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A New Runge-Kutta-Nyström Method With Phase-Lag of Order Infinity for the Numerical Solution of the Schrödinger Equation

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Abstract

In this paper a new approach for constructing efficient Runge-Kutta-Nyström methods is introduced. Based on this approach a new Runge-Kutta-Nyström fourth algebraic order method is developed for the numerical solution of the Schrödinger equation. The new method has phase-lag of order infinity and extended interval of periodicity. Numerical illustrations using the radial Schrödinger equation indicate that the new method is more efficient than older ones.
Keywords: Runge-Kutta-Nyström methods, radial Schrödinger equation, resonance problems, scattering problems, phase shift problems, phase-lag, oscillating solutions.

1 Introduction

In this paper we study a special Runge-Kutta-Nystrom (RKN) method of Fehlberg for the integration of system of ODEs of the form

$$\frac{d^k u(t)}{dt^k} = f\left(t, u(t)\right), \ k = 1, 2 \tag{1}$$

for which it is known in advance that their solution is oscillatory. The study of such systems begins with the test equation

$$\frac{d^k u(t)}{dt^k} = (iv)^k u(t) + c \exp\left(iv_f t\right), \ k = 1, 2, \tag{2}$$

where c,v and v_f are real constants. In the case $k = 1$, van der Houwen and Sommeijer [1] proposed second-order m-stage Runge-Kutta and Runge-Kutta-Nyström methods with $m = 4, 5, 6$ and phase-lag order $q = 6, 8, 10$, respectively. They also derived some third-order methods with phase-lag order 6,8,10. Finally, they derived some specific fourth order Runge-Kutta-Nyström methods. The disadvantage of these methods is the slow convergence, and their inefficiency, especially in the case of forced oscillating solutions. For the case $k = 2$ there is an extensive literature (see [2], [3] - [36]). However, it is worth elaborating a bit more on the theory underlying these methods, especially in the light of the new accurate methods to be presented in this paper. When a numerical method is applied to the test equation (2), a numerical approximation u_n of the exact solution $u(t_n)$ is obtained, where n is an integer and gives the actual step number and $t_n = t_0 + n\,h$ (where t_0 is the initial point of integration and h is the stepsize of integration). This approximation is of the form

$$u_n = \sum_{j=1}^{s} k_j \left[\rho_j\left(vh\right)\right]^n + ch^k A_n\left(vh, v_f h\right) \exp\left(iv_f nh\right), \tag{3}$$

where s is the number of distinct roots of the characteristic polynomial of the method, ρ_j are the s distinct roots of the characteristic polynomial of the method, and k_j are the constants determined by the initial conditions.
The functions ρ_j^n and $ch^k A_n\left(vh, v_f h\right) \exp\left(iv_f nh\right)$ are called the homogeneous and inhomogeneous components of the numerical solution (3), respectively.
On the other hand, the exact solution of (2) is given by

$$u(t) = \sigma_1 \exp\left(ivt\right) + \sigma_2 \exp\left(-ivt\right) + \frac{c \exp\left(iv_f t\right)}{\left(iv_f\right)^k - \left(iv\right)^k}, \tag{4}$$

where σ_1 and σ_2 are constants with $\sigma_2 = 0$ when $k = 1$.
The functions $\exp\left(\pm ivt\right)$ and $ch^k A_e \exp\left(iv_f t\right)$ are called the homogeneous and inhomogeneous components of the exact solution, respectively, where $A_e = 1/\left[\left(iv_f h\right)^k - \left(ivh\right)^k\right]$.

In the phase analysis of the homogeneous components of (3) and (4) we have to compare the arguments (or phases) of $\exp(\pm iv t)$ with the arguments of the principal characteristic roots the set $\{\rho_1, \rho_2, ..., \rho_s\}$. These phase errors are time-dependent and therefore accumulate as n increases.

In the phase analysis of the inhomogeneous components of (3) and (4), we have to compare the phases of A_n and A_e. These phase errors are constant in time. For this reason our study will be confined in minimizing the phase errors of the homogeneous components.

