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A variant of the matrix Numerov method for the solution of coupled differential equations of the Schrodinger type.

M.Benfatto and C.R.Natoli

Laboratori Nazionali di Frascati dell'I.N.F.N.- C.P.13 - 00044 Frascati (ITALY)

Abstract

A variant of the matrix Numerov method for the solution of coupled differential equations arising from the Schrodinger equation is proposed. It allows a faster generation of the wanted solution, with accuracy comparable to the more traditionally applied method , and it is especially suitable for large system of order $N \gg 10$.

1. Introduction

Many problems of theoretical physics can be reduced to a set of coupled differential equations for which more or less accurate numerical solutions are sought for. As a consequence, it turns out quite useful, if not compelling sometime, to device fast numerical methods to find these solutions, especially for large sets.

For systems of coupled differential equations arising from the Schrodinger equation in scattering theory(either scattering from a non spherically symmetric potential or multichannel scattering theory), the matrix method of Numerov [1-3], an extension of the similarly named algorithm for single channel Schrodinger equations, is superior to any other that has been suggested for a step-by-step integrations of the system of equations. It is a three-points method with the smallest truncation error within this class. The two inherent disadvantages of the method, starting the integration and changing mesh size, can be readily overcome. However what makes this method rather time consuming for large sets of coupled equations is the fact that each integration step requires the inversion of

a large matrix. The observation that this matrix is strongly diagonally dominant, save possibly for integration steps near the origin of the coordinates, led Allison [2] to propose the iterative Numerov method, which he finds to be more efficent in generating the wanted solutions. The same observation motivates this note in that it allows a simplification of the matrix method which avoids the need of inverting a matrix, while preserving a comparable accuracy.

2. The matrix Numerov method and its simplified version.

We consider the set of N coupled differential equations

$$\sum_{j=1}^{N}\left(\left[\frac{d^2}{dr^2}+k_i^2-\frac{l_i(l_i+1)}{r^2}\right]\delta_{ij}-V_{ij}(r)\right)f_j^k(r)=0 \quad (i,j,k=1,N) \tag{2.1}$$

k labelling the N indipendent vector solutions $\vec{f^k}\equiv(f_j^k)$ regular at the origin, i.e. $\lim_{r\to 0} f_j^k(r)=0$. By introducing the matrices $F=(f_j^k)$ and $G\equiv\left(\left[\frac{l_i(l_i+1)}{r^2}-k_i^2\right]\delta_{ij}+V_{ij}(r)\right)$ we can write Eq.(2.1) in matrix form

$$F''=GF \tag{2.2}$$

With the notation $h=r_{n+1}-r_n$ and

$$F_n\equiv(f_j^k(r_n)) \tag{2.3}$$

where r_n is the n-th mesh point, the matrix Numerov method takes the form [3]

$$F_{n+1}=\left[I-\frac{h^2}{12}G_{n+1}\right]^{-1}\left[(2I+\frac{10}{12}h^2G_n)F_n-(I-\frac{h^2}{12}G_{n-1})F_{n-1}-\frac{h^6}{240}F_n^{\text{VI}}+h.o.\right] \tag{2.4}$$

where F_n^{VI} indicates a sixth derivate matrix at point r_n.

Negleting the term $-\frac{1}{240}h^6F_n^{\text{VI}}$, which therefore rapresent the truncation error proportional to h^6, one may use Eq.(2.4) together with the knowledge of the solution at two points to generate the wanted solution for all values of r. Now the usual statement that one encounters in the literature [2,3] is that one can use the first terms of a Frobenius expansion near the origin, if the solution for (2.4) is started closed enough to the origin . It is easily shown that the regular solutions for small r that satisfy Eq.(2.1) are given by

$$f_j^k\simeq r^{l_k+1}\delta_{kj} \tag{2.5}$$

provided the matrix elements $V_{ij}(r)$ have no singularities of order two or greater at the origin. Deferring some comments on this point later in the Appendix, let us assume for the moment that

one can start the recurrence procedure in Eq.(2.4) by using $F_0 = 0$ and $F_1 = (h^{l_h+1}\delta_{ij})$. As is stands however, Eq.(2.4) requires inversion of the matrix $(I - \frac{1}{12}h^2G_{n+1})$ at each step.

