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ORIGINAL PAPER

A family of two-stage two-step methods for the numerical integration of the Schrödinger equation and related IVPs with oscillating solution

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Abstract We develop a family of six methods for the numerical integration of the Schrödinger equation and related initial value problems with oscillating solution. Three of the methods are constructed so that they are P-stable, using the methodology of Wang (Comp Phys Comm 171(3):162–174, 2005). Also two of these three methods are trigonometrically fitted with trigonometric orders one and two. The other three methods are constructed so that they are trigonometrically fitted with orders one, two and three. We show that there is an equivalence between the three pairs of methods, as if the property of P-stability can be substituted by an extra trigonometric order, that is the P-stable method is equivalent to the method with trigonometric order one, the P-stable method with trigonometric order one is equivalent to the method with order two, and the P-stable method with order two is equivalent to the method with order three. There is a condition that we choose the same frequency for the P-stability test problem $y'' = -\theta^2 y$ and the functions that the method has to integrate exactly, in order to be trigonometrically fitted: $\{cos(\omega x),\ sin(\omega x),\ x\,cos(\omega x),\ x\,sin(\omega x),\ x^2\,cos(\omega x),\ x^2\,sin(\omega x)\}$. A stability analysis and a local truncation error analysis are performed on the methods and also the v–s diagrams are produced, where $v = \omega h$ and

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This work is dedicated to the memory of Gene H. Golub. A part of this work has been presented in the two days Conference "Gene Around the World", Tripolis, 29 February–1 March 2008, which was dedicated to 76th birthday of Gene Golub.

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$s = \theta h$. Finally the methods are applied to IVPs with oscillating solutions, such as the one-dimensional time independent Schrödinger equation and the nonlinear problem.

Keywords Numerical integration · Hybrid methods · Schrödinger equation · P-stability

1 Introduction

The one-dimensional time-independent 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 $\lim_{x\to\infty} V(x) = 0$ 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

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

The numerical solution of the Schrödinger equation and related problems has attracted many researchers the last decades. Some multistep methods have been constructed by Raptis and Allison, who have developed a two-step exponentially-fitted method of order four in [49], by Kalogiratou and Simos, who have constructed a two-step P-stable exponentially-fitted method of order four in [30], by Anastassi and Simos, who have constructed a six-step P-stable trigonometrically-fitted method in [6] and by Panopoulos, Anastassi and Simos, who have constructed two optimized eight-step methods with high or infinite order of phase-lag in [40].

Some other notable multistep methods for the numerical solution of oscillating IVPs have been developed by Chawla and Rao [20], who produced a three-stage, two-Step P-stable method with minimal phase-lag and order six and by Henrici [23], who produced a four-step symmetric method of order six.

Van de Vyver has developed some optimized Numerov-type methods in [89–91].

Also some recent research work in numerical methods can be found in [1,15–19,24,25,37,43,71,73,88] and [2–5,7–14,22,27–29,31–34,38,39,41,42,44–48,50–70,72,74–77,79–87,92,93,95].

2 Theory

2.1 Exponential symmetric multistep methods

For the numerical solution of the initial value problem

$$y = f(x, y), \quad \text{where} \quad y'(x) \text{ is omitted} \tag{3}$$

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 $h = |x_{i+1} - x_i|$, $i = 0(1)m - 1$.

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

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 (or exponential) of order p if the associated linear operator L vanishes for any linear combination of the linearly independent functions $1, x, x^2, \ldots, x^{p+1}$ (or $e^{\omega_0 x}, e^{\omega_1 x}, \ldots, e^{\omega_{p+1} x}$, where $\omega_i | i = 0(1)p + 1$ are real or complex numbers).

Remark 1 [36] If $\omega_i = \omega$ for $i = 0, 1, \ldots, n$, $n \leqslant p+1$, then the operator L vanishes for any linear combination of $e^{\omega x}, xe^{\omega x}, x^2 e^{\omega x}, \ldots, x^n e^{\omega x}, e^{\omega_{n+1} x}, \ldots, e^{\omega_{p+1} x}$.

Remark 2 [36] Every exponential multistep method corresponds in a unique way to an algebraic method (by setting $\omega_i = 0$ for all i), which is called the *classical method*.

When we use an imaginary number for frequency, that is $I\omega$, then $e^{I\omega x}$ can be expanded to $\cos(\omega x) + I \sin(\omega x)$, so we refer to a method that integrates exactly these functions as a trigonometrical multistep method with trigonometric order p. However we may refer to such a method as an exponential method, being a more general case that includes the special case of complex ω.

2.2 Stability analysis of symmetric multistep methods

We give the definitions for the stability of symmetric linear multistep methods according to Lambert and Watson theory [35] as well as some definitions from the paper of Coleman and Ixaru for the stability of methods with variable coefficients [21].

We apply the symmetric linear m-step method (4) to the scalar test equation

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

and then we solve the corresponding characteristic equation, which has m characteristic roots λ_i, $i = 0(1)m-1$.

Definition 2 [35] If the characteristic roots satisfy the conditions $|\lambda_i| \leqslant 1$, $i = 0(1)m-1$ for all $s < s_0$, where $s = \theta h$, then we say that the method has interval of periodicity $(0, s_0^2)$.

Definition 3 [35] Method (4) is called P-stable if its *interval of periodicity* is $(0, \infty)$.

We deliberately use frequency θ for the stability analysis that is different from frequency ω used for exponential-fitting. In this way we will be able to produce the v–s plane, which gives the stability regions of the method.

Definition 4 [21] A *region of stability* for a multistep method is a region of the v–s plane, throughout which the roots of the corresponding characteristic equation satisfy the conditions of Definition 2. If the conditions are valid for the equality only then that curve is called *stability boundary*.

If we set $r = \frac{v}{s} = \frac{\omega}{\theta}$, then we can say that the *principal interval of periodicity* is represented by the line segment from the beginning of the axes to the intersection of line $v = rs$ and the stability boundary. *Secondary intervals of periodicity* can be defined along the line $v = rs$ further from the beginning of the axes, but they are less important since the method must always be stable around the area where $h \to 0$.

2.3 A Methodology for developing P-stable symmetric multistep methods

A methodology, developed by Wang (see [94]), for producing P-stable symmetric multistep methods is given below. For a symmetric $2m$-step method of the form

$$\begin{aligned} &y(x+mh) + y(x-mh) - 2ay(x) \\ &= \sum_{i=1}^{m-1} c_i \left(y(x+ih) + y(x-ih)\right) + h^2 \sum_{i=0}^{m} b_i \left(y''(x+ih) + y''(x-ih)\right) \end{aligned} \tag{7}$$

we force the $2m-1$ characteristic roots to have the form

$$\{\lambda_{2k}, \lambda_{2k+1}\} = e^{I\frac{2k\pi}{m}} \{e^{Ih\theta}, e^{-Ih\theta}\}, \quad k = 0, 1, \ldots, m-1 \tag{8}$$

3 Development

We will construct a family of methods with two stages and two steps.

The general form of the method is given below:

$$\overline{y}(x) = y(x) - a_0 h^2 \, (f(x+h) - 2\, f(x) + f(x-h))$$
$$y(x+h) = 2\, y(x) - y(x-h) + h^2 \, (b_0 \, \left(f(x+h) + f(x-h)\right) + b_1 \, \overline{f}(x)\big) \quad (9)$$

and it's applied to the IVP $y'' = f(x, y)$, where $y'(x)$ is omitted.

3.1 Construction of a P-stable method

According to Wang's methodology for developing P-stable symmetric $2m$-step methods [94], and as it was briefly mentioned in (2.3), if λ_i, $i = 1 \dots n$ are the n characteristic roots of the method, then we force the roots to have the form

$$\{\lambda_{2k}, \lambda_{2k+1}\} = e^{I \frac{2k\pi}{m}} \{e^{Ih\theta}, e^{-Ih\theta}\}, \quad k = 0, 1, \dots, m-1. \tag{10}$$

In this case we have a 2-step method, as seen in (9), even though the method has a second stage. This will be clearer, when we see the characteristic equation. If we substitute $\overline{f}(x) = \overline{y}''(x)$ into the second stage, then the method will have the following form

$$y(x+h) + y(x-h) - 2\, y(x) + a_0 b_1 h^4 \left(y^{(4)}(x+h) - 2\, y^{(4)}(x) + y^{(4)}(x-h)\right) + \left(-b_0 y''(x+h) - b_0 y''(x-h) - b_1 y''(x)\right) h^2 = 0 \tag{11}$$

It is more efficient to satisfy the conditions for algebraic order first and then the conditions for all other properties, including P-stability. All the information we need is how many coefficients will be necessary for the other properties other than the algebraic order. We know in advance that, for this type of method, due its symmetry, we only need one coefficient to satisfy the condition of P-stability.[1]

We use two of the three coefficients, in order to increase the algebraic order: b_0 and b_1. By requiring that the method integrates exactly the sequence of monomials

$$\{1,\ x,\ x^2,\ \dots,\ x^p\}$$

for the highest possible p, then we acquire these two equations

$$2\, b_0 + b_1 - 1 = 0 \quad \text{and} \quad b_0 - \frac{1}{12} = 0,$$

which give

$$b_0 = \frac{1}{12} \quad \text{and} \quad b_1 = \frac{5}{6}. \tag{12}$$

[1] Even if we used only one coefficient for the algebraic conditions, leaving two for the P-stability, we would end up having a free parameter, which again would be used to increase the algebraic order.

