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**Title:**

## P-stability, TF and VSDPL technique in Obrechkoff methods for the numerical solution of the Schrödinger equation

**Author(s):**

A. Shokri and H. Saadat

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# P-STABILITY, TF AND VSDPL TECHNIQUE IN OBRECHKOFF METHODS FOR THE NUMERICAL SOLUTION OF THE SCHRÖDINGER EQUATION

A. SHOKRI* AND H. SAADAT

(Communicated by Mohammad Asadzadeh)

Abstract. Many simulation algorithms (chemical reaction systems, differential systems arising from the modeling of transient behavior in the process industries and etc.) contain the numerical solution of systems of differential equations. For the efficient solution of the above mentioned problems, linear multistep methods or Runge-Kutta technique are used. For the simulation of chemical procedures the radial Schrödinger equation is used frequently. In the present paper we will study a symmetric two-step Obrechkoff method, in which we will use of technique of VSDPL (vanished some of derivatives of phase-lag), for the numerical integration of the one-dimensional Schrödinger equation. We will show superiority of new method in stability, accuracy and efficiency. So we present a stability analysis and an error analysis based on the radial Schrödinger equation. Also we will apply the new proposed method to the resonance problem of the radial Schrödinger equation.
**Keywords:** P-stable, Phase-lag, Schrödinger equation, trigonometrically fitted.
**MSC(2010):** Primary: 65L05; Secondary: 65L06.

## 1. Introduction

The time-independent Schröodinger equation is one of the basic equations of quantum mechanics. Its solutions are required in the studies of atomic and molecular structure and spectra, molecular dynamics and quantum chemistry. Large research on the construction of numerical methods for the solution of the Schrödinger equation has been done the last years. The aim and scope of this research is the construction of fast and reliable methods for the solution of the Schrödinger equation and related problems.

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*Corresponding author.

Specially, in this subject the following works have been done in recent years:

- Phase-fitted methods and numerical methods with minimal phase-lag are developed in [1–4, 11].
- In [5, 9, 10, 13–19] exponentially and trigonometrically fitted methods are obtained.

We can divide the numerical methods for the numerical solution of the Schrödinger equation and related problems into two main categories:

The radial time-independent Shorödinger equation can be written as:

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

The boundary conditions are $y(0) = 0$, and a second boundary condition, for large values of $x$, determined by physical considerations. The function $W(x) = l(l+1)/x^2 + V(x)$ is called *the effective potential*, which satisfies $\lim_{x\to\infty} W(x) = 0$. The quantity $E = k^2$ is a real number denoting *the energy*, $l$ is a given integer representing the *angular momentum*, $V$ is a given function which denotes the *potential*.

The numerical methods for the approximate solution of the Schrödinger equation and related problems can be divided into two main categories:

(1) Methods with constant coefficients.
(2) Methods with coefficients depending on the frequency of the problem. [1]

Large research on the algorithmic development of numerical methods for the solution of the Schrödinger equation has been done during the last decades . The earliest method to solve (1.1) numerically is the Numerov's method. Recently Simos have developed 10th algebraic order Obrechkoff method [12]. In [19] an improved trigonometrically fitted P-stable of 12th algebraic order Obrechkoff method have developed by Wang, Daele and Berghe [17], Sujatha D. Achar [1] and Vanden Berghe [18] have been developed Obrechkoff method to solve Second order initial value problems. The purpose of this paper is to study the importance of the properties of P-stability, trigonometrically-fitting and VSDPL technique for the numerical integration of the one-dimensional Schrödinger equation. This will be done via the study of the error analysis, stability region and the application of the investigated methods to the numerical solution of the radial Schrödinger equation. We will investigate all of the three categories of methods, i.e.:

(1) the category of the VSDPL technique, for linear multistep methods,
(2) the category of P-stable linear multistep methods,
(3) the category of trigonometrically-fitted linear multistep methods.

[1] When using a functional fitting algorithm for the solution of the radial Schrödinger equation, the fitted frequency is equal to: $\sqrt{|l(l+1)/x^2 + V(x) - k^2|}$.

In this paper we will use a recent methodology for the development of numerical methods for the approximate solution periodic initial-value problems. The new methodology is based on the requirement of vanishing the phase-lag and its derivatives. Based on this new methodology we will develop a two step Obrechkoff method which will have vanishing phase-lag and its first and fifth derivatives. We will apply the new developed method on the numerical solution of the radial Schrödinger equation. We will study the efficiency of the new obtained method via:

- a comparative error analysis
- a comparative stability analysis and finally
- the numerical results produced from the numerical solution of the radial Schrödinger with the application to the specific potential.

More specifically, we will develop a symmetric two step Obrechkoff method with twelfth algebraic order. The development of the new family of methods is based on the requirement of vanishing the phase-lag and its first and fifth derivatives. We will give a comparative error analysis and investigate region of periodicity in order to show the efficiency of the new proposed method. Finally, we will apply the new method to the resonance problem. This is one of the most difficult problems arising from the radial Schrödinger equation.

We have organized the paper as follows:
In Section 2, we present phase-lag analysis of Obrechkoff method. In Section 3, we present the development of the new method. Comparison of the new method with other methods in accordance to their local truncation error and their stability is made and remarks and theorems are given in Section 4. In Section 5, the numerical results are presented. Finally, in Section 6 conclusions are discussed.

## 2. Phase-lag analysis of Obrechkoff method

Consider Obrechkoff method of the form:

$$\sum_{j=0}^{k} \alpha_j y_{n-j+1} = \sum_{i=1}^{l} h^{2i} \sum_{j=0}^{k} \beta_{ij} y_{n-j+1}^{(2i)}, \tag{2.1}$$