To avoid this and in order to reduce the number of arithimetic operations per step we rewrite Eq.(2.4) as

$$\left[I - \frac{h^2}{12}G_{n+1}\right]F_{n+1} = \left[2I + \frac{10}{12}h^2G_n\right]F_n - \left[I - \frac{h^2}{12}G_{n-1}\right]F_{n-1} + 0(h^6) \tag{2.6}$$

and introduce the auxilary quantity

$$Y_n = \left[I - \frac{1}{12}h^2G_n\right]F_n \tag{2.7}$$

Then equation (2.6) can be rewritten as

$$Y_{n+1} = 12F_n - (10Y_n + Y_{n-1}) + 0(h^6) = 12\left[I - \frac{h^2}{12}G_n\right]^{-1}Y_n - (10Y_n + Y_{n-1}) + 0(h^6) \tag{2.8}$$

Now it is a well known theorem in matrix theory that for a NxN matrix A

$$[I - A]^{-1} = \sum_{k=0}^{\infty} A^k \tag{2.9}$$

provided $\rho(A) < 1$ where $\rho(A)$ is the spectral radius of A, defined as

$$\rho(A) \equiv \max_{1 \le i \le N} |\lambda_i|$$

where $\lambda_i (i = 1, N)$ are the eigenvalues of A. [4]

Given the expression for G, it is possible that, for small r, $\rho\left(\frac{h^2}{12}G(r)\right) > 1$. To avoid this inconvenience we rewrite $I - \frac{h^2}{12}G(r)$ as

$$I - \frac{h^2}{12}G(r) \equiv \Lambda(r) + \frac{h^2}{12}K(r) = \Lambda(r) + K'(r) \tag{2.10}$$

where

$$\Lambda_{ij}(r) = \left[1 - \frac{h^2}{12}\left(\frac{l_i(l_i+1)}{r^2} - k_i^2 + V_{ij}(r)\right)\right]\delta_{ij} \qquad K_{ij}(r) = (1 - \delta_{ij})V_{ij}(r)$$

so that $\Lambda(r)$ is completly diagonal and $K(r)$ completly off-diagonal ,i.e. with diagonal elements equal to zero. Hence

$$(\Lambda + K')^{-1} = (I + \Lambda^{-1}K')^{-1}\Lambda^{-1} = \sum_{m=0}^{\infty}(\Lambda^{-1}K')^m\Lambda^{-1} \tag{2.11}$$

if h is chosen so that $\frac{h^2}{12}\rho(\Lambda_n^{-1}K_n) < 1$ for all r_n in the range of integration.

Under these assumptions Eq.(2.8) can be rewritten as

$$Y_{n+1} = 12\left(\sum_{m=0}^{\infty}\frac{h^{2m}}{12^m}(\Lambda_n^{-1}K_n)^m\right)\Lambda_n^{-1}Y_n - (10Y_n + Y_{n-1}) + 0(h^6)$$

from which

$$Y_{n+1} = 12\left[I + \frac{h^2}{12}\Lambda_n^{-1}K_n + \frac{h^4}{12^2}(\Lambda_n^{-1}K_n)^2\right]\Lambda_n^{-1}Y_n - (10Y_n + Y_{n-1}) + 0(h^6) \qquad (2.12)$$

the last step being justified by the fact that we can truncate the expression at the fourth order in the mesh size h with little loss in accuracy since the truncation error is already $0(h^6)$. The development in powers of $\Lambda_n^{-1}K_n'$ is convenient only as long as $\rho(\Lambda_n^{-1}) > 1$. (A glance at definition (2.10) shows that this is to be expected for a number n of mesh points near the origin, such that roughly $n \approx \left[\frac{l_{max}(l_{max}+1)}{12}\right]^{\frac{1}{2}} \approx \frac{l_{max}}{3}$). When this condition is no longer satisfied, then is better to expand in power of $\frac{h^2}{12}G_n$ and choose h so that in the range of integration $\frac{h^2}{12}\rho(G_n) < 1$ for all r_n of interest. One way of avoiding the first mesh points is to use an accurate Froboenius expansion of the solution near the origin, so as to start Numerov iteration farther away from it. Alternatively one can use both developments, each one in its range of validity. For convenience we shall assume henceforth $\Lambda_n = I$ and $K_n = G_n$

3. Stability of the various methods.

In order to discuss the conditions of the stability for Eq. (2.8) and its approximate form (2.12) we use a comparison method with difference equation with constant coefficients.

As is well known, if in the difference equation

$$y_{n+1} - 2(1+\alpha)y_n + y_{n-1} = 0 \qquad (3.1)$$

$|1+\alpha| < 1$, then the method of integration of the original differential equation is locally stable. If instead $|1+\alpha| > 1$, the method is unstable. When the quantity $\alpha \equiv \alpha_n$ is point dependent, then the condition $|1+\alpha_n| \gtrless 1$ defines the intervals of local stability (instability) of the solution of the differential equations. Application of these considerations to a matrix difference equation, like the one in Eqs.(2.8) and (2.12), requires a preliminary discussion of the eigenvalues of G_n.

