A generalized Numerov method
for linear second-order differential equations
involving a first derivative term

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Abstract

The Numerov method for linear second-order differential equations is generalized
to include equations containing a first derivative term. The method presented has
the same degree of accuracy as the ordinary Numerov sixth-order method. A general
scheme of the application to the numerical solution of the Hartree-Fock equations is
considered.

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1 Introduction

The linear second-order differential equations of the type

\[ y''(x) + g(x) y'(x) + f(x) y(x) = 0 \]  \hspace{1cm} (1)

occur in various fields of physics. Here we shall mean the problem of the numerical self-consistent solution of the Hartree-Fock (HF) equations of motion deduced from the Skyrme energy functional \cite{9} describing ground-state properties of atomic nuclei. For spherical nuclei these equations can be reduced to the form (1), the first derivative term arising due to the radial dependence of the nucleon effective mass. Usually the task is solved by the Runge-Kutta method. But this method is not the best one for the HF self-consistency procedure because it requires the interpolation of functions \( g(x) \) and \( f(x) \) in Eq. (1) between the grid points where function \( y(x) \) is not calculated. Another well-known method (see, for example, Refs. \cite{2, 1}), which was proposed by B. V. Numerov in 1923, is free of the pointed difficulty but the first derivative term in Eq. (1) precludes from its immediate application. Several modifications of the Numerov method (NM) were developed \cite{4, 8} in order to include equations of the type (1) and more general nonlinear equations. Here another generalization of the NM is presented which is most suitable for the HF calculations \cite{7} and yields the same degree of accuracy as the initial Numerov method.

2 Generalized linear Numerov method

Let us introduce notations: \( y_0 = y(x_0) \), \( y_\pm = y(x_0 \pm h) \) and analogously for \( g(x) \) and \( f(x) \), where \( x_0 \) is the fixed grid point, \( h \) is the step length. Developing quantities \( y_\pm, y'_\pm, y''_\pm \) in powers of \( h \), we obtain

\[
y_+ + y_- = 2y_0 + h^2y_0'' + \frac{h^4}{12}y_0^{(4)} + \frac{h^6}{360}y_0^{(6)} + O(h^8),
\]

(2)

\[
y_+ - y_- = 2hy_0' + \frac{h^3}{3}y_0''' + \frac{h^5}{60}y_0^{(5)} + O(h^7),
\]

(3)

\[
y'_+ + y'_- = 2y_0' + h^2y_0''' + \frac{h^4}{12}y_0^{(5)} + O(h^6),
\]

(4)

\[
y'_+ - y'_- = 2hy_0'' + \frac{h^3}{3}y_0^{(4)} + \frac{h^5}{60}y_0^{(6)} + O(h^7),
\]

(5)

\[
y''_+ + y''_- = 2y_0'' + h^2y_0^{(4)} + \frac{h^4}{12}y_0^{(6)} + O(h^5),
\]

(6)

\[
y''_+ - y''_- = 2hy_0''' + \frac{h^3}{3}y_0^{(5)} + O(h^5).
\]

(7)

In addition, Eq. (1) yields:

\[
y''_0 = -gy_0' - f_0y_0,
\]

(8)

\[
y''_+ = -g_+y'_+ - f_+y_+,
\]

(9)

\[
y''_- = -g_-y'_- - f_-y_-.
\]

(10)
Let us consider Eqs. (3)–(10) as a system of eight linear equations for eight unknown quantities: $y_0''$, $y_0''$, $y_0^{(4)}$, $y_0'$, $y_0''$. Solving these equations and substituting the found quantities $y_0''$ and $y_0^{(4)}$ in Eq. (2) we get

$$T_0 y_0 = T_+ y_+ + T_- y_- + R^{(6)}, \quad (11)$$

where

$$T_0 = 2a - \frac{5h^2}{6}b_0 f_0, \quad (12)$$

$$T_\pm = a \pm \frac{h}{24}(10c g_0 + g_+ + g_-) + \frac{h^2}{12}b_\pm f_\pm, \quad (13)$$

