MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **60** (2008) 711-732

ISSN 0340 - 6253

Efficient one-step methods for the Schrödinger equation

Hans Van de Vyver
Department of Mathematics, Katholieke Universiteit Leuven,
Celestijnenlaan 200 B, B-3001 Heverlee, Belgium
e-mail: hans_vandevyver@hotmail.com

(Received November 6, 2007)

Abstract

Exponentially-fitted (EF) versions of the sixth-order one-step Obrechkoff method for the Schrödinger equation are constructed following the six-step flow-chart introduced in [1, 2]. The error analysis indicates that each version will be very different when big values of the energy are involved. The stability and phase properties are examined. It is found that the new methods are P-stable. The phase properties are in agreement with the error analysis. An application to the well-known Woods-Saxon resonance problem confirms the theory. Some additional tests show that one of the new methods is more efficient than sixth-order EF multistep algorithms.

1 Introduction

In theoretical physics no equation has been given more study than the Schrödinger equation. It is the fundamental equation of the nonrelativistic quantum mechanics, with direct applications in the description of various effects in nuclear, atomic and molecular physics [3]. The radial or one-dimensional Schrödinger equation has the form

$$y''(x) = \Big(\frac{l\,(l+1)}{x^2} + V(x) - E\Big)\, y(x). \tag{1.1}$$

The function $V(x)$ is denoted as the *potential* with $V(x) \to 0$ if $x \to \infty$. For a given integer l the term $\frac{l\,(l+1)}{x^2}$ is called the *centrifugal potential* and the function $W(x) = \frac{l\,(l+1)}{x^2} + V(x)$ is denoted as the *effective potential*. E is a real number which is called the *energy*. The two boundary conditions associated with this equation are $y(0) = 0$ together with a second condition imposed at large x, determined by physical considerations.

The past four decennia a lot of research has been performed in the area of the numerical integration of the Schrödinger equation. Standard algorithms (Runge-Kutta or Numerov, for example) for solving ordinary differential equations are satisfactory. However, when high lying bound states or resonance states are investigated, special techniques should chosen to adequately account for the oscillatory character of the solution. For such a case, finite difference methods based on *exponential fitting* are among the best candidates for use. A good theoretical foundation of exponentially-fitted (EF) multistep methods for oscillatory problems is given by Gautschi [4] and Lyche [5]. From technical point of view, the exponential fitting procedure relies on the replacement of power functions, which are taken for reference in the classical case, by a conveniently chosen mixture of powers and exponential or trigonometric functions. One should take in mind that exponential fitting can be applied only when a good estimate of the dominant frequency of the solution is known in advance. The coefficients of EF methods depend on the product of the frequency and the stepsize. An important property of EF algorithms is that they tend to the classical ones when the involved frequencies tend to zero, a fact which allows to say that exponential fitting represents a natural extension of the classical polynomial fitting. Exponential fitting may be regarded as a well-established field, the essential parts of this study are collected by Ixaru and Vanden Berghe [2]. Some recent work is included in [6, 7, 8, 9, 10]. The application of EF methods to the Schrödinger equation finds its origins in the work of

Raptis and Allison [11] and Ixaru and Rizea [12]. An exhaustive overview of available finite difference methods for the Schrödinger equation which are based on exponential fitting, phase fitting among other techniques is summarized by Simos and Williams [13].

Most finite difference methods for the Schrödinger equation are multistep methods possibly combined with hybrid techniques. A disadvantage of these methods is that additional start values are needed. The first is given by the problem while the rest are conditions that can produce errors that are larger than the error produced by the numerical method. Furthermore, the implementation of multistep codes with variable stepsizes may be time-consuming. Also multistep methods for $y'' = f(x, y)$ fail to deliver approximations of the derivative of the solution. These values are necessary for the computation of the eigen-energies [14]. All these difficulties are eliminated when selecting a one-step method. The most studied one-step methods are Runge-Kutta(-Nyström) (RK(N)) methods. Simos and coworkers [15, 16, 17, 18, 19, 20] have developed RK(N) methods which are specifically tuned on the Schrödinger equation. Some recent extensions to variable stepsizes among other references are included in [21, 22, 23]. A less known class are one-step Obrechkoff methods [24, 25]. These methods require higher-order derivatives of the solution. The purpose of this paper is to construct sixth-order Obrechkoff methods when it is formulated on the basis of exponential fitting. Only a few EF Obrechkoff method are in existence, see for example [26, 27, 28, 29]. Our new methods share the same form with the method from [28]. However, we show that the new methods are much more efficient. Some additional tests show that one of the new methods is more efficient than a sixth-order EF hybrid algorithm [30] and a sixth-order EF four-step method [31].

The paper is organized as follows. In Section 2 we discuss a class of one-step Obrechkoff methods. In Section 3 we present three different EF versions of the sixth-order Obrechkoff method. The construction is based on the six-step flow-chart for EF algorithms [1, 2]. The error analysis from Section 4 reveals that the performance of the methods will be very different when big values of the energy are involved. Such an error analysis was introduced by Ixaru and Rizea [12]. Section 5 provides a detailed stability and phase-lag analysis. The stability analysis is based on the work of Coleman and Ixaru [32] on the stability properties of methods whose coefficients depend on the product of the frequency and the stepsize. It is shown that the phase properties are in agreement with the error analysis of the Section 4. The numerical examples included

in Section 6 confirm the theory. Finally, in Section 7, some conclusions are drawn.