In fact the matrix $I - \frac{h^2}{12}G_n$ is, except for few mesh points near the origin, a strictly diagonally dominant hermitian matrix with positive eigenvalues centered around the value 1 if, as it usually the case, $\frac{h^2}{12}\rho(G_n) < 1$. If, morover, G_n itself is strictly or irreducibly diagonally dominant with positive (negative) diagonal entries [4], then all its eigenvalues are positive (negative) , so that the eigenvalues of $I - \frac{h^2}{12}G_n$ are either all < 1 or all > 1.

In such a case diagonalization of the matrix difference equation reduces the discussion to the case of the single difference equation.

Hence, indicating by ϵ the common sign(± 1) of the eigenvalues of G_n, the conditions of local stability for equation (2.8) becomes

$$|\frac{6}{1-\frac{h^2}{12}\rho(G_n)\epsilon}-5|<1 \qquad \mapsto \qquad -\frac{1}{2}<\frac{h^2}{12}\rho(G_n)\epsilon<0 \tag{3.2}$$

i.e. $\epsilon=-1$ and $\frac{h^2}{12}\rho(G_n)<\frac{1}{2}$

Similary for Eq. (2.12) the same condition takes the form, putting $h^2\rho(G_n)=\gamma>0$

$$|1+\epsilon\frac{\gamma}{2}+\frac{1}{24}\gamma^2|<1 \qquad \mapsto \qquad 0<\gamma<-12\epsilon \tag{3.3}$$

i.e. $\epsilon=-1$ and $\frac{h^2}{12}\rho(G_n)<1$

When $\epsilon=+1$ (i.e.G_n positive definite) or when there are eigenvalues of both signs, then there is local instability. In those intervals of integration where this happens, one can minimize the rate of accumulation of systematic or random errors by making $h^2\rho(G_n)\equiv 2\alpha_n \ll 1$. This is because, under this condition both Eqs. (2.8) and (2.12) take the form (3.1) with $\alpha=\alpha_n$

$$y_{n+1}-2(1+\alpha_n)y_n+y_{n-1}=0$$

By defining an average value $\bar{\alpha}$ for the α_n on the interval of instability we see that the rate of growth for the error ϵ_n at mesh point n goes like

$$\epsilon_n \approx C_1 e^{n\ lnr_1}+C_2 e^{n\ lnr_2}$$

where $r_{1,2}\equiv 1+\bar{\alpha}\pm[(1+\bar{\alpha})^2-1]^{\frac{1}{2}}\approx 1\pm(2\bar{\alpha})^{\frac{1}{2}}$ are the roots of the equation

$$m^2-2(1+\bar{\alpha})m+1=0$$

associated to (3.1) and C_1 and C_2 are constants depending on the initial conditions.
Hence $\epsilon_n \approx e^{n(2\alpha)^{\frac{1}{2}}}$, from which the above statement follows.

From the above discussion we see that the condition (3.2) of stability for Eq. (2.4) is even more restrictive than the condition $\frac{h^2}{12}\rho(G_n)<1$ required for the validity of the expansion in Eq. (2.11). Hence we can always use this latter to pass from Eq. (2.8) to Eq. (2.12).

Depending on the degree of accuracy for the wanted solution, we can further simplify Eq. (2.12) by simply dropping in this latter the term $\frac{h^4}{12^2}\rho(G_n)$. The percentage error introduced in such a way in the solution is of the order of $\frac{h^4}{24}\rho_{max}(G_n)$, where ρ_{max} is the upper bound of all the spectral radii of G_n in the range of integration . In this latter case the condition for stability becames $\frac{h^2}{12}\rho(G_n)<\frac{1}{3}$

4.Conclusion.

The three point matrix method of integration given by Eq. (2.8) and its variant Eq. (2.12), when expressed in terms of the auxiliary variable Y_n defined in Eq. (2.7), have the computational advantage that the coupling intervenes only through the coefficent multiplying Y_n, implying a minimum number of matrix multiplications at each step and the ability to generate the whole set of indipendent solutions in one go.

This is true even in the case when one needs the original variable F_n at all mesh points, since at each step in Eq. (2.8) we have to calculate anyway the quantity $\left[I - \frac{h^2}{12}G_n\right]^{-1} Y_n \equiv F_n$. One further advantage is the possibility of using the expansion (2.11) by choosing the variable mesh size h so that in the appropiate interval $\frac{h^2}{12}\rho(G_n) \ll 1$. Depending moreover on the accuracy needed one can further envisage to retain the first term in the above expansion, i.e. to put $\left[I - \frac{h^2}{12}G_n\right]^{-1} \approx I + \frac{h^2}{12}G_n$.