$$a = \left(1 + \frac{h}{3}g_+\right)\left(1 - \frac{h}{3}g_-\right) + \frac{h^2}{18}g_0(g_+ + g_-), \quad (14)$$

$$b_0 = \left(1 + \frac{4h}{15}g_+\right)\left(1 - \frac{4h}{15}g_-\right) + \left(\frac{h}{15}\right)^2 g_+ g_-, \quad (15)$$

$$b_\pm = \left(1 \pm \frac{5h}{6}g_0\right)\left(1 + \frac{h}{3}g_\mp\right) + \left(\frac{h}{3}\right)^2 g_0 g_\mp, \quad (16)$$

$$c = \left(1 + \frac{7h}{20}g_+\right)\left(1 - \frac{7h}{20}g_-\right) + \left(\frac{3h}{20}\right)^2 g_+ g_-, \quad (17)$$

$$R^{(6)} = \frac{h^6}{240}(y_0^{(6)} + 3g_0 y_0^{(5)}) + O(h^8). \quad (18)$$

In more detail this result can be obtained by the following way. Making use of Eqs. (8)–(10), we get from Eqs. (7) and (6)

$$y_0''' = g_+ y_- - g_- y_+ - 2 \frac{h^2}{6} y_0^{(5)} + O(h^4), \quad (19)$$

$$y_0^{(4)} = \frac{2(g_0 y_0' + f_0 y_0) - g_+ y_+ - 2 g_- y_- - 2 y_0^{(5)}}{h^2}$$

$$- \frac{h^2}{12} y_0^{(6)} + O(h^4). \quad (20)$$

Substituting these equalities into Eqs. (3)–(5) we obtain

$$y_+ - y_- = 2h y_0 + \frac{h^2}{6}(g_+ y_- + f_- y_- - g_+ y_+ - f_+ y_+)$$

$$- \frac{7h^5}{180} y_0^{(5)} + O(h^7), \quad (21)$$

$$y_+ + y_- = 2y_0' + \frac{h}{2}(g_+ y_- + f_- y_- - g_+ y_+ - f_+ y_+)$$

$$- \frac{h^4}{12} y_0^{(5)} + O(h^6), \quad (22)$$

$$y_+ - y_- = \frac{h}{3}(4 g_0 y_0' + 4 f_0 y_0 + g_+ y_+ + f_+ y_+ + g_- y_- + f_- y_-)$$

$$- \frac{h^5}{90} y_0^{(6)} + O(h^7). \quad (23)$$
It is useful to rewrite Eq. (21) in the form:

\[ y_0' = \frac{y_+ - y_-}{2h} + \frac{h}{12}(g_+y_+ + f_+y_+ - g_-y_- - f_-y_-) \]

\[ + \frac{7h^4}{360}y_0^{(5)} + O(h^6). \]  

(24)

Substitution for this formula into Eqs. (22) and (23) leads to the following system of two equations for quantities \( y'_\pm \)

\[ \alpha_+y'_+ + \alpha_-y'_- = u, \]

\[ \beta_+y'_+ - \beta_-y'_- = v, \]  

(25)

where

\[ \alpha_\pm = 1 \pm \frac{h}{3}g_\pm, \quad \beta_\pm = \alpha_\pm + \frac{h^2}{9}g_0g_\pm, \]  

(27)

\[ u = \frac{1}{h}(y_+ - y_-) + \frac{h}{3}(f_-y_- - f_+y_+) - \frac{2h^4}{45}y_0^{(5)} + O(h^6), \]  

(28)

\[ v = \frac{2}{3}g_0(y_- - y_+) - \frac{h}{3}(4f_0y_0 + f_+y_+ + f_-y_-) \]

\[ - \frac{h^2}{9}g_0(f_-y_- - f_+y_+) - \frac{7h^5}{270}y_0^{(5)} - \frac{h^5}{90}y_0^{(6)} + O(h^7). \]  

(29)

The solution of the system (25), (26) is as follows:

\[ y'_\pm = \frac{\beta_\pm u \pm \alpha_\pm v}{2a}, \]  

(30)

where \( a = \frac{1}{2}(\alpha_+\beta_- + \alpha_-\beta_+) \), that coincides with the definition (14).