2 A one-step Obrechkoff method

For the numerical solution of the initial value problem (IVP) related to the scalar linear second-order differential equation (ODE)

$$y''(x) = f(x)\,y(x), \qquad y(x_0) = y_0, \qquad y'(x_0) = y'_0, \tag{2.2}$$

we consider the family of one-step Obrechkoff methods

$$y_{n+1} - y_n = h\,\alpha\left(y'_{n+1} + y'_n\right) + h^2\,c_1\left(y''_{n+1} - y''_n\right) + h^3\,c_2\left(y^{(3)}_{n+1} + y^{(3)}_n\right). \tag{2.3}$$

In particular, the choice of the free parameters

$$c_1 = -\frac{1}{10}, \qquad c_2 = \frac{1}{120}, \qquad \alpha = \frac{1}{2}, \tag{2.4}$$

represents the classical sixth-order method. The higher-order derivatives occurring in (2.3) can be found by differentiation of the right-hand side of (2.2):

$$\begin{aligned} y^{(3)}(x) &= f'(x)\,y(x) + f(x)\,y'(x), \\ y^{(4)}(x) &= \left(f''(x) + f^2(x)\right)y(x) + 2\,f'(x)\,y'(x), \\ &\ldots \end{aligned} \tag{2.5}$$

To find the values of y' which occur in method (2.3) and in the higher-order derivatives (2.5), Wang and Chen [28] proposed the following formula

$$y'_{n+1} - y'_n = h\,\alpha\left(y''_{n+1} + y''_n\right) + h^2\,c_1\left(y^{(3)}_{n+1} - y^{(3)}_n\right) + h^3\,c_2\left(y^{(4)}_{n+1} + y^{(4)}_n\right). \tag{2.6}$$

This is obtained by differentiating (2.3) with respect to x. Finally, (2.3), (2.5) and (2.6) lead to the following one-step method for (2.2)

$$\begin{pmatrix} y_{n+1} \\ \\ y'_{n+1} \end{pmatrix} = Q^{-1}_{n+1}\,P_n \begin{pmatrix} y_n \\ \\ y'_n \end{pmatrix}, \tag{2.7}$$

where

$$P_n = \begin{pmatrix} 1 - h^2\,c_1\,f_n + h^3\,c_2\,f'_n & h\,\alpha + h^3\,c_2\,f_n \\ h\,\alpha\,f_n - h^2\,c_1\,f'_n + h^3\,c_2\,(f''_n + f^2_n) & 1 - h^2\,c_1\,f_n + 2\,h^3\,c_2\,f'_n \end{pmatrix},$$

and

$$Q_{n+1} = \begin{pmatrix} 1 - h^2\, c_1\, f_{n+1} - h^3\, c_2\, f'_{n+1} & -h\,\alpha - h^3\, c_2\, f_{n+1} \\ -h\,\alpha\, f_{n+1} - h^2\, c_1\, f'_{n+1} - h^3\, c_2\, (f''_{n+1} + f^2_{n+1}) & 1 - h^2\, c_1\, f_{n+1} - 2\, h^3\, c_2\, f'_{n+1} \end{pmatrix}.$$

We observe that the computational cost is dominated by the evaluation of f, f' and f''.

3 An exponential fitting approach

In this section we follow the six-step procedure from [1, 2] for the construction of EF formulae. The reader is referred to [2] for the mathematical properties and technical details of the EF approach.

Step 1

We associate with method (2.3) the following linear operator

$$\begin{aligned} \mathcal{L}[h, \alpha, c_1, c_2]y(x) &= y(x+h) - y(x) - h\,\alpha \Big(y'(x+h) + y'(x)\Big) \\ &\quad -h^2\, c_1 \Big(y''(x+h) - y''(x)\Big) - h^3\, c_2 \Big(y^{(3)}(x+h) + y^{(3)}(x)\Big). \end{aligned}$$

The expressions of the so-called starred classical moments are

$$\begin{aligned} &L^*_0(\alpha, c_1, c_2) = 0, \qquad L^*_1(\alpha, c_1, c_2) = 1 - 2\,\alpha, \qquad L^*_2(\alpha, c_1, c_2) = 1 - 2\,\alpha, \\ &L^*_3(\alpha, c_1, c_2) = 1 - 3\,\alpha - 6\,c_1 - 12\,c_2, \qquad L^*_4(\alpha, c_1, c_2) = 1 - 4\,\alpha - 12\,c_1 - 24\,c_2, \\ &L^*_5(\alpha, c_1, c_2) = 1 - 5\,\alpha - 20\,c_1 - 60\,c_2, \qquad L^*_6(\alpha, c_1, c_2) = 1 - 6\,\alpha - 30\,c_1 - 120\,c_2, \\ &\qquad \ldots \end{aligned}$$

Step 2

Examine the algebraic system

$$L^*_m(\alpha, c_1, c_2) = 0, \qquad m = 0, \ldots, M-1,$$

to find out the maximal M for which it is compatible. In our case we have found that $M = 7$.

Step 3

Let $z := \mu\, h$. We construct the formal expression $E_0^*(z, \alpha, c_1, c_2)$ by applying $\mathcal{L}$ on $y(x) = \exp(\mu\, x)$ to obtain

$$E_0^*(z, \alpha, c_1, c_2) = \exp(\nu) - 1 - \nu\,(\exp(\nu) + 1)\,\alpha - \nu^2\,(\exp(\nu) - 1)\,c1 - \nu^3\,(\exp(\nu) + 1)\,c_2,$$

and then

$$\begin{aligned} G^+(Z, \alpha, c_1, c_2) &:= \frac{1}{2}\left(E_0^*(z, \alpha, c_1, c_2) + E_0^*(-z, \alpha, c_1, c_2)\right) \\ &= \xi(Z) - 1 - Z\,\eta_0(Z)\,\alpha + Z\,(-\xi(Z) + 1)\,c_1 - Z^2\,\eta_0(Z)\,c_2, \\ G^-(Z, \alpha, c_1, c_2) &:= \frac{1}{2\,z}\left(E_0^*(z, \alpha, c_1, c_2) - E_0^*(-z, \alpha, c_1, c_2)\right) \\ &= \eta_0(Z) - (\xi(Z) + 1)\,\alpha - Z\,\eta_0(Z)\,c_1 - Z\,(\xi(Z) + 1)\,c_2, \end{aligned}$$

where $Z = z^2$. The definition and properties of the functions ξ and η_0 are summarized in Appendix A. In addition, we denote by $G^{\pm(p)}(Z, \alpha, c_1, c_2)$, $p = 1, 2, \ldots$ the derivatives of $G^{\pm}(Z, \alpha, c_1, c_2)$ with respect to Z.

Step 4

Choose the reference set of M functions which is appropriate for the given form of $y(x)$. In general for a hybrid set one considers

$$\{1, x, x^2, \ldots, x^K, \exp(\pm\mu\, x), x\, \exp(\pm\mu\, x), \ldots, x^P\, \exp(\pm\mu\, x)\}, \tag{3.8}$$

with $K+2\,P = M-3$. The reference set is thus characterized by two integer parameters, K and P. The set in which there is no classical component is identified by $K = -1$ while the set in which there is no EF component (the classical case) is identified by $P = -1$. Parameter P will be called the *level of tuning*.