The method (2.1) is symmetric when $\alpha_j = \alpha_{k-j}$, $\beta_{ij} = \beta_{ik-j}$, $j = 0(1)k$. To investigate the stability properties of the methods for solving the initial value problem, Lambert and Watson [8] introduced the scalar test equation

$$y'' = -\omega^2 y, \quad \omega, y \in \mathbb{R}. \tag{2.2}$$

When a symmetric 2-step Obrechkoff method, is applied to the scalar test equation (2.2), a difference equation of the form:

$$A(v)\, y_{n+1} - 2\, B(v)\, y_n + A(v)\, y_{n-1} = 0, \tag{2.3}$$

is obtained, where $h$ is the step length and $A(v)$, $B(v)$ are polynomials of $v$. The characteristic equation associated with (2.3) is given by:

$$\Omega(\xi, v) = A(v)\xi^2 - 2\,B(v)\xi + A(v) = 0, \tag{2.4}$$

where $A(v) = 1 + \sum_{i=1}^{l} (-1)^{i-1}\,\beta_{i0} v^{2\,i}$, and $B(v) = 1 - \frac{1}{2}\,\sum_{i=1}^{l} (-1)^{i-1}\,\beta_{i1} v^{2\,i}$, with $v = \omega h$. The roots of (2.4) are complex and of modulus one if

$$\left|\frac{B(v)}{A(v)}\right| < 1. \tag{2.5}$$

Let the roots of (2.4) be $\xi_{1,2} = e^{\pm\theta(v)}$, when (2.5) is satisfied. The exact solution of the test equation (2.2) with the initial conditions $y(t_0) = y_0$ and $y'(0) = y_0'$ is given by

$$y(t) = y_0 \cos(\omega t) + \frac{y_0'}{\omega} \sin(\omega t) \tag{2.6}$$

Evaluating (2.6) at $t_{n+1}$, $t_n$ and $t_{n+1}$ and eliminating $y_0$ and $y_0'$, we obtain $y(t_{n+1}) - 2\cos(\omega h) y(t_n) + y(t_{n-1}) = 0$, whose characteristic equation is

$$\xi^2 - 2\,\cos(v)\,\xi + 1 = 0, \quad v = \omega h. \tag{2.7}$$

The characteristic equation of (2.4) may be written as

$$\xi^2 - 2\,\cos(\theta(v))\,\xi + 1 = 0, \quad v = \omega h. \tag{2.8}$$

where $\cos(\theta(v)) = B(v)/A(v)$.

**Definition 2.1.** (see [2]) We define the phase-lag error of the method (2.1) as the leading coefficient in the expansion of

$$\frac{(A(v)\cos(v) - B(v))}{v^2}, \tag{2.9}$$

and denote it by $P(v)$ (The motivation of this definition may be easily noted to be the difference in the frequency distortion of the characteristic equations (2.8) and (2.7).). $P(s)$ gives us a direct formula to calculate the phase-lag of any symmetric 2-step Obrechkoff method.

## 3. Construction of the new method

From the form (2.1) with $l = 3$ we get

$$\begin{aligned} y_{n+1} - 2y_n + y_{n-1} \;=\; & h^2 \left[\beta_{10}(y_{n+1}^{(2)} + y_{n-1}^{(2)}) + \beta_{11} y_n^{(2)}\right] \\ & + h^4 \left[\beta_{20}(y_{n+1}^{(4)} + y_{n-1}^{(4)}) + \beta_{21} y_n^{(4)}\right] \\ & + h^6 \left[\beta_{30}(y_{n+1}^{(6)} + y_{n-1}^{(6)}) + \beta_{31} y_n^{(6)}\right]. \end{aligned} \tag{3.1}$$

Recently Simos [12] and Daele [17] have developed tenth order methods also Wang [19], Achar [1] and Berghe [18] have developed twelfth order methods. The coefficients due to Wang are given by

$$\begin{aligned} \beta_{10} &= \frac{229}{7788}, \quad \beta_{20} = \frac{-1}{2360}, \\ \beta_{21} &= \frac{711}{12980}, \quad \beta_{30} = \frac{127}{39251520}, \quad \beta_{31} = \frac{2923}{3925152}, \end{aligned} \tag{3.2}$$

where

$$\beta_{11} = 2v^{-2} + \beta_{21}v^2 - \beta_{31}v^4 - 2\cos(v)\left(v^{-2} + \beta_{10} - \beta_{20}v^2 + \beta_{30}v^4\right). \tag{3.3}$$

Simos's coefficients are given by

$$\begin{aligned} \beta_{10} &= \frac{89}{1878} - \frac{7560}{313}\beta_{31}, \quad \beta_{11} = \frac{850}{939} + \frac{15120}{313}\beta_{31}, \\ \beta_{20} &= -\frac{1907}{1577520} + \frac{330}{313}\beta_{31}, \quad \beta_{21} = \frac{30257}{788760} + \frac{6900}{313}\beta_{31}, \\ \beta_{30} &= \frac{59}{3155040} - \frac{13}{626}\beta_{31}, \quad \beta_{31} = \frac{1}{1784160}\frac{\varphi}{v^2}, \end{aligned} \tag{3.4}$$

where

$$\begin{aligned} \varphi &= 190816819200\,(1-\cos(v)) - 95408409600v^2 + 7950700800v^4 \\ &\quad -265023360v^6 + 47322560v^8 - 52584v^{10} + 1727v^{12}. \end{aligned}$$

Daele's coefficients are given by

$$\begin{aligned} \beta_{10} &= 1/39 + \frac{15120}{13}\beta_{30}, \quad \beta_{11} = \frac{37}{39} - \frac{30240}{13}\beta_{30}, \quad \beta_{20} = -\frac{660}{13}\beta_{30} - \frac{17}{65520}, \\ \beta_{21} &= \frac{1907}{32760} - \frac{13800}{13}\beta_{30}, \quad \beta_{31} = \frac{59}{65520} - \frac{626}{13}\beta_{30} \\ \beta_{30} &= \frac{\left(131040 + 3360\,v^2 + 34\,v^4\right)\cos(v) - 131040 + 62160\,v^2 - 3814\,v^4 + 59\,v^6}{(15120 + 660\,v^2 + 13\,v^4)\cos(v) - 15120 + 6900\,v^2 - 313\,v^4}. \end{aligned}$$

In the method which proposed by Achar, when letting $r = 1(1)6$ in below form, Achar has obtained the coefficients $\beta_{10}$, $\beta_{11}$, $\beta_{20}$, $\beta_{21}$, $\beta_{30}$ and $\beta_{31}$. Because of its long length we refuse to write it (see [1]).

$$\begin{aligned} \left[\frac{\sin(r\sigma)}{r\sigma}\right]^2 &= 2\cos(2r\sigma)\beta_{10} + \beta_{11} - 8r^2\sigma^2\cos(2r\sigma)\beta_{20} \\ &\quad -4r^2\sigma^2\beta_{21} + 32r^4\sigma^4\cos(2r\sigma)\beta_{30} + 16r^4\sigma^4\beta_{31}, \end{aligned}$$

where $\sigma = \dfrac{\omega h}{2}$.

