Fourth Order Compact Finite Difference Scheme for Two Dimension Schrödinger Equation

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الفروقات المحددة المضغوطة من الرتبة الرابعة لحل معادلة شرودنكر ثنائية البعد

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الخلاصة

في هذا البحث قمنا بتحسين دقة التقريبات العددية المستخدمة لحل معادلة شرودنكر ثنائية البعد والغير مستقرة مع الزمن. لقد قدم (Subasi, 2002) ثلاث طرق مختلفة لحل هذه المعادلة . لذلك فأننا استخدمنا اسلوب الفروقات المحددة المضغوطة للحصول على حل من الرتبة الرابعة وقد قمنا بمقارنة النتائج العددية لاسلوبنا مع بقية الاساليب وتبين من خلال النتائج ان اسلوبنا هو اكثر دقة من الاساليب التي استخدمت في (Subasi, 2002) .

Abstract:

In this paper we improve the accuracy of the numerical approximation used to solve the two dimensions unsteady Schrödinger equation. Subasi in (Subasi, 2002) present three different finite difference schemes to solve this equation. In this paper, we use compact finite difference scheme to get fourth order solution. The computational accuracy is demonstrated by comparing the results of these schemes. The results appeared that the compact fourth order finite difference scheme is more accurate than the schemes of Subasi.

Keyword: compact finite difference, Schrödinger equation, fourth order, time dependent.

1.INTRODUCTION

The Schrödinger equation is one of the fundamental equations in mathematical physics. It occurs in a broad range of applications as quantum dynamics calculations (Ixaru 1997, Hajj 1985) and has received considerable attention because of its usefulness as a model that describes several important physical and chemical phenomena (Subasi, 2002).

The two dimensions unsteady Schrödinger equation with the potential $v(x, y)$ is written by

$$i\frac{\partial\psi}{\partial t}+\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+v(x,y)\psi=0 \qquad 0\le x,y\le 1,\quad 0\le t\le T \tag{1}$$

With the initial conditions

$$\psi(x,y,0)=\psi_0(x,y) \tag{2}$$

and the boundary condition

$$\begin{aligned}&\psi(0,y,t)=\psi_2(y,t), && \psi(x,0,t)=\psi_3(x,t),\\ &\psi(1,y,t)=\psi_4(x,t), && \psi(x,1,t)=\psi_5(x,t)\ .\end{aligned} \tag{3}$$

Various numerical finite difference schemes have been proposed to solve Schrödinger equation problems, in the late 1960's Gldberg,Schey and Schwartz (Goldberg et al , 1967) considered the solution of the time dependent Schrödinger equation by using explicit and implicit scheme.
Recently, due to the difficulty by introducing a dissipative term in the conventional explicit schemes, Chen,Lee,and Shen (Chan et al , 1986) obtaining a class of new explicit two- level finite difference schemes which are
Conditionally stable. The three-level explicit scheme is derived in (Dai 1989, Dai 1992) for solving Schrödinger equation with constant coefficient and with a variable coefficient which are un conditionally stable. Subasi solve the Schrödinger equation in three methods. The first is the fully explicit finite difference method, the second is the Noye-Hayman implicit finite difference method and he applied the Paceman-Rachford ADI method (Subasi, 2002), all these method are second accurate in space and time, the second and third scheme is un conditionally stable (Mitchell et al 1980, Noye et al 1993).

2. Fourth order compact scheme

Let us consider a rectangular domain $\Omega=[0,1]\times[0,1]$. We discretize Ω with uniform mesh sizes Δx and Δy respectively in the x and y coordinate directions. denote $N_x=1/\Delta x$ and $Ny=1/\Delta y$ be the numbers of uniform intervals along the x and y coordinate directions, respectively. The mesh point are (x_i, y_j) with $x_i=i\Delta x$ and $y_j=j\Delta y$, $0\le i\le Nx$, $0\le j\le Ny$.
In the sequel, we may also use the index pair (i, j) to represent the mesh point (x_i, y_j). In this paper we take $\Delta x=\Delta y=h$ .and $N_x=N_y=N$. Also, we discretize the time interval with uniform mesh sizes Δt . Let $N_t = T/\Delta t$ the numbers of uniform intervals along the time T.

