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Two New Optimized Eight-Step Symmetric Methods for the Efficient Solution of the Schrödinger Equation and Related Problems

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Abstract

In this paper we construct two optimized eight-step symmetric methods with phase-lag order infinite and eight. The methods are constructed to solve numerically the radial time-independent Schrödinger equation during the resonance problem with use of the Woods-Saxon potential. They can also be used to integrate related IVPs with oscillating solutions such as orbital problems. We compare the two new methods to some recently constructed optimized methods from the literature. We measure the efficiency of the methods and conclude that the new method with infinite order of phase-lag is the most efficient of all the compared methods and for all the problems solved.

1 Introduction

The radial Schrödinger equation is given by:

$$y''(x) = \left(\frac{l(l+1)}{x^2} + V(x) - E\right) y(x) \tag{1}$$

where $\frac{l(l+1)}{x^2}$ is the *centrifugal potential*, $V(x)$ is the *potential*, E is the *energy* and $W(x) = \frac{l(l+1)}{x^2} + V(x)$ is the *effective potential*. It is valid that $\lim\limits_{x\to\infty} V(x) = 0$

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and therefore $\lim_{x\to\infty} W(x) = 0$.

We consider $E > 0$ and divide $[0, \infty)$ into subintervals $[a_i, b_i]$ so that $W(x)$ is a constant with value $\bar{W}_i$. After this the problem (1) can be expressed by the approximation

$$\begin{aligned} &y_i'' = (\bar{W} - E)\, y_i, \qquad \text{whose solution is} \\ &y_i(x) = A_i \exp\left(\sqrt{\bar{W} - E}\, x\right) + B_i \exp\left(-\sqrt{\bar{W} - E}\, x\right), \\ &A_i,\ B_i\ \in \mathbb{R}. \end{aligned} \tag{2}$$

Many numerical methods have been developed for the efficient solution of the Schrödinger equation and related problems. For example Raptis and Allison have developed a two-step exponentially-fitted method of order four in [6]. More recently Kalogiratou and Simos have constructed a two-step P-stable exponentially-fitted method of order four in [7]. Also Anastassi and Simos have constructed exponentially-fitted Runge-Kutta methods of various orders in [8], [9] and [10].

Some other notable multistep methods for the numerical solution of oscillating IVPs have been developed by Chawla and Rao in [4], who produced a three-stage, two-Step P-stable method with minimal phase-lag and order six and by Henrici in [5], who produced a four-step symmetric method of order six.

Also some recent research work in numerical methods can be found in [18], [19], [20], [21], [22], [23], [24], [25], [26], [27], [28], [29], [30], [31], [32], [33], [34] and [35].

2 Phase-lag analysis of symmetric multistep methods

For the numerical solution of the initial value problem

$$y'' = f(x, y) \tag{3}$$

multistep methods of the form

$$\sum_{i=0}^{m} a_i y_{n+i} = h^2 \sum_{i=0}^{m} b_i f(x_{n+i}, y_{n+i}) \tag{4}$$

with m steps can be used over the equally spaced intervals $\{x_i\}_{i=0}^{m} \in [a, b]$ and $h = |x_{i+1} - x_i|, \quad i = 0(1)m - 1$.

If the method is symmetric then $a_i = a_{m-i}$ and $b_i = b_{m-i}, \quad i = 0(1)\lfloor \frac{m}{2} \rfloor$.

Method (4) is associated with the operator

$$L(x) = \sum_{i=0}^{m} a_i u(x + ih) - h^2 \sum_{i=0}^{m} b_i u''(x + ih) \tag{5}$$

where $u \in C^2$.

Definition 1 The multistep method (5) is called algebraic of order p if the associated linear operator L vanishes for any linear combination of the linearly independent functions $1, x, x^2, \ldots, x^{p+1}$.

When a symmetric $2k$-step method, that is for $i = -k(1)k$, is applied to the scalar test equation

$$y'' = -\omega^2 y \tag{6}$$

a difference equation of the form

$$\begin{aligned} A_k(v)y_{n+k} + ... + A_1(v)y_{n+1} + A_0(v)y_n \\ +A_1(v)y_{n-1} + ... + A_k(v)y_{n-k} = 0 \end{aligned} \tag{7}$$

is obtained, where $v = \omega h$, h is the step length and $A_0(v), A_1(v), \ldots, A_k(v)$ are polynomials of v.