3.1. **Development of the method.** In order to find the phase-lag and its derivatives, we use the formula (2.9). Then we have

$$\begin{aligned} P(v) &= (\cos(v)\beta_{30} + 1/2\,\beta_{31})v^4 + (-\cos(v)\beta_{20} - 1/2\,\beta_{21})v^2 \\ &\quad + \cos(v)\beta_{10} + 1/2\,\beta_{11} + \frac{\cos(v) - 1}{v^2}. \end{aligned} \tag{3.5}$$

We demand that the phase-lag and its first, second, third, fourth and fifth derivatives to be equal to zero, the coefficients $\beta_{10}$, $\beta_{11}$, $\beta_{20}$, $\beta_{21}$, $\beta_{30}$ and $\beta_{31}$ are the solution of the system of equations, which arises when we set $P(v)$, $P^{(j)}(v)$, $j = 1(1)5$ equal to zero. So we have

$$\begin{aligned} \beta_{10} &= \frac{\gamma_1}{\vartheta v^3}, \quad \beta_{11} = \frac{\gamma_2}{\vartheta v^3}, \quad \beta_{20} = \frac{\gamma_3}{\vartheta v^5}, \\ \beta_{21} &= \frac{\gamma_4}{\vartheta v^5}, \quad \beta_{30} = \frac{\gamma_5}{\vartheta v^7}, \quad \beta_{31} = \frac{\gamma_6}{\vartheta v^7}, \end{aligned} \tag{3.6}$$

where

$$\begin{aligned} \gamma_1 = {} & \Big(-9450-7290v^2-18v^6-540v^4\Big)(\cos(v))^3+\Big(\Big(-405v^3-3v^7 \\ & -405v-54v^5\Big)\sin(v)-1260v^4+4590v^2+6v^6+9450\Big)(\cos(v))^2 \\ & +\Big(\big(-4500v^3+144v^5-7020v\big)\sin(v)-9180v^2+9450+3870v^4 \\ & +168v^6\Big)\cos(v)+\big(-9810v^3-1170v^5+84v^7+7425v\big)\sin(v) \\ & -9450+2520\,v^4+11880\,v^2+24\,v^6, \end{aligned}$$

$$\begin{aligned} \gamma_2 = {} & \big(12v^6+9180v^2-2520v^4+18900\big)\,(\cos(v))^4+\Big(\Big(14040v-288v^5 \\ & +9000v^3\Big)\sin(v)-1080v^4-14580v^2-36v^6-18900\Big)(\cos(v))^3 \\ & +\Big(\Big(810v^3+810v+6v^7+108v^5\Big)\sin(v)-24480v^4+34560v^2 \\ & -18900+816v^6\Big)(\cos(v))^2+\Big(\big(-8064v^5-28080v+36000v^3\big)\sin(v) \\ & +4500v^4+336v^6-18360v^2+18900\Big)\cos(v)-168v\Big(\Big(\frac{213}{14}v^4-\frac{315}{4} \\ & +\frac{195}{2}v^2+v^6\Big)\sin(v)-4v^5+\frac{450}{7}v-\frac{600}{7}v^3\Big), \end{aligned}$$

$$\begin{aligned} \gamma_3 = {} & \big(11340-648v^4+4140v^2-36v^6\big)\,(\cos(v))^3+\Big(\Big(90v^5+3915v^3 \\ & +6075v-3v^7\Big)\sin(v)-792v^4-5220v^2-11340+12v^6\Big)(\cos(v))^2 \\ & +\Big(\Big(192v^5+360v^3+3240v\Big)\sin(v)-4302v^4+336v^6+10440v^2 \\ & -11340\Big)\cos(v)+\big(8550v^3-1722v^5-9315v+84v^7\big)\sin(v)+11340 \\ & +48v^6-9360v^2+1152v^4, \end{aligned}$$

$$\begin{aligned}
\gamma_4 &= \left(-22680+24v^6-1584v^4-10440v^2\right)(\cos(v))^4+\Big(\Big(-384v^5\\
&-720v^3-6480v\Big)\sin(v)+22680-72v^6+8280v^2-1296v^4\Big)(\cos(v))^3\\
&+\Big(\left(-7830v^3-180v^5+6v^7-12150v\right)\sin(v)+22680+1632v^6\\
&-14400v^2-13536v^4\Big)(\cos(v))^2+\Big(\Big(-2880v^3-10752v^5\\
&+12960v\Big)\sin(v)+672v^6-22680+14076v^4+20880v^2\Big)\cos(v)\\
&-168\left(\left(v^6+\frac{1185}{14}v^2-\frac{135}{4}+\frac{257}{14}v^4\right)\sin(v)-8v^5-\frac{480}{7}v^3+\frac{180}{7}v\right)v,
\end{aligned}$$

$$\begin{aligned}
\gamma_5 &= \left(-810-18v^6+372v^4+1350v^2\right)(\cos(v))^3+\Big(\Big(-v^7+126v^5\\
&-135v^3-2295v\Big)\sin(v)+810+270v^2+6v^6-12v^4\Big)(\cos(v))^2\\
&+\Big(\Big(48v^5+540v^3+1620v\Big)\sin(v)+810+168v^6-540v^2\\
&-1182v^4\Big)\cos(v)+\Big(-534v^5+28v^7+810v^3+675v\Big)\sin(v)\\
&-810-1080v^2+24v^6+552v^4,
\end{aligned}$$

$$\begin{aligned}
\gamma_6 &= \Big(12v^6-24v^4+1620+540v^2\Big)(\cos(v))^4+\Big(\Big(-96v^5-1080v^3\\
&-3240v\Big)\sin(v)-1620-36v^6+2700v^2+744v^4\Big)(\cos(v))^3\\
&+\Big(\Big(270\,v^3-252\,v^5+2\,v^7+4590\,v\Big)\sin(v)-1620+816\,v^6\\
&-8640\,v^2-2496\,v^4\Big)(\cos(v))^2+\Big(\Big(-4320v^3-2688v^5\\
&+6480v\Big)\sin(v)+336\,v^6+1620+5196\,v^4-1080\,v^2\Big)\cos(v)\\
&+\left(-56v^7-7830v+2700v^3-564v^5\right)\sin(v)+672v^6\\
&-2880v^4+6480v^2,
\end{aligned}\tag{3.7}$$

$$\begin{aligned}
\vartheta &= \sin(v)\left(18v^4+135v^2+135+v^6\right)(\cos(v))^2\\
&-270\cos(v)v^3+\sin(v)\left(-28v^6-18v^4+270v^2-135\right).
\end{aligned}$$