In this latter form, the matrix Numerov method in the coupled case becomes comparable in speed to the more traditional method used for the uncoupled case.

A test run for a 100 mesh points integration of a 9x9 system of equations, with potentials $V_{ij}(r)$ of the atomic type, has shown a reduction of 20 % of CPU time when using the simplest variant of the Numerov method Eq. (2.12), with h^4 terms discarded, over the traditional method Eq. (2.8).

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It is a plesaure to acknowledge illuminating discussions with Dr. F.Palumbo on the Frobenius method of integration in series for systems of differential equations.

Appendix

In this appendix we want to write explicity, for convenience of the reader, the first few terms of the Frobenius expansion for the system of equations (2.1) which we now write as

$$\left(r^2\frac{d^2}{dr^2} - L(L+I) - A(r)\right)\vec{f}^k(r) = 0 \qquad (A.1)$$

where $\vec{f}^k(r)$ is the k-th indipendent regular vector solution ($k = 1, ...N$), $\mathcal{L} \equiv l_i\delta_{ij}$ $(i, j = 1, ...N)$ and

$$A(r) \equiv r^2[V_{ij}(r) - k^2\delta_{ij}] = \sum_{\nu=0}^{\infty} A_\nu r^\nu \tag{A.2}$$

assuming that all the functions $r^2V_{ij}(r)$ are analytical near the origin and that $\lim_{r\to 0} r^2V_{ij}(r) = 0$, so that $A_0 = 0$. We shall also assume that $l_i < l_j$ if $i < j$. From the explicit expansion we shall derive the conditions under which one can use Eq. (2.5) in the text to start the recurrence procedure in Eq. (2.4).

The method of Frobenius for the solution of linear differential equations is a standard method [5,6] that demands the definition of the vector series

$$\vec{\Lambda}^k(\sigma, r) = r^{l_k+1+\sigma} \sum_{\nu=0}^{\infty} \vec{\phi}_\nu^k(\sigma) r^\nu \tag{A.3}$$

of the two variables σ and r. Formal insertion of this into (A.1) shows that

$$\left[r^2\frac{d^2}{dr^2} - \mathcal{L}(\mathcal{L}+I) - A\right]\vec{\Lambda}^k(\sigma, r) = [(l_k+1+\sigma)(l_k+\sigma)I - \mathcal{L}(\mathcal{L}+I)]\vec{\phi}_0^k(\sigma) r^{l_k+1+\sigma} \tag{A.4}$$

provided for $\nu > 0$ the functions $\vec{\phi}_\nu^k(\sigma)$ are determined by the recurrence relations

$$[(l_k+1+\sigma+\nu)(l_k+\sigma+\nu)I - \mathcal{L}(\mathcal{L}+I)]\vec{\phi}_\nu^k(\sigma) = \sum_{\mu=0}^{\nu} A_\mu \vec{\phi}_{\nu-\mu}^k(\sigma) = \sum_{\mu=1}^{\nu} A_\mu \vec{\phi}_{\nu-\mu}^k(\sigma) \tag{A.5}$$

and $\vec{\phi}_0^k(\sigma)$ is arbitrary.

Under these assumption, Ref [5] shows that the series (A.3) is analytical in both σ and r, for $0 \leq \sigma \leq 1$ and r sufficently near the origin. Hence by choosing $\vec{\phi}_0^k(\sigma) = \sigma^D\vec{E}^k$ where $\vec{E}^k = \delta_{kj}$ and $D = l_{max} = l_N$ we see from (A.4) that

$$\lim_{\sigma\mapsto 0} \frac{d^D}{d\sigma^D}\vec{\Lambda}^k(\sigma, r) = r^{l_k+1} \sum_{\tau=0}^{D} (ln\ r)^\tau \frac{D!}{\tau!(D-\tau)!} \lim_{\sigma\mapsto 0} \frac{d^{D-\tau}}{d\sigma^{D-\tau}} \sum_{\nu=0}^{\infty} \vec{\phi}_\nu^k(\sigma) r^\nu \tag{A.6}$$

is a vector solution of (A.1). By taking in turn $\vec{\phi}_0^k(\sigma)$ proportional to different vectors $\vec{E}^{k'} \equiv \delta_{k'j}$, $k' \# k$ one can show that in this way all the N indipendent regular vector solutions of (A.1) are generated.