The characteristic equation associated with (7) is

$$A_k(v)s^k + ... + A_1(v)s + A_0(v) + A_1(v)s^{-1} + ... + A_k(v)s^{-k} = 0 \tag{8}$$

Theorem 1 [1] *The symmetric $2k$-step method with characteristic equation given by* (8) *has phase-lag order q and phase-lag constant c given by*

$$-cv^{q+2} + O(v^{q+4}) = \frac{2A_k(v)\cos(kv) + ... + 2A_j(v)\cos(jv) + ... + A_0(v)}{2k^2A_k(v) + ... + 2j^2A_j(v) + ... + 2A_1(v)} \tag{9}$$

The formula proposed from the above theorem gives us a direct method to calculate the phase-lag of any symmetric $2k$- step method.

3 Construction of the new optimized multistep methods

We consider the multistep symmetric method of Quinlan-Tremaine [16], with eight steps and eighth algebraic order:

$$\begin{aligned} y_4 = -y_{-4} - a_3(y_3 + y_{-3}) - a_2(y_2 + y_{-2}) - a_1(y_1 + y_{-1}) \\ +h^2\left(b_3(f_3 + f_{-3}) + b_2(f_2 + f_{-2}) + b_1(f_1 + f_{-1}) + b_0f_0\right) \end{aligned} \tag{10}$$

where $a_3 = -2, \qquad a_2 = 2, \qquad a_1 = -1,$

$b_3 = \frac{17671}{12096}, \qquad b_2 = -\frac{23622}{12096}, \qquad b_1 = \frac{61449}{12096}, \qquad b_0 = -\frac{50516}{12096},$

$y_i = y(x + ih)$ and $f_i = f(x + ih, y(x + ih))$

Based on the a_i coefficients of this method, we will construct two new optimized methods.

3.1 First optimized method with infinite order of phase-lag

We want the first method to have infinite order of phase-lag, that is the phase-lag will be nullified using b_3 coefficient.

First we satisfy as many algebraic equations as possible, but leaving b_3 free. After achieving 8th algebraic order, the coefficients depend now on b_3:

$$b_0 = -20\, b_3 + \frac{601}{24}, \qquad b_2 = -6\, b_3 + \frac{109}{16}, \qquad b_1 = 15\, b_3 - \frac{101}{6}$$

and the phase-lag becomes:

$$\begin{aligned} PL = \frac{1}{10}\frac{A}{B}, \qquad \text{where} \\ A = 192\, (\cos(v))^4 - 192\, (\cos(v))^3 + 96\, (\cos(v))^3\, v^2 b_3 \\ -288\, (\cos(v))^2\, v^2 b_3 - 96\, (\cos(v))^2 + 327\, (\cos(v))^2\, v^2 + 120\, \cos(v) \\ -404\, \cos(v)\, v^2 + 288\, \cos(v)\, v^2 b_3 + 137\, v^2 - 96\, v^2 b_3 - 24 \quad \text{and} \\ B = 12 + 25\, v^2 \end{aligned}$$

so by satisfying $PL = 0$, we derive

$$\begin{aligned} b_3 = \frac{1}{96}\frac{C}{D}, \qquad \text{where} \\ C = -192\, (\cos(v))^4 + 192\, (\cos(v))^3 + \left(96 - 327\, v^2\right) (\cos(v))^2 \\ + \left(-120 + 404\, v^2\right) \cos(v) - 137\, v^2 + 24 \\ D = v^2\, (\cos(v) - 1)^3 \end{aligned} \tag{11}$$

where $v = \omega\, h$, ω is the frequency and h is the step length used.

3.2 Second optimized method with eighth order of phase-lag

For this method we use all b_i coefficients for achieving maximum algebraic order or maximum phase-lag order. After achieving maximum algebraic order, that is eighth, the coefficients become:

$$b_0 = -\frac{12629}{3024}, \qquad b_1 = \frac{20483}{4032}, \qquad b_2 = -\frac{3937}{2016}, \qquad b_3 = \frac{17671}{12096} \tag{12}$$

If we repeat the procedure of the previous section and expand phase-lag using the Taylor series, we can nullify the leading term (that is the coefficient of h^8). However we obtain the same method as (12). The same method will be produced if we attempt any combination of algebraic order and phase-lag order. This happens due to the symmetry of the specific a_i chosen.

4 Numerical results

4.1 The problems

The efficiency of the two newly constructed methods will be measured through the integration of four initial value problems with oscillating solution.