The behavior of coefficients of the method are shown in figures 1, to 3. Based on this procedure we obtain the following expansion for the LTE:

$$\begin{aligned}
LTE &= -\frac{45469}{1697361329664000}\Big(15\omega^8y_n^{(6)}+15\omega^4y_n^{(10)}\\
&+6\omega^2y_n^{(12)}+y_n^{(14)}+20\omega^6y_n^{(8)}+\omega^{12}y_n^{(2)}+6\omega^{10}y_n\Big)h^{14},
\end{aligned}$$

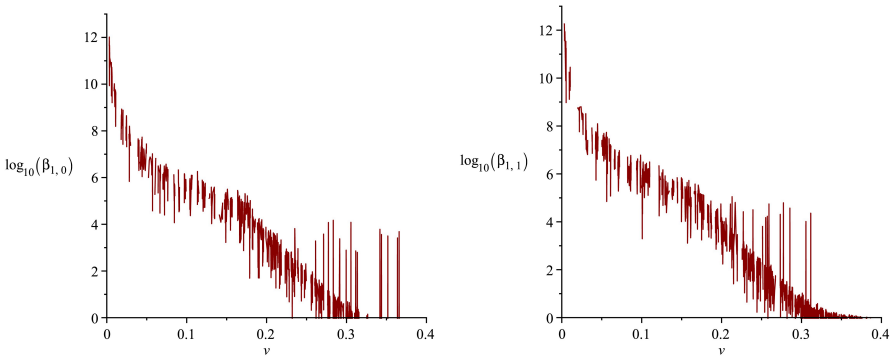


FIGURE 1. Behavior of the coefficients $\beta_{10}$ and $\beta_{11}$ in new method.

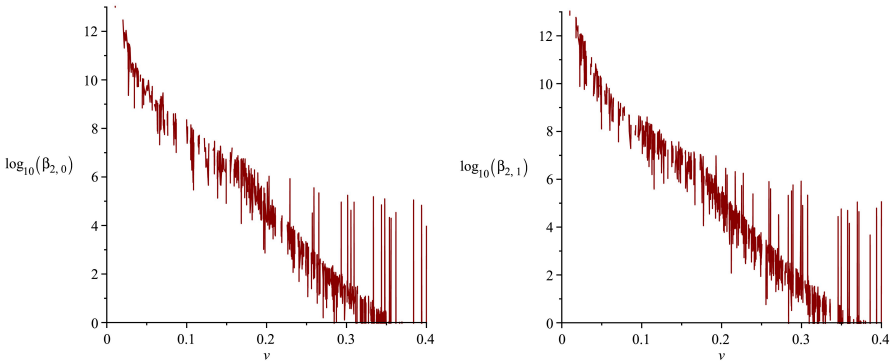


FIGURE 2. Behavior of the coefficients $\beta_{20}$ and $\beta_{21}$ in new method.

## 4. **Comparative error and stability analysis**

In this section we will study the following methods:

- The symmetric two-step Obrechkof tenth algebraic order method developed by Simos [12].
- The trigonometrically-fitted symmetric two-step P-stable Obrechkof twelfth algebraic order method developed by Wang [19].
- The symmetric two-step Obrechkof tenth algebraic order method developed by Daele [17].
- The trigonometrically-fitted symmetric two-step Obrechkof twelfth algebraic order method developed by Achar [1] with the set $\{\cos(P\,\omega\,h)\}$ where $P = 1(1)6$.

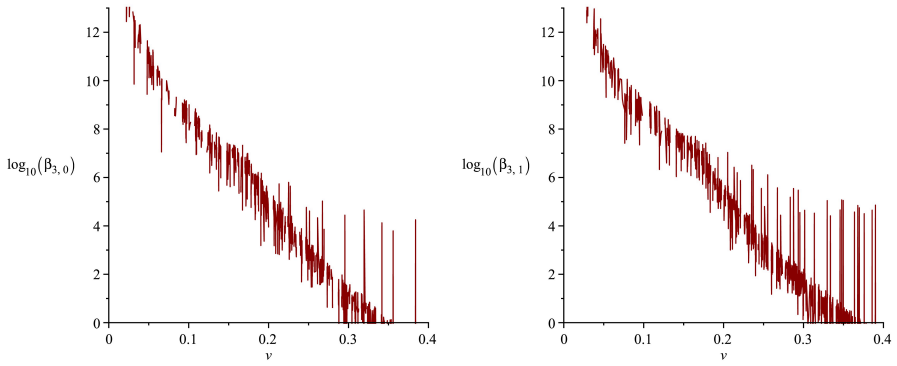


FIGURE 3. Behavior of the coefficients $\beta_{30}$ and $\beta_{31}$ in new method.

- The exponentially-fitted two-step Obrechkoff twelfth algebraic order method developed by Vanden Berghe [18] with the set $\{1, x, \ldots, x^5, \exp(\pm\omega h), x\exp(\pm\omega h)\}$.
- The new developed two-step Obrechkof twelfth algebraic order method with use of VSDPL technique in which we derive method with vanished the set $\{p(v), p^{(i)}(v), i = 1(1)5\}$ where $P(v)$ is phase-lag of new method and $v = \omega h$.