Step 5

Solve the algebraic systems

$$L_k^*(\alpha, c_1, c_2) = 0, \qquad 0 \le k \le K, \qquad G^{\pm(p)}(Z, \alpha, c_1, c_2) = 0, \qquad 0 \le p \le P,$$

for the Z-dependent coefficients α, c_1 and c_2. Note that in our case $L_0^*(\alpha, c_1, c_2)$ is identically equal to 0. The solution of the classical case $(K, P) = (6, -1)$ corresponds

to (2.4). Beside this classical solution three options of tuning are available: $(K,P) = (4,0)$, $(K,P) = (2,1)$ and $(K,P) = (0,2)$. This leads to the schemes EXPFIT1, EXPFIT2 and EXPFIT3, respectively. For abbreviation we define $\xi := \xi(Z)$ and $\eta_0 := \eta_0(Z)$.

EXPFIT1: exact for $\{1, x, x^2, x^3, x^4, \exp(\pm\mu\, x)\}$

The system to be solved is $L_k^*(\alpha, c_1, c_2) = 0$ $(k = 1, \ldots, 4)$ and $G^{\pm}(Z, \alpha, c_1, c_2) = 0$. The unique solution is given by

$$\alpha = \frac{1}{2}, \qquad c_1 = \frac{-24\,(\xi - 1) + Z\,(12 - Z)\,\eta_0}{N}, \qquad c_2 = \frac{12\,(\xi - 1) - Z\,(1 + 6\,\eta_0 - \xi)}{N},$$

where $N = 12\,Z\,(-2\,(\xi - 1) + Z\,\eta_0)$.

EXPFIT2: exact for $\{1, x, x^2, \exp(\pm\mu\, x), x\, \exp(\pm\mu\, x)\}$

The system to be solved is $L_1^*(\alpha, c_1, c_2) = L_2^*(\alpha, c_1, c_2) = 0$ and $G^{\pm}(Z, \alpha, c_1, c_2) = G^{\pm(1)}(Z, \alpha, c_1, c_2) = 0$. The unique solution is given by

$$\alpha = \frac{1}{2}, \qquad c_1 = \frac{(\xi - 1)\,(\xi + 3\,\eta_0) - 2\,Z\,\eta_0^2}{N},$$
$$c_2 = \frac{-4\,(\xi - 1)^2 + Z\,(\xi - 1)\,(\eta_0 - \xi) + Z^2\,\eta_0^2}{2\,Z\,N},$$

where $N = Z\left((\xi - 1)\,(\xi + \eta_0) - Z\,\eta_0^2\right)$.

EXPFIT3: exact for $\{1, \exp(\pm\mu\, x), x\, \exp(\pm\mu\, x), x^2\, \exp(\pm\mu\, x)\}$

The system to be solved is $G^{\pm(p)}(Z, \alpha, c_1, c_2) = 0$ $(p = 0, 1, 2)$. The unique solution is given by

$$\alpha = \frac{-(\xi - 1)^2\,(5\,\xi + 3\,\eta_0) + Z\,\eta_0\,(\xi - 1)\,(2\,\xi + 1 + 5\,\eta_0) - 2\,Z^2\,\eta_0^3}{N},$$
$$c_1 = \frac{(\xi - 1)\,(2\,\xi^2 + 3\,\eta_0\,\xi + 3\,\eta_0^2) - Z\,\eta_0^2\,(3\,\eta_0 - 1 + 2\,\xi)}{N},$$
$$c_2 = \frac{(\xi - 1)^2\,(\xi - \eta_0) - Z\,\eta_0\,(\xi - 1)\,(2\,\xi + \eta_0 + 1) + 2\,Z^2\,\eta_0^3}{Z\,N},$$

where $N = Z\left((\xi - 1)\,(2\,\xi + \eta_0)\,(\xi - \eta_0) - Z\,\eta_0^2\,(-\eta_0 + 2\,\xi - 1)\right)$.

Remark 1 *For small values of $|Z|$ the coefficients are subject to heavy cancellation. In that case the Taylor expansions should be preferred, see Appendix B. It can be seen that for $Z \to 0$ the method is reduced to the classical method (2.4).*

Step 6

The leading term of the error ($PLTE$) of the formula obtained in this way reads

- EXPFIT1: $$PLTE = \frac{h^7}{100800}\,(y^{(7)} - \mu^2\, y^{(5)}).$$
- EXPFIT2: $$PLTE = \frac{h^7}{100800}\,(y^{(7)} - 2\,\mu^2\, y^{(5)} + \mu^4\, y^{(3)}).$$
- EXPFIT3: $$PLTE = \frac{h^7}{100800}\,(y^{(7)} - 3\,\mu^2\, y^{(5)} + 3\,\mu^4\, y^{(3)} - \mu^6\, y^{(1)}).$$

Note that the error constant is very small. For comparison, the sixth-order four-step method of Raptis [31] has error constant $-19/6048$.

Remark 2 *To obtain the expressions of the PLTE of the EF versions of method (2.6) one has to differentiate the PLTE's given above with respect to x.*

4 Error analysis

We take into account that in this paper our interest lies in solving the Schrödinger equation. The error formulae from Section 3 (Step 6) are still not sufficiently transparent to enable drawing quantitative conclusions on the merits of each method. We follow a similar approach as that of Ixaru and Rizea [12] (p. 24-25) that was developed for EF Numerov methods in order to find the asymptotic expressions of the $PLTE$ for large energies E. The knowledge of the potential $W(x)$ and the energy E is sufficient to get reasonable approximations of the frequency. If we partition the integration interval in subintervals on which we approximate the effective potential $W(x)$ by a constant $\bar{W}$, then (1.1) is approximated in by the equation $y'' = (\bar{W} - E)\, y$. Obviously, a good choice of the fitted frequency in such a subinterval is $\mu = \sqrt{\bar{W} - E}$. The Schrödinger equation (1.1) is equivalent to $y'' = (\Delta W + \mu^2)\, y$, where $\Delta W = W(x) - \bar{W}$. Now the higher-order derivatives of y can be written as a function of y, y', E, ΔW and the

derivatives of ΔW. We introduce them in the error formulae obtained in Section 3 (Step 6). The same task has to be performed for the EF versions of method (2.6). To compare the errors when E is a large value it is then sufficient to organize the expressions as polynomials in E and to retain only the terms with the highest power. Altogether we arrive to the following asymptotic expressions for large E.