The purpose of this paper is to construct a four-stage RKN method of Fehlberg of fourth algebraic order with phase-lag of order infinity. Since our study is confined the homogeneous phase errors, we will use as test equation

$$\frac{d^2u(t)}{dt^2} = -v^2 u(t) \tag{5}$$

2 Phase-lag analysis of RKN methods and periodicity interval

The general m-stage method for the equation ($k = 2$)

$$\frac{d^2u(t)}{dt^2} = f(t, u(t)) \tag{6}$$

is of the form

$$\begin{aligned}
t_{n+1} &= t_n + h \\
u_n^{(0)} &= u_{n-1} \\
u_n^{(i)} &= u_{n-1} + a_i h \dot{u}_{n-1} + h^2 \sum_{j=0}^{i-1} \gamma_{i,j} f\left(t_{n-1} + a_j h, u_n^{(j)}\right), \ i = 0..m-1, \\
\dot{u}_n &= \dot{u}_{n-1} + h \sum_{j=0}^{m-1} \dot{c}_j f\left(t_{n-1} + a_j h, u_n^{(j)}\right), \\
u_n &= u_{n-1} + h \dot{u}_{n-1} + h^2 \sum_{j=0}^{m-1} c_j f\left(t_{n-1} + a_j h, u_n^{(j)}\right)
\end{aligned} \tag{7}$$

where $a_0 = 0$.

By applying the general method (7) to the test equation (5) we obtain the numerical solution

$$\begin{bmatrix} u_n \\ h\dot{u}_n \end{bmatrix} = D^n \begin{bmatrix} u_0 \\ h\dot{u}_n \end{bmatrix}, \ D = \begin{bmatrix} A(z^2) & B(z^2) \\ A'(z^2) & B'(z^2) \end{bmatrix}, \quad z = vh, \tag{8}$$

where A, A', B, B' are polynomials in z^2, completely determined by the parameters of the method (7).

The analytical solution of (5) is given by

$$u(t_n) = \sigma_1 [\exp(iv)]^n + \sigma_2 [\exp(-iv)]^n, \tag{9}$$

where $\sigma_{1,2} = \frac{1}{2}\left[u_0 \mp \left(i\dot{u}_0\right)/v\right]$ or $\sigma_{1,2} = |\sigma| \exp\left(\pm i\chi\right)$, where $|\sigma| = |\sigma_1| = |\sigma_2|$. Substituting in (9), we have

$$u(t_n) = 2\,|\sigma| \cos\left(\chi + nv\right). \tag{10}$$

Now let us assume that the eigenvalues of D are ρ_1, ρ_2 and the corresponding eigenvectors are $[1, v_1]^T$, $[1, v_2]^T$, $v_i = A'/\left(\rho_i - B'\right), i = 1, 2$. The solution of (8) is

$$u_n = c_1\rho_1^n + c_2\rho_2^n, \tag{11}$$

where

$$c_1 = -\frac{v_2u_0 - h\dot{u}_0}{v_1 - v_2}, c_2 = \frac{v_1u_0 - h\dot{u}_0}{v_1 - v_2} \tag{12}$$

If ρ_1, ρ_2 are complex conjugate, then $c_{1,2} = |c| \exp\left(\pm iw\right)$ and $\rho_{1,2} = |\rho| \exp\left(\pm ip\right)$, where w and p are the frequencies of the solution of the test equation. By substituting in (11), we have

$$u_n = 2\,|c|\,|\rho|^n \cos\left(w + np\right). \tag{13}$$

Eqs. (10) and (13) lead us to the following definition.

Definition 1 *(Phase-lag) Apply the RKN method (7) to (5). We define the phase-lag* $\Phi\left(z\right) = z - p$. *If* $\Phi\left(z\right) = O\left(z^{q+1}\right)$, *then the RKN method is said to have phase-lag order* q.