Now we need to determine a_0, in order to satisfy the condition for P-stability according to Wang. So, if we substitute $y''(x) = -\theta^2 y(x)$ and then $\theta h = s$, so the method takes the form

$$\frac{1}{12}\, y(x+h)\left(s^2 + 10\, a_0 s^4 + 12\right) + y(x)\left(-\frac{5}{3}\, a_0 s^4 + \frac{5}{6}\, s^2 - 2\right) + \frac{1}{12}\, y(x-h)\left(s^2 + 10\, a_0 s^4 + 12\right) = 0 \qquad (13)$$

The characteristic equation of (13) is

$$\frac{1}{12}\,\lambda^2\left(s^2 + 10\, a_0 s^4 + 12\right) + \lambda\left(-\frac{5}{3}\, a_0 s^4 + \frac{5}{6}\, s^2 - 2\right) + \frac{1}{12}\left(s^2 + 10\, a_0 s^4 + 12\right) = 0 \qquad (14)$$

We now substitute $\lambda_1 = e^{I\theta h} = e^{Is}$ and $\lambda_2 = e^{-I\theta h} = e^{-Is}$ and we have two equations that must be satisfied:

$$\begin{aligned} \frac{5}{3}\left(\left(\frac{6}{5} + \frac{1}{10}\, s^2 + a_0 s^4\right)\cos(s) - a_0 s^4 + \frac{1}{2}\, s^2 - \frac{6}{5}\right)(\cos(s) + I\sin(s)) = 0 \\ \frac{5}{3}\left(\left(\frac{6}{5} + \frac{1}{10}\, s^2 + a_0 s^4\right)\cos(s) - a_0 s^4 + \frac{1}{2}\, s^2 - \frac{6}{5}\right)(\cos(s) - I\sin(s)) = 0 \end{aligned} \qquad (15)$$

As we can see, when solving for a_0, only one equation is necessary, so we have

$$a_0 = -\frac{1}{10}\,\frac{12\,\cos(s) + \cos(s)\, s^2 + 5\, s^2 - 12}{s^4\,(\cos(s) - 1)} \qquad (16)$$

We remind that $s = \theta h$, where θ is the frequency used in the test problem $y'' = -\theta^2 y$.

After determining all three coefficients, we conclude that the order of the method is six. For the error analysis of the method see 3.11.

3.2 Construction of a method with trigonometric order one

Beginning with the same general form (9), we develop a trigonometrically fitted method with trigonometric order one. We already know, because of the symmetry of the method, that we only need one equation, so that the method integrates exactly the functions $\{cos(\omega x), sin(\omega x)\}$. This means that only one free coefficient is necessary, so that the method has trigonometric order one.

We substitute $\overline{f}(x) = \overline{y}''(x)$ into the final stage, then the method will have the following form

$$y(x+h) + y(x-h) - 2\,y(x) + a_0 b_1 h^4 \left(y^{(4)}(x+h) - 2\,y^{(4)}(x) + y^{(4)}(x-h)\right) + \left(-b_0 y''(x+h) - b_0 y''(x-h) - b_1 y''(x)\right) h^2 = 0 \quad (17)$$

As in 3.1, we use two of the three coefficients, b_0 and b_1, in order to increase the algebraic order. By requiring that the method integrates exactly the sequence of monomials

$$\{1,\ x,\ x^2,\ \ldots,\ x^p\}$$

for the highest possible p, then we acquire these two equations

$$2\,b_0 + b_1 - 1 = 0 \quad \text{and} \quad b_0 - \frac{1}{12} = 0,$$

which give

$$b_0 = \frac{1}{12} \quad \text{and} \quad b_1 = \frac{5}{6}. \quad (18)$$

Now we need to determine a_0, so that the method integrates exactly $e^{I\omega x}$ or equivalently $\{cos(\omega x), sin(\omega x)\}$. By applying $y(x) = e^{I\omega x}$ to method (17) and then by dividing by $e^{I\omega x}$ we get:

$$\left(2\,b_1 a_0 v^4 + 2\,b_0 v^2 + 2\right)\cos(v) + b_1 v^2 - 2\,b_1 a_0 v^4 - 2 = 0 \quad (19)$$

and if we also apply the values of b_0 and b_1, then we get:

$$\frac{1}{6}\left(12 + 10\,a_0 v^4 + v^2\right)\cos(v) - \frac{5}{3}\,a_0 v^4 - 2 + \frac{5}{6}\,v^2 \quad (20)$$

By solving the above equation, we determine a_0:

$$a_0 = -\frac{1}{10}\,\frac{12\,\cos(v) + \cos(v)\,v^2 + 5\,v^2 - 12}{v^4\,(\cos(v) - 1)} \quad (21)$$

Please note that even if we choose another coefficient other than a_0 for the trigonometric fitting, a_0 will still be the only variable coefficient, while the other two remain constant, and all three will have the same values as above. This happens because of the way the three coefficients depend on each other through the three equations.

3.3 Equivalence between the P-stable method and the trigonometrically fitted method

We can see that by using two different techniques, one introduced by Wang [94] for developing P-stable methods and another for developing trigonometrically fitted methods, we constructed the same method.

The coefficients of the trigonometrically fitted method developed in 3.2 are the same as the coefficients of the P-stable method developed 3.1, assuming that we use the same frequency $\theta = \omega \Rightarrow s = v$.

We remind that $s = \theta h$, where θ is the frequency used in the test problem $y'' = -\theta^2 y$, while $v = \omega h$, where ω is the frequency used in $e^{I\omega x}$, which is the function that the trigonometrically fitted method integrates exactly.

As it comes to the equivalence of the two methods, the choice of the frequency θ or ω and thus s or v is irrelevant, since a_0 (the only variable coefficient) depends only on either s or v.

The Taylor expansion series of a_0 is of course the same for the two methods:

$$
\begin{aligned}
a_0 = & \frac{1}{200} + \frac{1}{5{,}040}v^2 + \frac{1}{144{,}000}v^4 + \frac{1}{4{,}435{,}200}v^6 + \frac{691}{99{,}066{,}240{,}000}v^8 \\
& + \frac{1}{4{,}790{,}016{,}000}v^{10} + \frac{3{,}617}{592{,}812{,}380{,}160{,}000}v^{12} \\
& + \frac{43{,}867}{250{,}445{,}794{,}959{,}360{,}000}v^{14}
\end{aligned} \tag{22}
$$

3.4 Construction of a P-stable method with trigonometric order one

Following the same concept as in 3.1, we develop a P-stable method using Wang's methodology, but we also provide the method with trigonometric order one.

After the substitution of $\overline{f}(x) = \overline{y}''(x)$ into the final stage, the method will have the following form, which of course is the same as in 3.1:

$$
\begin{aligned}
& y(x+h) + y(x-h) - 2\,y(x) + a_0 b_1 h^4 \left(y^{(4)}(x+h) - 2\,y^{(4)}(x) + y^{(4)}(x-h)\right) \\
& \quad + \left(-b_0 y^{(2)}(x+h) - b_0 y^{(2)}(x-h) - b_1 y^{(2)}(x)\right) h^2 = 0
\end{aligned} \tag{23}
$$

For the construction of this method, apart from a_0, that it is needed for the satisfaction of the P-stability condition, we will use another coefficient, b_0, for the achievement of trigonometric fitting. Again, due to the symmetry of the method, only one condition is capable of making the method integrate exactly both necessary functions for trigonometric order one: $\{cos(\omega x), sin(\omega x)\}$.