- Classical method (2.4):

$$PLTE(y) \approx -y'\,E^3, \qquad PLTE(y') \approx y\,E^4.$$

- Method of Wang and Chen [28]:

$$PLTE(y) \approx [9\,W'\,y + 3\,\Delta W\,y']\,E^2, \qquad PLTE(y') \approx -3\,\Delta W\,y\,E^3.$$

- EXPFIT1:

$$PLTE(y) \approx [5\,W'\,y + \Delta W\,y']\,E^2, \qquad PLTE(y') \approx -\Delta W\,y\,E^3.$$

- EXPFIT2:

$$PLTE(y) \approx 2\,W'\,y\,E^2, \qquad PLTE(y') \approx [9\,W^{(2)}\,y + 2\,W'\,y' + (\Delta W)^2\,y]\,E^2.$$

- EXPFIT3:

$$PLTE(y) \approx [-8\,W^{(3)}\,y - 4\,W^{(2)}\,y' - 6\,W'\,\Delta W\,y]\,E, \qquad PLTE(y') \approx 4\,W^{(2)}\,y\,E^2.$$

It was explained in [2] (p. 197) that the amplitude of the derivative y' is bigger by a factor $E^{1/2}$ than that of the solution y itself. Thus the increase of the error on the numerical solution of y produced by the classical method is proportional to $E^{7/2}$ while the error on the derivative y' is proportional to E^4. One should take in mind that the derivative y' has an influence on y. Thus in total, the error increases with E^4. Likewise, the errors produced by the method of Wang and Chen [28] and EXPFIT1 are proportional to E^3 but the performance of EXPFIT1 is better. The errors produced by EXPFIT2 and EXPFIT3 are proportional to $E^{5/2}$ and E^2, respectively. To summarize, EXPFIT 3 is the version to choose and this is indeed confirmed by the numerical results reported in Section 6.

5 Stability and phase-lag analysis

To investigate the stability properties of methods for solving $y'' = f(x, y)$, Lambert and Watson [33] introduced the scalar test equation

$$y'' = -\omega^2\, y, \tag{5.9}$$

where ω is a real constant, which may be assumed non-negative for notational convenience in latter inequalities. The concepts of stability analysis and P-stability for EF methods was given by Coleman and Ixaru [32]. Accordingly to their approach we have to consider the trigonometric versions of the EF methods, i.e. the methods are exact for trigonometric functions instead of exponentials. This is accomplished by considering purely imaginary frequencies $\mu = i\,k$. The coefficients of the methods are then depending on $\theta = k\,h$. An application of a θ-dependent method (2.7) to the test equation (5.9) leads to the difference equation

$$\begin{pmatrix} y_{n+1} \\ h\,y'_{n+1} \end{pmatrix} = M\,(\nu^2;\theta) \begin{pmatrix} y_n \\ h\,y'_n \end{pmatrix}, \qquad \nu = \omega\,h, \tag{5.10}$$

where $M(\nu^2;\theta) = M_1^{-1}(\nu^2;\theta)\,M_2(\nu^2;\theta)$ with

$$M_1(\nu^2;\theta) = \begin{pmatrix} 1 + c_1(\theta)\,\nu^2 & -(\alpha(\theta) - c_2(\theta)\,\nu^2) \\ (\alpha(\theta) - c_2(\theta)\,\nu^2)\,\nu^2 & 1 + c_1(\theta)\,\nu^2 \end{pmatrix},$$

and

$$M_2(\nu^2;\theta) = \begin{pmatrix} 1 + c_1(\theta)\,\nu^2 & \alpha(\theta) - c_2(\theta)\,\nu^2 \\ -(\alpha(\theta) - c_2(\theta)\,\nu^2)\,\nu^2 & 1 + c_1(\theta)\,\nu^2 \end{pmatrix}.$$

The eigenvalues of the *amplification matrix* $M(\nu^2;\theta)$ are the roots of the characteristic equation

$$\zeta^2 - 2\,R(\nu^2;\theta)\,\zeta + 1 = 0, \tag{5.11}$$

where $R(\nu^2;\theta) := \frac{1}{2}$ trace $M(\nu^2;\theta)$. Of particular interest of periodic motion is the situation where the roots are on the unit circle. Then the numerical solution preserves the amplitude. Obviously, this periodicity condition is equivalent to $|R(\nu^2;\theta)| < 1$. For this reason $R(\nu^2;\theta)$ is called the *stability function*. For a method with the stability function $R(\nu^2;\theta)$ the *region of stability* is a region of the $\nu - \theta$ plane, throughout which $|R(\nu^2;\theta)| < 1$. Any closed curve defined by $|R(\nu^2;\theta)| = 1$ is a stability boundary. In short, an EF method is P-stable if the whole $\nu - \theta$ plane is covered but the presence of a

set of curves which corresponds to critical values (where the method is undefined) or to stability boundaries is tolerated. To show that at least one such family of methods can be found Coleman and Ixaru [32] have constructed a second-order example. For a long time, the question if there exist higher-order P-stable EF methods remains without a definitive answer [2]. This problem is recently solved by the present author [7, 8]. In particular, we have shown the existence of arbitrary high order P-stable EF formulae. The methods considered here will serve new examples: condition $|R(\nu^2;\theta)| < 1$ is equivalent to

$$(\alpha(\theta) - c_1(\theta)\,\nu^2)^2 > 0 \qquad \text{and} \qquad (\alpha(\theta) - c_2(\theta)\,\nu^2)^2 > 0,$$

which is always satisfied except on the stability boundaries defined by

$$\nu^2 = \frac{\alpha(\theta)}{c_1(\theta)} \qquad \text{and} \qquad \nu^2 = \frac{\alpha(\theta)}{c_2(\theta)}.$$

In fact, every method of the form (2.7) is P-stable. This establishes

Theorem 1 *The new EF methods are P-stable.*

For any method with the stability function $R(\nu^2;\theta)$ the quantity

$$\phi(\nu^2;\theta) = \nu - arccos\Big(R(\nu^2;\theta)\Big),$$

is called the *phase-lag*. The ratio $r = \theta/\nu = k/\omega$ plays an important role in what follows. The *phase-lag order* is s if

$$\phi(\nu^2; r\,\nu) = \gamma(r)\,\nu^{s+1} + \mathcal{O}(\nu^{s+3}).$$

When $r = 1$, EF methods solve the test equation (5.9) exactly. So there is no phase-lag when the fitted frequency k is equal to the test frequency ω. It follows that $\gamma(1) = 0$. We investigate the phase properties of the following methods.

