# An Exponentially Fitted Method for the Numerical Solution of the Schrödinger Equation†

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We present here a new method for the numerical integration of the radial Schrödinger eq. The formula considered contains free parameters which are defined in order to integrate exponential functions. Numerical results also indicate that the new methods are much more accurate than other Numerov-type methods.

## 1. INTRODUCTION

In many scientific areas there is a real need for the numerical solution of the Schrödinger eq. Some of these areas include nuclear physics, physical chemistry, theoretical physics, and chemistry (see refs 1 and 2).

The one dimensional Schrödinger eq has the form

$$y''(x) = [l(l+1)/x^2 + V(x) - k^2]y(x) \qquad (1.1)$$

where $k^2$ is a real number denoting *the energy*, $l$ is an integer, and $V$ is *the potential*. The function $W(x) = l(l+1)/x^2 + V(x)$ denotes *the effective potential*, which satisfies $W(x) \rightarrow 0$ as $x \rightarrow \infty$. The boundary conditions are

$$y(0) = 0 \qquad (1.2)$$

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

Boundary value methods based on either collocation or finite differences are not very popular for the solution of (1.1) due to the fact that the problem is posed on an infinite interval. Initial value methods, such as shooting, also need to take into account the fact that $|y'(x)|$ may be very large near $x = 0$. The aim of this paper is to derive more efficient integrators to solve eq 1 in a shooting approach.

One of the most popular methods for the solution of (1.1) is Numerov's method. This method is only of order four, but in practice it has been found to have a superior performance to certain higher order four-step methods. (We mention here that the Cashion's version of the Numerov−Cooley method[3] gives more accurate results than the classical Numerov's method.) The reason for this, as proved in ref 4, is that the Numerov method has the same phase-lag order as the four-step methods, but it has a larger interval of periodicity. Another disadvantage of the four-step methods is that with these methods we need more starting values. These reasons suggest that the investigation of linear multistep methods is not a fruitful way of deriving efficient high order methods. We note here that when we apply the technique of the Richardson extrapolation to any method we can have more accurate results.

An alternative approach to deriving higher order methods for (1.1) was given by Cash and Raptis.[5] In ref 5, a sixth order Runge−Kutta type method with a large interval of periodicity was derived. This method has a phase-lag of order six (while Numerov's method has phase-lag of order four) and a much larger interval of periodicity than the method of Numerov. More recently Simos[6] has derived a sixth order method with phase-lag of order eight and with a large interval of periodicity.

Another approach for developing efficient methods for the solution of (1.1) is to use exponential fitting. Raptis and Allison[7] have derived a Numerov type exponentially fitted method. Numerical results presented in ref 7 indicate that these fitted methods are much more efficient than Numerov's method for the solution of (1.1). Many authors have investigated the idea of exponential fitting, since Raptis and Allison. Perhaps the most significant work in this general area was that of Ixaru and Rizea.[8] They showed that for the resonance problem defined by (1.1) it is generally more efficient to derive methods which exactly integrate functions of the form

$$\{1,x,x^2,...,x^p, \exp(\pm\upsilon x), x\exp(\pm\upsilon x),...,x^m\exp(\pm\upsilon x)\} \qquad (1.3)$$

where $\upsilon$ is the frequency of the problem than to use classical exponential fitting methods. From the error analysis developed in ref 9, the main reason for this is that, when the classical exponential fitting methods are applied to Schrödinger's eq, the leading coefficients in the asymptotic expansion of their local truncation errors depend on the energy $k^2$. For many problems of interest, these leading coefficients are large in modulus. For the method obtained by Ixaru and Rizea[8] we have $m = 1$ and $p = 1$. A powerful low order method of this type (with $m = 2$ and $p = 0$) was developed by Raptis.[10] Simos[11] has derived a four-step method of this type which integrates more exponential functions and gives much more accurate results than the four-step methods of Raptis.[12,13] For this method we have $m = 3$ and $p = 0$. Simos[14] has derived a family of four-step methods which give more efficient results than other four-step methods. In particular, he has derived methods with $m = 0$ and $p = 5$, $m = 1$ and $p = 3$, $m = 2$ and $p = 1$, and finally $m = 3$ and $p = 0$. Also Raptis and Cash[15] have derived a two-step method fitted to (1.3) with $m = 0$ and $p$

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= 5 based on the well-known Runge−Kutta-type sixth order formula of Cash and Raptis.[5] The method of Cash, Raptis, and Simos[16] is also based on the formula proposed in ref 5 and is fitted to (1.3) with $m = 1$ and $p = 3$.

