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Some embedded modified Runge–Kutta methods for the numerical solution of some specific Schrödinger equations

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Some embedded Runge–Kutta methods for the numerical solution of the eigenvalue Schrödinger equation are developed. More specifically, a new embedded modified Runge–Kutta 4(6) Fehlberg method with minimal phase-lag and a block embedded Runge–Kutta–Fenlberg method are developed. For the numerical solution of the eigenvalue Schrödinger equation we investigate two cases. (i) The specific case, in which the potential $V(x)$ is an even function with respect to x. It is assumed, also, that the wavefunctions tend to zero for $x \to \pm\infty$. (ii) The general case for the well-known cases of the Morse potential and Woods–Saxon or Optical potential. Numerical and theoretical results show that the new approaches are more efficient compared with the well-known Runge–Kutta–Fehlberg 4(5) method.

1. Introduction

In recent years, the Schrödinger equation has been the subject of great activity, the aim being to achieve a fast and reliable algorithm that generates a numerical solution (see [20] and references therein).

The one-dimensional Schrödinger equation has the form

$$y''(x) = \big[V(x) - E\big]y(x). \tag{1}$$

Equations of this type occur very frequently in theoretical physics (see, for example, [18]), and there is a real need to be able to solve them both efficiently and reliably by numerical methods. In (1), E is a real number denoting the *energy* and V is a given function which denotes the potential. We investigate two cases.

In the first specific case, $V(x)$ is an even function and $y(x) \to 0$ for $x \to \pm\infty$. As example of potentials which satisfy these properties, we present the following, which is well known in several areas of physics:

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The one-dimensional anharmonic oscillator potential

$$V_{\mathrm{i}}(x) = x^2 + \frac{\lambda x^2}{1+\gamma x^2}, \quad \lambda \text{ and } \gamma \text{ parameters}. \tag{2}$$

For the numerical solution of the specific eigenvalue Schrödinger equation (1), the following group of algorithms are available: (1) Rayleigh–Ritz methods [19], (2) perturbation methods [2,14,15], (3) methods using Padé approximants [17], (4) direct numerical integration techniques or boundary value techniques [6–9] and (5) an operator method based upon the SO(2,1) dynamic group [5]. Analytical approaches to the Schrödinger equation (1) have been obtained for $V_{\mathrm{i}}(x)$ by Flessas [11,12], Varma [25], Whitehead et al. [26]. The most popular methods (for the reasons fully described in [4,21]) for the numerical integration of the eigenvalue Schrödinger equation are the shooting techniques. A well-known method of this category is the *Numerov's method*.

In the second case, $V(x)$ is a general function and $y(x) \to 0$ for $x \to 0$. As examples of potentials which satisfy these properties, we present the following potentials, which are well known in several areas of physics:

(i) The Morse potential (Kobeissi and Kobeissi [16], Yano et al. [27]):

$$V_{\mathrm{gi}}(x) = D\big[1 - \exp(-aX)\big]^2, \tag{3}$$

where $X = x - x_{\mathrm{e}}$, $x_{\mathrm{e}} = 0$, $a = 1$, and $D = 1000$.

(ii) The Woods–Saxon potential (Adam et al. [1]):

$$V_{\mathrm{gii}}(x) = \frac{u_0}{1+t} - \frac{u_0 t}{a_0(1+t)^2}, \tag{4}$$

where $t = \exp((x - x_{\mathrm{e}})/a_0)$, $u_0 = -50$, $x_{\mathrm{e}} = 7$ and $a_0 = 0.6$.

The Schrödinger equation of the form (1) can be analyzed to a set of equations which belong to the general category of differential equations of the form

$$\mathbf{y}' = f(\mathbf{x}, \mathbf{y}), \tag{5}$$

which have solution with periodical or oscillating behavior. For the solution of the problems of the form (5), Runge–Kutta methods are very popular. Many packages which are used for the numerical solution of the Schrödinger equation consist of Runge–Kutta methods. One of the most popular Runge–Kutta method of these packages is the Runge–Kutta–Fehlberg 4(5) method.

Brusa and Nigro [3] introduced the *phase-lag* as an important property of methods for solving problems of the form (5) especially in the cases where its solution is periodic or has an oscillatory behavior. Two-step methods with minimal phase-lag have been developed for the numerical solution of problem (1) (see [23] and references therein).

In section 2 we will develop the basic theory for the phase-lag analysis of the Runge–Kutta methods. Based on this theory, we will describe in section 3 the derivation of the modified Runge–Kutta–Fehlberg method with minimal phase-lag. In sec-

tion 4, the basic theory for the phase-lag analysis of the block Runge–Kutta methods is introduced. In section 5 we develop a block embedded Runge–Kutta–Fehlberg method based on the second-order Runge–Kutta–Fehlberg scheme. In section 6, the error estimation procedure is described for the embedded methods and for the block embedded methods. Finally, in section 7, the application of the developed methods to problem (1) is presented, and extended numerical results based on the potentials V_{i}, V_{gi} and V_{gii} are produced to show the efficiency of the new approach.

