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Abstract: A new Runge-Kutta-Nystr^m method, with phase-lag and amplification error of order infinity, for the numerical solution of the Schr^{dinger} equation is developed in this paper. The new method is based on the Runge-Kutta-Nystr^m method with fourth algebraic order, developed by Dormand, El-Mikkawy and Prince. Numerical illustrations indicate that the new method is much more efficient than other methods derived for the same purpose.

Response to Reviewers: Reviewer #1: The authors modified the fourth order Runge-Kutta-Nystrom method. The numerical approach to me is OK. However, I think that efficiency evaluation of the method is too brief and more measurement is needed for a complete comparison with other methods. I suggest the authors use other ways to evaluate the performance of the new method. Moreover, it is of interest to know the efficiency at different orders.

We have read the reviewer's comments and we made the following changes:

- We added the bound states problem using eight eigenenergies. We present the figures with the efficiency of the methods for these eigenenergies and some remarks on the results. There are no other RKN methods of the same order that are used for the solution of the Schrodinger equation so that we can compare with.

We have also changed Theorem 1, so that it is more clear and precise.

A modified phase-fitted and amplification-fitted Runge-Kutta-Nyström method for the numerical solution of the Radial Schrödinger equation

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Abstract. A new Runge-Kutta-Nyström method, with phase-lag and amplification error of order infinity, for the numerical solution of the Schrödinger equation is developed in this paper. The new method is based on the Runge-Kutta-Nyström method with fourth algebraic order, developed by Dormand, El-Mikkawy and Prince. Numerical illustrations indicate that the new method is much more efficient than other methods derived for the same purpose.

Keywords: Runge-Kutta-Nyström methods, Phase-fitted, Amplification-fitted, Schrödinger, Phase-lag infinity.

PACS: 0.260, 95.10.E

1. Introduction

The one-dimensional or radial Schrödinger equation has the form

$$y''(x) + \left(E - \frac{l(l+1)}{x^2} - V(x) \right) y(x) = 0, \quad \text{where } 0 \leq x < \infty \quad (1)$$

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We call the term $l(l+1)/x^2$ the *centrifugal potential*, and the function $V(x)$ the *electric potential*. In (1), E is a real number denoting the *energy*, and l is a *quantum number*. The function $W(x) = l(l+1)/x^2 + V(x)$ denotes the *effective potential*, where $\lim_{x \rightarrow \infty} V(x) = 0$ and so $\lim_{x \rightarrow \infty} W(x) = 0$. The boundary conditions are $y(0) = 0$ together with a second boundary condition, for large values of x , determined by the physical considerations.

This type of equations appears in many scientific areas including, theoretical physics, nuclear physics, molecular physics, physical chemistry, quantum chemistry. For the numerical solution of equation (1) there is a high demand. The last three decades a lot of researchers have developed new methods to solve numerically the Schrödinger equation [3 – 14].

The purpose of this paper is to construct an explicit Runge-Kutta-Nyström with fourth algebraic order, phase lag of order infinity and amplification error of order infinity. The new method is based on the coefficients of the well-known fourth algebraic order Dormand, El-Mikkawy and Prince Runge-Kutta-Nyström method [1]. It is also based on the FSAL (first stage as last) technique, which means that the number of stages is four but it effectively uses only three stages at each step.

2. Modified Runge-Kutta-Nyström method

The general m -stage method for the equation

$$\frac{d^2u(t)}{dt^2} = f(t, u(t)) \quad (2)$$

is of the form

$$\begin{aligned} u_n &= u_{n-1} + h\hat{u}_{n-1} + h^2 \sum_{i=1}^m b_i f(t_{n-1} + c_i h, f_i), \\ \hat{u}_n &= \hat{u}_{n-1} + h \sum_{i=1}^m \hat{b}_i f(t_{n-1} + c_i h, f_i), \end{aligned} \quad (3)$$

where

$$f_i = u_{n-1} + hg_i c_i \hat{u}_{n-1} + h^2 \sum_{j=1}^{i-1} \alpha_{ij} f(t_{n-1} + c_j h, f_j), \quad i = 1, \dots, m \quad (4)$$

especially for the explicit Runge-Kutta-Nyström methods $c_1 = 0$ and more specifically for an FSAL explicit RKN method $c_m = 1$ and $c_{m,j} = b_j$ for $j = i$.

Table I. m-stage Runge-Kutta-Nyström method

c_1	1	0				
c_2	g_2	α_{21}				
c_3	g_3	α_{31}	α_{32}			
\vdots	\vdots	\vdots	\vdots			
c_m	g_m	$\alpha_{m,1}$	$\alpha_{m,2}$	\dots	$\alpha_{m,m-1}$	
		b_1	b_2	\dots	b_{m-1}	b_m
		\hat{b}_1	\hat{b}_2	\dots	\hat{b}_{m-1}	\hat{b}_m

The above expressions are presented in Table I.