So, we have the following methods:
The symmetric two-step Obrechkof method developed by Simos

$$LTE_{Simos} = -\frac{2923}{209898501120}\, y_n^{(12)} h^{12}. \tag{4.1}$$

The P-stable trigonometrically-fitted symmetric two-step Obrechkof method developed by Wang

$$LTE_{Wang} = \frac{45469}{1697361329664000}\, \left(-y_n^{(14)} + \omega^{12} y_n''\right) h^{14}. \tag{4.2}$$

The symmetric two-step Obrechkof method developed by Daele

$$LTE_{Daele} = \frac{127}{43589145600}\, y_n{}^{(12)} h^{12}. \tag{4.3}$$

The trigonometrically-fitted symmetric two-step Obrechkof method developed by Achar

$$LTE_{Achar} = -\frac{45469}{1697361329664000}\, (T)\, h^{14}, \tag{4.4}$$

where

$$\begin{aligned} T \;=\; & 296296\,\omega^8 y_n^{(6)} + 3003\,\omega^4 y_n^{(10)} + 91\,\omega^2 y_n^{(12)} + y_n^{(14)} + 44473\,\omega^6 y_n^{(8)} \\ & + 773136\,\omega^{10} y_n^{(4)} + 518400\,\omega^{12} y_n^{(2)}. \end{aligned}$$

The Exponentially-fitted two-step Obrechkof method developed by Vanden Berghe

$$LTE_{VanBer} = -\frac{45469}{1697361329664000}\left(\omega^4 y_n^{(10)} + y_n^{(14)} + 2\,\omega^2 y_n^{(12)}\right) h^{14} \tag{4.5}$$

The new two-step Obrechkof method of this paper

$$LTE_{New} = -\frac{45469}{1697361329664000}\,(T)\,h^{14}, \tag{4.6}$$

where

$$\begin{aligned} T &= 15\omega^8 y_n^{(6)} + 15\omega^4 y_n^{(10)} + 6\omega^2 y_n^{(12)} + y_n^{(14)} + 20\omega^6 y_n^{(8)} \\ &\quad +\omega^{12} y_n^{(2)} + 6\omega^{10} y_n^{(4)}. \end{aligned}$$

**Theorem 4.1.** *For the numerical solution of the time independent radial Schrödinger equation the new proposed method produced in this paper is the most accurate method, especially for large values of* $|G| = |Vc - E|$.

*Proof.* The radial time independent Schrödinger equation is of the form

$$y''(x) = f(x)\,y(x). \tag{4.7}$$

Based on the paper of Ixaru and Rizea [6], the function $f(x)$ can be written in the form $f(x) = g(x) + G$, where $g(x) = V(x) - V_c = g$, and $V_c$ is the constant approximation of the potential and $G = v^2 = V_c - E$. We express the derivatives $y_n^{(i)}, i = 2, 3, 4, \cdots$, which are terms of the local truncation error formulae, in terms of Eq. (4.7). The expressions are presented as polynomials of $G$. Finally, we substitute the expressions of the derivatives, into the local truncation error formulae. We use the procedure mentioned above and the formulae:

$$\begin{aligned} y_n^{(2)} &= (V(x) - V_c + G)y(x), \\ y_n^{(4)} &= \left(\frac{d^2}{dx^2}V(x)\right)y(x) + 2\left(\frac{d}{dx}V(x)\right)\left(\frac{d}{dx}y(x)\right) \\ &\quad +(V(x) - V_c + G)\left(\frac{d^2}{dx^2}y(x)\right), \end{aligned}$$

$$\begin{aligned} y_n^{(6)} &= \left(\frac{d^4}{dx^4}V(x)\right)y(x) + 4\left(\frac{d^3}{dx^3}V(x)\right)\left(\frac{d}{dx}y(x)\right) \\ &\quad +3\left(\frac{d^2}{dx^2}V(x)\right)\left(\frac{d^2}{dx^2}y(x)\right) + 4\left(\frac{d}{dx}V(x)\right)^2 y(x) \\ &\quad +6(V(x) - V_c + G)\left(\frac{d}{dx}V(x)\right)\left(\frac{d}{dx}y(x)\right) \\ &\quad +4(V(x) - V_c + G)\left(\frac{d^2}{dx^2}V(x)\right)y(x) \\ &\quad +(V(x) - V_c + G)^2\left(\frac{d^2}{dx^2}y(x)\right)\cdots. \end{aligned}$$

We consider two cases in terms of the value of E:
1-The energy is close to the potential, i.e. $G = V_c - E \approx 0$. So only the free terms of the polynomials in $G$ are considered. Thus for these values of $G$, the methods are of comparable accuracy. This is because the free terms of the polynomials in $G$, are the same for the cases of the classical method and of the new developed methods and of comparable accuracy for the method of Wang [19].
2- $G \gg 0$ or $G \ll 0$. Then $|G|$ is a large number.
So, we have the following asymptotic expansions of the local truncation errors:
*The method produced by Simos [12]*

$$LTE_{\,Simos} = h^{12}\left(-\frac{2923}{209898501120}\,y(x)\,G^6 + \cdots\right). \tag{4.8}$$

*The P-stable trigonometrically-fitted method produced by Wang [19]*

$$LTE_{\,Wang} = h^{14}\left(-\frac{45469}{282893554944000}\,g(x)\,y(x)\,G^6 + \cdots\right). \tag{4.9}$$

*The method produced by Daele [17]*

$$LTE_{\,Daele} = h^{12}\left(-\frac{45469}{282893554944000}\,y(x)\,G^6 + \cdots\right). \tag{4.10}$$

*The method produced by Achar [1]*

$$LTE_{\,Achar} = h^{14}\left(\left(\frac{45469}{5612967360}\,g(x)\,y(x)\right)\,G^6 + \cdots\right). \tag{4.11}$$

*The method produced by Van den Berghe in [18]*

$$LTE_{Van} = -\frac{45469}{1697361329664000}h^{14}\left[T_{Van}\right]. \tag{4.12}$$

where

$$T_{Van} = \left(\left((g(x))^2 + 21\frac{d^2}{dx^2}g(x)\right)y(x) + 2\left(\frac{d}{dx}g(x)\right)\left(\frac{d}{dx}y(x)\right)\right)G^5 + \cdots. \tag{4.13}$$

*The new method produced in this paper*

$$\begin{aligned} LTE_{New} &= -\frac{45469}{17680847184000}\,h^{14}\left(\psi(x)G^3 + \cdots\right), \\ \psi(x) &= \left(\left(\frac{d^4}{dx^4}g(x)\right)g(x) + \frac{5}{2}\left(\frac{d}{dx}g\,(x)\right)\frac{d^3}{dx^3}g(x)\right. \\ &\quad \left. + \frac{5}{3}\left(\frac{d^2}{dx^2}g(x)\right)^2 + \frac{3}{2}\,\frac{d^6}{dx^6}g\,(x)\right)y(x) \\ &\quad + \frac{1}{3}\left(\frac{d^5}{dx^5}g(x)\right)\frac{d}{dx}y(x). \end{aligned} \tag{4.14}$$

| method | Algebraic order | Order of G | CFAE |
|---|---|---|---|
| Simos | 12 | 6 | $-\frac{2923}{2098985011120}$ |
| Daele | 12 | 6 | $\frac{127}{43589145600}$ |
| Achar | 14 | 6 | $\frac{45469}{5612967360}$ |
| Wang | 14 | 6 | $-\frac{45469}{282893554944000}$ |
| Vanden Berghe | 14 | 5 | $-\frac{45469}{1697361329664000}$ |
| New method | 14 | 3 | $-\frac{45469}{17680847184000}$ |

TABLE 1. Comparative error analysis for the methods. CFAE is the coefficient of the maximum power of $G$ in the asymptotic expansion and order of $G$ is the order of the maximum power of $G$ in the asymptotic expansion of the local truncation error.