2. Phase-lag analysis of the Runge–Kutta methods

To develop the new method we use the test equation

$$y' = \mathrm{i}vy, \quad v \text{ real}. \tag{6}$$

Based on the reasons fully described in Houwen et al. [13], we shall confine our considerations to homogeneous phase-lag, and, based on its definition given in that work, it is convenient to use a test equation with an exact solution of the form $\mathrm{e}^{\mathrm{i}vx}$. However, as is shown by our numerical results, inhomogeneous problems can successfully be dealt with by increasing the order of homogeneous phase-lag. By comparing the exact and the numerical solution for this equation and by requiring that these solutions are in phase with maximal order in the step-size h, we derive the so-called *phase-lag relation*.

For first-order equations we write the m-stage explicit Runge–Kutta method in the matrix form given in table 1.

Based on the table 1, we have that for an explicit m-stage s-block Runge–Kutta method the quantity y_{n+1} is given by

$$\begin{aligned} y_{n+1}^{(0)} &= y_n, \\ y_{n+1}^{(q)} &= y_n + h \sum_{p=0}^{q-1} g_{q,p} f\bigl(x_{n-1} + a_p h, y_{n+1}^{(p)}\bigr), \quad q = 1, \ldots, s, \\ y_{n+1} &= y_{n+1}^{(s)}, \end{aligned} \tag{7}$$

Table 1
m-stage explicit Runge–Kutta method.

0					
a_1	b_{10}				
a_2	b_{20}	b_{21}			
$\vdots$	$\vdots$	$\vdots$			
a_m	$b_{m,0}$	$b_{m,1}$	$\ldots$	$b_{m,m-1}$	
	$d_{0,0}$	$d_{0,1}$	$\ldots$	$d_{0,m-1}$	$d_{0,m}$

where $a_j = 1$ for $j > m$, $g_{i,j} = b_{i,j}$ for $i = 1, \ldots, m$, $j = 1, \ldots, i-1$, $g_{i,j} = d_{i,j}$ for $i = m+1$, $j = 1, \ldots, i-1$ and $g_{i,j} = c_{r,t}$ for $i = m+2, \ldots, m+k$, $j = 1, \ldots, i-1$, $r = 0, \ldots, k$, $t = 0, \ldots, m+k$.

Application of the above method to (6) yields the numerical solution

$$y_n = a_*^n y_0 \quad \text{and} \quad a_* = A_m\big(H^2\big) + \mathrm{i}H B_m\big(H^2\big), \quad H = vh, \tag{8}$$

where

$$\begin{aligned} A_m\big(H^2\big) &= 1 - t_2 H^2 + t_4 H^4 + t_6 H^6 + \cdots, \\ B_m\big(H^2\big) &= 1 - t_3 H^2 + t_5 H^4 + t_7 H^6 + \cdots \end{aligned} \tag{9}$$

are polynomials in H^2, completely defined by Runge–Kutta parameters a_i and b_{ij}, $i = 0, \ldots, m$, $j = 1, \ldots, i-1$. The dissipative factor is $a_* = a_*(H)$, and y_n denotes the approximation to $y(x_n)$, where $x_n = nh$, $n = 0, 1, \ldots$.

A comparison of (8) with the solution of (6) leads to the following definition of the *dispersion or phase error or phase-lag and the dissipative error*.

Definition 1 (see [13] and [22]). In the explicit m-stage Runge–Kutta method, presented in table 1, the quantities

$$t(H) = H - \arg\big[a_*(H)\big], \qquad a(H) = 1 - \big|a_*(H)\big| \tag{10}$$

are, respectively, called the phase-lag and the dissipative error. If $t(H) = \mathrm{O}(H^{r+1})$ and $a(H) = \mathrm{O}(H^{s+1})$, then the method is said to be of phase-lag order r and dissipative order s.

We also have the following theorem (for the detailed proof, see Simos [22]):

Theorem 1. For the Runge–Kutta method, given by table 1 and (8), we have the following formula for the direct calculation of the phase-lag order r and the phase-lag constant c:

$$\tan(H) - H\left[\frac{B_m(H^2)}{A_m(H^2)}\right] = cH^{r+1} + \mathrm{O}\big(H^{r+3}\big). \tag{11}$$

Using formulas (11) and (9) we derive the phase-lag relations for a fourth-algebraic-order method. The results are shown in table 2. It is clear from this table that we have a considerable extension to the table given by Houwen et al. [13]. We also note that for a fourth-order method we have that $t_4 = 1/24$ and $t_5 = 1/120$. In table 3 we present the results for the second-order Runge–Kutta methods.

Table 2
Phase-lag conditions of the RK method of algebraic order four.

Phase-lag order	Phase-lag conditions
4	$t_2 = \frac{1}{2},\ t_3 = \frac{1}{6}$
6	$t_4 - t_5 = \frac{1}{30}$
8	$t_4 + 3t_6 - 3t_7 = \frac{4}{105}$
10	$2t_4 + 5t_6 + 15t_8 - 15t_9 = \frac{29}{378}$
12	$17t_4 + 42t_6 + 105t_8 + 315t_{10} - 315t_{11} = \frac{323}{495}$
14	$62t_4 + 153t_6 + 378t_8 + 945t_{10} + 2835t_{12} - 2835t_{13} = \frac{1021}{429}$
16	$1382t_4 + 3410t_6 + 8415t_8 + 20790t_{10} + 51975t_{12} + 155925t_{14} - 155925t_{15} = \frac{217241}{4095}$
18	$21844t_4 + 53898t_6 + 132990t_8 + 328185t_{10} + 810810t_{12} + 2027025t_{14} + 6081075t_{16} - 6081075t_{17} = \frac{2993509}{3570}$
20	$929569t_4 + 2293620t_6 + 5659290t_8 + 13963950t_{10} + 34459425t_{12} + 85135050t_{14} + 212837625t_{16} + 638512875t_{18} - 638512875t_{19} = \frac{103730599}{2907}$

Table 3
Explicit Runge–Kutta–Fehlberg method of order four (RKF4). The coefficients are defined in [10].