Substituting the formulas (30) into right-hand side of Eq. (24) we obtain after some algebra with taking into account Eqs. (27)–(29)

\[ y'_0 = \frac{S_+y_+ - S_-y_- - S_0y_0}{2ah} + R^{(4)}, \]  

(31)

where

\[ S_0 = \frac{h^3}{9}(g_+ + g_-)f_0, \]  

(32)

\[ S_\pm = \left(1 + \frac{5h}{12}g_+\right)\left(1 - \frac{5h}{12}g_-\right) + \left(\frac{h}{12}\right)^2g_+g_- + \frac{h^2}{6}\left(1 \pm \frac{h}{3}g_\pm\right)f_\pm, \]  

(33)

\[ R^{(4)} = \frac{7h^4}{360}y_0^{(5)} + O(h^6). \]  

(34)

Finally, substitution for the found solutions \( y'_\pm, y'_0 \) (Eqs. (30), (31)) into Eqs. (8) and (24) yields the explicit formulas for the quantities \( y''_0 \) and \( y^{(4)}_0 \) in terms of \( y_0, y_\pm \). After substitution for these formulas into Eq. (2) and a series of lengthy but straightforward algebraic transformations we arrive at the result (11)–(18). Omitting the term \( R^{(6)} \) in Eq. (11) we obtain the recurrence three-point formula of the generalized Numerov method for linear
second-order differential equations or, for brevity, of the generalized linear NM (GLNM). Clearly this method reduces to the ordinary NM if \( g(x) = 0 \) in Eq. (1). The local truncation error of the GLNM, which is contained in the term \( R^{(6)} \), is one of the same order \( h^6 \) as the error of the ordinary NM.

The formula (31) enables one to calculate the first derivative if the function \( y(x) \) is known at the grid points. The local truncation error of order \( h^4 \) is determined by the term \( R^{(4)} \). The more precise formula follows immediately from Eq. (23)

\[
y'(x) = \frac{(3 \mp h g(x)) y'(0) \mp h (4g_0 y_0 + 4f_0 y_0 + f_+ y_+ + f_- y_-) \mp 3R^{(5)}}{3 \pm h g(x)},
\]

where

\[
R^{(5)} =\frac{h^5}{90} y_0^{(6)} + O(h^7).
\]

The presence of the derivatives in the right-hand side is a shortcoming of this formula, nevertheless Eq. (35) is practical for the evaluation of \( y'(x) \) at the endpoints of the grid.

### 3 Application to the Hartree-Fock calculations

Consider a general scheme within which the method proposed can be applied to the numerical solution of the HF equations. The HF approximation is a basis of numerous microscopic physical theories describing the quantum many-body systems. In general formulation, the HF method leads to a system of nonlinear integrodifferential equations. We shall consider a special case of the HF equations of motion deduced from the energy functional constructed on the base of the zero-range Skyrme forces \( \mathcal{H} \) which are widely used for the description of atomic nuclei properties (see, for example, Ref. \( [3] \)). The variational principle applied to the Skyrme energy functional leads in the case of spherical nuclei to the following system of equations (in proper units):

\[
z''(x) - \frac{m'_q(x)}{m_q(x)} z'(x) + 2m_q(x)[e_\lambda(x) - V_\lambda(x)] z_\lambda(x) = 0 ,
\]

where \( q \) denotes a sort of nucleon (proton or neutron), the index \( \lambda \) stands for the set of orbital quantum numbers (including \( q \)), \( x \) denotes the radial coordinate, \( z_\lambda(x) \) is the radial wave function, \( e_\lambda \) is the eigenvalue playing the role of single-particle energy, \( V_\lambda(x) \) is the state-dependent mean-field potential, \( m_q(x) \) is the nucleon effective mass.