The purpose of this paper is to develop a simple and accurate exponentially fitted numerical method for the solution of the radial Schrödinger eq. The new method has a phase-lag of order infinity (phase-fitted) and is almost P-stable. We have applied the new method to *the resonance problem* (which arises from the one-dimensional Schrödinger eq) with two different types of potential. Note that *the resonance problem* is one of the most difficult to solve of all the problems based on the one-dimensional Schrödinger eq, because it has highly oscillatory solutions, especially for large resonances (see section 4).

## 2. THE NEW METHOD

Consider the method

$$\bar{y}_n = y_n - ah^2(y''_{n+1} - 2y''_n + y''_{n-1}) \tag{2.1}$$

$$\bar{y}_n = y_n - bh^2(y''_{n+1} - 2\bar{y}''_n + y''_{n-1}) \tag{2.2}$$

$$y_{n+1} + a_1 y_n + y_{n-1} = h^2[b_0(y''_{n+1} + y''_{n-1}) + b_1\bar{y}''_n] \tag{2.3}$$

where, for example, $y''_{n+1} = f(x_{n+1})y_{n+1}$ with $x_{n+1} = x_n + h$, $f(x_{n+1}) = l(l+1)/x^2_{n+1} + V(x_{n+1}) - k^2$.

We have chosen to consider this family of methods, because it has five free parameters. This is sufficient to allow the construction of methods which integrate more exponential functions than the analogous Numerov-type method, with algebraic order four, proposed by Raptis.[10]

We require that the family of methods 2.1−2.3 should integrate exactly any linear combination of the functions

$$\{\exp(\pm\upsilon x), x\exp(\pm\upsilon x), x^2\exp(\pm\upsilon x), x^3\exp(\pm\upsilon x), x^4\exp(\pm\upsilon x)\} \tag{2.4}$$

To construct a method of the form 2.1−2.3 which integrates exactly the functions 2.4, we require that the method 2.1−2.3 integrates exactly (see refs 4 and 17)

$$\{1, x, \exp(\pm\upsilon_0 x), \exp(\pm\upsilon_1 x), \exp(\pm\upsilon_2 x), \exp(\pm\upsilon_3 x), \exp(\pm\upsilon_3 x), \exp(\pm\upsilon_4 x)\} \tag{2.5}$$

and then put

$$\upsilon_0 = \upsilon_1 = \upsilon_2 = \upsilon_3 = \upsilon_4 = \upsilon \tag{2.6}$$

Demanding that (2.1−2.3) integrate (2.5) exactly, we obtain the following system of equations for $b_0$, $b_1$, $a$, and $a_1$

$$-a_1 + 2b_0 w_j^2 \cosh(w_j) + b_1 w_j^2 + 2bb_1 w_j^4[1 - \cosh(w_j)] + 4abb_1 w^6[1 - \cosh(w_j)] = 2\cosh(w_j) \tag{2.7}$$

where $w_j = \upsilon_j h$, $j = 0(1)4$.

Solving for $b_i$, $i = 0, 1$, for $a$, $b$, and $a_1$ and requiring the satisfaction of (2.6) we obtain

$$a_1 = \frac{2T_0}{Denom_1}, \quad b_0 = \frac{3T_1}{-w^2 Denom_1}$$

$$b_1 = \frac{6T_2}{-w^2 Denom_1}, \quad b = \frac{T_3}{2wT_2}, \quad a = \frac{T_4}{-6w^3 T_3} \tag{2.8}$$

where

$$T_0 = 12w(9 - w^2)\cosh(4w) + 12w(9 + 2w^2)\sinh(4w) + w(w^4 - 171w^2 + 171)\cosh(3w) + 3(5w^4 + 142w^2 - 144)\sinh(3w) - 2w(w^4 + 363w^2 + 603)\cosh(2w) + 6(5w^4 + 6w^2 + 108)\sinh(2w) + w(59w^4 + 807w^2 + 1557)\cosh(w) + 3(85w^4 - 482w^2 - 144)\sinh(w) + 2w(7w^4 - 652w^2 - 315)$$