0					
a_1	b_{10}				
a_2	b_{20}	b_{21}			
a_3	b_{30}	b_{31}	b_{32}		
a_4	b_{40}	b_{41}	b_{42}	b_{43}	
	c_0	c_1	c_2	c_3	c_4

3. Derivation of the modified Runge–Kutta–Fehlberg method with minimal phase-lag

We will derived here the modified Runge–Kutta–Fehlberg method with phase-lag of order six based on the well-known Runge–Kutta fourth-order Fehlberg method.

In table 3 we present the well-known fourth-order Runge–Kutta–Fehlberg method.

If we apply the method parametrised by table 3 to the test equation (6), we have the following theorem:

Theorem 2. The method, parameterised by table 3 with coefficients $a_i, b_{i,j}, c_k$, $i = 1(1)4$, $j = 0(1)i - 1$, $k = 0(1)4$, given in [10], is a fourth-order Runge–Kutta method with phase-lag of order 6.

Proof. Application of the method RKF4 to (6) leads to (8) with

$$\begin{aligned} A_4\big(H^2\big) &= 1 - t_2H^2 + t_4H^4, \\ B_4\big(H^2\big) &= 1 - t_3H^2 + t_5H^4, \end{aligned} \tag{12}$$

where

$$t_2 = \frac{1}{2}, \qquad t_4 = \frac{1}{24}, \qquad t_3 = \frac{1}{6}, \qquad t_5 = \frac{a_2(1-2a_2)H^4}{48(5a_2^2-4a_2+1)}. \tag{13}$$

Based on equations (13) and on table 2 (with the notation that $t_4 = 1/24$) and $t_5 = 1/120$ for a fourth-order Runge–Kutta method), we have that the method is of phase-lag order six if the following equation is satisfied:

$$t_4 - t_5 = \frac{1}{30}. \tag{14}$$

Solving this equation we have that

$$a_2 = \frac{1}{4} \quad \text{or} \quad a_2 = \frac{2}{5}. \tag{15}$$

We choose the value $a_2 = 1/4$. A similar result without proof and analysis can be found in [24]. □

From (11) and for the value of parameter a_2 given above and the parameters of the method given in the appendix, we have that the phase-lag of the method is equal to

$$t(H) = \tan(H) - \frac{HB_4(H^2)}{A_4(H^2)} = -\frac{H^7}{840} + \mathrm{O}\big(H^9\big). \tag{16}$$

Definition 2. We call a Runge–Kutta method an embedded method when a local phase-lag error estimate is included. This local phase-lag error estimate is obtained from the difference between the m-stages of the method which produce a numerical solution y_{n+1}^L of phase-lag order q and the $(m+1)$-stages of the method which produce a numerical solution y_{n+1}^H of phase-lag order $q+2$.

Based on the above definition, we have produced an embedded Runge–Kutta–Fehlberg 4(6) method. This, because the embedded method, consists by two methods – one with phase-lag of order four (which is equal to algebraic order of the method) and the other with minimal phase-lag of order six (see equation (16)).

4. Block Runge–Kutta methods

For first-order equations we introduce the m-stage $(k+1)$-block explicit Runge–Kutta method in the matrix form given in table 4.

We have the following definition:

Definition 3. We call a Runge–Kutta method a k-block method when consists of k embedded Runge–Kutta schemes.

Table 4
m-stage $(k+1)$-block explicit Runge–Kutta method.

0											
a_1	b_{10}										
a_2	b_{20}	b_{21}									
$\vdots$	$\vdots$	$\vdots$									
a_m	$b_{m,0}$	$b_{m,1}$	$\dots$	$b_{m,m-1}$							
	$d_{m+1,0}$	$d_{m+1,1}$	$\dots$	$d_{m+1,m-1}$	$d_{m+1,m}$						
	$c_{0,0}$	$c_{0,1}$	$\dots$	$c_{0,m-1}$	$c_{0,m}$	$c_{0,m+1}$					
	$c_{1,0}$	$c_{1,1}$	$\dots$	$c_{1,m-1}$	$c_{1,m}$	$c_{1,m+1}$	$c_{1,m+2}$				
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$			
	$c_{s,0}$	$c_{s,1}$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$c_{s,m+s-1}$	$c_{s,m+s}$		
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	
	$c_{k,0}$	$c_{k,1}$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$c_{k,m+k-1}$	$c_{k,m+k}$

The phase-lag error estimate is given by

$$TEC = \left|y_{n+1}^{(s)} - y_{n+1}^{(s-2)}\right|, \tag{17}$$

where s is the phase-lag order.

So it is obvious that the *block method* is very useful for cases, in which we want to use a variable-step procedure.