The only free coefficient for the increase of the algebraic order is b_1. By requiring that the method integrates exactly the sequence of monomials

$$\{1,\, x,\, x^2,\, \ldots,\, x^p\}$$

for the highest possible p, then we acquire one equation:

$$2\,b_0 + b_1 - 1 = 0 \tag{24}$$

We need the method to integrate exactly $e^{I\omega x}$ or equivalently $\{cos(\omega x), sin(\omega x)\}$. By applying the substitution $y(x) = e^{I\omega x}$ to method (23) and then by dividing by $e^{I\omega x}$ we get:

$$\begin{aligned}&\left(2 + (2 - 4\,b_0)\,a_0 v^4 + 2\,b_0 v^2\right)\cos(v) - 2\\&\quad + (-2 + 4\,b_0)\,a_0 v^4 + (1 - 2\,b_0)\,v^2 = 0\end{aligned} \tag{25}$$

For the achievement of P-stability we substitute $y''(x) = -\theta^2 y(x)$ and then $\theta h = s$, so the method takes the form

$$\begin{aligned}&\left(1 + a_0\,(1 - 2\,b_0)\,s^4 + b_0 s^2\right) y\,(x + h)\\&+4\,y\,(x)\left(-\frac{1}{2} + \left(-\frac{1}{2} + b_0\right) a_0 s^4 + \left(\frac{1}{4} - \frac{1}{2}\,b_0\right) s^2\right)\\&+\left(1 + a_0\,(1 - 2\,b_0)\,s^4 + b_0 s^2\right) y\,(x - h) = 0\end{aligned} \tag{26}$$

The characteristic equation of (26) is

$$\begin{aligned}&\left(b_0 s^2 + a_0 s^4 - 2\,a_0 s^4 b_0 + 1\right)\lambda^2 + \left(s^2 - 2\,a_0 s^4 + 4\,a_0 s^4 b_0 - 2 - 2\,b_0 s^2\right)\lambda\\&+b_0 s^2 + a_0 s^4 - 2\,a_0 s^4 b_0 + 1 = 0\end{aligned} \tag{27}$$

We now substitute $\lambda_1 = e^{I\theta h} = e^{Is}$ and $\lambda_2 = e^{-I\theta h} = e^{-Is}$ and we have two equations that must be satisfied:

$$\begin{aligned}&-4\ (\cos(s) + I\sin(s))\ A = 0 \quad \text{and}\\&-4\ (\cos(s) - I\sin(s))\ A = 0, \quad \text{where}\end{aligned} \tag{28}$$

$$\begin{aligned}A = &\left(\left(-\frac{1}{2} + \left(-\frac{1}{2} + b_0\right) a_0 s^4 - \frac{1}{2}\,b_0 s^2\right)\cos(s)\right.\\&\left. + \frac{1}{2} - \left(-\frac{1}{2} + b_0\right) a_0 s^4 + \left(\frac{1}{2}\,b_0 - \frac{1}{4}\right) s^2\right)\end{aligned} \tag{29}$$

which are both satisfied for $A = 0$. By solving the system of (28) and (25) we get:

$$
\begin{aligned}
dsa_0 &= \frac{a_{0,num}}{a_{0,den}}, \quad b_0 = \frac{b_{0,num}}{b_{0,den}}, \quad b_1 = \frac{b_{1,num}}{b_{1,den}}, \quad \text{where} \\
a_{0,num} &= \left(\left(-2\,v^2+2\,s^2\right)\cos(s)+\left(2-s^2\right)v^2-2\,s^2\right)\cos(v) \\
&\quad +\left(\left(2+s^2\right)v^2-2\,s^2\right)\cos(s)-2\,v^2+2\,s^2 \\
a_{0,den} &= \left(\left(2\,s^2+4\right)v^4-4\,s^4\right)\cos(s)+4\,s^4-4\,v^4 \\
&\quad +\left(\left(\left(-2\,s^2-4\right)v^4+2\,s^4v^2+4\,s^4\right)\right. \\
&\qquad \left.\cos(s)+4\,v^4-2\,s^4v^2-4\,s^4\right)\cos(v) \\
b_{0,num} &= \left(\left(2\,v^4-2\,s^4\right)\cos(s)+\left(-2+s^2\right)v^4+2\,s^4\right)\cos(v) \\
&\quad +\left(-2\,v^4+2\,s^4-s^4v^2\right)\cos(s)+\left(2-s^2\right)v^4+s^4v^2-2\,s^4 \\
b_{0,den} &= 2\,v^2\,(-v+s)\,(v+s)\,(\cos(s)-1)\,(\cos(v)-1)\,s^2 \\
b_{1,num} &= \left(\left(\left(-2-s^2\right)v^4+s^4v^2+2\,s^4\right)\cos(s)+2\,v^4-s^4v^2-2\,s^4\right)\cos(v) \\
&\quad +\left(\left(2+s^2\right)v^4-2\,s^4\right)\cos(s)+2\,s^4-2\,v^4 \\
b_{1,den} &= v^2\,(-v+s)\,(v+s)\,(\cos(s)-1)\,(\cos(v)-1)\,s^2
\end{aligned} \tag{30}
$$

We remind that $s=\theta h$, where θ is the frequency used in the test problem $y''(x) = -\theta^2 y(x)$.

After determining all three coefficients, we conclude that the order of the method is six. For the error analysis see 3.11.

3.5 Construction of a method with trigonometric order two

Beginning with the same general form (9), we develop a trigonometrically fitted method with trigonometric order two. We need two equations, so that the method integrates exactly the set of functions $\{cos(\omega x), sin(\omega x), x\,cos(\omega x), x\,sin(\omega x)\}$. This means that two (due to symmetry) free coefficients are necessary for trigonometric fitting.

By requiring that the simplified form of the method

$$
\begin{aligned}
&y(x+h)+y(x-h)-2\,y(x)+a_0b_1h^4\left(y^{(4)}(x+h)-2\,y^{(4)}(x)+y^{(4)}(x-h)\right) \\
&\quad +\left(-b_0y''(x+h)-b_0y''(x-h)-b_1y''(x)\right)h^2=0
\end{aligned} \tag{31}
$$

integrates exactly the sequence of monomials $\{1,\ x,\ x^2,\ \ldots,\ x^p\}$ for the highest possible p, we acquire one equation:

$$
2\,b_0+b_1-1=0 \tag{32}
$$

Now we apply $y(x) = e^{I\omega x}$ to method (31) and divide by $e^{I\omega x}$ and get the equation:

$$\left(2 + (2 - 4\,b_0)\,a_0 v^4 + 2\,b_0 v^2\right)\cos(v) - 2 + (-2 + 4\,b_0)\,a_0 v^4 + (1 - 2\,b_0)\,v^2 = 0 \tag{33}$$

and we also apply $y(x) = x\,e^{I\omega x}$ and after the division by $e^{I\omega x}$ we get:

$$\frac{1}{2}\,\frac{A}{v\,(\cos(v) - 1)} = 0, \quad \text{where}$$

$$\begin{aligned} A = {} & \left(4I\left(2 + b_0 v^2\right)h\cos(v) + \left(-8I + v^3 + (-4Ib_0 + 4I)\,v^2\right)h - xv^3\right)e^{-Iv} \\ & + \left(4I\left(2 + b_0 v^2\right)h\cos(v) + \left(-8I - v^3 + (-4Ib_0 + 4I)\,v^2\right)h - xv^3\right)e^{Iv} \\ & + \left(\left(-16I + (-4I - 8Ib_0)\,v^2\right)h + 2\,xv^3\right)\cos(v) \\ & + 8I\left(2 + (-1/2 + b_0)\,v^2\right)h \end{aligned} \tag{34}$$

This expression has only imaginary part, which can be simplified to

$$\frac{h\left(\left(\left(8 + 4\,b_0 v^2\right)\cos(v) - 8 + (2 - 4\,b_0)\,v^2\right)\sin(v) + v^3\,(\cos(v) + 1)\right)}{v\sin(v)} = 0 \tag{35}$$

By solving the above equation, we determine the three coefficients:

$$\begin{aligned} a_0 &= \frac{1}{2}\,\frac{v^3\cos(v) + v^3 + 4\,\sin(v)\cos(v) - 4\,\sin(v)}{\left(8\,\sin(v)\cos(v) + 2\,v^2\sin(v)\cos(v) - 8\,\sin(v) + v^3\cos(v) + v^3\right)v^2} \\ b_0 &= -\frac{1}{4}\,\frac{v^3\cos(v) + v^3 + 2\,\sin(v)\,v^2 + 8\,\sin(v)\cos(v) - 8\,\sin(v)}{\sin(v)\,v^2\,(\cos(v) - 1)} \\ b_1 &= \frac{1}{2}\,\frac{8\,\sin(v)\cos(v) + 2\,v^2\sin(v)\cos(v) - 8\,\sin(v) + v^3\cos(v) + v^3}{\sin(v)\,v^2\,(\cos(v) - 1)} \end{aligned} \tag{36}$$

3.6 Equivalence between the P-stable method with trigonometric order one and the method with trigonometric order two

We can see that the coefficients of the trigonometrically fitted method developed in 3.5 are the same as the coefficients of the P-stable method developed 3.4, assuming that we use the same frequency $\theta = \omega \Rightarrow s = v$.