Additionally, the quantity $a\left(z\right) = 1 - |\rho|$ is called the *amplification error.*
Let us denote

$$R\left(z^2\right) = A\left(z^2\right) + B'\left(z^2\right) \text{ and } Q\left(z^2\right) = A\left(z^2\right)B'\left(z^2\right) - A'\left(z^2\right)B\left(z^2\right). \tag{14}$$

where $z = vh$. ¿From Definition 1 it follows that

$$\Phi\left(z\right) = z - \arccos\left(\frac{R\left(z^2\right)}{2\sqrt{Q\left(z^2\right)}}\right), |\rho| = \sqrt{Q\left(z^2\right)}. \tag{15}$$

If at a point $z, a(z) = 0$, then the RKN method has zero dissipation at this point. Thus we arrive at the following useful definition.

Definition 2 *(Interval of periodicity) The interval of periodicity is the interval* $z^2 \in [0, \gamma^2]$ *on which* $\left|\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right| \leq 1$ *or* $R^2 \leq 4\,|Q|$.

3 The New Method

In the following we shall derive a special four-stage fourth-order accurate Runge-Kutta-Nyström Fehlberg method with phase-lag of order infinity. Let us represent the general m-stage RKN method with the array given in Table 1. The parameters above must satisfy

0					
a_1	γ_{10}				
a_2	γ_{20}	γ_{21}			
$\vdots$	$\vdots$	$\vdots$			
a_{m-1}	$\gamma_{m-1,0}$	$\gamma_{m-1,1}$	$\cdots$	$\gamma_{m-1,m-2}$	
	c_0	c_1	$\cdots$	c_{m-2}	c_{m-1}
	$\dot{c}_0$	$\dot{c}_1$	$\cdots$	$\dot{c}_{m-2}$	$\dot{c}_{m-1}$

Table 1: m-stage explicit Runge-Kutta-Nyström method

the following relations in order to obtain fourth-order accuracy: (See [38])

$$\begin{aligned}
c_0 + c_1 + c_2 + c_3 &= \frac{1}{2} \\
c_1 a_1 + c_2 a_2 + c_3 a_3 &= \frac{1}{6}, \\
c_1 a_1^2 + c_2 a_2^2 + c_3 a_3^2 &= \frac{1}{12}, \\
c_1 \gamma_{10} + c_2(\gamma_{20} + \gamma_{21}) + c_3(\gamma_{30} + \gamma_{31} + \gamma_{32}) &= \frac{1}{24} \\
\dot{c}_0 + \dot{c}_1 + \dot{c}_2 + \dot{c}_3 &= 1, \\
\dot{c}_1 a_1 + \dot{c}_2 a_2 + \dot{c}_3 a_3 &= \frac{1}{2}, \\
\dot{c}_1 a_1^2 + \dot{c}_2 a_2^2 + \dot{c}_3 a_3^2 &= \frac{1}{3}, \\
\dot{c}_1 \gamma_{10} + \dot{c}_2(\gamma_{20} + \gamma_{21}) + \dot{c}_3(\gamma_{30} + \gamma_{31} + \gamma_{32}) &= \frac{1}{6} \\
\dot{c}_1 a_1^3 + \dot{c}_2 a_2^3 + \dot{c}_3 a_3^3 &= \frac{1}{4}, \\
\dot{c}_1 a_1 \gamma_{10} + \dot{c}_2 a_2(\gamma_{20} + \gamma_{21}) + \dot{c}_3 a_3(\gamma_{30} + \gamma_{31} + \gamma_{32}) &= \frac{1}{8} \\
\dot{c}_2 a_1 \gamma_{2,1} + \dot{c}_3(a_1 \gamma_{31} + a_2 \gamma_{32}) &= \frac{1}{24}
\end{aligned} \tag{16}$$

In order to simplify the order relations Fehlberg has added the following relations

$$\begin{aligned}
\gamma_{10} &= \frac{1}{2} a_1^2 \\
\gamma_{20} + \gamma_{21} &= \frac{1}{2} a_2^2 \\
\gamma_{30} + \gamma_{31} + \gamma_{32} &= \frac{1}{2} a_3^2
\end{aligned} \tag{17}$$