Application of the above method to (6) yields the numerical solution

$$y_n = a_*^n y_0 \quad \text{and} \quad a_* = A_{m,k}\left(H^2\right) + \mathrm{i}HB_{m,k}\left(H^2\right), \quad H = vh, \tag{18}$$

where

$$\begin{aligned} A_{m,k}\left(H^2\right) &= 1 - t_2H^2 + t_4H^4 + t_6H^6 \cdots, \\ B_{m,k}\left(H^2\right) &= 1 - t_3H^2 + t_5H^4 + t_7H^6 \cdots \end{aligned} \tag{19}$$

are polynomials in H^2, completely defined by Runge–Kutta parameters a_i, b_{ij} and $c_{k,l}$, $i = 1, \dots, m$, $j = 1, \dots, i-1$, $l = 0, \dots, m+k$. The dissipative factor is $a_* = a_*(H)$, and y_n denotes the approximation to $y(x_n)$, where $x_n = nh$, $n = 0, 1, \dots$.

A comparison of (18) with the solution of (6) leads to the definition of the *dispersion or phase error or phase-lag and the dissipative error* given above.

We have, now, the following theorem for the block methods which is similar to the previous theorem 1 for the simple Runge–Kutta methods (for the detailed proof, see Simos [22]):

Theorem 3. For the m-stage $(k+1)$-block Runge–Kutta method, given by table 4, we have the following formula for the direct calculation of the phase-lag order r and the phase-lag constant c:

$$\tan(H) - H\left[\frac{B_{m,k}(H^2)}{A_{m,k}(H^2)}\right] = cH^{r+1} + \mathrm{O}\left(H^{r+3}\right). \tag{20}$$

Table 5
Phase-lag conditions of the RK method of algebraic order two.

Phase-lag order	Phase-lag conditions
4	$\frac{1}{3} + t_3 - t_2 = 0$
6	$\frac{2}{15} + t_2 t_3 + t_4 - t_5 - t_2^2 = 0$
8	$\frac{17}{315} + t_6 - t_4 t_3 + 2t_4 t_2 - t_2 t_5 + t_2^2 t_3 - t_2^3 - t_7 = 0$
10	$-t_6 t_3 + t_4 t_5 + \frac{62}{2835} + t_8 + 3t_4 t_2^2 - t_2 t_7 - t_2^2 t_5 + 2t_6 t_2 + t_2^3 t_3 - t_2^4 - t_4^2 - t_9$ $- 2t_4 t_2 t_3 = 0$
12	$t_4 t_7 + \frac{1382}{155925} + 4t_4 t_2^3 - 2t_6 t_4 - 3t_4^2 t_2 + 3t_6 t_2^2 - t_8 t_3 + t_{10} - t_2^2 t_7 - t_2 t_9 - t_2^3 t_5 + t_4^2 t_3$ $+ t_2^4 t_3 + 2t_8 t_2 + t_6 t_5 - t_2^5 - t_{11} - 2t_6 t_2 t_3 + 2t_4 t_2 t_5 - 3t_4 t_2^2 t_3 = 0$
14	$t_{12} - t_{13} - t_{10} t_3 + 2t_{10} t_2 - 2t_8 t_2 t_3 + 2t_6 t_4 t_3 - 6t_6 t_4 t_2 + 2t_6 t_2 t_5 - 3t_6 t_2^2 t_3 + 3t_4^2 t_2 t_3$ $+ 2t_4 t_2 t_7 + 3t_4 t_2^2 t_5 - 4t_4 t_2^3 t_3 + t_4^3 - t_2^6 - 2t_8 t_4 + t_8 t_5 + 3t_8 t_2^2 - t_6^2 + t_6 t_7 + 4t_6 t_2^3$ $+ t_4 t_9 - t_4^2 t_5 - 6t_4^2 t_2^2 + 5t_4 t_2^4 - t_2 t_{11} - t_2^2 t_9 - t_2^3 t_7 - t_2^4 t_5 + t_2^5 t_3 + \frac{21844}{6081075} = 0$
16	$t_{14} - t_{15} - 12t_6 t_4 t_2^2 + 2t_6 t_2 t_7 + 3t_6 t_2^2 t_5 - 4t_6 t_2^3 t_3 - 3t_4^2 t_2 t_5 + 6t_4^2 t_2^2 t_3 + 2t_4 t_2 t_9$ $+ 3t_4 t_2^2 t_7 + 4t_4 t_2^3 t_5 - 5t_4 t_2^4 t_3 - t_2^7 - t_{12} t_3 + 2t_{12} t_2 - 2t_{10} t_4 + t_{10} t_5 + 3t_{10} t_2^2$ $- 2t_8 t_6 + t_8 t_7 + 4t_8 t_2^3 + t_6 t_9 + t_6^2 t_3 - 3t_6^2 t_2 + 3t_6 t_4^2 + 5t_6 t_2^4 + t_4 t_{11} - t_4^2 t_7 - t_4^3 t_3$ $+ 4t_4^3 t_2 - 10t_4^2 t_2^3 + 6t_4 t_2^5 - t_2 t_{13} - t_2^2 t_{11} - t_2^3 t_9 - t_2^4 t_7 - t_2^5 t_5 + t_2^6 t_3 - 2t_{10} t_2 t_3$ $+ 2t_8 t_4 t_3 - 6t_8 t_4 t_2 + 2t_8 t_2 t_5 - 3t_8 t_2^2 t_3 - 2t_6 t_4 t_5 + 6t_6 t_4 t_2 t_3 + \frac{929569}{638512875} = 0$

Based on formula (20) and from (19), we derived in table 5 the phase-lag relations for a second-algebraic-order method.