We remind that $s = \theta h$, where θ is the frequency used in the test problem $y'' = -\theta^2 y$, while $v = \omega h$, where ω is the frequency used in $x^n\,e^{I\omega x}$, which are the functions that the trigonometrically fitted method integrates exactly.

If c_{PS} are the coefficients of the P-stable method and c_{EF} are the corresponding coefficients of the exponentially fitted method, then $\lim\limits_{s \to v} c_{PS} = c_{EF}$.

The Taylor expansion series of the coefficients are given below:

$$\begin{aligned}
a_0 &= \frac{1}{200} + \frac{1}{2{,}520}\,v^2 + \frac{19}{1{,}008{,}000}\,v^4 + \frac{21{,}149}{34{,}927{,}200{,}000}\,v^6 \\
&\quad + \frac{10{,}471}{1{,}089{,}728{,}640{,}000}\,v^8 - \frac{149{,}711}{457{,}686{,}028{,}800{,}000}\,v^{10} \\
&\quad - \frac{840{,}406{,}661}{23{,}341{,}987{,}468{,}800{,}000{,}000}\,v^{12} - \frac{24{,}605{,}927{,}681}{13{,}659{,}731{,}066{,}741{,}760{,}000{,}000}\,v^{14} \\
b_0 &= \frac{1}{12} - \frac{1}{6{,}048}\,v^4 - \frac{1}{86{,}400}\,v^6 - \frac{1}{1{,}774{,}080}\,v^8 - \frac{691}{29{,}719{,}872{,}000}\,v^{10} \\
&\quad - \frac{1}{1{,}149{,}603{,}840}\,v^{12} - \frac{3{,}617}{118{,}562{,}476{,}032{,}000}\,v^{14} \\
b_1 &= \frac{5}{6} + \frac{1}{3{,}024}\,v^4 + \frac{1}{43{,}200}\,v^6 + \frac{1}{887{,}040}\,v^8 + \frac{691}{14{,}859{,}936{,}000}\,v^{10} \\
&\quad + \frac{1}{574{,}801{,}920}\,v^{12} + \frac{3{,}617}{59{,}281{,}238{,}016{,}000}\,v^{14} \qquad (37)
\end{aligned}$$

3.7 Construction of a P-stable method with trigonometric order two

This new method will have P-stability along with trigonometric order two.

After the substitution of $\overline{f}(x) = \overline{y}''(x)$ into the final stage, the method will take the form:

$$\begin{aligned}
&y(x+h) + y(x-h) - 2\,y(x) + a_0 b_1 h^4 \left(y^{(4)}(x+h) - 2\,y^{(4)}(x) + y^{(4)}(x-h)\right) \\
&\quad + \left(-b_0 y^{(2)}(x+h) - b_0 y^{(2)}(x-h) - b_1 y^{(2)}(x)\right) h^2 = 0 \qquad (38)
\end{aligned}$$

We need the method to integrate exactly the functions $\{cos(\omega x),\ sin(\omega x),\ x\,cos(\omega x),\ x\,sin(\omega x)\}$. By applying $y(x) = e^{I\omega x}$ and $y(x) = x\,e^{I\omega x}$ to method (38) and then by dividing by $e^{I\omega x}$ we get two equations that must be satisfied:

$$\begin{aligned}
&\left(2\,b_1 a_0 v^4 + 2\,b_0 v^2 + 2\right)\cos(v) + b_1 v^2 - 2\,b_1 a_0 v^4 - 2 = 0 \\
&2\,b_1 a_0 v^4 \sin(v) + 2\,\sin(v)\,b_0 v^2 + 2\,\sin(v) - 4\,\cos(v)\,b_0 v \\
&\quad -2\,b_1 v - 8\,b_1 a_0 v^3 \cos(v) + 8\,b_1 a_0 v^3 = 0 \qquad (39)
\end{aligned}$$

For the achievement of P-stability we substitute $y''(x) = -\theta^2 y(x)$ and then $\theta h = s$, so the method takes the form

$$\begin{aligned}
&y\,(x-h)\left(b_0 s^2 + b_1 a_0 s^4 + 1\right) + y\,(x+h)\left(b_0 s^2 + b_1 a_0 s^4 + 1\right) \\
&\quad -2\,y\,(x)\left(-\frac{1}{2}\,b_1 s^2 + b_1 a_0 s^4 + 1\right) = 0 \qquad (40)
\end{aligned}$$

The characteristic equation of (40) is

$$\lambda^2\left(b_0s^2+b_1a_0s^4+1\right)+\left(-2\,b_1a_0s^4-2+b_1s^2\right)\lambda+b_0s^2+b_1a_0s^4+1 \quad (41)$$

We now substitute $\lambda_1 = e^{I\theta h} = e^{Is}$ and $\lambda_2 = e^{-I\theta h} = e^{-Is}$ and we have one equation that must be satisfied:

$$2\left(\left(b_0s^2+b_1a_0s^4+1\right)\cos(s)-1-b_1a_0s^4+\frac{1}{2}\,b_1s^2\right)\cos(s) \quad (42)$$

$$a_0=\frac{1}{2}\,\frac{a_{0,num}}{a_{0,den}},\quad b_0=-\frac{b_{0,num}}{b_{0,den}},\quad b_1=2\,\frac{b_{1,num}}{b_{1,den}},\quad \text{where}$$

$$\begin{aligned}
a_{0,num} &= -\cos(s)s^2\sin(v)v-2\,\cos(s)s^2\cos(v)+2\,\cos(s)s^2\\
&\quad+\cos(s)\sin(v)v^3+s^2\sin(v)v+2\,s^2(\cos(v))^2-2\,s^2\cos(v)-\sin(v)v^3\\
a_{0,den} &= 4\,\cos(s)s^2v^2(\cos(v))^2-8\,\cos(s)s^2v^2\cos(v)+4\,\cos(s)s^2v^2\\
&\quad-\cos(s)s^4\sin(v)v-2\,\cos(s)s^4(\cos(v))^2+2\,\cos(s)s^4\cos(v)\\
&\quad+\cos(s)v^5\sin(v)-2\,\cos(s)v^4(\cos(v))^2+2\,\cos(s)v^4\cos(v)+s^4\sin(v)v\\
&\quad+2\,s^4(\cos(v))^2-2\,s^4\cos(v)-v^5\sin(v)+2\,v^4(\cos(v))^2-2\,v^4\cos(v)\\
b_{0,num} &= \cos(s)v^5\sin(v)-v^5\sin(v)-2\,\cos(s)v^4\cos(v)+2\,v^4\cos(v)\\
&\quad+2\,v^4\cos(s)-2\,v^4-8\,s^2v^2\cos(v)+4\,s^2v^2(\cos(v))^2+4\,s^2v^2\\
&\quad+s^4\sin(v)v-\cos(s)s^4\sin(v)v-2\,s^4+2\,\cos(s)s^4+2\,s^4\cos(v)\\
&\quad-2\,\cos(s)s^4\cos(v)\\
b_{0,den} &= s^2v^3(\sin(v)\cos(s)v^2-v^2\sin(v)+2\,v\cos(s)-2\,\cos(v)v\cos(s)\\
&\quad+2\,v(\cos(v))^2-2\,v\cos(v)+s^2\sin(v)-\cos(s)s^2\sin(v))\\
b_{1,num} &= 4\,\cos(s)s^2v^2(\cos(v))^2-8\,\cos(s)s^2v^2\cos(v)+4\,\cos(s)s^2v^2\\
&\quad-\cos(s)s^4\sin(v)v-2\,\cos(s)s^4(\cos(v))^2+2\,\cos(s)s^4\cos(v)\\
&\quad+\cos(s)v^5\sin(v)-2\,\cos(s)v^4(\cos(v))^2+2\,\cos(s)v^4\cos(v)\\
&\quad+s^4\sin(v)v+2\,s^4(\cos(v))^2-2\,s^4\cos(v)\\
&\quad-v^5\sin(v)+2\,v^4(\cos(v))^2-2\,v^4\cos(v)\\
b_{1,den} &= s^2v^3(\sin(v)\cos(s)v^2-v^2\sin(v)+2\,v\cos(s)-2\,\cos(v)v\cos(s)\\
&\quad+2\,v(\cos(v))^2-2\,v\cos(v)+s^2\sin(v)-\cos(s)s^2\sin(v))
\end{aligned} \quad (43)$$

We remind that $s = \theta h$, where θ is the frequency used in the test problem $y''(x) = -\theta^2 y(x)$.

After determining all three coefficients, we conclude that the order of the method is six. For the error analysis see 3.11.