We look for a solution with

$$a_1 = \frac{1}{3},\ a_2 = \frac{2}{3},\ a_3 = 1 \tag{18}$$

and then satisfying the order relations (16), and simplifying conditions (17) the following values of coefficients are obtained:

$$c_0 = \frac{13}{120},\ c_1 = \frac{3}{10},\ c_2 = \frac{3}{40},\ c_3 = \frac{1}{60},$$

$$\dot{c}_0 = \frac{1}{8},\ \dot{c}_1 = \frac{3}{8},\ \dot{c}_2 = \frac{3}{8},\ \dot{c}_3 = \frac{1}{8} \tag{19}$$
$$\gamma_{10} = \frac{1}{18},\ \gamma_{20} = 0,\ \gamma_{21} = \frac{2}{9}$$
$$\gamma_{30} = \frac{1}{6} + \gamma_{32},\ \gamma_{31} = \frac{1}{3} - 2\gamma_{32}.$$

Applying the obtained method to the scalar test equation (5), the following expressions for the polynomials A, B, A' and B' are obtained :

$$\begin{aligned}
A\left(z^2\right) &= 1 - \frac{1}{2}z^2 + \frac{1}{24}z^4 - \left(\frac{1}{810} + \frac{1}{540}\gamma_{32}\right)z^6 + \frac{1}{4860}\gamma_{32}z^8 \\
B\left(z^2\right) &= 1 - \frac{1}{6}z^2 + \frac{1}{135}z^4 - \frac{1}{810}\gamma_{32}z^6 \\
A'\left(z^2\right) &= -z^2 + \frac{1}{6}z^4 - \left(\frac{1}{144} + \frac{1}{72}\gamma_{32}\right)z^6 + \frac{1}{648}\gamma_{32}z^8 \\
B'\left(z^2\right) &= 1 - \frac{1}{2}z^2 + \frac{1}{24}z^4 - \frac{1}{108}\gamma_{32}z^6
\end{aligned} \tag{20}$$

Using (14) we have

$$\begin{aligned}
R\left(z^2\right) &= 2 - z^2 + \frac{1}{12}z^4 - \left(\frac{1}{810} + \frac{1}{90}\gamma_{32}\right)z^6 + \frac{1}{4860}\gamma_{32}z^8 \\
Q\left(z^2\right) &= 1 - \left(\frac{1}{1296} - \frac{1}{360}\gamma_{32}\right)z^6 - \left(\frac{1}{25920} - \frac{13}{19440}\gamma_{32}\right)z^8
\end{aligned} \tag{21}$$

In order that the method has phase-lag of order infinity, the following relation must hold:

$$\Phi(z) = z - arccos\left(\frac{R\left(z^2\right)}{2\sqrt{Q\left(z^2\right)}}\right) \Rightarrow R\left(z^2\right)^2 = 4cos(z)^2 Q\left(z^2\right) \tag{22}$$

Solving the above equation (22) we obtain:

$$\gamma_{32} = \frac{p - 54\sqrt{q}}{(z^4 - 108z^2 + 2916)z^6} \tag{23}$$

where

$$p = 12z^8 - 1458z^6 + 53460z^4 + 63180z^2\cos^2 z - 544320z^2 + 262440\cos^2 z + 1049760 \tag{24}$$

and

$$\begin{aligned}
q = &-64800z^8\cos^2 z + 1762560z^6 cos^2 z + 566870400\cos^2 z + 960z^{10}\cos^2 z \\
&+1368900z^4\cos^4 z + 11372400z^2 cos^4 z - 5z^{12}\cos^2 z + 23619600\cos^4 z \\
&-66484800z^2\cos^2 z - 13834800z^4\cos^2 z
\end{aligned} \tag{25}$$

For small values of z the above formulae are subject to heavy cancelations. In this case the following Taylor series expansions must be used.