- Method of Wang and Chen [28]:

$$\phi(\nu^2; r\,\nu) = \frac{(1-r^2)(r^4+r^2+1)}{100800}\,\nu^7 + \mathcal{O}(\nu^9).$$

- EXPFIT1: $\qquad \phi(\nu^2; r\,\nu) = \dfrac{(1-r^2)}{100800}\,\nu^7 + \mathcal{O}(\nu^9).$

- EXPFIT2: $\phi(\nu^2; r\,\nu) = \dfrac{(1-r^2)^2}{100800}\,\nu^7 + \mathcal{O}(\nu^9)$.
- EXPFIT3: $\phi(\nu^2; r\,\nu) = \dfrac{(1-r^2)^3}{100800}\,\nu^7 + \mathcal{O}(\nu^9)$.

All the methods remain phase-lag order six, the same as the algebraic order. When an acceptable estimate of the dominant frequency is available (i.e. $r \approx 1$) the magnitude of the phase-lag is then much smaller than that of the corresponding classical method (i.e. $r = 0$). Furthermore, the more accurate the estimate of the dominant frequency is, the smaller the phase-lag is. It is remarkable to see that the power of $(1 - r^2)$ increases as the level of tuning increases. When $r \approx 1$ it turns out that EXPFIT3 is the most accurate method. This is in accordance with the error analysis of Section 4 because the test equation (5.9) is very similar to the Schrödinger equation.

6 Numerical illustrations

For a positive energy $E = k^2 > 0$ the equation (1.1) effectively reduces to

$$y''(x) = \Big(\frac{l\,(l+1)}{x^2} - k^2\Big)\,y(x), \tag{6.12}$$

in the asymptotic region. This 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*, respectively. Thus the solution of (1.1) has the asymptotic form (when $x \to \infty$)

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

where δ_l is the *scattering phase-shift* that must be determined. This can be expressed as

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

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 $S(x) = k\,x\,j_l(k\,x)$ and $C(x) = -k\,x\,n_l(k\,x)$.

We consider the Schrödinger equation (1.1) with $l = 0$ in the case of the well-known *Woods-Saxon* potential

$$V(x) = \frac{u_0}{1+q} + \frac{u_1\,q}{(1+q)^2}, \qquad q = \exp(\frac{x - x_0}{a}), \tag{6.13}$$

with

$$u_0 = -50, \qquad a = 0.6, \qquad x_0 = 7 \qquad \text{and} \qquad u_1 = -\frac{u_0}{a}. \tag{6.14}$$

The domain of numerical integration is $[0, 15]$. The so-called *resonance problem* consists of finding those energies (or resonances) $E > 0$, at which the phase-shift is equal to $\frac{\pi}{2}$. It may be regarded as the inverse problem of the calculation of the phase-shifts. The boundary conditions for this eigenvalue problem are

$$y(0) = 0 \qquad \text{and} \qquad y(x) = \cos(\sqrt{E}\, x) \text{ for large } x.$$

We consider a rather large domain of resonance eigen-energies $E \in [0, 1000]$. For the determination of the resonances we use the shooting method which has been described by Blatt [14]. This strategy consists of splitting up the boundary-value problem into two initial-value problems. Using a trial eigenvalue one integrates forwards from the origin, and backwards from large value of x, and attempts to match the solution at some internal point $x = x_c$. Here we take as matching point $x_c = 6.5$. An iterative process then uses the degree of mismatch to calculate a correction of the eigenvalue until we reach the desired accuracy. For the numerical comparisons we select the classical method (2.4), the method of Wang and Chen [28], EXPFIT1, EXPFIT2 and EXPFIT3. An acceptable estimate of the frequency is (see [12])

$$\mu = \begin{cases} \sqrt{-50 - E} & \text{for } x \in [0, 6.5[, \\ \sqrt{-E} & \text{for } x \in [6.5, 15]. \end{cases}$$

The numerical results obtained are compared with the analytical solution of the Woods-Saxon potential, rounded to six decimal places. Four resonances are considered [12]: 53.588872, 163.215341, 341.495874 and 989.701916. The outline of the results are presented in Figures 1–2.

It is interesting to make a comparison with multistep methods. We have selected the sixth-order EF hybrid method of Simos [30] (labeled as EFHYBRID) and the sixth-order EF four-step method of Raptis [31] (labeled as EF4STEP). The efficiency curves of the methods for resonances 163.215341 and 341.495874 are shown in Figure 3. The computational effort is measured with the CPU-time. Although the methods share approximately the same exactness, we observe that, to reach a certain accuracy, EXPFIT3 is faster than EFHYBRID and EF4STEP.

7 Conclusions

The great advantage of Obrechkoff methods is that they are one-step methods and thus will not require additional start values. On the other hand, they require higher-order derivatives of the solution. However, in the case of the Schrödinger equation the sixth-order scheme, as introduced by Wang and Chen [28], is simple and efficient. This scheme requires only the evaluation of f, f' and f'' of (2.2). We have derived three EF versions of this method following the six-step procedure introduced by Ixaru [1, 2]. It turns out that this procedure is more appropriate for the Schrödinger equation than the fitting technique applied by Wang and Chen [28]. A comparative error analysis indicates that the higher the level of tuning the more accurate the EF version is, in particular when large energies are involved. The same phenomenon was also established for EF multistep methods and EF hybrid methods in [12, 34, 35]. The error of EXPFIT3 increases quadratic with E. For comparison, it is recalled that the increase is proportional to E^4 for its classical companion. The phase-lag analysis agrees with the error analysis: the magnitude of the phase-lag decreases when the level of tuning increases. We have proved that the new methods are P-stable in the approach of [32]. The practical consequence is that stability problems will never occur. The numerical experiments carried out on the Woods-Saxon resonance problem are understandable in terms of the predictions from all the theoretical considerations. Finally, we have pointed out that the new one-step methods are, remarkably enough, more efficient than multistep algorithms. This came as a surprise to us since, in general, one-step methods are known to be less efficient than the rival multistep algorithms.