Expression (A.6) for the solutions shows that logarithmic terms appear whenever some $\vec{\phi}_\nu^k(\sigma)$ have zeros of order less then $D = l_{max}$ in the limit $\sigma \mapsto 0$. From the recurrence relations (A.5) we see that this happens whenever for some index j and some ν

$$\lim_{\sigma\mapsto 0} [(l_k+1+\sigma+\nu)(l_k+\sigma+\nu)I - \mathcal{L}(\mathcal{L}+I)]_{jj} = 0 \tag{A.7}$$

Notice that for $l_k = l_{max} = l_N$ this can never occur for any $\nu \geq 1$, so that the vector solution corresponding to the index N in (A.6) does not contain logarithmic terms.

For any other index $k < N$,Eq. (A.7) may be verified for some ν . In such a case the appearance of logarithms depends on the structure of the matrices A_ν.

Indeed let us take an index k so that already for $\nu = 1$ condition (A.7) occurs once, for a certain index j necessarily different from k. Then from the recurrence relations (A.5) we derive, remembering that

$$\vec{\phi}_1^k(\sigma) = [(l_k + 1 + \sigma + 1)(l_k + \sigma + 1)I - \mathcal{L}(\mathcal{L} + I)]^{-1} A_1 \vec{E}^k \sigma^D \qquad (A.8a)$$

$$\vec{\phi}_2^k(\sigma) = [(l_k + 1 + \sigma + 2)(l_k + \sigma + 2)I - \mathcal{L}(\mathcal{L} + I)]^{-1} [A_1 \vec{\phi}_1^k(\sigma) + A_2 \vec{E}^k \sigma^D] \qquad (A.8b)$$

.....

$$\vec{\phi}_\nu^k(\sigma) = [(l_k + 1 + \sigma + \nu)(l_k + \sigma + \nu)I - \mathcal{L}(\mathcal{L} + I)]^{-1} \sum_{\mu=1}^{\nu} A_\mu \vec{\phi}_{\nu-\mu}^k(\sigma) \qquad (A.8c)$$

Provided now that the matrix element $(A_1)_{jk}$ is different from zero, i.e. $\lim_{r \to 0} rV_{jk}(r) \neq 0$,we see from Eq. (A.8a) that the j-th component of the vector $\vec{\phi}_1^k(\sigma)$ has a zero of order $D - 1$ in the $lim\ \sigma \mapsto 0$,whereas all the other components have a zero of order D. Consequetly in this istance the first few terms of the Frobenius expansion for the k-th solution $\vec{f}^k(r)$ are given by

$$\vec{f}^k(r) = r^{l_k+1}[\vec{E}^k + (A_1 \vec{E}^k - a_{jk} \vec{E}^j) r + a_{jk} \vec{E}^j l_{max}\ r\ \ ln\ r + ...] \qquad (A.9)$$

where, for simplicity $a_{jk} \equiv (A_1)_{jk}$

This expression clearly shows that, although in the limit $r \mapsto 0$ only the first term $\vec{E}^k$ within brakets survives, the approximation of the solutions near the origin by only this term is a poor one, even for such a small mesh size $h \approx 10^{-3}$ as usually chosen near $r = 0$. In other words the percentage of error introduced in the solution by neglecting the second term in brackets with respect to the first, especially in the presence of logarithms, can be much higher than the ratio $r(\approx h)$ to 1. This fact, if overlooked may prevent an accurate solution of the system (2.1), all the more that near $r = 0$ the solution is instable and the error increase at least until a turning point is met.

The correct procedure to follow is then to fix an a priori error within which one wants to know the solution and then use as many terms in the Frobenius expansion (A.9) as necessary to obtain the desidered accuracy.

The above is not at all an exhaustive treatment of the Frobenius method for the series integration of systems of differential equations . The interested reader is referred to ref [5] for rigorous

presentation of the subject and to ref [6] for a very useful discussion on the implications of the method as applied to systems of the type shown in (A.1), arising in problems of nuclear physics. We have used much of the material contained in this latter reference for the discussion in this Appendix.

References

1) B.Numerov, Publs.Observ. central astrophys. Russ. 2,188 (1933) ; D.R.Hartee, 'The calculation of Atomic Structure' John Wiley and Sons, New York (1957)

2) A.C. Allison, J.Comput. Phys. 6 (1970) 378

3) L.L.Barnes,N.F.Lane and C.C.Lin, Phys. Rev.A 137 (1965) 388 ; K.Smith,R.J.W.Henry ; P.G.Burke, Phys. Rev. 147 (1966) 21

4) R.S.Varga, Matrix Iterative Analysis (Prentice Hall,1968)

5) E.L.Ince, Ordinary Differential Equations (Dover, 1956)

6) F.Palumbo, Phys. Lett. 69B, 275 (1977)