$$Denom_1 = w(w^4 + 93w^2 + 387)\cosh(3w) + 3(5w^4 + 94w^2 + 72)\sinh(3w) - 2w(w^4 - 171w^2 + 171)\cosh(2w) + 6(5w^4 + 142w^2 - 144)\sinh(2w) + w(59w^4 - 225w^2 - 2115)\cosh(w) + 15(17w^4 - 170w^2 + 72)\sinh(w) + 2w(7w^4 - 105w^2 + 1035)$$

$$T_1 = w(w^4 + 37w^2 - 105)\cosh(3w) + (11w^4 + 6w^2 - 120)\sinh(3w) - 2w(w^4 - 51w^2 + 15)\cosh(2w) + 2(11w^4 - 138w^2 + 240)\sinh(2w) + w(59w^4 - 9w^2 + 1065)\cosh(w) + (187w^4 + 534w^2 - 600)\sinh(w) + 2w(7w^4 - 65w^2 - 465)$$

$$T_2 = -4w(15 + w^2)\cosh(4w) - 12(5 + 2w^2)\sinh(4w) + w(w^4 - 51w^2 + 15)\cosh(3w) + (11w^4 - 138w^2 + 240)\sinh(3w) - 2w(w^4 - 115w^2 - 225)\cosh(2w) + 2(11w^4 + 270w^2 - 180)\sinh(2w) + w(59w^4 + 335w^2 - 975)\cosh(w) + (187w^4 - 570w^2 + 240)\sinh(w) + 2w(7w^4 - 255w^2 + 285)$$

$$T_3 = (w^4 + 5w^2 - 45)\cosh(3w) + w(30 - 7w^2)\sinh(3w) - 2(w^4 + 5w^2 - 45)\cosh(2w) + 2w(30 - 7w^2)\sinh(2w) + (59w^4 + 55w^2 + 45)\cosh(w) - 7w(17w^2 + 30)\sinh(w) + 2w(7w^4 - 25w^2 - 45)$$

$$T_4 = (w^4 - 3w^2 - 9)\cosh(3w) + 3w(6 - w^2)\sinh(3w) - 2(w^4 - 3w^2 - 9)\cosh(2w) + 6w(6 - w^2)\sinh(2w) + (59w^4 - 33w^2 + 9)\cosh(w) - 3w(17w^2 + 42)\sinh(w) + 2w(7w^4 + 15w^2 - 9)$$

The above formulas are subject to heavy cancellations for small values of $w = \upsilon h$. In this case it is much more convenient to use the following series expansion for the coefficients $b_i$, $i = 0, 1$, $a$, $b$, and $a_1$ of the method:

$$a_1 = -2 + \frac{w^{10}}{172800} - \frac{w^{12}}{1064448}$$

$$b_0 = \frac{1}{12} - \frac{w^6}{17280} + \frac{347w^8}{31933440} - \frac{10001w^{10}}{8895744000} + \frac{9553w^{12}}{112086374400}$$

$$b_1 = \frac{5}{6} + \frac{w^6}{8640} + \frac{23w^8}{3193344} - \frac{2669w^{10}}{972972000} + \frac{1411w^{12}}{4483454976}$$

$$b = \frac{1}{200} - \frac{w^4}{14400} + \frac{923w^6}{110880000} - \frac{1637w^8}{2594592000} + \frac{509141w^{10}}{10378368000000} - \frac{11798837w^{12}}{2470051584000000}$$

$$a = -\frac{5}{252} + \frac{w^2}{288} - \frac{35w^4}{57024} + \frac{29539w^6}{272432160} - \frac{25049w^8}{1307674368} + \frac{1418843537w^{10}}{419203040256000} - \frac{2074827233w^{12}}{3469138048696320} \quad (2.9)$$