5. Derivation of the block Runge–Kutta–Fehlberg method

Based on the simple second-algebraic-order Runge–Kutta–Fehlberg method (see [10]), we introduce the new explicit block Runge–Kutta–Fehlberg (BRKF) method given in table 6.

If we apply any stage of the method of table 6 to the test equation (6), we have the following theorem:

Theorem 4. The method, described in table 6 with coefficients $c_{k,l}$, $l = 1, \ldots, m+k$, given in the appendix, is a 3-block 3-stage Runge–Kutta method with phase-lag orders given in table 7.

See the appendix for a detailed proof.

6. Numerical illustration

6.1. Local phase-lag error estimate

The embedded methods described in this paper are used for the solution of the Schrödinger equation, which is analyzed on a set of first-order equations.

To estimate the error we use the other stage of the Runge–Kutta–Fehlberg 4(6) method (of phase-lag order four) (for coefficients, see [10]). The definition of these

Table 6
A 3-block 3-stage Runge–Kutta–Fehlberg method (BRKF).

0						
1/4	1/4					
27/40	−189/800	729/800				
	$c_{0,0}$	$c_{0,1}$	$c_{0,2}$	$c_{0,3}$		
	$c_{1,0}$	$c_{1,1}$	$c_{1,2}$	$c_{1,3}$	$c_{1,4}$	
	$c_{2,0}$	$c_{2,1}$	$c_{2,2}$	$c_{2,3}$	$c_{2,4}$	$c_{2,5}$

Table 7
Phase-lag for the 3-block 3-stage Runge–Kutta–Fehlberg method given in table 6.

Stage	Phase-lag
0	$\frac{H^9}{99225}$
1	$\frac{H^{11}}{9823275}$
2	$\frac{H^{13}}{1404728325}$

Table 8
Embedded Runge–Kutta–Fehlberg method 4(6). The coefficients are defined in [10] with the free parameter a_2 defined in previous section.

0						
1/6	1/6					
1/4	1/16	3/16				
2/5	14/125	−12/125	48/125			
1	17/20	6/5	−24/5	15/4		
1/2	1/10	−3/10	34/45	−5/72	1/72	
c	1/4	0	−16/27	125/108	5/27	
error	1/4	0	−16/9	125/36	1/18	−2

coefficients is based on the fact that $a_2 = 1/4$. The resulting method is presented in table 8.

Our error control strategy is simple. At every x_n, we control the estimate of the *local phase-lag error TEC* from (17).

If *TEC* is less than the maximum allowable local error *TOL*, given by the user, then the new step-size is given by

$$h_{\text{new}} = 0.9 h_{\text{old}} \left\{ \frac{TOL}{\|TEC\|_\infty} \right\}^{1/q}, \tag{21}$$

where $q = 1/6$. If *TEC* is greater than the maximum allowable local error *TOL*, then this step-size is rejected and we repeat the step.

6.2. Block methods

For the block method introduced in section 5 the error control strategy is simple. At every x_n we control, for the k-block, the estimate of the *local phase-lag error TEC*

from (17). The *TEC* is, for every block, i.e., for an embedded method, the difference between the approximation of the solution $y(x_n)$, y_{n+1}^L, which is obtained using the method with *phase-lag of low order* and the approximation of the solution $y(x_n)$, y_{n+1}^H, which is obtained using the method with *phase-lag of high order* (see definition 1 and formula (17)).

If *TEC* is less than the maximum allowable local error *TOL* given by the user, then we use this block to calculate the solution at x_n and the new step-size is given by (21), where q is the phase-lag order of the successful k-block. If *TEC* is greater than the maximum allowable local error *TOL* then we repeat the previous developed strategy for the $(k+1)$-block.

6.3. Numerical tests

To test the validity of the proposed new methods we have applied the new methods to potential (2) for specific choices of the parameters, for the first case. Based on previous works (see Fack et al. [6–9]), we choose appropriate values of R, the cut-off value for which we assume that $f(R) = 0$. These are given in the tables. For the second case, we have applied the new method to the potentials (3) and (4). For comparison purposes, we have used the well-known classical Runge–Kutta–Fehlberg 4(5) method.

In table 9 we present the absolute errors $|E^{\text{calculated}} - E^{\text{exact}}|$ and of real time of computation for the energy values E_n, $n = 1, \ldots, 4$, for the potential (2) with $\lambda = \gamma = 0$ using the following methods:

(1) MI: the classical Runge–Kutta–Fehlberg 4(5) method;

(2) MII: the modified Runge–Kutta–Fehlberg 4(6) method produced in this paper and presented in table 8;

(3) MIII: the block Runge–Kutta–Fehlberg method (BRKF) introduced in section 5 for initial step-size $h_0 = 0.1$.

In table 10 we present the absolute errors $|E^{\text{calculated}} - E^{\text{exact}}|$ and of real time of computation for the energy values E_n, $n = 1, \ldots, 4$, for the potential (2) with $\lambda = \gamma = 10$ using the methods mentioned above for initial step-size $h_0 = 0.1$.

In table 11 we present the absolute errors $|E^{\text{calculated}} - E^{\text{exact}}|$ and of real time of computation for the energy values E for the potential (3) using the methods mentioned above. $R = 10.0$ and $h_0 = 0.125$.

In table 12 we present the absolute errors $|E^{\text{calculated}} - E^{\text{exact}}|$ and of real time of computation for the energy values E for the potential (4) using the methods mentioned above. $R = 15.0$ and $h_0 = 0.125$.