3.8 Construction of a method with trigonometric order three

Here we develop a trigonometrically fitted method with trigonometric order three. We need the method to integrate exactly the set of functions $\{cos(\omega x), sin(\omega x), x\ cos(\omega x), x\ sin(\omega x), x^2\ cos(\omega x), x^2\ sin(\omega x)\}$.

The simplified form of the method is given below:

$$y(x+h)+y(x-h)-2\,y(x)+a_0b_1h^4\left(y^{(4)}(x+h)-2\,y^{(4)}(x)+y^{(4)}(x-h)\right)$$
$$+\left(-b_0y''(x+h)-b_0y''(x-h)-b_1y''(x)\right)h^2=0 \quad (44)$$

Now we apply $y(x)=e^{I\omega x}$ to method (44) and divide by $e^{I\omega x}$ and get the equation:

$$\left(2\,b_1a_0v^4+2\,b_0v^2+2\right)\cos(v)+b_1v^2-2\,b_1a_0v^4-2=0 \quad (45)$$

and solve for a_0. Then we apply $y(x)=x\,e^{I\omega x}$ and after some simplifications we get:

$$\left(4\,\cos(v)+2\,\cos(v)\,b_0v^2+b_1v^2-4\right)\sin(v)$$
$$+v^3\,(b_0+1/2\,b_1)\,(\cos(v)+1)=0 \quad (46)$$

and solve for b_0. Then we apply $y(x)=x^2\,e^{I\omega x}$ and after some simplifications we get:

$$-16\,(\cos(v))^2+\left(b_1v^4+16-4\,v^2\right)\cos(v)$$
$$+\left(v^3b_1+4\,v\right)\sin(v)+2\,b_1v^4-8\,v^2=0 \quad (47)$$

After solving the system of the three equations 47–49, we determine the three coefficients:

$$a_0=-4\,\frac{\sin(v)\,v-4\,(\cos(v))^2-\cos(v)\,v^2+4\,\cos(v)-2\,v^2}{v^3\,(v\cos(v)+\sin(v)+2\,v)}$$
$$b_0=\frac{1}{4}\,\frac{-v\cos(v)+3\,\sin(v)-2\,v}{\left(\sin(v)\,v-4\,(\cos(v))^2-\cos(v)\,v^2+4\,\cos(v)-2\,v^2\right)v}$$
$$b_1=2\,\frac{-\cos(v)\,v^2-4\,\cos(v)-2\,v^2+\sin(v)\,v+4}{v^3\,(v\cos(v)+\sin(v)+2\,v)} \quad (48)$$

3.9 Equivalence between the P-stable method with trigonometric order two and the method with trigonometric order three

We can see that the coefficients of the trigonometrically fitted method developed in 3.8 are the same as the coefficients of the P-stable method developed 3.7, assuming that we use the same frequency $\theta=\omega\Rightarrow s=v$.

We remind that $s=\theta h$, where θ is the frequency used in the test problem $y''=-\theta^2y$, while $v=\omega h$, where ω is the frequency used in $x^n\,e^{I\omega x}$, which are the functions that the trigonometrically fitted method integrates exactly.

If c_{PS} are the coefficients of the P-stable method and c_{EF} are the corresponding coefficients of the exponentially fitted method, then $\lim_{s\to v}c_{PS}=c_{EF}$.

The Taylor expansion series of the coefficients are given below:

$$\begin{aligned}
a_0 &= \frac{1}{200} + \frac{1}{1{,}680}\, v^2 + \frac{1}{28{,}000}\, v^4 + \frac{961}{970{,}200{,}000}\, v^6 - \frac{491}{12{,}972{,}960{,}000}\, v^8 \\
&\quad - \frac{68{,}479}{10{,}594{,}584{,}000{,}000}\, v^{10} - \frac{66{,}150{,}629}{162{,}097{,}135{,}200{,}000{,}000}\, v^{12} \\
&\quad - \frac{264{,}415{,}429}{21{,}890{,}594{,}658{,}240{,}000{,}000}\, v^{14} \\
b_0 &= \frac{1}{12} - \frac{1}{2{,}016}\, v^4 - \frac{109}{1{,}814{,}400}\, v^6 - \frac{227}{53{,}222{,}400}\, v^8 - \frac{8{,}251}{54{,}486{,}432{,}000}\, v^{10} \\
&\quad + \frac{7{,}963}{1{,}046{,}139{,}494{,}400}\, v^{12} + \frac{547{,}123}{296{,}406{,}190{,}080{,}000}\, v^{14} \\
b_1 &= \frac{5}{6} + \frac{1}{1{,}008}\, v^4 - \frac{41}{907{,}200}\, v^6 - \frac{47}{5{,}322{,}240}\, v^8 - \frac{44{,}923}{54{,}486{,}432{,}000}\, v^{10} \\
&\quad - \frac{24{,}067}{523{,}069{,}747{,}200}\, v^{12} - \frac{83{,}023}{148{,}203{,}095{,}040{,}000}\, v^{14}
\end{aligned} \tag{49}$$

3.10 The corresponding classical method

The corresponding classical methods is derived by requiring that the method integrates exactly the sequence of monomials

$$\{1,\ x,\ x^2,\ \ldots,\ x^p\}$$

for the highest possible p.

By solving the three equations $2\,b_0 + b_1 - 1 = 0$, $b_0 - \frac{1}{12} = 0$ and $a_0 - \frac{1}{200} = 0$, we get the values of the three coefficients:

$$a_0 = \frac{1}{200}, \quad b_0 = \frac{1}{12}, \quad b_1 = \frac{5}{6},$$

which of course are the same as the limit of the coefficients of every method produced above when $s, v \to 0$.

3.11 Error analysis

The principal terms of the local truncation error of the methods constructed in 3 are given below.

In (50) we present the P.L.T.E. of the P-stable method developed with the methodology of Wang in 3.1. The method is equivalent to the exponentially fitted method of exponential order one, whose P.L.T.E. is the same as in (50), after the substitution $\theta = \omega$. We remind that θ denotes the frequency used in the test P-stability problem $y'' = -\theta^2\, y$ and ω denotes the frequency used in the functions that the exponentially fitted method integrates exactly, here $e^{I\omega x}$.

$$P.L.T.E._{PS} = \frac{h^8}{6048}\left(\theta^2 y^{(6)} + y^{(8)}\right) \tag{50}$$

In (51) we present the P.L.T.E. of the P-stable exponentially fitted method with exponential order one developed with the methodology of Wang. The P.L.T.E. of the equivalent method, that is exponentially fitted with exponential order two, is given from the same formula given below, if we make the substitution $\theta = \omega$.

$$P.L.T.E._{PSEF_1} = \frac{h^8}{6048} \left(\omega^2 \theta^2 y^{(4)} + \left(\theta^2 + \omega^2\right) y^{(6)} + y^{(8)}\right) \tag{51}$$

In (52) we present the P.L.T.E. of the P-stable exponentially fitted method with exponential order two developed with the methodology of Wang. The P.L.T.E. of the equivalent method, that is exponentially fitted with exponential order three, is given from the same formula given below, if we make the substitution $\theta = \omega$.

$$\begin{aligned} P.L.T.E._{PSEF_2} = \frac{h^8}{6048} &\left(\theta^2 \omega^4 y'' + \left(2\,\theta^2 + \omega^2\right) \omega^2 y^{(4)}\right. \\ &\left. + \left(\theta^2 + 2\,\omega^2\right) y^{(6)} + y^{(8)}\right) \end{aligned} \tag{52}$$

The P.L.T.E. of the classical method is given if substitute $\omega = \theta = 0$, that is

$$P.L.T.E._{Classical} = \frac{h^8}{6{,}048}\, y^{(8)} \tag{53}$$

We also present the principal term of the local truncation error for the special case of the one-dimensional time-independent Schrödinger equation, which reveals the relation to the value of energy. In (54) we can see that the P.L.T.E. of the classical method is proportional to the fourth power of the energy, which results in large error when energy gets high values. In (55) we see that the P.L.T.E. of the method with trigonometric order one is proportional to the third power of energy. As the exponential order increases, the higher power of the energy found in the P.L.T.E. reduces from 3 to 2 for the cases (56) and (57). Finally when comparing the last two cases, we notice a different coefficient of E^2 which is generally smaller for the case with third exponential order (57).

