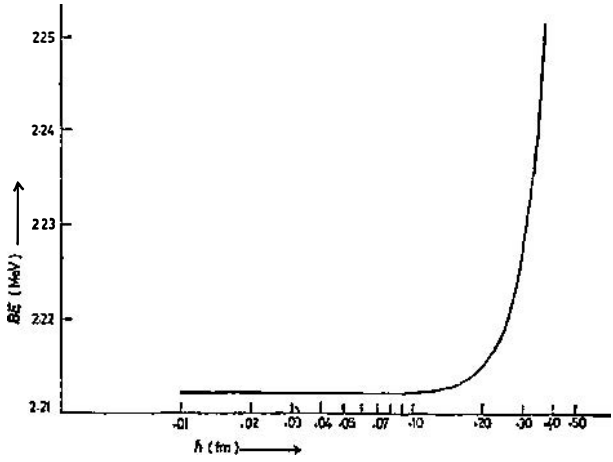

Fig. 1. Binding energy (*BE*) as a function of step size (h) for RN method with exponential tail for S3 potenatial.

TABLE 1.

Step size (h) (fm)	RK method		RN method with sharp cut-off tail		RM method with exponential tail	
	BE (MeV)	CPU time (s)	*BE* (MeV)	CPU time (s)	*BE* (MeV)	CPU time (s)
0.01	2.22277	90.38	2.19764	29.14	2.21209	33.29
0.02	2.22277	33.87	2.19764	14.57	2.21209	15.20
0.03	2.22277	29.09	2.19764	10.14	2.21209	10.14
0.04	2.22277	19.62	2.19764	7.61	2.21209	7.62
0.05	2.22277	18.21	2.19765	6.37	2.21210	6.12
0.06	2.22277	18.18	2.19766	5.10	2.21211	5.74
0.10	2.22277	17.03	2.19781	3.18	2.21226	3.22
0.15	2.22277	17.86	2.19853	2.04	2.21297	2.05
0.20	2.22277	17.08	2.20051	1.74	2.21491	1.56
0.25	2.22277	17.58	2.20477	1.38	2.21911	1.40
0.30	2.22277	17.91	2.21262	1.16	2.22685	1.16
0.35	2.22277	17.71	2.22544	0.94	2.23916	1.03
0.37	2.22277	18.66	2.23251	0.94	2.24782	0.98
0.40	2.22277	18.41	2.25673	0.83	2.27167	0.85

Binding energy and CPU time for Runge-Kutta (RK) and Renormalized Numerov (RN) methods for different step sizes for S3 potential.

we present the convergence behaviour of BE as a function of step size (h) for the RN method. One can see from Table 1 that the RK method attains convergence for quite large values of h, while RN method has a rather peculiar behaviour, as h is reduced, BE decreases gradually and attains convergence (Fig. 1). The gradual *decrease* of binding energy with decrease of h is an unexpected behaviour; although there is a clear indication of convergence (Fig. 1). The RK method has a very stable value of BE even for quite large values of h. This apparently strange behaviour can be understood easily, since the standard subroutine RKGS for integration of a differential equation by the Runge-Kutta method actually bisects the given step size, until it reaches the prescribed accuracy. For this reason the CPU time taken for the RK method attains almost a constant value ($\cong 17$ s) for $h \geqslant 0.10$ fm. In comparing the CPU time required by the two methods one should compare this value with the CPU time for the RN method when convergence is first attained ($h \approx 0.04$ fm). This shows that the RN method is about three times faster than the RK method.

From Table 1 we can also see that the RN method with the wave function having an exponential tail gives a better binding energy (as can be seen by comparison with RK method) than when the wave function has a sharp cut off in the asymptotic region.

5. *Conclusions*

1) RN method is about three times faster than RK method.

2) The convergence behaviour of the RN method is rather strange: *BE decreases* with decrease of h and attains a convergence.

3) Requirement of a correct exponential tail of the wave function improves the BE over the sharp cut-off asymptotic form, which is usually adopted[2].

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PONAŠANJE KONVERGENCIJE PRI NUMERIČKOJ INTEGRACIJI DIFERENCIJALNIH JEDNADŽBI METODOM RUNGE-KUTTA I RENORMALIZACIJE NUMEROVA

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Istraživano je ponašanje konvergencije Runge-Kuttove metode (RK) i renormalizacione metode Numerova (RN). Riješeno je $^3s_1$ stanje deuterona s Afnan Tang S3 potencijalom. Iako je RN metoda znatno brža od RK metode, prva ima neobično ponašanje pri konvergenciji, npr. za manje vrijednosti koraka, energija vezanja (*BE*) opada brže k pravoj vrijednosti. Izbor eksponencijalne valne funkcije u asimptotskom području poboljšava *BE* u usporedbi s obično prihvaćenim oblikom naglog rezanja.