From the above-mentioned results, it is easy to see that the new methods are more accurate and efficient compared with the well-known Runge–Kutta–Fehlberg 4(5) method.

Table 9
Comparison of absolute errors $|E^{\text{calculated}} - E^{\text{exact}}|$ and of real time of computation for potential (2) with $\lambda = \gamma = 0$, produced by the classical Runge–Kutta–Fehlberg 4(5) method (MI), the present modified Runge–Kutta–Fehlberg 4(6) method with phase-lag of order 6 (MII) and the block Runge–Kutta–Fehlberg method (BRKF) (MIII). $R = 10$.

Exact eigenvalues E_n	Absolute errors		
	MI	MII	MIII
$E_0 = 1$	7.9×10^{-8}	1.0×10^{-10}	9.3×10^{-12}
$E_6 = 7$	5.9×10^{-6}	1.2×10^{-8}	8.3×10^{-10}
$E_{14} = 15$	6.3×10^{-5}	1.5×10^{-6}	7.3×10^{-8}
$E_{22} = 23$	2.1×10^{-4}	1.7×10^{-5}	8.8×10^{-7}
Total time of computation (in s)	8.3	6.5	5.3

Table 10
Comparison of absolute errors $|E^{\text{calculated}} - E^{\text{exact}}|$ and of real time of computation for potential (2) with $\lambda = \gamma = 10$, produced by the classical Runge–Kutta–Fehlberg 4(5) method (MI), the present modified Runge–Kutta–Fehlberg 4(6) method with phase-lag of order 6 (MII) and the block Runge–Kutta–Fehlberg method (BRKF) (MIII). $R = 10$.

Exact eigenvalues E_n	Absolute errors		
	MI	MII	MIII
$E_0 = 1.580022327$	2.8×10^{-6}	1.0×10^{-8}	9.9×10^{-10}
$E_6 = 3.879036830$	4.0×10^{-7}	3.2×10^{-8}	9.8×10^{-10}
$E_{14} = 5.832767530$	9.7×10^{-7}	5.0×10^{-8}	8.7×10^{-10}
$E_{22} = 7.903154152$	8.1×10^{-6}	3.1×10^{-7}	9.1×10^{-9}
Total time of computation (in s)	9.0	7.4	6.1

Table 11
Comparison of absolute errors $|E^{\text{calculated}} - E^{\text{exact}}|$ and of real time of computation for potential (3), produced by the classical Runge–Kutta–Fehlberg 4(5) method (MI), the present modified Runge–Kutta–Fehlberg 4(6) method with phase-lag of order 6 (MII) and the block Runge–Kutta–Fehlberg method (BRKF) (MIII). $R = 10$.

Exact eigenvalues E_n	Absolute errors		
	MI	MII	MIII
$E_0 = 31.3727766017$	4.4×10^{-4}	1.6×10^{-6}	9.1×10^{-8}
$E_2 = 151.8638830084$	7.1×10^{-3}	3.1×10^{-4}	8.7×10^{-6}
$E_4 = 264.3549894152$	4.0×10^{-2}	2.1×10^{-3}	8.5×10^{-5}
$E_6 = 368.8460958219$	6.1×10^{-3}	4.2×10^{-4}	9.1×10^{-6}
$E_8 = 465.3372022286$	7.2×10^{-2}	4.0×10^{-3}	8.8×10^{-5}
Total time of computation (in s)	13.2	11.5	10.0

Table 12
Comparison of absolute errors $|E^{\text{calculated}} - E^{\text{exact}}|$ and of real time of computation for potential (4), produced by the classical Runge–Kutta–Fehlberg 4(5) method (MI), the present modified Runge–Kutta–Fehlberg 4(6) method with phase-lag of order 6 (MII) and the block Runge–Kutta–Fehlberg method (BRKF) (MIII). $R = 10$.

Exact eigenvalues E_n	Absolute errors		
	MI	MII	MIII
$E_0 = -49.457788728$	3.2×10^{-3}	4.3×10^{-5}	8.8×10^{-7}
$E_4 = -41.232607772$	2.1×10^{-4}	5.4×10^{-6}	7.9×10^{-8}
$E_9 = -22.588602257$	6.2×10^{-3}	4.8×10^{-5}	8.1×10^{-7}
$E_{13} = -3.9082324808$	7.8×10^{-2}	6.4×10^{-4}	7.7×10^{-6}
Total time of computation (in s)	8.8	7.2	6.3

7. Conclusions

In this paper, some new numerical methods for the numerical solution of the Schrödinger equation are developed. The methods are based on the minimization of the phase-lag. More specifically, a Runge–Kutta method with minimal phase-lag is produced based on the fourth-order Runge–Kutta–Fehlberg method. Based on this method, we have constructed a modified Runge–Kutta–Fehlberg method with phase-lag of order six. Based on the new method and the appropriate fifth-algebraic-order method with phase-lag of order four, we have constructed a new modified embedded Runge–Kutta–Fehlberg scheme.

The block Runge–Kutta methods with minimal phase-lag are, also, introduced in the present work. A block Runge–Kutta–Fehlberg method is obtained.

The numerical results indicate that the new methods are significantly more efficient than the classical fourth-order Runge–Kutta–Fehlberg method for the solution of the Schrödinger equation.