Comparing Eqs. (1) and (37), we see that they have the same form and would be identical if we put

\[
y(x) = z_\lambda(x), \quad g(x) = -\frac{m'_q(x)}{m_q(x)} , \quad f(x) = 2m_q(x)[e_\lambda(x) - V_\lambda(x)].
\]

The essential difference consists in the following: actually formula (37) stands for the system of \( N \) coupled nonlinear integrodifferential equations because the quantities \( m_q(x) \) and \( V_\lambda(x) \) are functionals of the densities which depend in turn on the set \( \{z_\lambda, z'_\lambda\} \) of all the wave functions and their derivatives with \( \lambda \in \{\lambda_1, \ldots, \lambda_N\} \) (see \( [3] \)). In practice, the system of equations (37) is solved by making use of some iteration procedure. The convergence is
achieved by averaging of the densities calculated on two successive iterations. The description and the analysis of the procedure in more detail are outside the scope of the present paper (see, e. g., Ref. [3], and references therein where some relevant methods are discussed). Here it is important only that on each fixed HF iteration one has to solve the set of \( N \) uncoupled linear differential equations which have the same form (37) but with already known functions \( m_q(x) \) and \( V_{\lambda}(x) \) determined by the results of previous iterations.

The numerical integration of Eq. (37) in this case can be performed by means of the GLNM described above. For the sake of simplicity it is convenient to come back to the notations of the preceding section taking into account Eqs. (38). Setting

\[
Y_{\text{out}}^0 = y_0 / y_+, \quad Y_{\text{out}}^+ = y_- / y_0, \quad (39)
\]

we obtain the following recurrence relations from Eq. (11) (omitting the term \( R^{(6)} \)):

\[
Y_{\text{out}}^0 = T_+/ (T_0 - T_- Y_{\text{out}}^-), \quad (41)
\]

\[
Y_{\text{in}}^0 = T_- / (T_0 - T_+ Y_{\text{in}}^+). \quad (42)
\]

Note that these transformations of Eq. (11) are similar but not identical to ones of the renormalized Numerov method developed in Ref. [3].

In the proposed scheme Eqs. (41) and (42) are used for the outward and the inward integrations, respectively. The outward integration starts from a point near \( x = 0 \). The initial value of \( Y_{\text{out}}^0 \) in Eq. (11) is calculated using analytic expansions of the regular solutions \( z_{\lambda}(x) \) about \( x = 0 \). To improve the accuracy of calculations it is practical to decrease the step length of the grid near this point. The inward integration starts from an outside endpoint of the grid where the irregular solutions of Eq. (37) are known analytically. The initial value of \( Y_{\text{in}}^+ \) in Eq. (12) is calculated as the ratio of the Whittaker functions for protons and of the spherical Hankel ones for neutrons. The eigenvalue \( e_{\lambda} \) is found from the condition \( Y_{\text{out}}^0 = 1 / Y_{\text{in}}^0 \) at some matching point \( x_0 = x_m \). The reasonable choice for this point is (see, e. g., Ref. [4]) the approximate position of the last extremum of the wave function \( z_{\lambda}(x) \). In the end of this procedure, which is performed for each \( z_{\lambda}(x) \) separately, the function \( z_{\lambda}(x) \) is calculated at the grid points using the ratios \( Y_{\text{out}}^0, Y_{\text{in}}^0 \), and the normalization condition:

\[
\int_0^\infty dx z_{\lambda}^2(x) = 1. \quad (43)
\]

Finally, the derivatives \( z'_{\lambda}(x) \) are calculated employing Eq. (31) at the inside points of the grid and Eq. (35) at the endpoints. After this, new approximations to the functions \( m_q(x), V_{\lambda}(x) \), which are used in the next HF iteration, are calculated.

The algorithm, that was briefly outlined above, has been realized in the computer code [7] intended for the Skyrme-Hartree-Fock calculations. The convergence and stability of the procedure described were tested in the calculations of ground-state properties of all doubly magic atomic nuclei using most of the present Skyrme-force parametrizations. It was obtained that the algorithm based on the GLNM reproduce the known reference results within their accuracy.
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