4.1.1 The resonance problem

We will integrate problem (1) with $l = 0$ at the interval $[0, 15]$ using the well known Woods-Saxon potential

$$V(x) = \frac{u_0}{1+q} + \frac{u_1\, q}{(1+q)^2}, \qquad q = \exp\left(\frac{x - x_0}{a}\right), \quad \text{where} \tag{13}$$
$$u_0 = -50, \quad a = 0.6, \quad x_0 = 7 \quad \text{and} \quad u_1 = -\frac{u_0}{a}$$

and with boundary condition $y(0) = 0$.

The potential $V(x)$ decays more quickly than $\frac{l\,(l+1)}{x^2}$, so for large x (asymptotic region) the Schrödinger equation (1) becomes

$$y''(x) = \left(\frac{l(l+1)}{x^2} - E\right) y(x) \tag{14}$$

The last equation has two linearly independent solutions $k\,x\,j_l(k\,x)$ and $k\,x\,n_l(k\,x)$, where j_l and n_l are the *spherical Bessel* and *Neumann* functions. When $x \to \infty$ the solution takes the asymptotic form

$$\begin{aligned} y(x) &\approx A\,k\,x\,j_l(k\,x) - B\,k\,x\,n_l(k\,x) \\ &\approx D[sin(k\,x - \pi\,l/2) + \tan(\delta_l)\,\cos(k\,x - \pi\,l/2)], \end{aligned} \tag{15}$$

where δ_l is called *scattering phase shift* and it is given by the following expression:

$$\tan(\delta_l) = \frac{y(x_i)\,S(x_{i+1}) - y(x_{i+1})\,S(x_i)}{y(x_{i+1})\,C(x_i) - y(x_i)\,C(x_{i+1})}, \tag{16}$$

where $S(x) = k\,x\,j_l(k\,x)$, $C(x) = k\,x\,n_l(k\,x)$ and $x_i < x_{i+1}$ and both belong to the asymptotic region. Given the energy we approximate the phase shift, the accurate value of which is $\pi/2$ for the above problem.

We will use two different values for the energy: i) 989.701916 and ii) 341.495874. As for the frequency ω we will use the suggestion of Ixaru and Rizea [13]:

$$\omega = \begin{cases} \sqrt{E-50}, & x \in [0,\, 6.5] \\ \sqrt{E}, & x \in [6.5,\, 15] \end{cases} \tag{17}$$

4.1.2 Two-Body Problem

$y'' = -\frac{y}{(y^2+z^2)^{\frac{3}{2}}}$, $z'' = -\frac{z}{(y^2+z^2)^{\frac{3}{2}}}$, with $y(0) = 1$, $y'(0) = 0$, $z(0) = 0$, $z'(0) = 1, t \in [0, 1000\,\pi]$. Theoretical solution: $y(t) = \cos(t)$ and $z(t) = \sin(t)$. We used the estimation $w = \frac{1}{(y^2+z^2)^{\frac{3}{4}}}$ as frequency of the problem.

4.1.3 Inhomogeneous Equation

$y'' = -100\,y + 99\,\sin(t)$, with $y(0) = 1, y'(0) = 11$, $t \in [0, 1000\,\pi]$.
Theoretical solution: $y(t) = \sin(t) + \sin(10\,t) + \cos(10\,t)$.
Estimated frequency: $w = 10$.

4.1.4 Orbital Problem by Franco and Palacios

The "almost" periodic orbital problem studied by [17] can be described by

$$y'' + y = \epsilon\, e^{i\,\psi\, x}, \quad y(0) = 1, \quad y'(0) = i, \quad y \in \mathcal{C}, \tag{18}$$

or equivalently by

$$\begin{array}{ll} u'' + u = \epsilon\, \cos(\psi\, x), & u(0) = 1, \quad u'(0) = 0, \\ v'' + v = \epsilon\, \sin(\psi\, x), & v(0) = 0, \quad v'(0) = 1, \end{array} \tag{19}$$

where $\epsilon = 0.001$ and $\psi = 0.01$.

The theoretical solution of the problem (18) is given below:

$$\begin{aligned} y(x) &= u(x) + i\, v(x), \quad u, v \in \mathcal{R} \\ u(x) &= \tfrac{1-\epsilon-\psi^2}{1-\psi^2}\, \cos(x) + \tfrac{\epsilon}{1-\psi^2}\, \cos(\psi\, x) \\ v(x) &= \tfrac{1-\epsilon\psi-\psi^2}{1-\psi^2}\, \sin(x) + \tfrac{\epsilon}{1-\psi^2}\, \sin(\psi\, x) \end{aligned}$$

The system of equations (19) has been solved for $x \in [0, 1000\,\pi]$. The estimated frequency is $w = 1$.