The derivatives in Eq.(1) can be approximated as

$$\left.\begin{aligned}\left.\frac{\partial^2\psi}{\partial x^2}\right|_{ij}^{n} &= \left[\delta_x^2\psi-\frac{h^2}{12}\frac{\partial^4\psi}{\partial x^4}\right]_{ij}^{n}+O(h^4)\\ \left.\frac{\partial^2\psi}{\partial y^2}\right|_{ij}^{n} &= \left[\delta_y^2\psi-\frac{h^2}{12}\frac{\partial^4\psi}{\partial y^4}\right]_{ij}^{n}+O(h^4)\end{aligned}\right\} \qquad (4)$$

$$\left.\frac{\partial\psi}{\partial t}\right|_{ij}^{n}=\left[\delta_t\,\psi-\frac{\Delta t}{2}\frac{\partial^2\psi}{\partial t^2}\right]_{ij}^{n}+O(\Delta t)^2 \qquad (5)$$

The finite difference formula described in this section and to be applied at interior grid points in the solution domain using the standard second order central difference operators (Mitchell et al, 1980) and the approximation given in equation (4) and (5).
Substituting the the standard second order central difference operators and equation (4) and (5) in equation (1) yields the following finite difference equation:

$$i\,\delta_t\,\psi_{ij}^n+\delta_x^2\psi_{ij}^n+\delta_y^2\psi_{ij}^n+v_{ij}\psi_{ij}^n-\tau_{ij}^n=0 \qquad (6)$$

where the truncation error is

$$\tau_{ij}^n=\left[i\frac{\Delta t}{2}\frac{\partial^2\psi}{\partial t^2}+\frac{h^2}{12}\frac{\partial^4\psi}{\partial x^4}+\frac{h^2}{12}\frac{\partial^4\psi}{\partial y^4}\right]_{ij}^{n}+O(h^4,(\Delta t)^2) \qquad (7)$$

We have include both $O(h^2)$ and $O(\Delta t)$ term in Eq.(7) because we wish to approximate all of them in order to construct an $O(h^4)$ and $O(\Delta t)^2$ scheme.

To obtain compact approximation to $O(h^2)$ and $O(\Delta t)$ terms in Eq.(7), we simply take the appropriate derivatives of Eq.(1),

$$\begin{aligned}
\frac{\partial^4\psi}{\partial x^4} &= -i\frac{\partial^3\psi}{\partial x^2\partial t} - \frac{\partial^4\psi}{\partial x^2\partial y^2} - v\frac{\partial^2\psi}{\partial x^2} - 2\frac{\partial\psi}{\partial x}\frac{\partial v}{\partial x} - \psi\frac{\partial^2 v}{\partial x^2}\\
\frac{\partial^4\psi}{\partial y^4} &= -i\frac{\partial^3\psi}{\partial y^2\partial t} - \frac{\partial^4\psi}{\partial y^2\partial x^2} - v\frac{\partial^2\psi}{\partial y^2} - 2\frac{\partial\psi}{\partial y}\frac{\partial v}{\partial y} - \psi\frac{\partial^2 v}{\partial y^2}\\
i\frac{\partial^2\psi}{\partial t^2} &= -\frac{\partial^3\psi}{\partial t\partial x^2} - \frac{\partial^3\psi}{\partial t\partial y^2} - v\frac{\partial\psi}{\partial t}
\end{aligned} \tag{8}$$