The local truncation error of the above scheme is given by

$$\mathrm{LTE}(h) = \frac{h^6(y_n^{(4)}F_nS_1S_0 - 205837632000000y_n^{(6)}S_2}{13842956331576852480000000000} + O(h^8) \quad (2.10)$$

where $F_n = \left(\frac{\partial f}{\partial y}\right)_n$ and

$$S_0 = 176375w^{12} - 1537344w^{10} + 4036500w^8 + 64864800w^6 + 467026560000$$

$$S_1 = 11798837w^{12} - 121175558w^{10} + 1558424000w^8 - 20561486400w^6 + 171531360000w^4 + 61751289600000w^2 - 389033124480000$$

$$S_2 = 47765w^{12} - 630063w^{10} + 6089850w^8 - 32432400w^6 + 28021593600$$

If $\omega = i\phi$, then the family of methods (4) is exact for any linear combination of the functions:

$$\{\sin(\phi x),\cos(\phi x),x\sin(\phi x),x\cos(\phi x),x^2\sin(\phi x), x^2\cos(\phi x),x^3\sin(\phi x),x^3\cos(\phi x),x^4\sin(\phi x),x^4\cos(\phi x)\} \quad (2.11)$$

## 3. STABILITY AND PHASE-LAG ANALYSIS

If we apply the method 2.1−2.3 to the scalar test eq $y'' = -v^2y$, we obtain the difference eq

$$y_{n+1} - 2Q(H^2)y_n + 1 = 0 \quad (3.1)$$

where $Q(H^2) = \frac{B(H^2)}{A(H^2)}$ and

$$A(H^2) = 1 + b_0H^2 + bb_1H^4 - 2abb_1H^6$$

$$B(H^2) = -\frac{a_1}{2} - \frac{b_1H^2}{2} + bb_1H^4 - 2abb_1H^6 \quad (3.2)$$

and $H = vh$.

The stability polynomial of the difference eq 3.1 is given by

$$C(t;H^2) = t^2 - 2Q(H^2)t + 1 \quad (3.3)$$

We have the following definitions.

**Definition 1.**[18] *A symmetric two-step method with a stability polynomial given by (3.3) is said to have a nonzero interval of periodicity* $(0, H_0^2)$ *if, for all* $H^2 \in (0, H_0^2)$, *the roots of the stability polynomial satisfy*

$$t_1 = e^{i\theta(H)}, \quad t_2 = e^{-i\theta(H)} \quad (3.4)$$

*where* $\theta$ *is a real function of* $H = vh$.

**Definition 2.**[19,20] *A method is said to be phase fitted (or complete in phase) if it has a phase-lag of order* $\infty$.

**Remark 1.** *A method is said to be phase fitted if* $Q(H^2) = \cos(H)$.

**Remark 2.** *A symmetric two-step method with stability polynomial given by (3.3) has an interval of periodicity* $(0, H_0^2)$ *if, for all* $H^2 \in (0, H_0^2)$, $1 \pm Q(H^2) > 0$.

**Remark 3.** *A symmetric two-step method with stability polynomial given by (3.3) is said to be almost P-stable if its interval of periodicity is equal to* $(0, \infty) - A$ *where A is a set of distinct points.*

For the method derived in section 2 we find that for the values of coefficients given by (2.8), $1 \pm B(H^2) = 1 \pm \cos(H) > 0$ for all $H^2 \in (0, \infty) - \{H^2 : H = sq\pi, q = 1, 2, ...\}$, i.e., the method is almost P-stable and $Q(H^2) = \cos(H)$ i.e., the method is phase fitted.

## 4. NUMERICAL ILLUSTRATIONS

In this section we present some numerical results to illustrate the performance of our new methods. We consider the numerical integration of the Schrödinger eq

$$y''(x) = (W(x) - E)y(x) \quad (4.1)$$

in the well-known case where the potential $V(x)$ is the Woods−Saxon potential

$$V(x) = V_w(x) = \frac{u_0}{(1+z)} - \frac{u_0z}{[a(1+z)^2]} \quad (4.2)$$

with $z = \exp[(x-X_0)/a]$, $u_0 = -50$, $a = 0.6$, and $X_0 = 7.0$. In order to solve this problem numerically we need to approximate the true (infinite) interval of integration $[0, \infty)$ by a finite interval. For the purpose of our numerical illustration we take the domain of integration as $0 \le x \le 15$. We consider (4.1) in a rather large domain of energies, i.e., $E \in [1,1000]$. The problem we consider is the so-called *resonance problem.*

**4.1. The Resonance Problem Woods−Saxon Potential.** In the case of positive energies $E = k^2$ the potential dies away faster than the term $l(l+1)/x^2$ and eq 1.1 effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right)y(x) = 0 \qquad (4.3)$$

for $x$ greater than some value X.