4.2 The methods

We have used several multistep methods for the integration of the Schrödinger equation. These are:

- The new method with infinite order of phase-lag shown in (11)

- The new method with eighth order of phase-lag shown in (12)
- The 8-step symmetric method of Quinlan-Tremaine of order eight [16]
- The 6-step symmetric method of Jenkins of order six [3]
- The P-stable method of Henrici with minimal phase-lag and order six [5]
- The exponentially-fitted method of Raptis and Allison of order four [6]
- The P-stable exponentially-fitted method of Kalogiratou and Simos of order four [7]
- The three-stage method of Chawla and Rao of order six [4]

4.3 Comparison

We are presenting the **accuracy** of the tested methods expressed by the $-\log_{10}$(max. error over interval) or $-\log_{10}$(error at the end point), depending on whether we know the theoretical solution or not, versus the $\log_{10}$(total function evaluations). The **function evaluations** per step are equal to the number of stages of the method multiplied by one, which is the dimension of the vector of the functions integrated for the problem. In Figures 1 and 2 we see the results for the Resonance problem for energies $E = 989.701916$ and $E = 341.495874$ respectively. In Figure 3 we see the results for the Franco-Palacios almost periodic problem, in Figure 4 the results for the Inhomogeneous equation and in Figure 5 the results for the Two-body problem.

Among all the methods used and especially compared to the original method of Quinlan-Tremaine, the new optimized method with infinite order of phase-lag was the most efficient. The difference from the other methods was about 1.5 decimal digits better for the Resonance problem for energy $E = 989.701916$ and about 1 d.d. for $E = 341.495874$. For the other three problems the difference was enormous, where there was an almost vertical increase in the accuracy compared to the other methods. There were no case where the efficiency dropped below the efficiency of the others.

An interesting remark is that the new optimized method with eighth order of phase-lag had almost identical results with the original method of Quinlan-Tremaine in all problems. This happens because of the special way of development of the specific classical method and its symmetry, where finite order of phase-lag does not give higher accuracy.

As regards to the other methods, the one of Henrici was the most efficient, with next the method of Jenkins, the method of Chawla and finally the methods of Raptis-Allison and Kalogiratou-Simos, with the exception of the Two-body problem, where the method of Chawla had the lowest efficiency.

5 Conclusions

We have constructed two optimized eight-step symmetric methods with phase-lag order infinite and eight. We have applied the new methods along with a group of recently developed methods from the literature to the Schrödinger equation and related problems. We concluded that the new methods are highly efficient compared to other optimized methods which also reveals the importance of phase-lag when solving ordinary differential equations with oscillating solutions.