Substituting Eqs.(8) into Eq.(7) yields

$$\tau_{ij}^n = \begin{bmatrix} i\frac{\Delta t}{2}\left(-\frac{\partial^3\psi}{\partial t\partial x^2} - \frac{\partial^3\psi}{\partial t\partial y^2} - v\frac{\partial\psi}{\partial t}\right) + \frac{h^2}{12}\left(-i\frac{\partial^3\psi}{\partial x^2\partial t} - \frac{\partial^4\psi}{\partial x^2\partial y^2} - v\frac{\partial^2\psi}{\partial x^2} - 2\frac{\partial\psi}{\partial x}\frac{\partial v}{\partial x}\right.\\ \left. -\psi\frac{\partial^2 v}{\partial x^2}\right) + \frac{h^2}{12}\left(-i\frac{\partial^3\psi}{\partial y^2\partial t} - \frac{\partial^4\psi}{\partial y^2\partial x^2} - v\frac{\partial^2\psi}{\partial y^2} - 2\frac{\partial\psi}{\partial y}\frac{\partial v}{\partial y} - \psi\frac{\partial^2 v}{\partial y^2}\right) \end{bmatrix}_{ij}^n + O(h^4, \Delta t^2) \tag{9}$$

Note that all term on the right hand side of Eq.(9) have compact $O(h^2,\ \Delta t,\ \Delta t\, h^2)$ approximations at noted ijn, and the approximation of these terms has the following forms:

$$\begin{aligned}
\left.\frac{\partial\psi}{\partial x}\right|_{ij}^n &= \delta_x\psi_{ij}^n = \frac{\psi_{i+1j}^n - \psi_{i-1j}^n}{2h},\\
\left.\frac{\partial\psi}{\partial y}\right|_{ij}^n &= \delta_y\psi_{ij}^n = \frac{\psi_{ij+1}^n - \psi_{ij-1}^n}{2h},\\
\left.\frac{\partial^4\psi}{\partial x^2\partial y^2}\right|_{ij}^n &= \delta_x^2\delta_y^2\psi_{ij}^n = \frac{1}{h^4}\left[4\psi_{ij}^n - 2(\psi_{i-1j}^n + \psi_{i+1j}^n + \psi_{ij-1}^n + \psi_{ij+1}^n) + \psi_{i-1j-1}^n + \psi_{i+1j-1}^n + \psi_{i-1j+1}^n + \psi_{i+1j+1}^n\right],\\
\left.\frac{\partial^3\psi}{\partial x^2\partial t}\right|_{ij}^n &= \delta_x^2\delta_t\,\psi_{ij}^n = \frac{1}{\Delta t\ h^2}\left[\psi_{i-1j}^{n+1} - 2\psi_{ij}^{n+1} + \psi_{i+1j}^{n+1} - (\psi_{i-1j}^n - 2\psi_{ij}^n + \psi_{i+1j}^n)\right],\\
\left.\frac{\partial^3\psi}{\partial y^2\partial t}\right|_{ij}^n &= \delta_y^2\delta_t\,\psi_{ij}^n = \frac{1}{\Delta t\ h^2}\left[\psi_{ij-1}^{n+1} - 2\psi_{ij}^{n+1} + \psi_{ij+1}^{n+1} - (\psi_{ij-1}^n - 2\psi_{ij}^n + \psi_{ij+1}^n)\right],
\end{aligned} \tag{10}$$

We can easily get an $O(h^4,(\Delta t)^2)$ method by substituting difference expressions for the $O(h^2,\ \Delta t,\ \Delta t\, h^2)$ term in Eq.(9) and including these in the finite difference approximation (6). The resulting higher-order scheme is as follows