Hence, for the Wang's, Achar's, Simos's and Daele's Methods the error increases as the sixth power of $G$. For the Van den Berghe's Method the error increases as the fifth power of $G$. For new method produced in this paper the error increases as the third power of $G$ (see Table 1.). So, for the numerical solution of the time independent radial Schrödinger equation the new proposed method produced in this paper is the most accurate Method, especially for large values of $|G| = |V_c - E|$. □

In order to define the interval of periodicity we follow the procedure:
(1) Application of the proposed method to the scalar test equation: The method (3.1) with the coefficients (3.2) is applied to the scalar test equation $y'' = -\vartheta^2 y$, where $\vartheta \neq \omega$.
(2) Definition of the difference equation and the corresponding characteristic equation: We obtain the following difference equation:

$$D_m(s^2; v)\, y_{n+1} - 2N_m(s^2; v)\, y_n + D_m(s^2; v)\, y_{n-1} = 0, \tag{4.15}$$

where $s = \vartheta h$, $h$ is the step length and $D_m(s^2; v)$ and $N_m(s^2; v)$ are polynomials of $s, v$ where $D_m(s^2; v) = 1 - \sum_{i=1}^{m} (-s^2)^i \beta_{i0}$ and $N_m(s^2; v) = 1 + \sum_{i=1}^{m} (-s^2)^i \beta_{i1}$. The rational function $R_{mm}(s^2; v) = \frac{D_m(s^2;v)}{N_m(s^2;v)}$ is the stability function of the method (remark that in the classical case $v = 0$ ). The characteristic equation arising from (4.15) is $v^2 - 2R_{mm}(s^2; v)v + 1 = 0$.

A polynomial-based or classical method with stability function $R_{mm}$ $(s^2; v = 0) = R_{mm}(s^2)$ has an interval of periodicity $(0, s_0^2)$ if $\left|R_{mm}(s^2)\right| < 1$ for $0 < s^2 < s_0^2$. The method is P-stable if $\left|R_{m\,m}(s^2)\right| < 1$ for all real $s \neq 0$. For the classic method we have

$$R_{3\,3}(s^2; v) = \frac{1 - \frac{3665}{7788}s^2 + \frac{711}{25960}s^4 - \frac{2923}{7850304}s^6}{1 + \frac{229}{7788}s^2 + \frac{1}{2360}s^4 + \frac{127}{39251520}s^6}. \tag{4.16}$$

For a method with coefficients depending on the frequency of the problem with stability function $R_{m\,m}(s^2;v)$ the corresponding question of practical interest is this for a given method (i.e., a given $\omega$) and a given test frequency (i.e., given each value of $\vartheta$ relevant to the problem), what restriction, if any, must be placed on the step length $h$ to ensure that the condition $R_{m\,m}(s^2;v)$ is satisfied. Coleman and Ixaru [5] have phrased this answer in three definitions for methods with general stability functions of the form $R_{n\,m}(s^2;v)$.

In Fig. 4, we present the $s-v$ plane for the new methods produced in this paper. A shadowed area denotes the $s-v$ region where the method is stable, while a white area denotes the region where the method is unstable.

**Definition 4.2.** (see [5])A method is called singularly almost P-stable if its interval of periodicity is equal to $(0,\infty)$- S[2] only when the frequency of the exponential fitting is the same as the frequency of the scalar test equation, i.e. $s=v$.

A method is P-stable if the $s-v$ plane is completely shadowed. It can be seen the following:

- The Wang's method [19] is P-stable only in the case in which $s=v$, i.e. if the frequency of the method is equal to the frequency of the scalar test equation then we can say that this method is a singularly P-stable method (see Definition 4.2) and we comprehend that Van den Berghe's and new methods are singularly P-stable methods.
- It is necessary to observe the surroundings of the first diagonal of the $s-v$ plane because for the solution of the Schrödinger equation the frequency of the method is equal to the frequency of the scalar test equation. For new method we see that the surroundings of the first diagonal of the $s-v$ plane is bigger than Wang's method with properties of P-stability and Van den Berghe's method with properties of trigonometrically-fitted.
- There are areas in Figs. 4 that are white and in which the conditions of stability are not satisfied. In the new symmetric two-step Obrechkoff method with vanished phase-lag and its derivatives this areas (white) are fewer than both Wang's and Van den Berghe's methods with property P-stable and trigonometrically-fitted respectively.

**Remark 4.3.** Stability region for method in which we use VSDPL technique is better than methods in which is used from property of trigonometrically-fitted and P-stable in a symmetric two-step Obrechkoff method for the numerical integration of the Schrödinger equation.

[2]Where S is a set of distinct points.

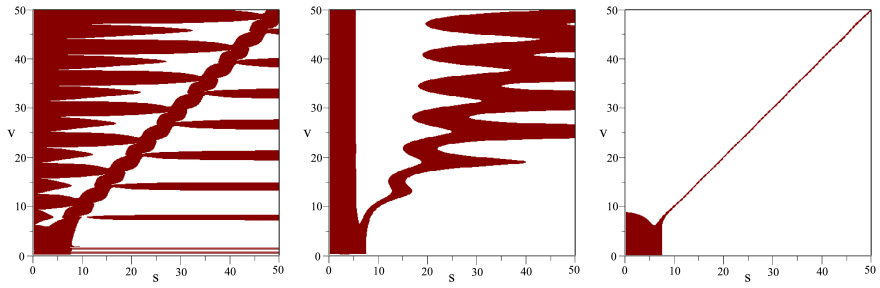


FIGURE 4. The stability plane for new method with VSDPL technique (left), trigonometrically-fitted (center) and P-stable method developed by Wang (right). The stable regions are colored in dark red.