This comparison reveals the importance of exponential fitting when solving the Schrödinger equation and especially the importance of high exponential order. This is the most vital property when it comes to the efficiency of numerical integration.

$$\begin{aligned} P.L.T.E._{Classical} &= \frac{h^8}{6{,}048}\, A_0, \quad \text{where} \\ A_0 = \Big[& y E^4 - 4\,W\,E^3 + ((6\,W^2 + 22\,W'')y + 12\,W'y')E^2 \\ & +((-44\,W W'' - 28\,(W')^2 - 4\,W^3 - 16\,(W^{(4)})y \\ & +(-24\,W W' - 24\,(W^{(3)})y')E + (28\,W(W')^2 + 22\,W^2 W'' \\ & +16\,W(W^{(4)} + 26\,W'(W^{(3)} + W^4 + (W^{(6)} + 15\,(W'')^2)y \\ & + 6\,(W^{(5)}y' + (24\,W(W^{(3)} + 12\,W'W^2 + 48\,W'W'')y' \Big] \end{aligned} \tag{54}$$

$$P.L.T.E._{EF1} = \frac{h^8}{6048} A_1, \quad \text{where}$$
$$\begin{aligned}A_1 = \Big[&(-W + \overline{W})yE^3 + ((-3\,W\overline{W} + 15\,W'' + 3\,W^2)y + 6\,W'y')E^2 \\ &+(((7\,W'' + 3\,W^2)\overline{W} - 3\,W^3 - 24\,(W')^2 - 15\,W^{(4)} - 37\,WW'')y \\ &+(-20\,W^{(3)} + 6\,W'\overline{W} - 18\,WW')y')E + ((-7\,WW'' - W^3 - 4\,(W')^2 \\ &-W^{(4)})\overline{W} + W^4 + 22\,W^2W'' + (28\,(W')^2 + 16\,W^{(4)})W + 26\,W^{(3)}W' \\ &+W^{(6)} + 15\,(W'')^2)y + ((-6\,WW' - 4\,W^{(3)})\overline{W} + 48\,W'W'' \\ &+6\,W^{(5)} + 24\,WW^{(3)} + 12\,W^2W')y'\Big]\end{aligned} \tag{55}$$

$$P.L.T.E._{EF2} = \frac{h^8}{36288} A_2, \quad \text{where}$$
$$\begin{aligned}A_2 = \Big[&((6\,W^2 + 6\,\overline{W}^2 - 12\,W\overline{W} + 54\,W'')y + 12\,y'W')E^2 \\ &+((-84\,W^{(4)} + (72\,\overline{W} - 180\,W)W'' + 24\,W^2\overline{W} - 12\,W^3 \\ &-12\,W\overline{W}^2 - 120\,(W')^2)y - 96\,y'W^{(3)} \\ &+(48\,\overline{W} - 72\,W)W'y')E + ((-12\,\overline{W} + 96\,W)W^{(4)} + 156\,W'W^{(3)} \\ &+90\,(W'')^2 + (6\,\overline{W}^2 - 84\,W\overline{W} + 132\,W^2)W'' \\ &+(-48\,\overline{W} + 168\,W)(W')^2 + 6\,W^4 + 6\,W^2\overline{W}^2 - 12\,W^3\overline{W} + 6\,W^{(6)})y \\ &+36\,y'W^{(5)} + (144\,W - 48\,\overline{W})y'W^{(3)} \\ &+(288\,W'W'' + (-72\,W\overline{W} + 12\,\overline{W}^2 + 72\,W^2)W')y'\Big]\end{aligned} \tag{56}$$

$$P.L.T.E._{EF3} = \frac{h^8}{6{,}048} A_3, \quad \text{where}$$
$$\begin{aligned}A_3 = \Big[&4\,W''yE^2 + ((-13\,W^{(4)} + (15\,\overline{W} - 23\,W)W'' - 16\,(W')^2 \\ &+3\,W^2\overline{W} + \overline{W}^3 - W^3 - 3\,\overline{W}^2W)y + (-12\,W^{(3)} + (-6\,W + 6\,\overline{W})W')y')E \\ &+(W^{(6)} + (-3\,\overline{W} + 16\,W)W^{(4)} + 26\,W'W^{(3)} + 15\,(W'')^2 \\ &+(3\,\overline{W}^2 + 22\,W^2 - 21\,W\overline{W})W'' + (28\,W - 12\,\overline{W})(W')^2 + 3\,W^2\overline{W}^2 + W^4 \\ &-\overline{W}^3W - 3\,W^3\overline{W})y + (6\,W^{(5)} + (-12\,\overline{W} + 24\,W)W^{(3)} + 48\,W'W'' \\ &+ (-18\,W\overline{W} + 6\,\overline{W}^2 + 12\,W^2)W')y'\Big]\end{aligned} \tag{57}$$

3.12 Stability analysis

The analysis of the P-stability property of the developed methods includes, first of all, the determination of the interval of periodicity. For the three P-stable methods of the family, the interval is of course $(0, \infty)$. This is also the case for the other three methods, since they are equivalent to the three P-stable methods. The interval of periodicity for the classical method is (0, 7.355).

Analytically, the characteristic equations for the problem $y'' = -\theta^2 y$ are given below:

$$
\begin{aligned}
C.E._{EF1} = {} & \Big(\Big(\Big(-1 - \lambda^2 - 10\,\lambda\Big)\, s^2 - 12\,(\lambda - 1)^2\Big)\, v^4 \\
& + \Big(\Big(\Big(10\,\lambda + 1 + \lambda^2\Big)\, s^2 + 12\,(\lambda - 1)^2\Big)\, v^4 - s^4\,(\lambda - 1)^2\, v^2 \\
& -12\, s^4\,(\lambda - 1)^2\Big)\cos(v) - 5\, s^4\,(\lambda - 1)^2\, v^2 + 12\, s^4\,(\lambda - 1)^2\Big) \Big/ \\
& \Big(12\, v^4\,(\cos(v) - 1)\Big)
\end{aligned}
\tag{58}
$$

$$
\begin{aligned}
C.E._{EF2} = {} & \Big(s^2 v^3\,(\lambda - 1)^2\,(s - v)\,(v + s)\,(\cos(v) + 1) + \Big(\Big(-2 - 2\,\lambda^2\Big)\, s^2 \\
& -4\,(\lambda - 1)^2\Big)\, v^4 + 8\, s^2\,(\lambda - 1)^2\, v^2 - 4\, s^4\,(\lambda - 1)^2\Big)\sin(v) \\
& + \Big(\Big(\Big(4\, s^2 \lambda + 4\,(\lambda - 1)^2\Big)\, v^4 - 8\, s^2\,(\lambda - 1)^2\, v^2 + 4\, s^4\,(\lambda - 1)^2\Big)\cos(v)\Big) \Big/ \\
& \Big(4\, v^4 \sin(v)\,(\cos(v) - 1)\Big) \\
C.E._{PS} = {} & C.E._{PSEF1} = \frac{\Big(-\lambda^2 - 1 + 2\,\cos(s)\,\lambda\Big)\, s^2}{2\,\cos(s) - 2}
\end{aligned}
\tag{59}
$$

$$
\begin{aligned}
& C.E._{PSEF2,num} \\
& = (v + s)^2 \Big(-\frac{2}{3}\,\lambda\,\cos(v + s) - \frac{1}{6}\,\cos(2\,v) - \frac{1}{6}\,\lambda^2 \cos(2\,v) \\
& \quad + \cos(s)\,\lambda + \frac{2}{3}\,\lambda^2 \cos(v) + \frac{1}{6}\,\lambda\,\cos(s + 2\,v) + \frac{1}{6}\,\cos(-s + 2\,v)\,\lambda - \frac{1}{2} \\
& \quad - \frac{2}{3}\,\lambda\,\cos(v - s) - \frac{1}{2}\,\lambda^2 + \frac{2}{3}\,\cos(v)\,(v - s)^2\Big) \\
& C.E._{PSEF2,den} \\
& = 12\,\Big(2\, v^4 \cos(v - s) + \Big(-v^5 + v^3 s^2\Big)\sin(v - s) \\
& \quad -2\, v^4 \cos(2\,v) + 2\, v^4 \cos(v + s) + \Big(-v^2 \sin(v + s) + s^2 \sin(v + s) \\
& \quad +2\,\sin(v)\, v^2 - 4\, v\cos(s) + 4\, v\cos(v) - 2\, v - 2\,\sin(v)\, s^2\Big)\, v^3\Big)
\end{aligned}
\tag{60}
$$

We omit the characteristic equation of the method with trigonometric order three due its very complex form.