Acknowledgments

The author wish to thank the anonymous referees for their careful reading of the manuscript. This research was supported by "Grant 0T/04/21 of Onderzoeksfonds K.U. Leuven" and "Scholarship BDB-B/05/06 of K.U. Leuven".

A Appendix

The functions $\xi(Z), \eta_0(Z), \eta_1(Z), \ldots$, were originally introduced in Section 3.4 of [36] and denoted there as $\bar{\xi}(Z), \bar{\eta}_0(Z), \bar{\eta}_1(Z), \ldots$ They are defined as follows. The functions

$\xi(Z)$ and $\eta_0(Z)$ are generated first by the formula:

$$\xi(Z) = \begin{cases} \cos(|Z|^{1/2}) & \text{if } Z < 0\,, \\ \cosh(Z^{1/2}) & \text{if } Z \geq 0\,, \end{cases}$$

$$\eta_0(Z) = \begin{cases} \sin(|Z|^{1/2})/|Z|^{1/2} & \text{if } Z < 0, \\ 1 & \text{if } Z = 0, \\ \sinh(Z^{1/2})/Z^{1/2} & \text{if } Z > 0, \end{cases}$$

while $\eta_s(Z)$ with $s > 0$ are further generated by recurrence

$$\eta_1(Z) = [\xi(Z) - \eta_0(Z)]/Z\,,$$

$$\eta_s(Z) = [\eta_{s-2}(Z) - (2s-1)\eta_{s-1}(Z)]/Z\,, \quad s = 2, 3, 4, \ldots$$

if $Z \neq 0$ and by following values at $Z = 0$:

$$\eta_s(0) = 1/(2s+1)!!, \quad s = 1, 2, 3, 4, \ldots$$

These functions satisfy the following differentiation property with respect to Z :

$$\xi'(Z) = \frac{1}{2}\eta_0(Z) \quad \text{and} \quad \eta_s'(Z) = \frac{1}{2}\eta_{s+1}(Z), \quad s = 0, 1, 2, \ldots$$

B Appendix

The Taylor expansions of the coefficients of the EF versions are given below.

EXPFIT1

$$c_1 = -\frac{1}{10} + \frac{1}{8400}\,Z - \frac{1}{756000}\,Z^2 + \frac{37}{2328480000}\,Z^3 - \frac{59}{302702400000}\,Z^4 + \ldots,$$
$$c_2 = \frac{1}{120} - \frac{1}{16800}\,Z + \frac{1}{1512000}\,Z^2 - \frac{37}{4656960000}\,Z^3 + \frac{59}{605404800000}\,Z^4 + \ldots.$$

EXPFIT2

$$c_1 = -\frac{1}{10} + \frac{1}{4200}\,Z + \frac{1}{126000}\,Z^2 - \frac{89}{388080000}\,Z^3 + \frac{1579}{454053600000}\,Z^4 + \ldots,$$
$$c_2 = \frac{1}{120} - \frac{1}{8400}\,Z + \frac{1}{1008000}\,Z^2 + \frac{31}{6985440000}\,Z^3 - \frac{89}{259459200000}\,Z^4 + \ldots.$$

EXPFIT3

$$\alpha = \frac{1}{2} - \frac{1}{201600}\,Z^3 + \frac{1}{6048000}\,Z^4 + \ldots,$$
$$c_1 = -\frac{1}{10} + \frac{1}{2800}\,Z + \frac{1}{36000}\,Z^2 + \frac{23}{129360000}\,Z^3 - \frac{31}{1029600000}\,Z^4 + \ldots,$$
$$c_2 = \frac{1}{120} - \frac{1}{5600}\,Z + \frac{1}{1008000}\,Z^2 - \frac{59}{1746360000}\,Z^3 + \frac{211}{67267200000}\,Z^4 + \ldots.$$

References

[1] L. Gr. Ixaru, Operations on oscillatory functions, *Comput. Phys. Commun.* **105** (1997) 1–19.

[2] L. Gr. Ixaru, G. Vanden Berghe, *Exponential fitting*, Kluwer Academic Publishers Dordrecht/Boston/London, 2004.

[3] L. D. Landau, F. M. Lifshitz, *Quantum mechanics*, Pergamon New York, 1965.

[4] W. Gautschi, Numerical integration of ordinary differential equations based on trigonometric polynomials, *Numer. Math.* **3** (1961) 381–397.

[5] T. Lyche, Chebyshevian multistep methods for ordinary differential equations, *Numer. Math* **19** (1972) 65–75.

[6] H. Van de Vyver, Frequency evaluation for exponentially-fitted Runge-Kutta methods, *J. Comput. Appl. Math.* **184** (2005) 442-463.

[7] H. Van de Vyver, On the generation of P-stable exponentially fitted Runge-Kutta-Nyström methods by exponentially fitted Runge-Kutta methods, *J. Comput. Appl. Math.* **188** (2006) 309–318.

[8] H. Van de Vyver, Erratum to "On the generation of P-stable exponentially fitted Runge-Kutta-Nyström methods by exponentially fitted Runge-Kutta methods", *J. Comput. Appl. Math.*, Corrected proof available online via ScienceDirect.

[9] H. Van de Vyver, A fourth-order symplectic exponentially fitted integrator, *Comput. Phys. Commun.* **174** (2006) 255-262.

[10] H. Van de Vyver, An embedded exponentially fitted Runge-Kutta-Nyström method for the numerical solution of orbital problems, *New Astronomy* **11** (2006) 577-587.

[11] A. Raptis, A. C. Allison, Exponential-fitting methods for the numerical solution of the Schrödinger equation, *Comput. Phys. Commun.* **14** (1978) 1–5.

[12] L. Gr. Ixaru, M. Rizea, A Numerov-like scheme for the numerical solution of the Schrödinger equation in the deep continuum spectrum of energies, *Comput. Phys. Commun.* **19** (1980) 23–27.

[13] T. E. Simos, P. S. Williams, On finite difference methods for the solution of the Schrödinger equation, *Comput. Chem.* **23** (1999) 513-554.

[14] J. M. Blatt, Practical points concerning the solution of the Schrödinger equation, *J. Comput. Phys* **1** (1967) 382–396.

[15] T. E. Simos, J. Vigo-Aguiar, A modified phase-fitted Runge-Kutta method for the numerical solution of the Schrödinger equation, *J. Math. Chem.* **30** (2001) 121-131.