Appendix: Construction of the BRKF scheme

Case I: Phase-lag of order 8

Application of the first block of the BRKF method to (6) leads to (18) with

$$\begin{aligned} A_{3,1}\big(H^2\big) &= 1 - t_2 H^2 + t_4 H^4, \\ B_{3,1}\big(H^2\big) &= b_{0,0} + b_{0,1} + b_{0,2} + b_{0,3} - t_3 H^2, \end{aligned} \tag{22}$$

where

$$t_2 = \frac{10b_{0,1} + 27b_{0,2} + 40b_{0,3}}{40}, \qquad t_3 = \frac{729b_{0,2} + 1600b_{0,3}}{3200}, \qquad t_4 = \frac{117b_{0,3}}{704}. \tag{23}$$

We note that a necessary relation from the algebraic order conditions is

$$b_{0,0} + b_{0,1} + b_{0,2} + b_{0,3} = 1. \tag{24}$$

The solution of the system of equations produced, based on the relations given in table 4 and in (23) and (24), is given by

$$b_{0,0} = -\frac{4477}{98415}, \qquad b_{0,1} = \frac{17756}{25515}, \qquad b_{0,2} = \frac{523520}{1791153}, \qquad b_{0,3} = \frac{704}{12285}. \tag{25}$$

From (20) and for the values of parameters given above, we have that the phase-lag of the method is equal to

$$t(H) = \tan(H) - \frac{HB_{3,1}(H^2)}{A_{3,1}(H^2)} = \frac{H^9}{99225} + \mathrm{O}\big(H^{11}\big). \tag{26}$$

Case II: Phase-lag of order 10

Application of the second block of the BRKF method to (6) leads to (18) with

$$\begin{aligned} A_{3,2}\big(H^2\big) &= 1 - t_2H^2 + t_4H^4, \\ B_{3,2}\big(H^2\big) &= b_{0,0} + b_{0,1} + b_{0,2} + b_{0,3} - t_3H^2 + t_5H^4, \end{aligned} \tag{27}$$

where

$$\begin{aligned} t_2 &= \frac{10b_{1,1} + 27b_{1,2} + 40(b_{1,3} + b_{1,4})}{40}, \qquad t_3 = \frac{5103b_{1,2} + 11200b_{1,3} + 9600b_{1,4}}{22400}, \\ t_4 &= \frac{2457b_{1,3} + 1408b_{1,4}}{14784}, \qquad t_5 = \frac{b_{1,4}}{105}. \end{aligned} \tag{28}$$

We note that a necessary relation from the algebraic order conditions is

$$b_{1,0} + b_{1,1} + b_{1,2} + b_{1,3} + b_{1,4} = 1. \tag{29}$$

The solution of the system of equations produced, based on the relations given in table 4 and in (28) and (29), is given by

$$\begin{aligned} b_{1,0} &= \frac{1076}{177147}, \qquad b_{1,1} = \frac{29492}{45927}, \qquad b_{1,2} = \frac{3366400}{16120377}, \\ b_{1,3} &= \frac{704}{22113}, \qquad b_{1,4} = \frac{1}{9}. \end{aligned} \tag{30}$$

From (20) and for the values of parameters given above, we have that the phase-lag of the method is equal to

$$t(H) = \tan(H) - \frac{HB_{3,2}(H^2)}{A_{3,2}(H^2)} = \frac{H^{11}}{9823275} + \mathrm{O}\big(H^{13}\big). \tag{31}$$

Case III: Phase-lag of order 12

Application of the third block of the BRKF method to (6) leads to (18) with

$$\begin{aligned} A_{3,3}\big(H^2\big) &= 1 - t_2H^2 + t_4H^4 + t_6H^6, \\ B_{3,3}\big(H^2\big) &= b_{0,0} + b_{0,1} + b_{0,2} + b_{0,3} - t_3H^2 + t_5H^4, \end{aligned} \tag{32}$$

where

$$\begin{aligned} t_2 &= \frac{10b_{2,1} + 27b_{2,2} + 40(b_{2,3} + b_{2,4} + b_{2,5})}{40}, \\ t_3 &= \frac{45927b_{2,2} + 100800b_{2,3} + 86400b_{2,4} + 89600b_{2,5}}{201600}, \\ t_4 &= \frac{22113b_{2,3} + 12672b_{2,4} + 14784b_{2,5}}{133056}, \qquad t_5 = \frac{3b_{2,4} + 5b_{2,5}}{315}, \qquad t_6 = -\frac{b_{2,5}}{945}. \end{aligned} \tag{33}$$

We note that a necessary relation from the algebraic order conditions is

$$b_{2,0} + b_{2,1} + b_{2,2} + b_{2,3} + b_{2,4} + b_{2,5} = 1. \tag{34}$$

The solution of the system of equations produced, based on the relations given in table 4 and in (33) and (34), is given by

$$\begin{aligned} b_{2,0} &= \frac{3652}{137781}, \qquad b_{2,1} = \frac{34376}{56133}, \qquad b_{2,2} = \frac{3616000}{19702683}, \\ b_{2,3} &= \frac{64}{2457}, \qquad b_{2,4} = \frac{2}{33}, \qquad b_{2,5} = \frac{1}{11}. \end{aligned} \tag{35}$$

From (20) and for the values of parameters given above, we have that the phase-lag of the method is equal to

$$t(H) = \tan(H) - \frac{HB_{3,3}(H^2)}{A_{3,3}(H^2)} = \frac{H^{13}}{1404728325} + \mathrm{O}\big(H^{15}\big). \tag{36}$$

References

[1] Gh. Adam, L.Gr. Ixaru and A. Corciovei, A first-order perturbative numerical method for the solution of the radial Schrödinger equation, J. Comput. Phys. 22 (1976) 1–33.