The roots of the three characteristic equations of the P-stable methods are

$$
\lambda_1 = \cos(s) + \sqrt{-(\sin(s))^2}, \quad \lambda_2 = \cos(s) - \sqrt{-(\sin(s))^2}
$$

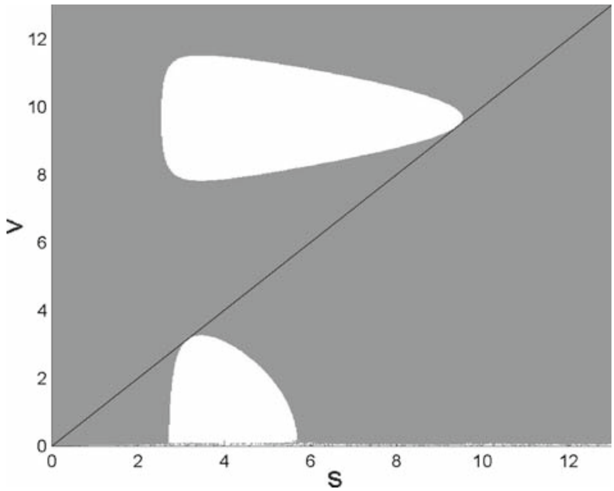

Fig. 1 v–s Plane for method 3.2 with exponential order one

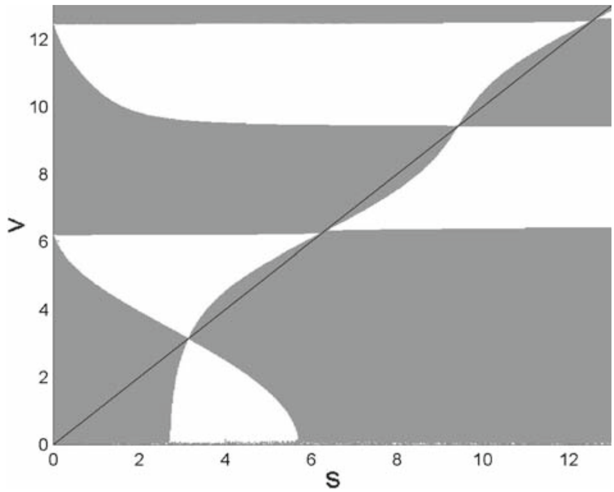

Fig. 2 v–s Plane for method 3.5 with exponential order two

which apparently give $|\lambda_{1,2}| = 1$, thus providing the three (originally developed as P-stable) methods with a stability region that includes the upper right quadrant.

We produce the v–s plane for the methods, where $v = \omega h$, $s = \theta h$, ω comes from trigonometric fitting and θ comes from the P-stability property. The v–s plane of a method shows the regions of stability of the method. In Figs. 1–3 we see the stability regions of the three trigonometrically fitted methods with the dark color. The stability region for the three P-stable methods includes the upper right quadrant, assuming that $v, s > 0$, since their coefficients depend on both v and s. The stability region for the classical method would be a rectangular with width $\sqrt{7.355} = 2.712$ and infinite height, since it doesn't depend on v.

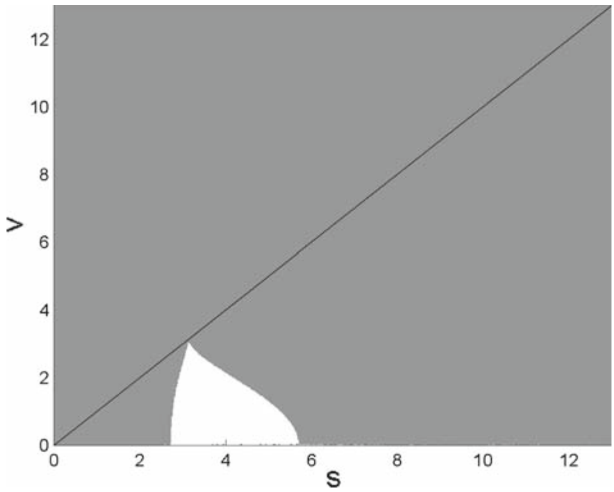

Fig. 3 v–s Plane for method 3.8 with exponential order three

The interval of periodicity of the methods can be seen on the v–s plane and more specifically on the diagonal of the plane, where $v = s$.

4 Applications and numerical results

4.1 The problems

4.1.1 The resonance problem

The efficiency of the new constructed methods will be measured through the integration of problem (1) with $l = 0$ at the interval [0, 15] using the well known Woods–Saxon potential

$$V(x) = \frac{u_0}{1+q} + \frac{u_1 q}{(1+q)^2}, \quad q = \exp\left(\frac{x - x_0}{a}\right), \quad \text{where}$$
$$u_0 = -50, \quad a = 0.6, \quad x_0 = 7 \quad \text{and} \quad u_1 = -\frac{u_0}{a} \tag{61}$$

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

$$y''(x) = \left(\frac{l(l+1)}{x^2} - E\right) y(x) \tag{62}$$

The previous 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

$x \rightarrow \infty$ the solution takes the asymptotic form

$$\begin{aligned} y(x) &\approx A\,k\,x\,j_l(k\,x) - B\,k\,x\,n_l(k\,x) \\ &\approx D[sin(k\,x - \pi\,l/2) + \tan(\delta_l)\,\cos(k\,x - \pi\,l/2)], \end{aligned} \tag{63}$$

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

$$\tan(\delta_l) = \frac{y(x_i)\,S(x_{i+1}) - y(x_{i+1})\,S(x_i)}{y(x_{i+1})\,C(x_i) - y(x_i)\,C(x_{i+1})}, \tag{64}$$

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 four different values for the energy: (i) 989.701916, (ii) 341.495874, (iii) 163.215341 and (iv) 53.588872. As for the frequency w we will use the suggestion of Ixaru and Rizea [26]:

$$w = \begin{cases} \sqrt{E-50} & x \in [0,\ 6.5] \\ \sqrt{E} & x \in [6.5,\ 15] \end{cases} \tag{65}$$

4.1.2 Nonlinear problem

The nonlinear problem is given by $y'' = -100\,y + \sin(y)$, with initial conditions: $y(0) = 0$, $y'(0) = 1$ and interval of integration $[0, 20\,\pi]$. We use $y(20\,\pi) = 3.92823991 \cdot 10^{-4}$, see [78]. We estimate the frequency $\omega = 10$.

4.2 The results

We are presenting the results of the produced methods for the two problems mentioned above. In Figs. 4–7 we can see the accuracy of the methods computed as $-\log_{10}$(max error at the end of interval) for the Schrödinger equation. We conclude, first of all, that when the value of energy increases, so does the error of the method. We also see that the higher the trigonometric order of the method, the more efficient the method is. The difference in efficiency between the methods of different trigonometric order is higher when the value of the energy used for the integration is higher. In Fig. 8 we can see the efficiency of the methods versus the value of the energy. The figure shows the difference in the efficiency of each method, while the energy changes values. We see that the decrease in accuracy, while the energy value increases, is lower when the trigonometric order increases, so the methods with high trigonometric order can be used effectively when a high value of energy is used.

These results confirm the local truncation error analysis of the methods, presented in the previous sections, revealing the critical role of high trigonometric order for the numerical integration of the Schrödinger equation.

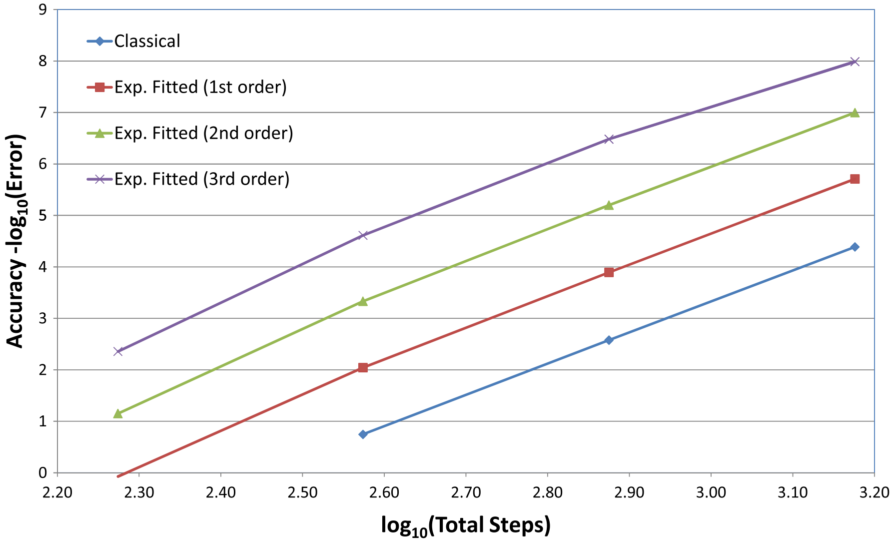

Fig. 4 Efficiency for the Schrödinger equation (E = 989.701916)