As we can see in Table I, the Butcher table has an extra column as compared to a classical m-stage Runge-Kutta-Nyström method. For the classical method $g_i = 1, i = 2(1)m$. In the present paper and based on the requirement of phase and amplification fitting, values $g_i, i = 2(1)m$ are variable and depend on z (which is the product of the frequency v and the step-size h). In section (4) we will present a development of a phase and amplification fitted four-stage Runge-Kutta-Nyström method of algebraic order four, based on the well-known DEP Runge-Kutta-Nyström [1].

3. Phase lag and amplification error analysis for Runge-Kutta-Nyström methods

To develop the new method we use the test equation,

$$\frac{d^2u(t)}{dt^2} = (iv)^2u(t) \implies u''(t) = -v^2u(t), \quad v \in R \quad (5)$$

By applying the general method (3) to the test equation (5) we obtain the numerical solution

$$\begin{bmatrix} u_n \\ h\hat{u}_n \end{bmatrix} = D^n \begin{bmatrix} u_0 \\ h\hat{u}_0 \end{bmatrix}, \quad D = \begin{bmatrix} A(z^2) & B(z^2) \\ \dot{A}(z^2) & \dot{B}(z^2) \end{bmatrix}, \quad z = vh, \quad (6)$$

where A, B, \dot{A}, \dot{B} are polynomials in z^2 , completely determined by the parameters of the method (3).

The exact solution of (5) is given by

$$u(t_n) = \sigma_1[\exp(iz)]^n + \sigma_2[\exp(-iz)]^n, \quad (7)$$

where

$$\sigma_{1,2} = \frac{1}{2} \left[u_0 \pm \frac{(i\hat{u}_0)}{v} \right] \quad \text{or} \quad \sigma_{1,2} = |\sigma| \exp(\pm i\chi).$$

Substituting in (7), we have

$$u(t_n) = 2|\sigma|\cos(\chi + nz). \quad (8)$$

Furthermore we assume that the eigenvalues of D are ρ_1, ρ_2 , and the consequent eigenvectors are $[1, v_1]^T, [1, v_2]^T$, where $v_i = \dot{A}/(\rho_i - \dot{B}), i = 1, 2$. The numerical solution of (5) is

$$u_n = c_1\rho_1^n + c_2\rho_2^n, \quad (9)$$

where

$$c_1 = -\frac{v_2u_0 - h\hat{u}_0}{v_1 - v_2}, \quad c_2 = \frac{v_1u_0 - h\hat{u}_0}{v_1 - v_2}.$$

If ρ_1, ρ_2 are complex conjugate, then $c_{1,2} = |c|\exp(\pm iw)$ and $\rho_{1,2} = |\rho|\exp(\pm ip)$. By substituting in (9), we have

$$u_n = 2|c||\rho|^n\cos(w + np). \quad (10)$$

The following definition is originally formulated by van der Houwen and Sommeijer [2].

DEFINITION 1. (Phase-lag). Apply the RKN method (3) to the general method (5). Then we define the phase-lag

$$\Phi(z) = z - \arccos(\text{tr}(D)/2\sqrt{\det(D)})$$

. If $\Phi(z) = O(z^{q+1})$, then the RKN method is said to have phase-lag order q . In addition, the quantity $a(z) = 1 - \sqrt{\det(D)}$ is called amplification error.

Let us denote

$$\begin{aligned} R(z^2) &= \text{tr}(D) = A(z^2) + \dot{B}(z^2) \\ Q(z^2) &= \det(D) = A(z^2)\dot{B}(z^2) - \dot{A}(z^2)B(z^2) \end{aligned} \quad (11)$$

where $z = vh$. From definition 1 it follows that

$$\Phi(z) = z - \arccos\left(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right), \quad a(z) = 1 - \sqrt{Q(z^2)}. \quad (12)$$

If at a point $z, a(z) = 0$, then the Runge-Kutta-Nyström method has zero dissipation at this point.

We can also put forward an alternative definition for the case of infinite order of phase lag.

DEFINITION 2. (Phase-lag of order infinity). To obtain phase-lag of order infinity the relation $\Phi(z) = z - \arccos\left(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right) = 0$ must be hold.

From definition 2 we have the following theorem.

THEOREM 1. If we have phase-lag of order infinity and at a point z , $\alpha(z) = 0$ then,

$$\left. \begin{array}{l} z - \arccos\left(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right) = 0 \\ 1 - \sqrt{Q(z^2)} = 0 \end{array} \right\} \Rightarrow \begin{array}{l} R(z^2) = 2\cos(z) \\ Q(z^2) = 1 \end{array}$$

Proof.

$$\begin{aligned} \Phi(z) = z - \arccos\left(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right) = 0 &\Leftrightarrow \\ \arccos\left(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right) = z &\Leftrightarrow \\ \cos\left(\arccos\left(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right)\right) = \cos(z) &\Leftrightarrow \\ \left(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\right) = \cos(z) &\Leftrightarrow \\ \left(\frac{R(z^2)}{\sqrt{Q(z^2)}}\right) = 2\cos(z). &\quad (13) \end{aligned}$$

Now for

$$a(z) = 0 \Leftrightarrow 1 - \sqrt{Q(z^2)} = 0 \Leftrightarrow Q(z^2) = 1. \quad (14)$$

From the above relation and the expression (13) we have

$$R(z^2) = 2\cos(z). \quad (15)$$

LEMMA 1. For the construction of a method with phase lag of order infinity and amplification error of order infinity, we must satisfy the conditions $R(z^2) = 2\cos(z)$ and $Q(z^2) = 1$.