[16] T. E. Simos, A fourth algebraic order exponentially-fitted Runge-Kutta method for the numerical solution of the Schrödinger equation, *IMA J. Numer. Anal.* **21** (2001) 919–931.

[17] T. E. Simos, P. S. Williams, a new Runge-Kutta-Nyström method with phase-lag of order infinity for the numerical solution of the Schrödinger equation, *MATCH Commun. Math. Comput. Chem.* **45** (2002) 123–137.

[18] Z. A. Anastassi, T. E. Simos, Trigonometrically fitted Runge-Kutta methods for the numerical solution of the Schrödinger equation, *J. Math. Chem.* **37** (2005) 281-293.

[19] Z. A. Anastassi, T. E. Simos, Trigonometrically fitted fifth-order Runge-Kutta methods for the numerical solution of the Schrödinger equation, *Math. Comput. Model.* **42** (2005) 877-886.

[20] Z. A. Anastassi, T. E. Simos, A family of exponentially-fitted Runge-Kutta methods with exponential order up to three for the numerical solution of the Schrödinger equation, *J. Math. Chem.*, in press.

[21] H. Van de Vyver, An embedded 5(4) pair of modified explicit Runge-Kutta methods for the numerical solution of the Schrödinger equation, *Int. J. Mod. Phys. C* **16** (2005) 879–894.

[22] H. Van de Vyver, An embedded phase-fitted modified Runge-Kutta method for the numerical solution of the Schrödinger equation, *Phys. Lett. A* **352** (2006) 278–285.

[23] H. Van de Vyver, Stability and phase-lag analysis of explicit Runge-Kutta methods with variable coefficients for oscillatory problems, *Comput. Phys. Commun.* **173** (2005) 115–130.

[24] J. D. Lambert, *Computational methods in ordinary differential equations*, London-Wiley, 1973.

[25] T. E. Simos, Multiderivative methods for the numerical solution of the Schrödinger equation, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 7-26.

[26] T. E. Simos, A P-stable complete in phase Obrechkoff trigonometric fitted method for periodic initial-value problems, *Proc. Roy. Soc. London A* **441** (1993) 283–289.

[27] D. P. Sakas, T. E. Simos, Trigonometrically-fitted multiderivative methods for the numerical solution of the radial Schrödinger equation, *MATCH Commun. Math. Comput. Chem.* **53** (2005) 299-320.

[28] Zhongcheng Wang, Qimang Chen, A trigonometrically-fitted one-step method with multi-derivative for the numerical solution of the one-dimensional Schrödinger equation, *Comput. Phys. Commun.* **170** (2005) 49–64.

[29] G. Vanden Berghe, M. Van Daele, Exponentially-fitted Obrechkoff methods for second-order differential equations, Extended abstracts of ICNAAM 2006 (2006) 11–14.

[30] T. E. Simos, Exponential fitted methods for the numerical solution of the Schrödinger equation, *J. Comput. Math.* **14** (1996) 120–134.

[31] A. D. Raptis, Exponentially-fitted solutions of the eigenvalue Schrödinger equation with automatic error control, *Comput. Phys. Commun.* **28** (1983) 427–431.

[32] J. P. Coleman, L. Gr. Ixaru, P-stability and exponential-fitting methods for $y'' = f(x, y)$, *IMA J. Numer. Anal.* **16** (1996) 179–199.

[33] J. D. Lambert, I. A. Watson, Symmetric multistep methods for periodic initial value problems, *J. Inst. Math. Appl.* **18** (1976) 189–202.

[34] L. Gr. Ixaru, M. Rizea, Comparison of some four-step methods for the numerical solution of the Schrödinger equation, *Comput. Phys. Commun.* **38** (1985) 329–337.

[35] T. E. Simos, Error analysis of exponential-fitted methods for the numerical solution of the one-dimensional Schrödinger equation, *Phys. Lett. A* **177** (1993) 345–350.

[36] L. Gr. Ixaru, *Numerical Methods for Differential Equations and Applications*, Reidel, Dordrecht, 1984.

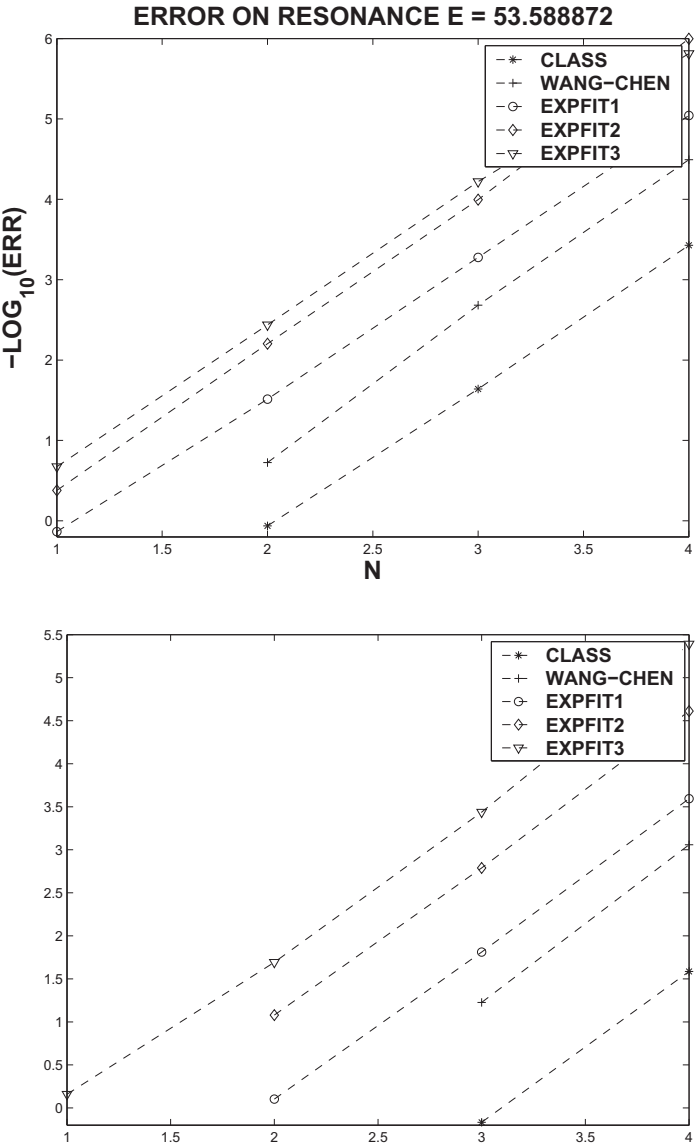

Figure 1: The decimal logarithm of ERR = $|E_{analytical} - E_{calculated}|$ as a function N where $h = 1/2^N$. The non-existence of a value indicates that the error (in absolute value) is greater than 1.