$$\frac{i}{\Delta t}\psi_{ij}^{n+1}+\frac{1}{2}(\delta_x^2+\delta_y^2)\psi_{ij}^{n+1}+\frac{1}{2}v_{ij}\psi_{ij}^{n+1}+\frac{i}{12s}(\delta_x^2+\delta_y^2)\psi_{ij}^{n+1}=\frac{i}{\Delta t}\psi_{ij}^{n}+(\frac{i}{12s}-\frac{1}{2}-\frac{h^2}{12}v_{ij})(\delta_x^2+\delta_y^2)\psi_{ij}^{n}$$
$$-\frac{1}{2}v_{ij}\psi_{ij}^{n}-\frac{h^2}{6}\delta_x^2\delta_y^2\psi_{ij}^{n}-\frac{h^2}{6}(\delta_x\psi_{ij}^{n}\delta_x v_{ij}+\delta_y\psi_{ij}^{n}\delta_y v_{ij})-\frac{h^2}{12}\psi_{ij}^{n}(\delta_x^2+\delta_y^2)v_{ij} \quad (11)$$

Equation (11) is called a high order compact difference scheme of order 4 (HOC-4).

3. Numerical Results

We now consider two test problems to compare the accuracy of fourth order compact scheme with other schemes.

Test problem 1(see[4]): The exact solution of this test problem is $\psi(x,y,t)=x^2y^2e^{it}$. The initial and boundary conditions are directly taken from this solution. The potential $v(x,y)=1-\frac{2}{x^2}-\frac{2}{y^2}$. The test problem were set the same as this in [4].

The results, obtained for ψ_{ij}^n at $T=1.0$, computed for $h=0.1,\ s=0.005$ using the fully explicit method, the Noye-Hayman (5, 5) implicit method, the Paceman-Rachford (3, 3) ADI method and the new fourth order compact finite difference scheme, are listed in Table I and Table II for real and imaginary parts of $\psi(x,y,t)$ respectively. The same problem is solved with values $h=0.1,\ s=0.007$ and the results are given in Table III and Table IV.

TABLE I: The real part results for $\psi(x,y,1)$ with h=0.1, s=0.005 for test-1

			Error			
x	y	exact	(1,5) Explicit	(5,5) N-H	(3,3) P-R ADI	HOC-4
0.1	0.1	5.40E-05	3.08E-05	4.80E-05	6.50E-05	6.25E-10
0.2	0.2	8.64E-04	8.25E-06	9.70E-05	9.00E-05	5.80E-09
0.3	0.3	4.38E-03	1.19E-06	7.30E-05	3.70E-04	1.20E-08
0.4	0.4	1.38E-02	1.59E-05	3.90E-04	9.70E-04	7.17E-09
0.5	0.5	3.38E-02	6.52E-05	4.20E-04	2.70E-03	7.55E-09
0.6	0.6	7.00E-02	1.18E-04	1.70E-03	4.60E-03	2.36E-09
0.7	0.7	1.30E-01	1.11E-04	2.60E-03	4.40E-03	6.02E-09
0.8	0.8	2.21E-01	5.81E-05	8.10E-04	3.60E-03	2.38E-08
0.9	0.9	3.54E-01	1.44E-05	7.00E-04	1.50E-03	1.72E-08

TABLE II: The imaginary part results for $\psi(x, y, 1)$ with h=0.1, s=0.005 for test-1

			Error			
x	y	exact	(1,5) Explicit	(5,5) N-H	(3,3) P-R ADI	HOC-4
0.1	0.1	8.41E-05	1.03E-05	1.30E-05	1.30E-05	1.98E-11
0.2	0.2	1.35E-03	1.87E-06	3.10E-05	4.40E-05	4.58E-11
0.3	0.3	6.82E-03	3.21E-06	1.10E-04	2.90E-04	1.50E-09
0.4	0.4	2.15E-02	1.22E-05	5.40E-04	8.00E-04	6.95E-09
0.5	0.5	5.26E-02	3.49E-07	6.30E-05	1.60E-03	8.86E-09
0.6	0.6	1.09E-01	4.16E-05	4.40E-04	4.00E-03	9.17E-09
0.7	0.7	2.02E-01	6.96E-05	5.40E-04	6.20E-03	1.22E-08
0.8	0.8	3.45E-01	5.44E-05	5.20E-04	4.90E-03	2.54E-08
0.9	0.9	5.52E-01	1.77E-05	4.10E-04	2.20E-03	2.49E-08