Table II. Fourth-order explicit Runge-Kutta-Nystöm method

0	1	0			
$\frac{1}{4}$	g_2	$\frac{1}{32}$			
$\frac{7}{10}$	g_3	$\frac{7}{1000}$	$\frac{119}{500}$		
1	1	$\frac{1}{14}$	$\frac{8}{27}$	$\frac{25}{189}$	
		$\frac{1}{14}$	$\frac{8}{27}$	$\frac{25}{189}$	0
		$\frac{1}{14}$	$\frac{32}{81}$	$\frac{250}{567}$	$\frac{5}{54}$

4. Derivation of the new Runge-Kutta-Nyström method

In this section we construct a four-stage explicit Runge-Kutta-Nyström method (presented in table I), based on $R(z^2) = 2\cos(z)$ and $Q(z^2) = 1$. Using the coefficients of DEP [1] and for $g_4 = 1$, the method can be seen in table II.

Now let us rewrite $R(z^2)$ and $Q(z^2)$ in the following form

$$\begin{aligned} R(z^2) &= 2 - r_1 z^2 + r_2 z^4 - r_3 z^6 + \dots + r_i z^{2i} = 0 \\ Q(z^2) &= 1 - q_1 z^2 + q_2 z^4 - q_3 z^6 + \dots + q_i z^{2i} = 0 \end{aligned} \quad (16)$$

By computing the polynomials A, \dot{A}, B, \dot{B} in terms of RKN parameters we obtain the expressions of $R(z^2)$ and $Q(z^2)$. Then by applying them to the equations (14) and (15) we lead to the following formulas for the coefficients g_2 and g_3 .

$$\begin{aligned} g_2 &= -1/20(-933120 + 459 z^6 - 19440 z^4 + 276480 z^2 - 18(-597196800 \\ &+ 597196800 \cos(z) - 576020 z^8 + 12913920 z^6 - 98858880 z^4 \\ &+ 349401600 z^2 + 8551 z^{10} + 7102080 z^4 \cos(z) - 50803200 z^2 \cos(z)) \\ &/ (-186624 + 31104 z^2 - 1332 z^4 + 17 z^6) + 648((-597196800 \\ &+ 597196800 \cos(z) - 576020 z^8 + 12913920 z^6 - 98858880 z^4 \\ &+ 349401600 z^2 + 8551 z^{10} + 7102080 z^4 \cos(z) - 50803200 z^2 \cos(z)) \\ &/ (z^2(-186624 + 31104 z^2 - 1332 z^4 + 17 z^6))) \\ &+ 933120 \cos(z) z^{-2} (17 z^4 - 772 z^2 + 2304)^{-1} \end{aligned}$$

$$\begin{aligned} g_3 &= \frac{9}{2000}(-597196800 + 597196800 \cos(z) - 576020 z^8 + 12913920 z^6 \\ &- 98858880 z^4 + 349401600 z^2 + 8551 z^{10} + 7102080 z^4 \cos(z)) \end{aligned}$$

$$- 50803200 z^2 \cos(z)) / (z^4 (-186624 + 31104 z^2 - 1332 z^4 + 17 z^6))$$

When $z < 0.5$ the following Taylor series expansions are used

$$g_2 = 1 - \frac{43}{1152} z^2 + \frac{13}{17920} z^4 - \frac{2603}{209018880} z^6 - \frac{22681}{14780620800} z^8 - \frac{1039043569}{5423187138969600} z^{10}$$

$$g_3 = 1 + \frac{43}{3600} z^2 - \frac{2183}{4838400} z^4 - \frac{1249}{373248000} z^6 - \frac{3577129}{4138573824000} z^8 - \frac{943612843}{8473729904640000} z^{10}$$

5. Numerical illustrations

In this section we will apply our method to the radial Schrödinger equation. For the purpose of our numerical illustration we take the domain of integration as $x \in [0, 15]$, using the Woods-Saxon potential:

$$V(x) = \frac{u_0}{1+q} + \frac{u_1 q}{(1+q)^2}, \quad q = \exp\left(\frac{x-x_0}{\alpha}\right), \quad \text{where} \quad (17)$$

$$u_0 = -50, \quad \alpha = 0.6, \quad x_0 = 7, \quad u_1 = -\frac{u_0}{\alpha}$$

5.1. RESONANCE PROBLEM

In the case of positive energies ($E = k^2$), the potential ($V(x)$) dies away faster than the centrifugal potential ($l(l+1)/x^2$), so for a large number for x , Schrödinger equation effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right)y(x) = 0 \quad (18)$$