$$\begin{aligned}
\gamma_{32} = \frac{1}{6} &- \frac{11}{630}z^2 + \frac{11}{4536}z^4 - \frac{8111}{22453200}z^6 + \frac{9374737}{183891708000}z^8 \\
&- \frac{122866049}{16550253720000}z^{10} + \frac{8829131489}{8440629397200000}z^{12} \\
&- \frac{2164252382659}{14433476269212000000}z^{14} + \ldots
\end{aligned} \tag{26}$$

Applying definition 2 to the new method we see that the interval of periodicity of the new method is equal to $(0, \infty) - S$ where S is a set of distinct points plus the interval $(2.8, 3.2)$. The internal interval $(2.8, 3.2)$ is excluded since there $q^2 < 0$ and the interval of periodicity is undefined. In Figure 1 (a) we present the stability function $ST = R^2 - 4|Q|$. In Figure 1 (b) we present a part of the stability function in which it is obvious that in the interval $(2.8, 3.2)$ we haven't values of stability polynomial since $q^2 < 0$.

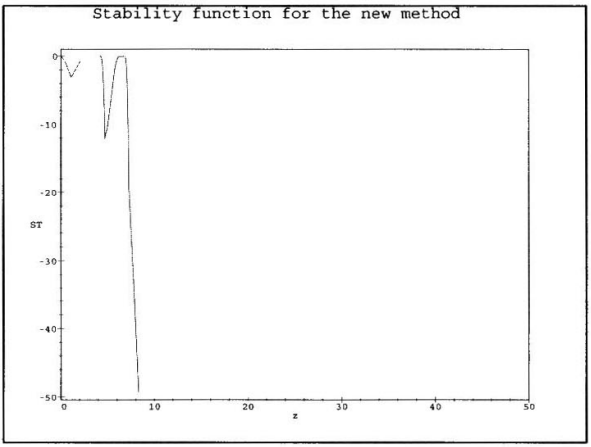

Figure 1: (a) Stability function $ST = R^2 - 4|Q|$.

4 Numerical Illustrations

In order to test the efficiency of the new method some illustrations are presented. Consider the numerical integration of the Schrödinger equation

$$y''(x) = [l(l+1)/x^2 + V(x) - k^2]y(x). \tag{27}$$

Equations of this type occur very frequently in theoretical physics and quantum chemistry (see for example [7], [8], [15],[28]), and it is needed to be able to solve them efficiently and reliably by numerical methods. In (27) the function $W(x) = l(l+1)/x^2 + V(x)$ denotes *the effective potential*, which satisfies $W(x) \to 0$ as $x \to \infty$, k^2 is a real number denoting *the*

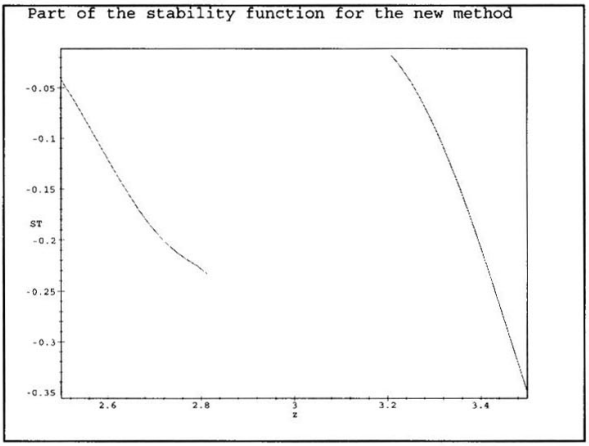

Figure 1: (b) Part of the stability function $ST = R^2 - 4|Q|$.

energy, l is a given integer, related to the angular momentum and V is a given function representing the potential. The boundary conditions are:

$$y(0) = 0 \tag{28}$$

and a second boundary condition, for large values of x, determined by physical considerations.