The above eq 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 eq 1 has (when $x \rightarrow 0$) the asymptotic form

$$y(x) \simeq Akxj_l(kx) - Bkxn_l(kx) \simeq AC[\sin(kx\text{-}\pi l/2) + \tan\delta_l \cos(kx\text{-}\pi l/2)] \quad (4.4)$$

where $\delta_l$ is the **phase shift** that may be calculated from the formula

$$\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)} \qquad (4.5)$$

for $x_1$ and $x_2$ distinct points on the asymptotic region (for which we have that $x_1$ is the right hand end point of the interval of integration and $x_2 = x_1 - h$, $h$ is the stepsize) with $S(x) = kxj_l(kx)$ and $C(x) = kxn_l(kx)$.

Since the problem is treated as an initial-value problem, one needs $y_0$ and $y_1$ before starting a two-step method. From the initial condition, $y_0 = 0$. It can be shown that, for values of $x$ close to the origin, the solution behaves like $y(x) \sim cx^{l+1}$ as $x \rightarrow 0$, where $c$ is an independent constant. In view of this we take $y_1 = h^{l+1}$.[4,5] With these starting values we evaluate at $x_1$ of the asymptotic region the phase shift $\delta_l$ and the normalization factor $C$ from the above relations.

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 $E$, for $E \in [1, 1000]$, at which $\delta$ equals $\pi/2$. We actually solve the latter problem, known as "*the resonance problem*" when *the positive eigenenergies lie under the potential barrier*.

The boundary conditions for this problem are

$$y(0) = 0,$$

$$y(x) \sim \cos[\sqrt{E}x] \text{ for large } x$$

The domain of numerical integration is [0, 15].

In our numerical illustration we find the positive *eigenenergies* or *resonances*. For comparison purposes we use the following fourth order methods:

Method MI: Numerov's method

Method MII: Numerov-type method of Ixaru and Rizea[8]

Method MIII: Numerov-type method of Raptis[10]

Method MIV: Numerov-type method of Simos and Mousadis[21]

Method MV: New exponentially-fitted method

We note here that Numerov's method with the exception of Chawla[22] gives better results when compared with Numerov's method.

The numerical results obtained for the four methods, with stepsizes equal to $h = \frac{1}{2^n}$, were compared with the analytic solution of the Woods−Saxon potential resonance problem, rounded to six decimal places. Figure 1 shows the errors

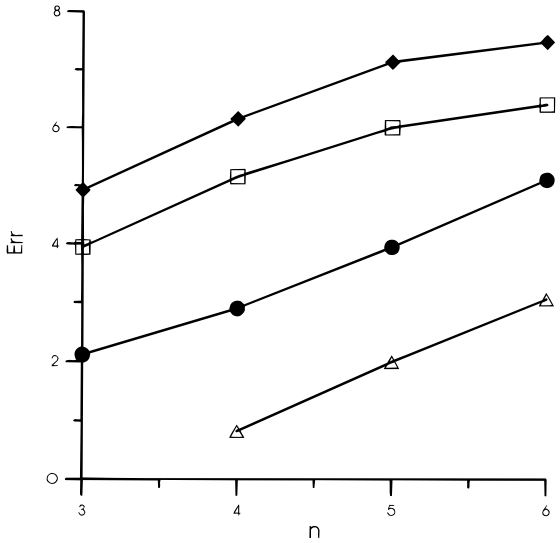


**Figure 1.** Values of Err for several values of $n$ for the resonance $E = 989.701916$. The nonexistence of the values of Err for the Method MI and the value of Err for $n = 3$ for the Method MII indicates that the value of Err is negative.