The above equation (18) has two linearly independent solutions, $kxj_l(kx)$ and $kxn_l(kx)$, where j_l and n_l are the spherical Bessel and Neumann functions, respectively. When $x \rightarrow \infty$, the solution of equation (1) take the following asymptotic form

$$y(x) \simeq Akxj_l(kx) - Bkxn_l(kx)$$

$$\simeq D \left[\sin\left(kx - \frac{l\pi}{2}\right) + \tan(\delta_l) \cos\left(kx - \frac{l\pi}{2}\right) \right], \quad (19)$$

where δ_l is the scattering phase shift that may be calculated from the bellow formula

$$\tan(\delta_l) = \frac{y(x_i)S(x_{i+1}) - y(x_{i+1})S(x_i)}{y(x_{i+1})C(x_i) - y(x_i)C(x_{i+1})}, \quad (20)$$

where $S(x) = kxj_l(kx)$, $C(x) = kxn_l(kx)$ and $x_i < x_{i+1}$ both exist in the asymptotic region.

For positive energies and for $l = 0$, we calculate the phase shift (δ_l) and then we compare it with the accurate value which is $\pi/2$. The boundary conditions for this eigenvalue problem are $y(0) = 0$ and $y(x) = \cos(\sqrt{E}x)$ for large x .

We use the following eigenenergies

$$E_1 = 53.588872$$

$$E_2 = 163.215341$$

$$E_3 = 341.495874$$

$$E_4 = 989.701916$$

5.2. BOUND-STATES PROBLEM

In the case of negative energies ($E < 0$), we consider the eigenvalue problem with boundary conditions $y(0) = 0$ and $y(x) = \exp(-\sqrt{-E}x)$ for large x .

In order to solve this problem numerically, by a chosen eigenvalue, we integrate forward from the point $x = 0$, backward from the point $x = 15$ and matching up the solution at some internal point in the range of integration.

For the Bound-states problem we use the following eigenenergies

$$E_1 = -49.457788728$$

$$E_2 = -48.148430420$$

$$E_3 = -41.232607772$$

$$E_4 = -38.122785096$$

$$E_5 = -26.873448915$$

$$E_6 = -22.588602257$$

$$E_7 = -8.676081670$$

$$E_8 = -3.908232481$$

We are going to compare our results to those derived by using the high order method of embedded Runge-Kutta-Nyström 4(3)4 method, of *DEP* (see [1]), as well as to other methods derived for the numerical solution of the Schrödinger equation. The methods used in the comparison have been denoted by:

- PAFRKN4: The new fourth-order RKN method with four stages (three effective stases with FSAL property), phase lag and amplification

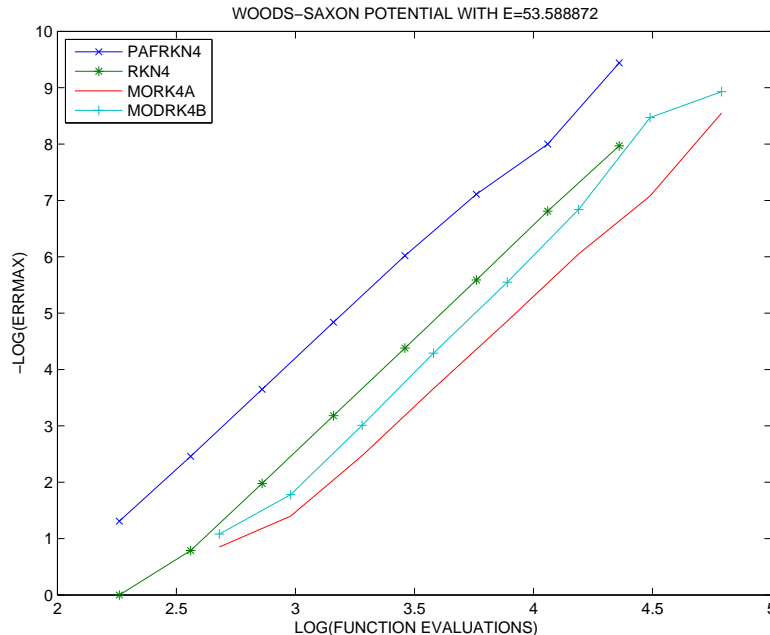


Figure 1. Efficiency for the Schrödinger equation using $E=53.588872$

error of order infinity derived in Section 4.

- RKN4: The high order method of pair RKN 4(3)4 method of *Dormand, El-Mikkawy and Prince* [1].
- MODRK4A: The modified exponentially fitted fourth order RK method with four stages of *H. Van de Vyver* [5] (Section 2.1).
- MODRK4B: The modified exponentially fitted fourth order RK method with four stages of *H. Van de Vyver* [5] (Section 2.2).

One way to measure the efficiency of the method is to compute the accuracy in the decimal digits, that is $-\log_{10}(\text{error at the end point})$ when comparing the phase shift to the actual value $\pi/2$ versus the computational effort measured by the $\log_{10}(\text{number of function evaluations required})$.

The frequency is given by the suggestion of *Ixaru and Rizea* [4]

$$v = \begin{cases} \sqrt{E + 50}, & x \in [0, 6.5] \\ \sqrt{E}, & x \in [6.5, 15] \end{cases}$$

In the figures we display the efficiency curves, that is the accuracy versus the computational cost measured by the number of function evaluations required by each method.