TABLE III: The real part results for $\psi(x, y, 1)$ with h=0.1, s=0.007 for test-1

			Error			
x	y	exact	(1,5) Explicit	(5,5) N-H	(3,3) P-R ADI	HOC-4
0.1	0.1	5.40E-05	1.36E-01	5.90E-02	1.10E-02	5.55E-10
0.2	0.2	8.64E-04	5.41E-02	5.40E-03	4.30E-03	5.75E-09
0.3	0.3	4.38E-03	2.04E-02	7.60E-04	7.90E-04	1.23E-08
0.4	0.4	1.38E-02	2.11E-02	9.30E-04	7.00E-04	7.65E-09
0.5	0.5	3.38E-02	3.79E-02	4.50E-04	2.70E-03	6.86E-09
0.6	0.6	7.00E-02	5.44E-02	5.70E-03	4.60E-03	1.75E-09
0.7	0.7	1.30E-01	5.36E-02	6.60E-03	4.20E-03	4.67E-09
0.8	0.8	2.21E-01	3.38E-02	6.20E-03	3.70E-03	1.74E-08
0.9	0.9	3.54E-01	1.02E-02	3.90E-03	1.50E-03	1.29E-08

TABLE IV: The imaginary part results for $\psi(x, y, 1)$ with h=0.1, s=0.007 for test-1

			Error			
x	y	exact	(1,5) Explicit	(5,5) N-H	(3,3) P-R ADI	HOC-4
0.1	0.1	8.41E-05	7.41E-02	2.30E-03	5.40E-03	3.51E-11
0.2	0.2	1.35E-03	4.06E-02	3.50E-04	1.80E-03	9.67E-11
0.3	0.3	6.82E-03	2.61E-02	2.60E-04	1.90E-04	1.45E-09
0.4	0.4	2.15E-02	2.44E-02	8.70E-03	7.20E-04	6.51E-09
0.5	0.5	5.26E-02	2.31E-02	6.90E-03	1.50E-03	9.53E-09
0.6	0.6	1.09E-01	1.60E-02	4.40E-04	4.10E-03	9.36E-09
0.7	0.7	2.02E-01	5.95E-03	5.90E-04	6.40E-03	1.13E-08
0.8	0.8	3.45E-01	2.06E-04	5.20E-03	5.00E-03	1.89E-08
0.9	0.9	5.52E-01	7.69E-04	4.50E-03	2.20E-03	2.02E-08

Test problem 2: The exact solution of this test problem is $\psi(x, y, t) = e^{it+x+y}$. The initial and boundary conditions are directly taken from this solution. The potential $v(x, y) = -1$.

For this test problem the results, obtained for ψ_{ij}^{n} at $T = 1.0$, computed for $h = 0.1, s = 0.005$ using the both the fully explicit method, the Noye-Hayman (5, 5) implicit method, the Paceman-Rachford (3, 3) ADI method and the new fourth order compact finite difference scheme are listed in Table V and TableVI for real and imaginary parts of $\psi(x, y, t)$ respectively The same problem is solved with values $h = 0.1, s = 0.007$ and the results are given in Table VII and Table VIII.