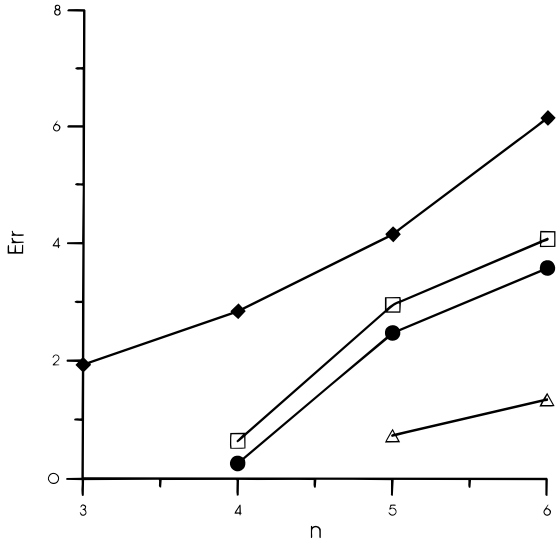


**Figure 2.** Values of Err for several values of $n$ for the resonance $E = 1002.768\,393$. The nonexistence of the values of Err for the Method MI for $n = 3$ and $n = 4$ for the method MII, for $n = 3$ for the Methods MIII and MIV, indicates that the value of Err is negative.

$Err = -log_{10}|E_{\text{calculated}} - E_{\text{analytical}}|$ of the highest eigenenergy $E_3 = 989.701\,916$ for several values of $n$.

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

$$v = \begin{cases} (-50-E)^{1/2} & \text{for } x \in [0, 6.5] \\ (-E)^{1/2} & \text{for } x \in (6.5, 15] \end{cases} \qquad (4.6)$$

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 ref 8, p 25.

**4.2. Modified Woods−Saxon Potential.** In Figure 2 some results for $Err = -log_{10}|E_{\text{calculated}} - E_{\text{analytical}}|$ of the highest eigenenergy $E_3 = 1002.768\,393$, for several values of $n$, obtained with another potential in (4.1) are shown. This potential is

$$V(x) = V_W(x) + \frac{D}{x} \tag{4.7}$$

where $V_W$ is the Woods−Saxon potential (4.2). For the purpose of our numerical experiments we use the same parameters as in ref 8, i.e., $D = 20$, $l = 2$.

Since $V(x)$ is singular at the origin, we use the special strategy of ref 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 ref 23). As in ref 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

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

**4.3. Error Estimation.** For the integration of systems of initial-value problems, several methods have been proposed for the estimation of the local truncation error (LTE) (see, for example, ref 15 and references therein).

In this paper we base our local error estimation technique on an embedded pair of integration methods and on the fact that when the local truncation error is of higher order, then the approximation of the solution for the problems with a periodical solution is better.

We denote the solution obtained with higher order as $y^H_{n+1}$ and the solution obtained with lower order as $y^L_{n+1}$, and then, we have the following definition.

**Definition 3.** *We define the* **local error** *estimate in the lower order solution $y^L_{n+1}$ by the quantity*

$$\text{LTE} = |y^H_{n+1} - y^L_{n+1}| \tag{4.8}$$

*Under the assumption that h is sufficiently small, the* **local error** *in $y^H_{n+1}$ can be neglected compared with that in $y^L_{n+1}$.*

We assume that the solution $y^L_{n+1}$ is obtained using the family of methods described in this paper and the solution $y^H_{n+1}$ is obtained using the exponentially fitted method developed by Simos.[24]

If the local error of acc is requested and the step size of the integration used for the $n$th step length is $h_n$, then the estimated step size for the $(n+1)$st step, which would give a local error of acc, must be

$$h_{n+1} = h_n\left(\frac{\text{acc}}{\text{LTE}}\right)^{1/q} \tag{4.9}$$

where $q$ is the order of the local truncation error.

However, for ease of programming we have restricted all step changes to halving and doubling. Thus, based on the procedure developed in ref 17 for the local truncation error (LTE), the step control procedure which we have actually used is

$$\text{If LTE} < \text{acc}, \quad h_{n+1} = 2h_n$$

$$\text{If } 100\,\text{acc} > \text{LTE} \geq \text{acc}, \quad h_{n+1} = h_n \tag{4.10}$$

$$\text{If LTE} \geq 100\,\text{acc}, \; h_{n+1} = \frac{h_n}{2} \text{ and repeat the step} \tag{4.11}$$

We note that the local error estimate is in the lower order solution $y^L_{n+1}$. So, it is the lower order solution $y^L_{n+1}$ which we actually accept at each point.