A fruitful way for developing efficient methods for the solution of (27) is to use exponential fitting. Many authors have contributed to this area (see [20], [8], [26], [17], [23], [16], [18], [24], [21], [4],[33])

In the asymptotic region the equation (27) effectively reduces to

$$y''(x) + (k^2 - \frac{l(l+1)}{x^2})y(x) = 0, \tag{29}$$

for x greater than some value X, where X defines the asymptotic region.

The above equation has linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$, where $j_l(kx), n_l(kx)$ are the **spherical Bessel and Neumann functions** respectively. Thus the solution of equation (1) has the asymptotic form (when $x \to \infty$)

$$\begin{aligned} y(x) &\sim Akxj_l(kx) - Bn_l(kx) \\ &\sim D[\sin(kx - \pi l/2) + \tan\delta_l \cos(kx - \pi l/2)] \end{aligned} \tag{30}$$

where δ_l is the **phase shift** which may be calculated from the formula

$$\tan \delta_l = \frac{y(x_i)S(x_{i+1}) - y(x_{i+1})S(x_i)}{y(x_{i+1})C(x_i) - y(x_i)C(x_{i+1})} \tag{31}$$

for x_i and x_{i+1} distinct points on the asymptotic region (for which we have that x_{i+1} is the right hand end point of the interval of integration and $x_i = x_{i+1} - h$, h is the stepsize) with $S(x) = kxj_l(kx)$ and $C(x) = kxn_l(kx)$.
We evaluate the phase shift δ_l from the above relation at x_i in the asymptotic region.

4.1 The Woods-Saxon Potential

As a test for the accuracy of our methods we consider the numerical integration of the Schrödinger equation (27) with $l = 0$ in the case where $V(x)$ is the Woods-Saxon potential :

$$V(x) = V_W(x) = \frac{u_0}{(1+z)} - \frac{u_0 z}{a(1+z)^2} \tag{32}$$

with $z = \exp[(x - R_0)/a]$, $u_0 = -50$, $a = 0.6$ and $R_0 = 7.0$.
For positive energies one has the so-called resonance problem. This problem consists either of finding the **phase shift** $\delta(E) = \delta_l$ or finding those $E \in [1, 1000]$, at which δ equals $\pi/2$. We actually solve the latter problem, using the technique fully described in [1], when *the positive eigenenergies lie under the potential barrier*.
The boundary conditions for this problem are:

$$\begin{aligned} y(0) &= 0, \\ y(x) &\sim \cos[\sqrt{E}x] \text{ for large } x. \end{aligned}$$

The domain of numerical integration is [0, 15].
For comparison purposes in our numerical illustration we use the Numerov's method (labeled as Method [a]), the method of Raptis and Allison [20] (labeled as Method [b]), the Runge-Kutta fourth algebraic order method developed by Houwen et. al. in [1] (labeled as Method [c]), the classical Runge-Kutta-Nystrom fourth algebraic order method [37] (labeled as Method [d]) and the new method (labeled as Method [e]).
The numerical results, which obtained using these three methods, with stepsizes $h = \frac{1}{2^m}, m = 3, 4, 5$, were compared with the analytic solution of the Woods-Saxon potential resonance problem, rounded to six decimal places. Figure 2 shows the errors $Err = log_{10}|E_{calculated} - E_{analytical}|$ for the highest eigenenergy $E_3 = 989.701916$ using several values of m.
The performance of the present method is dependent on the choice of the fitting parameter v. For the purpose of obtaining our numerical results it is appropriate to choose v in the way suggested by Ixaru and Rizea [8]. That is, we choose:

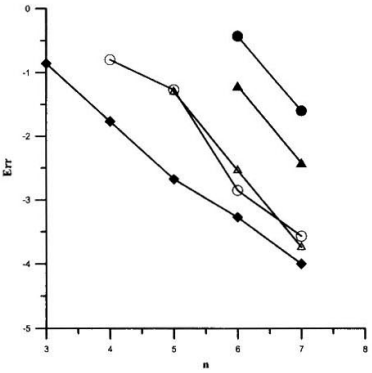

Figure 2: Values of Err for several values of n for the resonance E=989.701916. The nonexistance of the values of Err for the Methods [a-d] indicates that the values of Err are positive.
Method [a]
Method [b]
Method [c]
Method [d]
Method [e]

$$v = \begin{cases} (-50 - E)^{1/2} & \text{for } x \in [0, 6.5] \\ (-E)^{1/2} & \text{for } x \in (6.5, 15] \end{cases} \tag{33}$$