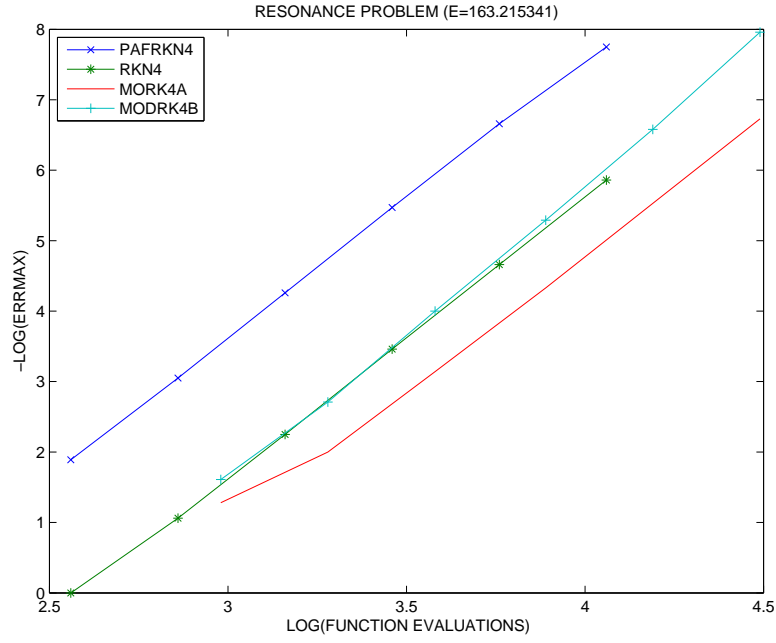


Figure 2. Efficiency for the Schrödinger equation using $E=163.215341$

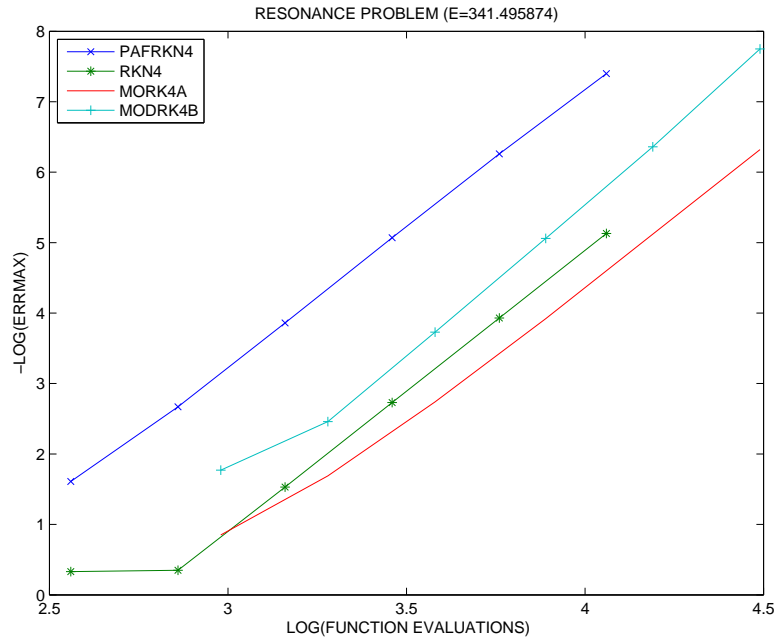


Figure 3. Efficiency for the Schrödinger equation using $E=341.495874$

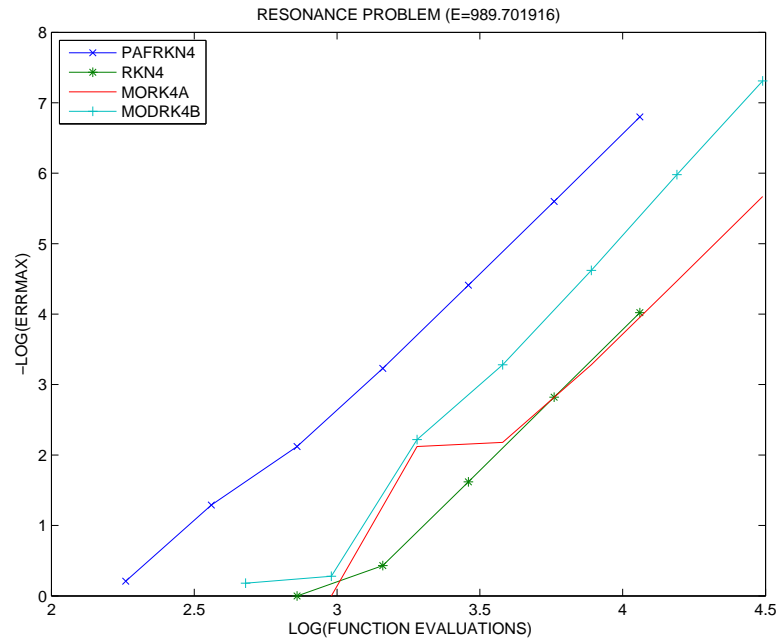


Figure 4. Efficiency for the Schrödinger equation using $E=989.701916$

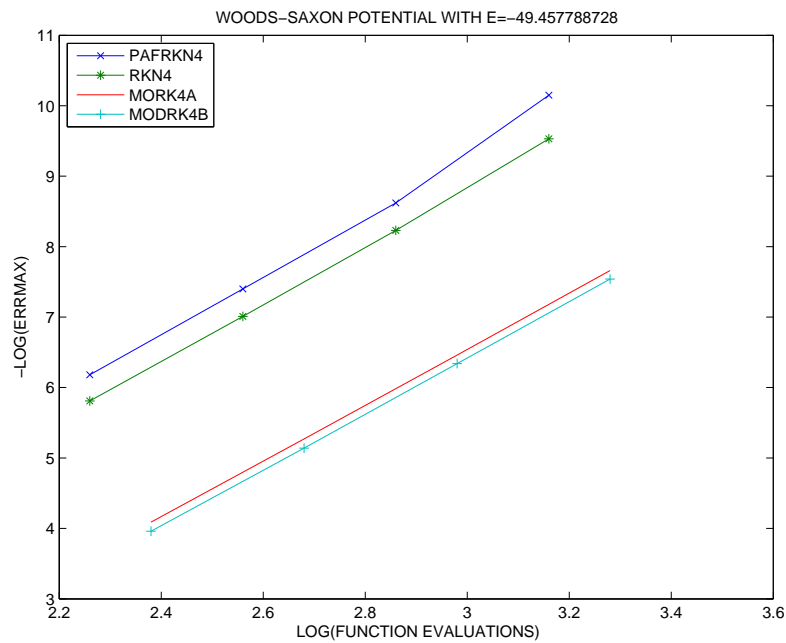


Figure 5. Efficiency for the Schrödinger equation using $E=-49.457788728$

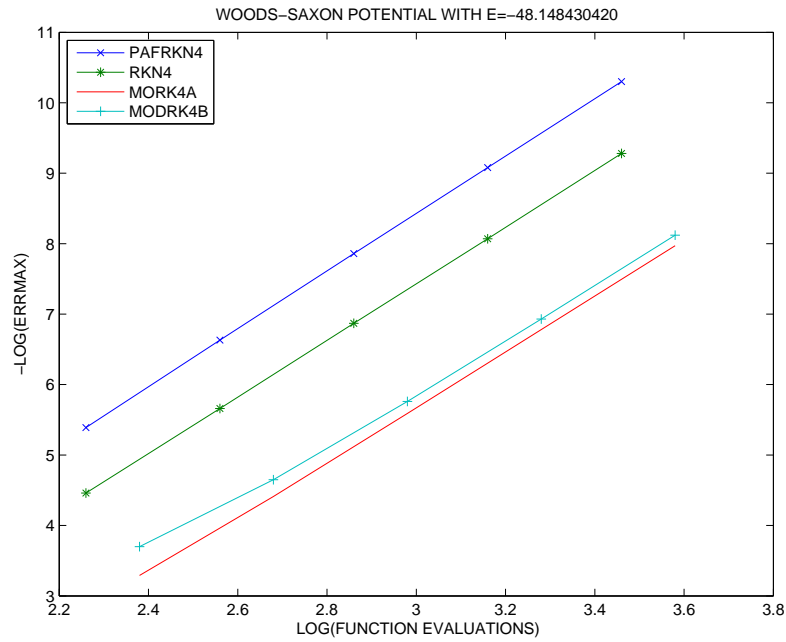


Figure 6. Efficiency for the Schrödinger equation using $E=-48.148430420$

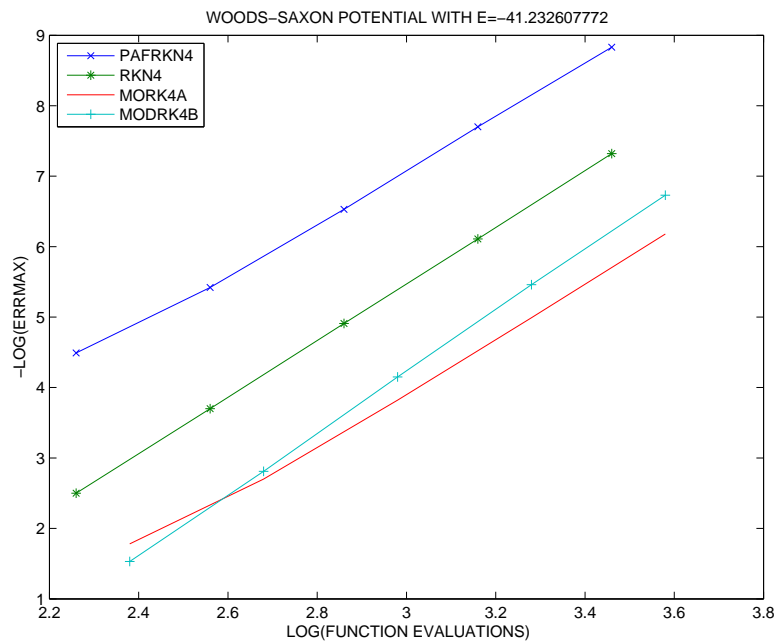


Figure 7. Efficiency for the Schrödinger equation using $E=-41.232607772$