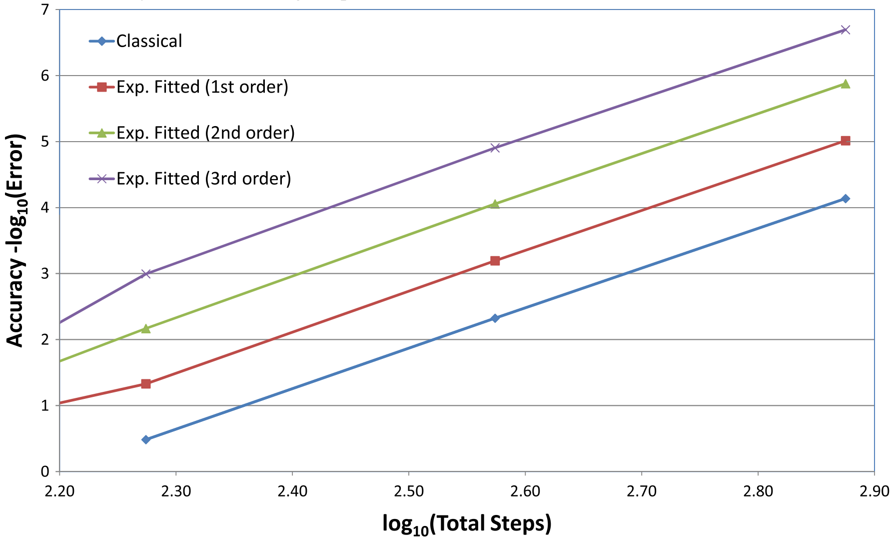

Fig. 5 Efficiency for the Schrödinger equation (E = 341.495874)

However high trigonometric order doesn't always give higher efficiency in all ODEs with oscillating solutions. For example at the integration of the nonlinear problem, we see that when increasing the trigonometric order from two to three, the efficiency decreases slightly, though it remains higher than in the classical case (Fig. 9).

The three P-stable methods, with coefficients that depend on both parameters $s = \theta h$ and $v = \omega h$, in problems that have one dominant frequency, can only be effective, when both θ and ω are equal to that frequency. Thus there is no point in giving θ a different value. So in the case when $\theta = \omega$, the derived method is the equivalent trigonometrically fitted method.

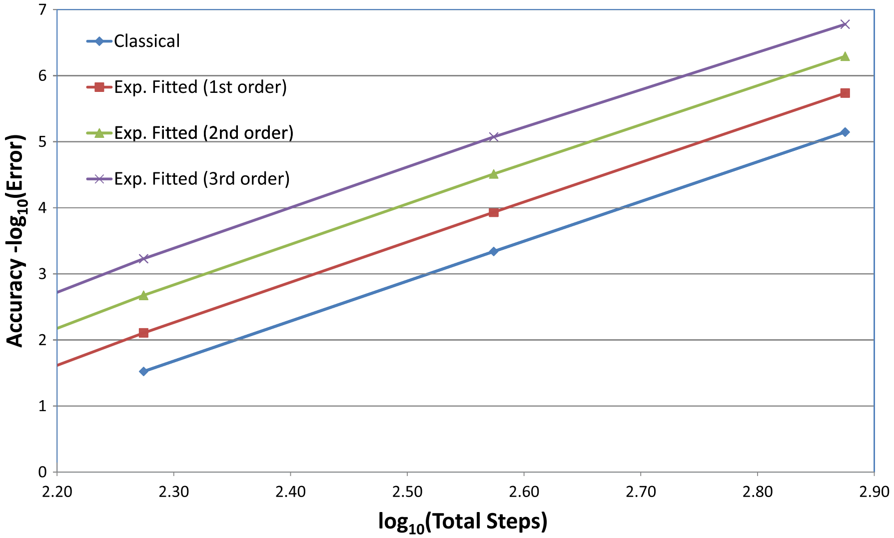

Fig. 6 Efficiency for the Schrödinger equation (E = 163.215341)

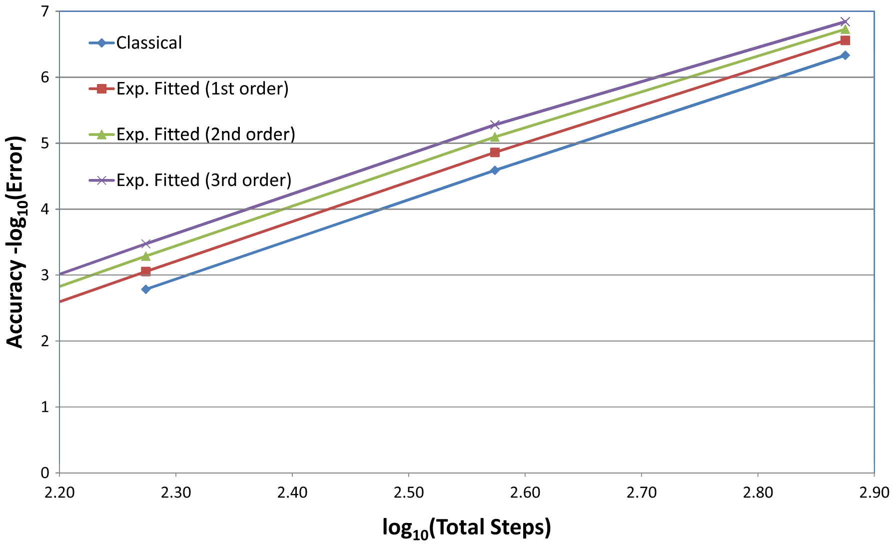

Fig. 7 Efficiency for the Schrödinger equation (E = 53.588872)

5 Conclusions

We developed a family of six methods, the three of which are P-stable with trigonometric orders 0,1,2 and the other have trigonometric orders 1,2,3. We showed the equivalency of the three pairs, as regards the coefficients, the error analysis and the stability analysis. We also showed the high efficiency gained by increasing

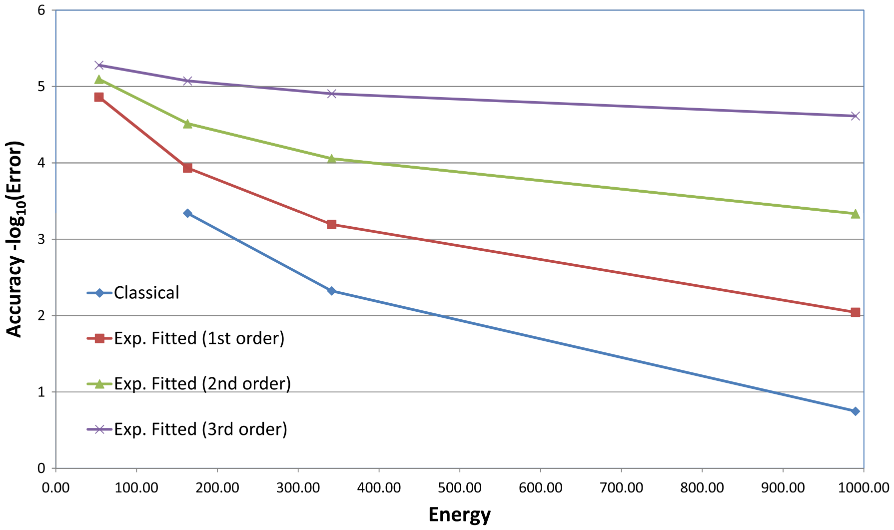

Fig. 8 Accuracy versus energy for the Schrödinger equation

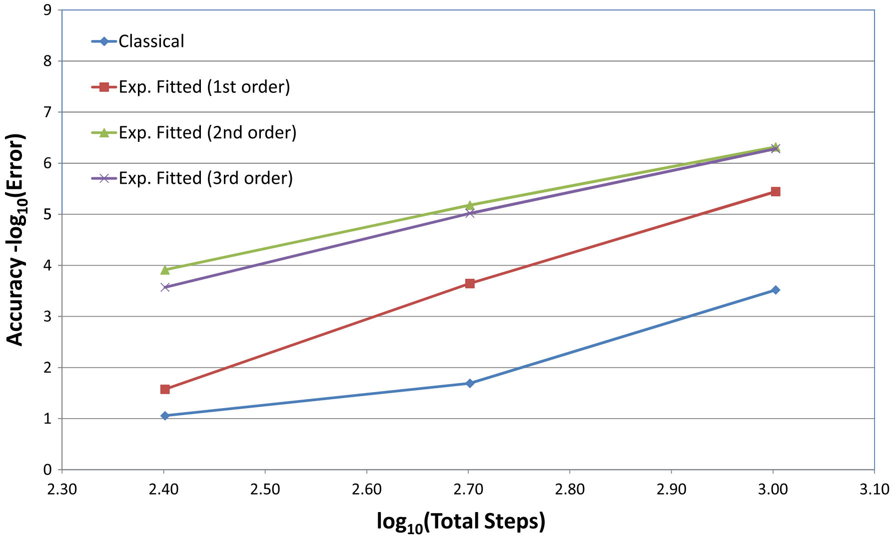

Fig. 9 Efficiency for the nonlinear problem

the exponential order of a method especially for the integration of the Schrödinger equation.

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