## 5. **Numerical results**

In order to illustrate the efficiency of the new method given by the coefficients in appendix A we apply it to the radial time independent Schrödinger equation. In order to apply the new method to the radial Schrödinger equation the value of parameter $v$ is needed. For every problem of the one-dimensional Schrödinger equation given by (1.1) the parameter $v$ is given by

$$v = \sqrt{|q(x)|} = \sqrt{|V(x) - E|}, \tag{5.1}$$

where $V(x)$ is the potential and E is the energy.

5.1. **Woods-Saxon potential.** We use as potential the well-known Woods-Saxon potential given by

$$V(x) = \frac{u_0}{1+z} - \frac{u_0 z}{a(1+z)^2}, \tag{5.2}$$

with $z = \exp[(x - X_0)/a]$, $u_0 = -50$, $a = 0.6$, and $X_0 = 7.0$.
The behavior of Woods-Saxon potential is shown in Fig. 5.

It is well known that for some potentials, such as the Woods - Saxon potential, the definition of parameter $v$ is not given as a function of $x$ but based on some critical points which have been defined from the investigation of the appropriate potential (see for details [7]).
For the purpose of obtaining our numerical results it is appropriate to choose

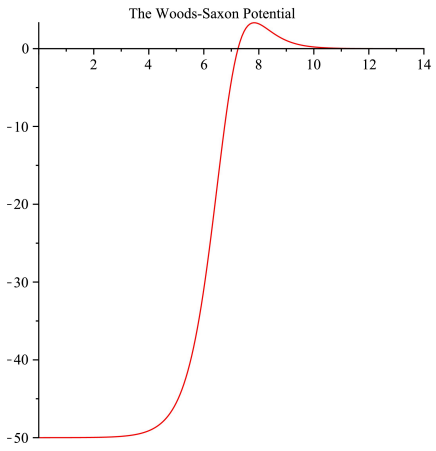


FIGURE 5. The Woods-Saxon potential.

$v$ as follows (see for details [7]):

$$v = \begin{cases} \sqrt{E-50}, & x \in [0, 6.5-2\,h], \\ \sqrt{E-37.5}, & x = 6.5-h, \\ \sqrt{E-25}, & x = 6.5, \\ \sqrt{E-12.5}, & x = 6.5+h, \\ \sqrt{E}, & x \in [6.5+2\,h, 15]. \end{cases}$$

5.2. **Schrödinger equation-resonance problem.** Consider the numerical solution of the radial time-independent Schrödinger equation (1.1) in the well-known case of the Woods- Saxon potential (5.2). In order to solve this problem numerically we need to approximate the true (infinite) interval of integration by a finite interval. For the purpose of our numerical illustration we take the domain of integration as $x \in [0, 15]$. We consider Eq. (1.1) in a rather large domain of energies, i.e. $E \in [1, 1000]$.
In the case of positive energies, $E = k^2$, the potential dies away faster than the term $\frac{l(l+1)}{x^2}$ and the Schrödinger equation effectively reduces to

$$y''(x) = \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x), \tag{5.3}$$

for $x$ greater than some value $X$.
The last equation has two linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$, where $j_l(kx)$ and $n_l(kx)$ are the spherical Bessel and Neumann functions respectively. Thus the solution of Eq. (1.1) has When $(x \to \infty)$ the solution

takes the asymptotic form

$$y(x) \approx A\,k\,x\,j_l(k\,x) - B\,k\,x\,n_l(k\,x) \approx D\,[\sin(k\,x - \pi l/2) + \tan(\delta_l)\cos(kx - \pi l/2)], \tag{5.4}$$

where $\delta_l$ is called *scattering phase-shift* that may be calculated from the formula

$$\tan(\delta_l) = \frac{y(x_i)S(x_{i+1}) - y(x_{i+1})S(x_i)}{y(x_{i+1})C(x_i) - y(x_i)C(x_{i+1})}, \tag{5.5}$$

for $x_1$ and $x_2$ distinct points in the asymptotic region (we choose $x_1$ as the right-hand end point of the interval of integration and $x_2 = x_1 - h$) with $S(x) = kxj_l(kx)$ and $C(x) = -kxn_l(kx)$. Since the problem is treated as an initial-value problem, we need $y_0$ before starting a one-step method. From the initial condition we obtain $y_0$. With these starting values we evaluate at $x_1$ of the asymptotic region the phase-shift $\delta_l$.

For positive energies we have the so-called resonance problem. This problem consists either of finding the phase-shift $\delta_l$ or finding those $E$, for $E \in [1, 1000]$, at which $\delta_l = \frac{\pi}{2}$. We actually solve the latter problem, known as the resonance problem when the positive eigenenergies lie under the potential barrier.

The boundary conditions for this problem are:

$$y(0) = 0, \quad y(x) = \cos(\sqrt{E}x), \quad \text{for large } x. \tag{5.6}$$

We compute the approximate positive eigenenergies of the Woods - Saxon resonance problem using:

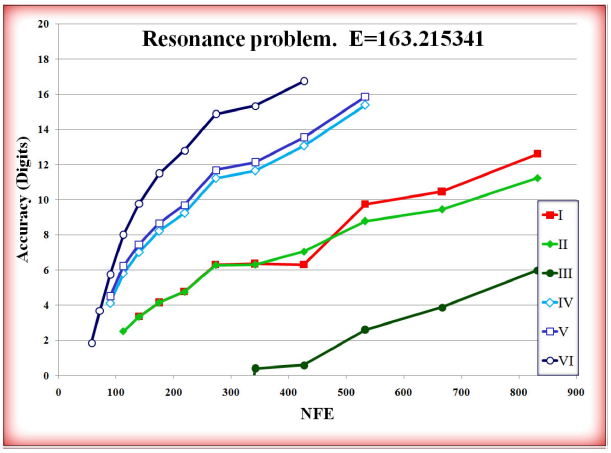


FIGURE 6. Error Errmax for several values of $n$ for the eigenvalue $E_3 = 163.215341$. The nonexistence of a value of Errmax indicates that for this value of $n$, Errmax is positive

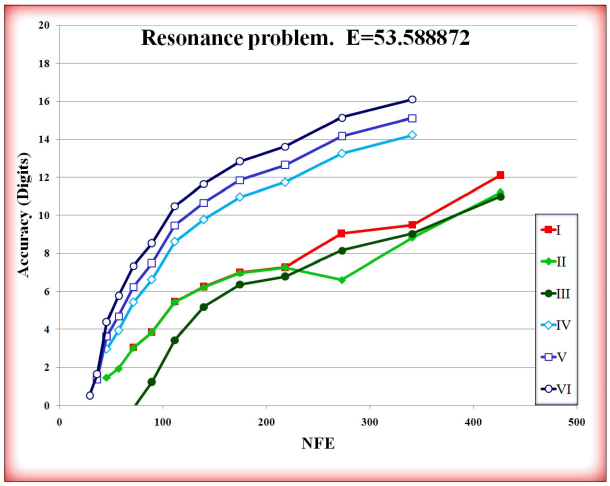


FIGURE 7. Error Errmax for several values of $n$ for the eigenvalue $E_4 = 53.588872$.