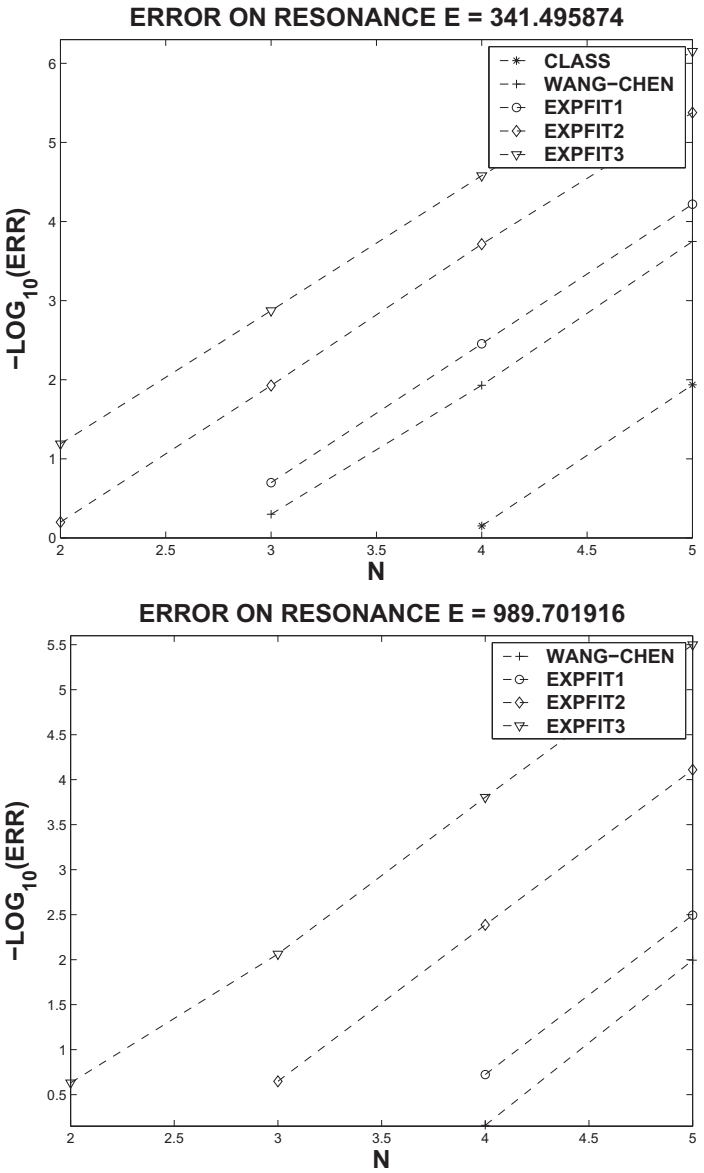

Figure 2: The decimal logarithm of ERR $= |E_{analytical} - E_{calculated}|$ as a function N where $h = 1/2^N$. The non-existence of a value indicates that the error (in absolute value) is greater than 1.

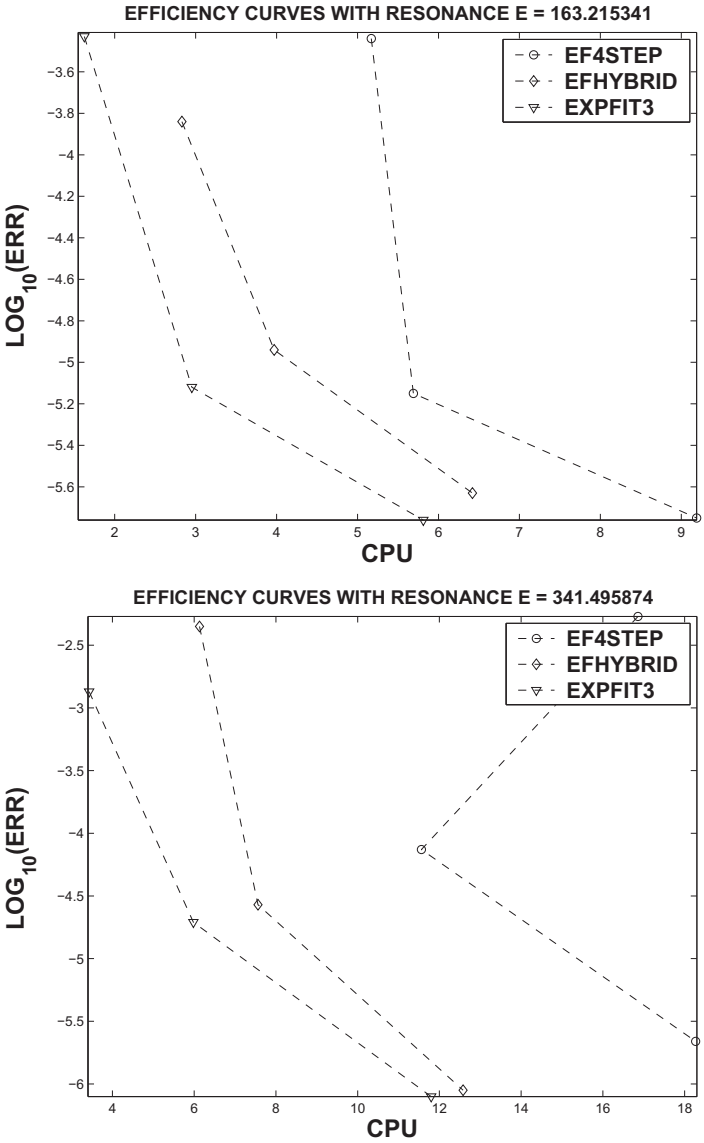

Figure 3: Efficiency curves: the decimal logarithm of ERR $= |E_{analytical} - E_{calculated}|$ as a function the CPU-time. The initial guesses for the resonances are $E_{init} = 164$ and $E_{init} = 340$, respectively. The stepsizes taken are $h = 1/2^N$ with $N = 5, 6, 7$ for EF4STEP and $N = 3, 4, 5$ for EFHYBRID and EXPFIT3.