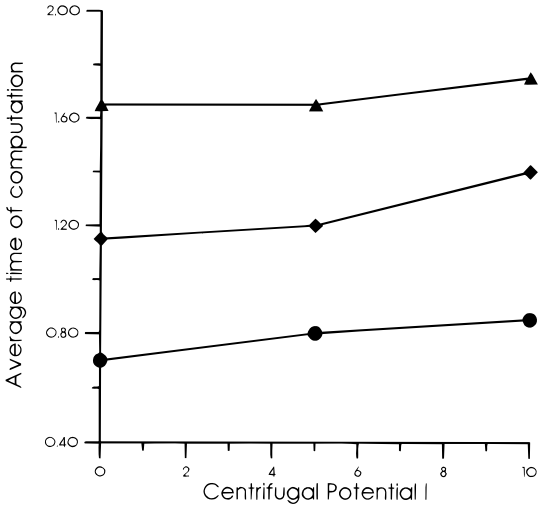


**Figure 3.** The average time of computation (in seconds) of the phase shifts for energy $k = 1$, 5, and 10.

**4.4. Phase Shift Problem. Lennard-Jones Potential.** In this section we present some numerical results to illustrate the performance of our methods on a problem of practical interest. We consider the numerical integration of the Schrödinger eq 1.1 in the well-known case where the potential $V(r)$ is the Lennard-Jones potential:

$$V(x) = m(1/x^{12} - 1/x^6), \quad \text{where } m = 500 \tag{4.12}$$

We solve this as an initial value problem and, in order to be able to use a two-step method we need an extra initial condition to be specified, e.g., $y_1$ (= $y(h)$). As we have described above, for values of $x$ close to the origin, the solution of (1.1) behaves like

$$y(x) \simeq Cx^{l+1} \text{ as } x \to 0 \tag{4.13}$$

Although this condition is not met for potential (4.12) we may use $y_1 = h^{l+1}$ as our extra initial condition since we are solving a homogeneous equation and this will be consistent with other cases where this condition is satisfied.

The problem we consider is the computation of the relevant phase shifts correct to four decimal places for energies $k = 1$, $k = 5$, and $k = 10$ and for $l = 0(1)10$. We consider the following **variable-step** approaches:

Method METHI: based on the variable step method of Raptis and Cash[15]

Method METHII: based on the variable step method of Avdelas and Simos[25]

Method METHIII: based on the variable-step method developed above

In Figure 3 we present the average time of computation of the phase shifts correct to four decimal places for energies $k = 1$, 5, and 10.

All computations were carried out on an IBM *PC*-AT compatible 80486 using double precision arithmetic (16 significant digits precision).

## 5. CONCLUSION

In this paper an exponentially-fitted method is developed. This method is much more accurate than the other well-known Numerov-type exponentially-fitted methods of Ixaru and Rizea[8] and Raptis[10] or general Numerov-type methods of Simos and Mousadis.[21] We note here that the method of Raptis is the most accurate Numerov-type method for the resonance problems of the Schrödinger eq. Based on the new exponentially-fitted method, a variable-step scheme is introduced. This scheme is much more efficient than the variable-step methods of Raptis and Cash[15] and Avdelas and Simos.[25] We note here that the method of Avdelas and Simos is the most efficient variable-step method for the numerical solution of the Schrödinger eq.

The crucial concern when solving the Schrödinger eq is that the numerical method should integrate exactly the functions (1.3) with $m$ as large as possible, as shown by refs 8 and 4. For our method we have obtained $m = 4$ and $p = 1$, i.e., a larger value of $m$ than all the well-known exponentially fitted methods.

As predicted by the analysis, the method MV is the most accurate of all the methods for the problems tested, and the variable-step method METHIII is the most efficient variable-step scheme for the numerical solution of the phase shift problem of the Schrödinger eq.

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