For a discussion of the reasons for choosing the values 50 and 6.5 and the extent to which the results obtained depend on these values see [8](pp. 25). We note here that we have defined in eq. (2) v as a real constant. It is obvious that eq. (2) is a test equation. In the real problems (as in the case of the Schrödinger equation), the parameter v is not a constant in the whole interval but only in subintervals. So, with the procedure presented above we have divided the interval of integration in two subintervals. In these subintervals v is a constant.

4.2 Modified Woods-Saxon Potential

A second example of this method is illustrated by solving a similar problem using the modified Woods-Saxon potential, given by

$$V(x) = V_W(x) + \frac{D}{x} \tag{34}$$

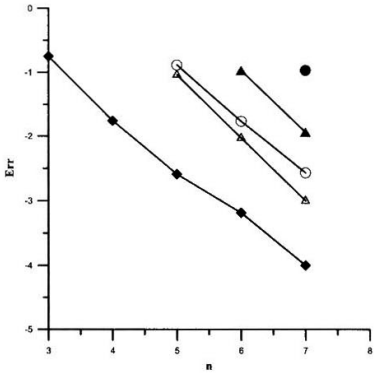

Figure 3:Values of Err for several values of n for the resonance E=1002.768.393. The nonexistance of the values of Err for the Methods |a-d| indicates that the values of Err are positive.

Method |a|
Method |b|
Method |c|
Method |d|
Method |e|

where V_W is the Woods-Saxon potential (32). For the purpose of our numerical experiments we use the same parameters as in [8], i.e. $D = 20$, $l = 2$. In Figure 3 results are shown for $Err = log_{10}|E_{calculated} - E_{analytical}|$ of the highest eigenenergy $E_3 = 1002.768393$, for several values of m.

Since $V(x)$ is singular at the origin, we use the special strategy of [8]. We start the integration from a point $\epsilon > 0$ and the initial values $y(\epsilon)$ and $y(\epsilon + h)$ for the integration scheme are obtained using a perturbative method (see [7]). As in [8] we use the value $\epsilon = \frac{1}{4}$ for our numerical experiments.

For the purpose of obtaining our numerical results it is appropriate to choose v in the way suggested by Ixaru and Rizea [8]. That is, we choose:

$$v = \begin{cases} \frac{[V(a_1)+V(\epsilon)]}{2} \text{ for } x \in [\epsilon, a_1] \\ \frac{V(a_1)}{2} \text{ for } x \in (a_1, a_2] \\ V(a_3) \text{ for } x \in (a_2, a_3] \\ V(15) \text{ for } x \in (a_3, 15]. \end{cases}$$

where a_i, $i = 1, 2, 3$ are fully defined in [8]. Based on the the procedure presented for the Woods-Saxon potential we have divided the interval of integration in four subintervals. In these subintervals v is a constant.
In all cases considered, the new method developed in this paper is more accurate than the other well known ones.

5 Conclusions

A new approach for constructing efficient Runge-Kutta-Nyström methods is introduced in this paper. Using this new approach we can construct Runge-Kutta-Nyström methods which phae-lag of order infinity . A Runge-Kutta-Nyström fourth algebraic order method with phase-lag of order infinity is thus obtained. Numerical and theoretical results show that this method is much more accurate than the similar well known methods. We note here that the method needs the knowledge of the frequency of the problem v. So, the method is appropriate for the problems for which the frequency is known or approximately known.
All computations were carried out on a IBM PC-AT compatible 80486 using double precision arithmetic with 16 significant digits accuracy (IEEE standard).

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