[2] N. Bessis and G. Bessis, A note on the Schrödinger equation for the $x^2 + \lambda x^2/(1 + gx^2)$ potential, J. Math. Phys. 21 (1980) 2780–2785.

[3] L. Brusa and L. Nigro, A one-step method for direct integration of structural dynamical equations, Internat. J. Numer. Methods Engrg. 15 (1980) 685–699.

[4] J.R. Cash, A.D. Raptis and T.E. Simos, A sixth-order exponentially fitted method for the numerical solution of the radial Schrödinger equation, J. Comput. Phys. 91 (1990) 413–423.

[5] V. Fack, H. De Meyer and G. Vanden Berghe, Dynamic-group approach to the $x^2 + \lambda x^2/(1 + gx^2)$, J. Math. Phys. 27 (1986) 1340–1343.

[6] V. Fack, H. De Meyer and G. Vanden Berghe, Some finite difference methods for computing eigenvalues and eigenvectors of special two-point boundary value problems, J. Comput. Appl. Math. 20 (1987) 211–217.

[7] V. Fack and G. Vanden Berghe, A finite difference approach for the calculation of perturbed oscillator energies, J. Phys. A: Math. Gen. 18 (1985) 3355–3363.
[8] V. Fack and G. Vanden Berghe, A programme for the calculation of energy eigenvalues and eigenstates of a Schrödinger equation, Comput. Phys. Commun. 39 (1986) 187–196.
[9] V. Fack and G. Vanden Berghe, (Extended) Numerov method for computing eigenvalues of specific Schrödinger equations, J. Phys. A: Math. Gen. 20 (1987) 4153–4160.
[10] E. Fehlberg, Low-order classical Runge–Kutta formulas with stepsize control and their application to some heat transfer problems, NASA Technical Report 315, USA (1969).
[11] G.P. Flessas, On the Schrödinger equation for the $x^2 + \lambda x^2/(1 + gx^2)$ interaction, Phys. Lett. 83A (1981) 121–122.
[12] G.P. Flessas, Definite integrals as solutions for the $x^2 + \lambda x^2/(1 + gx^2)$ potential, J. Phys. A: Math. Gen. 15 (1982) L97–L101.
[13] P.J. van der Houwen and B.P. Sommeijer, Explicit Runge–Kutta(–Nyström) methods with reduced phase errors for computing oscillating solutions, SIAM J. Numer. Anal. 24 (1987) 595–617.
[14] R.S. Kaushal, Small g and large λ solution of the Schrödinger equation doe the interaction $x^2 + \lambda x^2/(1 + gx^2)$, J. Phys. A: Math. Gen. 12 (1979) L253–L258.
[15] J.P. Killingbeck, Some applications of perturbation theory to numerical integration methods for the Schrödinger equation, Comput. Phys. Commun. 18 (1979) 211–214.
[16] H. Kobeissi and M. Kobeissi, On testing difference equations for the diatomic eigenvalue problem, J. Comput. Chem. 9 (1988) 844–850.
[17] C.S. Lai and H. Lin, On the Schrödinger equation for the interaction $x^2 + \lambda x^2/(1 + gx^2)$, J. Phys. A: Math. Gen. 15 (1982) 1495–1502.
[18] L.D. Landau and F.M. Lifshitz, *Quantum Mechanics* (Pergamon Press, New York, 1965).
[19] A. Mitra, On the interaction of the type $\lambda x^2/(1 + gx^2)$, J. Math. Phys. 19 (1978) 2018–2022.
[20] T.E. Simos, Numerical solution of ordinary differential equations with periodical solution, Doctoral dissertation, National Technical University of Athens (1990).
[21] T.E. Simos, Exponential fitted methods for the numerical integration of the Schrödinger equation, Comput. Phys. Commun. 71 (1992) 32–38.
[22] T.E. Simos, Runge–Kutta interpolants with minimal phase-lag, Comput. Math. Appl. 26 (1993) 43–49.
[23] T.E. Simos, Eighth order methods with minimal phase-lag for accurate computations for the elastic scattering phase-shift problem, J. Math. Chem. 21 (1997) 359–372.
[24] T.E. Simos and A.B. Sideridis, Accurate numerical approximations to initial value problems with periodical solutions, Computing 50 (1993) 87–92.
[25] V.S. Varma, On the $x^2 + \lambda x^2/(1 + gx^2)$ interaction, J. Phys. A: Math. Gen. 14 (1981) L489–L492.
[26] R.R. Whitehead, A. Watt, G.P. Flessas and M.A. Nagarajan, Exact solutions of the Schrödinger equation $(-\mathrm{d}^2/\mathrm{d}x^2 + x^2 + \lambda x^2/(1 + gx^2))y(x) = Ey(x)$, J. Phys. A: Math. Gen. 15 (1982) 1217–1226.
[27] T. Yano, K. Kitani, M. Otsuka, S. Tomiyoshi, S. Matsushima, T. Wada and Y. Ezawa, A high speed method for eigenvalue problems III. Case of unsymmetrical potentials in Milne's method, Comput. Phys. Commun. 81 (1994) 409–424.