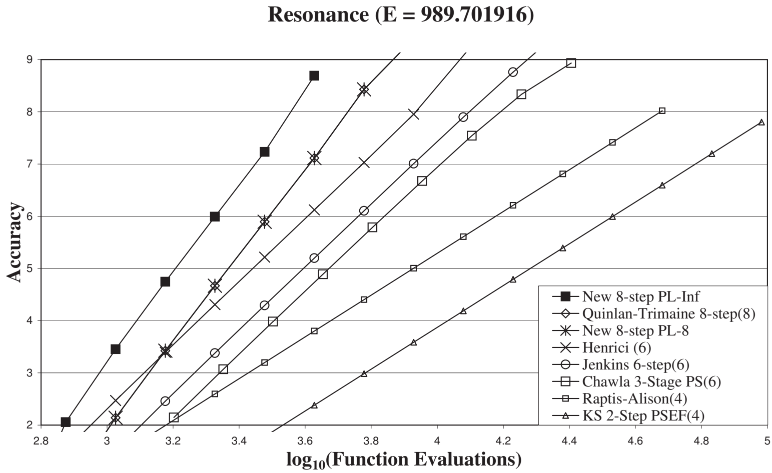

Figure 1: Efficiency for the Resonance Problem using E = 989.701916

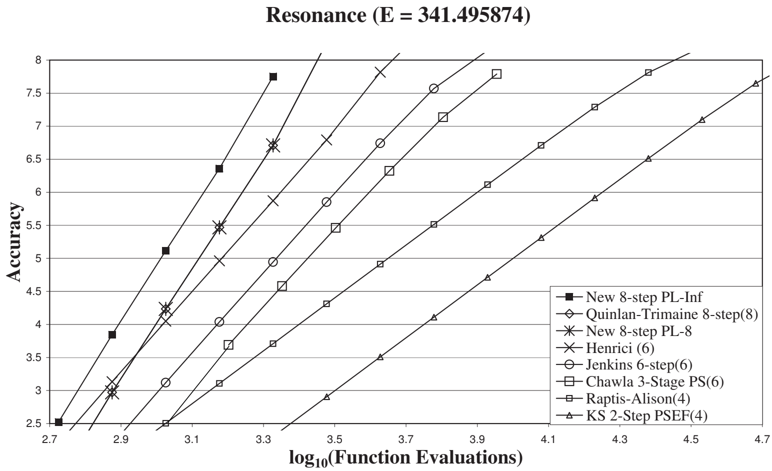

Figure 2: Efficiency for the Resonance Problem using E = 341.495874

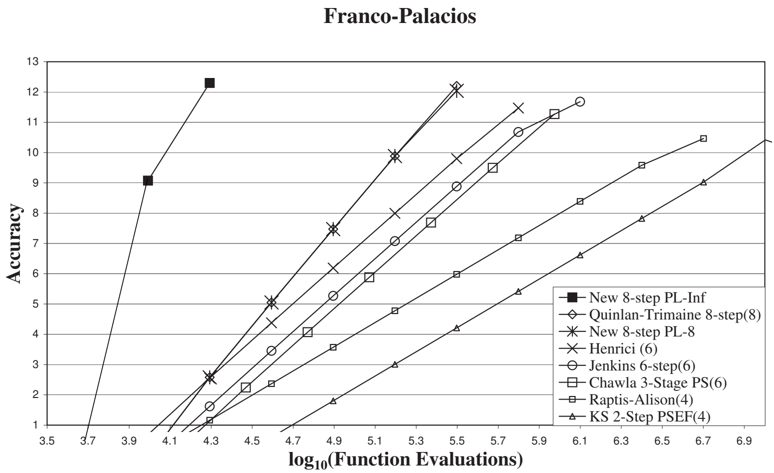

Figure 3: Efficiency for the Franco-Palacios problem

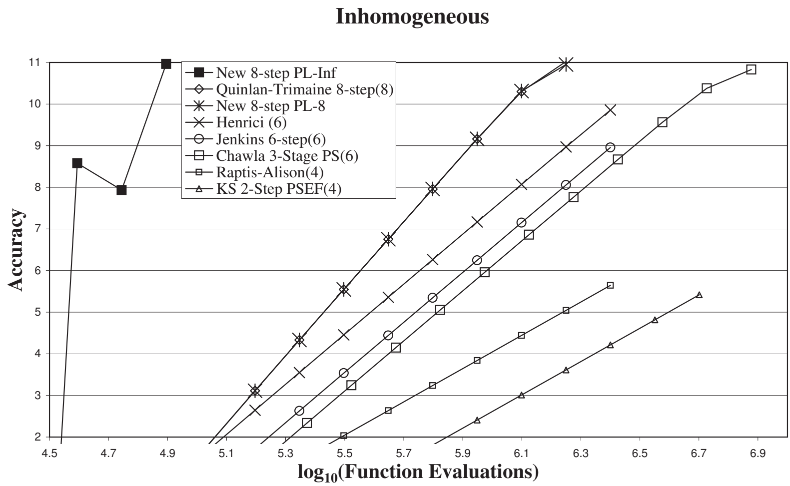

Figure 4: Efficiency for the Inhomogeneous equation

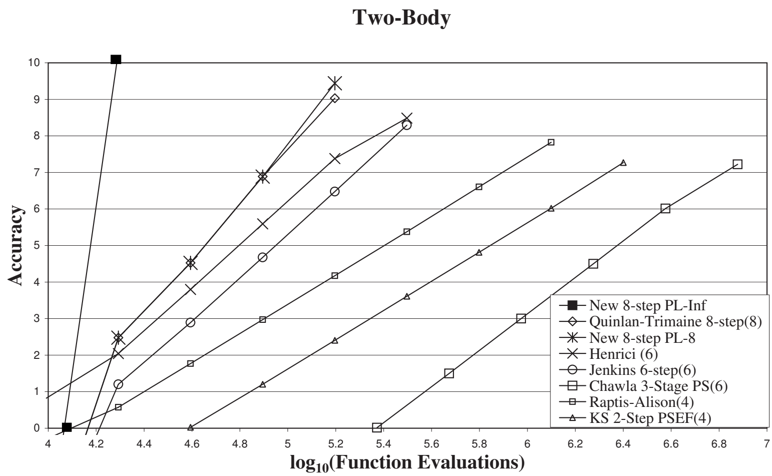

Figure 5: Efficiency for the Two-body problem

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