- The symmetric two-step Obrechkof tenth algebraic order method developed by Simos [12] which is indicated as Method**I**.
- The symmetric two-step Obrechkof tenth algebraic order method developed by Daele [17] which is indicated as Method**II**.
- The trigonometrically-fitted symmetric two-step Obrechkof twelfth algebraic order method developed by Achar [1] with the set $\{\cos(P\,\omega\,h)\}$ where $P = 1(1)6$ which is indicated as Method**III**.
- The trigonometrically-fitted symmetric two-step P-stable Obrechkof twelfth algebraic order method developed by Wang [19] with phase-lag (frequency distortion) infinity which is indicated as Method**IV**.
- The Exponentially-fitted two-step Obrechkof twelfth algebraic order method developed by Van den Berghe [18] with the set $\{1, x, \cdots, x^5, \exp(\pm\omega h), x\,\exp(\pm\,\omega\,h)\}$ which is indicated as Method**V**.
- The new developed two-step Obrechkof twelfth algebraic order method with use of VMDPL technique in which we derive method with vanished set $\{p(v), p^{(i)}(v)\,,\ i = 1(1)5\}$ where $P(v)$ is phase-lag of new method and $v = \omega h$ which is indicated as Method**VI**.

The computed eigenenergies are compared with exact ones. In Figs. 6 and 7 we present the maximum absolute error $\log_{10}(Err)$ where

$$Err = \|E_{calculated} - E_{accurate}\| \tag{5.7}$$

of the eigenenergy $E_3 = 163.215341$ and $E_4 = 53.588872$ respectively, for several values of NFE= Number of Function Evaluations. Also in Figs. 8

and 9 we present the maximum absolute error $\log_{10}(Err)$, of the eigenenergy $E_1 = 989.701916$ and $E_2 = 341.495874$ respectively, for several values of NFE.

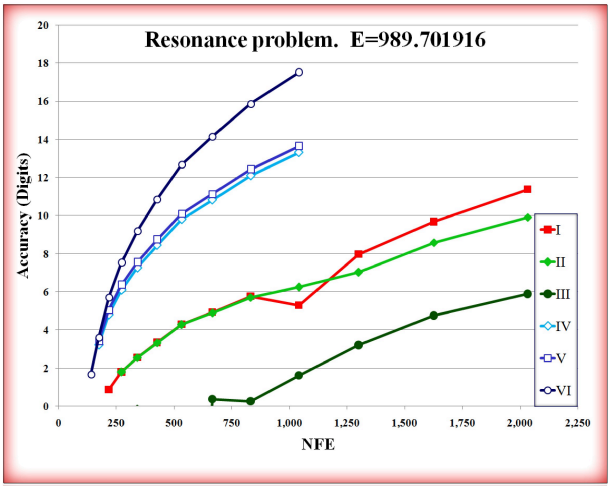


FIGURE 8. Error Errmax for several values of $n$ for the eigenvalue $E_1 = 989.701916$.

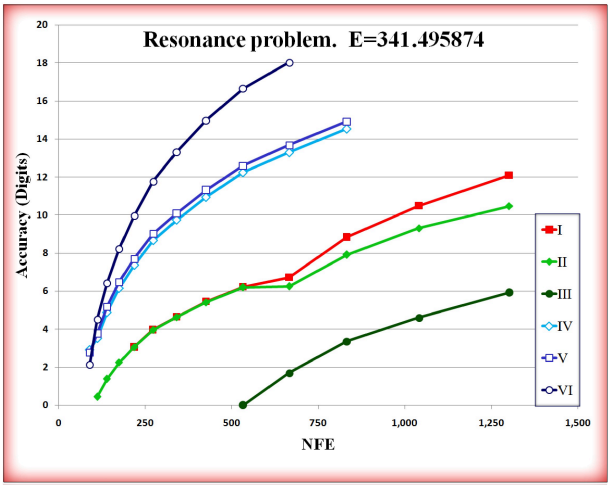


FIGURE 9. Error Errmax for several values of $n$ for the eigenvalue $E_2 = 341.495874$.

## 6. Conclusions

In the present paper we have developed a new P-stable method of twelfth algebraic order for the numerical solution of the radial Schrödinger equation.

We have applied the new method to the resonance problem of the one-dimensional Schrödinger equation. Based on the results presented above we have the following conclusions:

- The Wang's method (IV) is more efficient than the Simos's, Daele's and Achar's methods (I,II,III).
- The second trigonometrically-fitted method developed by Vanden Berghe (V) in [18] is more efficient than the Wang's method (IV) with properties of P-stable and also is much more efficient than the method developed by Simos, Achar and Daele.
- The new developed method (VI) is much more efficient than all the other methods.

**Remark 6.1.** Using the technique of vanished phase-lag and its derivatives in multistep Obrechkoff methods for the numerical solution of the Schrödinger equation, insure us that the principal term of the local truncation error contains the energy with a minimum power, which renders the method highly efficient for the problem and especially for high values of eigenenergies. So, technique of VSDPL is more important than property of trigonometrically-fitted and P-stable in multistep Obrechkoff methods for the numerical solution of the Schrödinger equation.

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(Ali Shokri) Department of Mathematics, Faculty of Basic Science, University of Maragheh, P.O. Box 55181-83111, Maragheh, Iran.
*E-mail address*: shokri@maragheh.ac.ir

(Hosein Saadat) Department of Mathematics, Faculty of Basic Science, University of Maragheh, P.O. Box 55181-83111, Maragheh, Iran.
*E-mail address*: hosein67saadat@yahoo.com