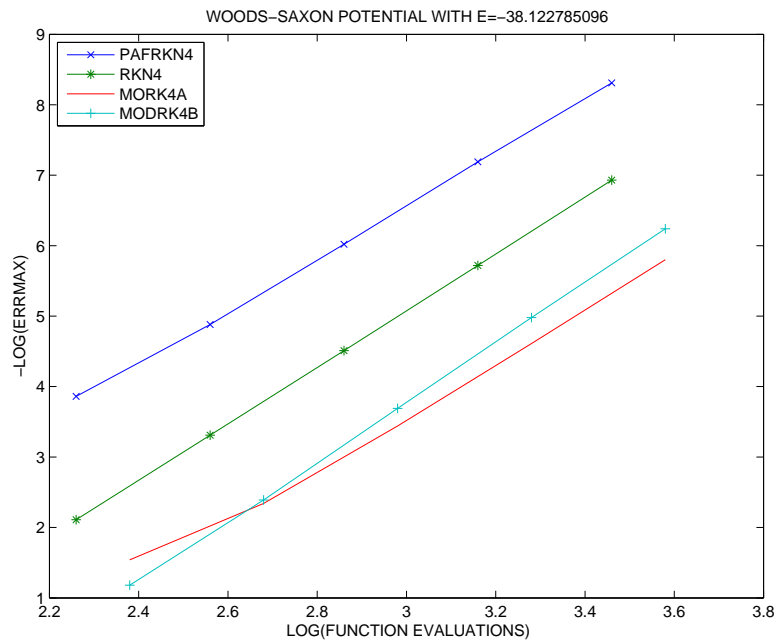


Figure 8. Efficiency for the Schrödinger equation using $E=-38.122785096$

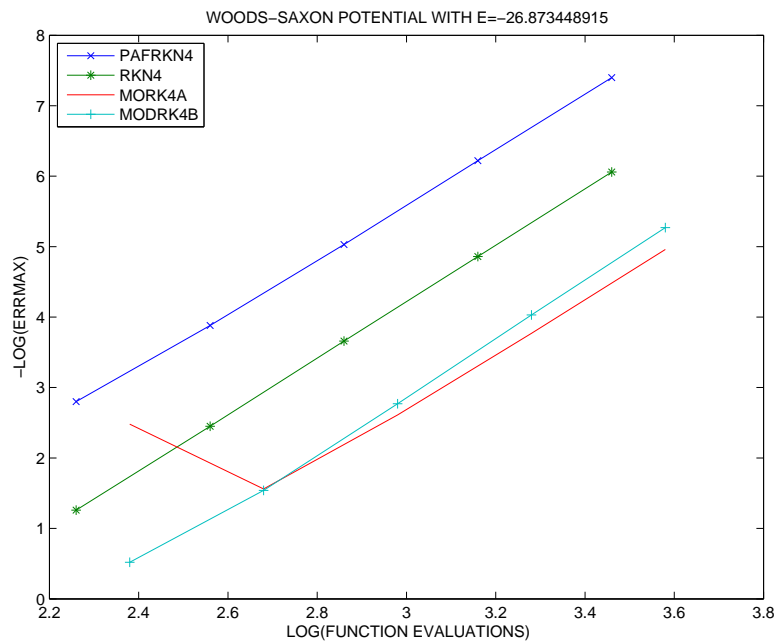


Figure 9. Efficiency for the Schrödinger equation using $E=-26.873448915$

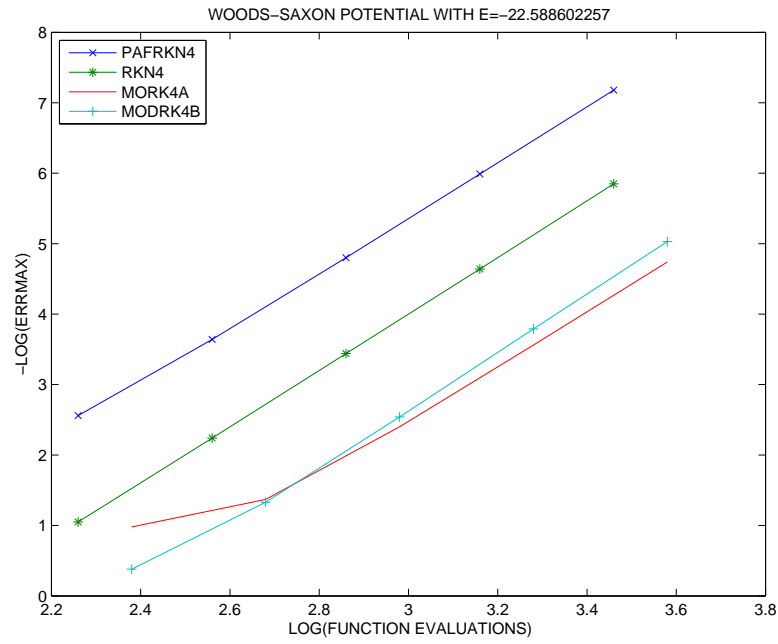


Figure 10. Efficiency for the Schrödinger equation using $E=-22.588602257$

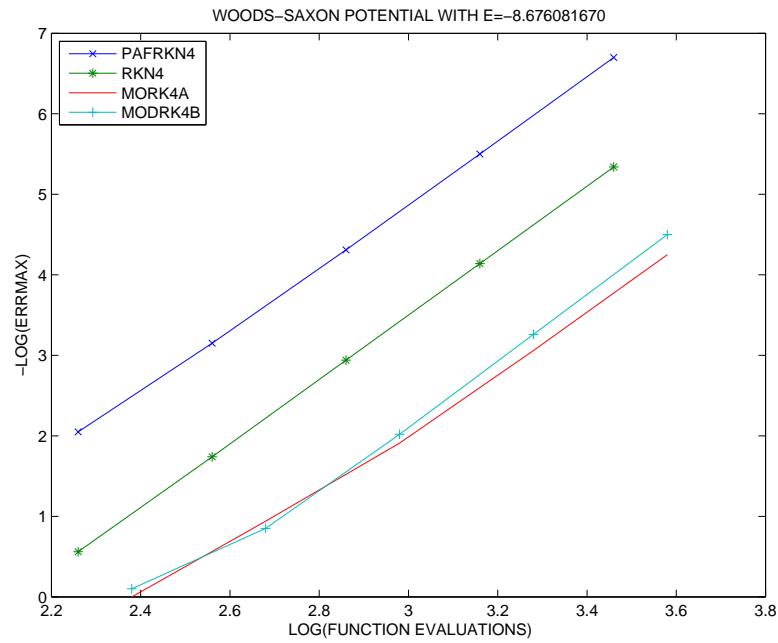


Figure 11. Efficiency for the Schrödinger equation using $E=-8.676081670$

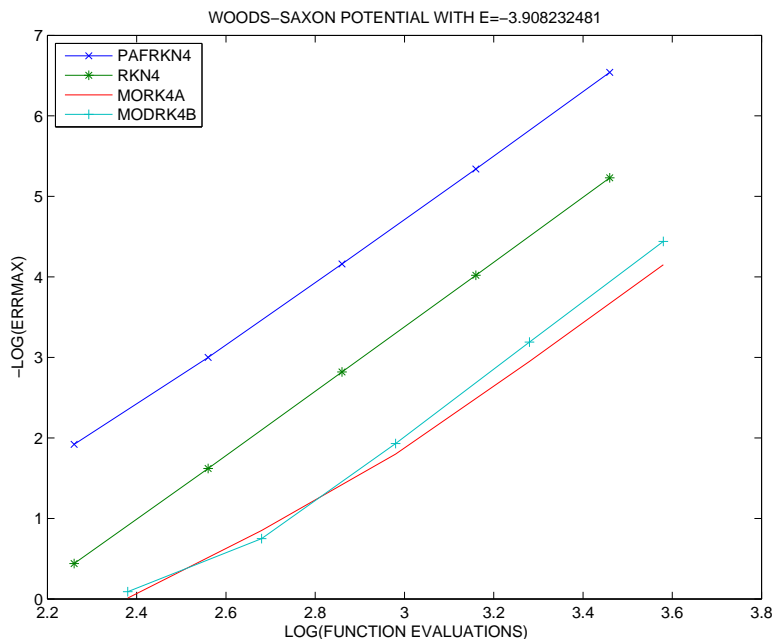


Figure 12. Efficiency for the Schrödinger equation using $E=-3.908232481$

Numerical results indicate that the new method derived in section 4, is very efficient for solving numerically the Schrödinger equation. More specifically we observe that, in the case of resonance problem our method is more accurate than MODRKB4 and MODRKA4 by two and three decimals respectively. Moreover the new method is more accurate by two decimals than RKN4 for the eigenvalues $E = \{53.588872, 163.215341, 341.495874\}$ and by three decimals for the eigenvalue $E = 989.701916$. In the case of bound-states problem, PAFRKN4 is more accurate than MODRKB4 and MODRKA4 by three decimals. Also our method maintained more accurate than the classical RKN4 method, by two decimals for the eigenvalues $E = \{-49.457788728, -48.148430420\}$ and by three decimals for the rest six eigenvalues.

6. Conclusion

A new Runge-Kutta-Nyström method of fourth algebraic order with four stages (three effective stages with FSAL property), is developed in the present paper. The new method is based on the very well known classical Dormand, El-Mikkawy and Prince fourth algebraic order Runge-Kutta-Nyström method and it has phase lag of order infinity and ampli-

fication error of order infinity. The numerical results show that the new method is more efficient for the numerical solution of the Schrödinger equation than other methods derived for the same purpose, including the corresponding classical method of DEP.

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