TABLE V: The real part results for $\psi(x, y, 1)$ with h=0.1, s=0.005 for test-2

			Error			
x	y	exact	(1,5) Explicit	(5,5) N-H	(3,3) P-R ADI	HOC-4
0.1	0.1	6.60E-01	1.98E-03	6.36E-07	2.30E-05	8.62E-09
0.2	0.2	8.06E-01	6.98E-03	2.58E-06	7.21E-05	2.91E-08
0.3	0.3	9.84E-01	1.15E-02	4.68E-06	1.38E-04	2.13E-08
0.4	0.4	1.202465	1.19E-02	6.12E-06	2.23E-04	9.76E-09
0.5	0.5	1.468694	1.01E-02	7.09E-06	2.67E-04	7.18E-08
0.6	0.6	1.7938669	8.67E-03	7.52E-06	2.28E-04	8.24E-08
0.7	0.7	2.191034	3.72E-03	6.64E-06	1.64E-04	3.51E-08
0.8	0.8	2.676135	2.29E-04	4.58E-06	1.18E-04	9.81E-09
0.9	0.9	3.2686387	7.39E-05	1.75E-06	5.12E-05	3.16E-08

TABLE VI: The imaginary results for $\psi(x, y, 1)$ with h=0.1, s=0.005 for test-2

			Error			
x	y	exact	(1,5) Explicit	(5,5) N-H	(3,3) P-R ADI	HOC-4
0.1	0.1	1.027775	3.11E-03	1.08E-06	6.61E-05	1.13E-08
0.2	0.2	1.2553272	1.36E-02	3.37E-06	2.26E-04	4.87E-08
0.3	0.3	1.5332601	3.17E-02	5.71E-06	4.27E-04	1.03E-07
0.4	0.4	1.8727281	4.84E-02	7.36E-06	5.92E-04	1.43E-07
0.5	0.5	2.2873553	4.65E-02	7.36E-06	6.43E-04	1.05E-07
0.6	0.6	2.7937821	2.51E-02	5.37E-06	5.86E-04	8.97E-08
0.7	0.7	3.4123331	5.36E-03	3.32E-06	4.16E-04	8.07E-08
0.8	0.8	4.1678331	1.32E-03	1.76E-06	2.44E-04	3.93E-08
0.9	0.9	5.0906029	1.04E-03	5.70E-07	9.47E-05	3.97E-08

TABLE VII: The real part results for $\psi(x, y, 1)$ with h=0.1, s=0.007 for test-2

			Error			
x	y	exact	(1,5) Explicit	(5,5) N-H	(3,3) P-R ADI	HOC-4
0.1	0.1	6.60E-01	3.04E-02	9.19E-07	2.30E-05	9.63E-09
0.2	0.2	8.06E-01	2.86E-01	3.69E-06	7.20E-05	2.85E-08
0.3	0.3	9.84E-01	9.37E-01	6.72E-06	1.38E-04	2.10E-08
0.4	0.4	1.202465	1.57356104	8.87E-06	2.22E-04	9.31E-09
0.5	0.5	1.468694	1.44039369	1.03E-05	2.66E-04	7.19E-08
0.6	0.6	1.7938669	6.18E-01	1.09E-05	2.28E-04	8.28E-08
0.7	0.7	2.191034	1.74E-02	9.61E-06	1.64E-04	3.68E-08
0.8	0.8	2.676135	7.02E-02	6.56E-06	1.18E-04	5.11E-09
0.9	0.9	3.2686387	1.59E-02	2.47E-06	5.12E-05	3.12E-08

TABLE VIII: The imaginary part results for $\psi(x, y, 1)$ with h=0.1, s=0.007 for test-2

			Error			
x	y	exact	(1,5) Explicit	(5,5) N-H	(3,3) P-R ADI	HOC-4
0.1	0.1	1.027775	1.8917665	1.27E-06	6.61E-05	1.23E-08
0.2	0.2	1.2553272	6.96802521	4.07E-06	2.26E-04	4.82E-08
0.3	0.3	1.5332601	13.1448211	7.10E-06	4.27E-04	1.03E-07
0.4	0.4	1.8727281	16.9793478	9.43E-06	5.93E-04	1.41E-07
0.5	0.5	2.2873553	15.7596525	9.72E-06	6.43E-04	1.06E-07
0.6	0.6	2.7937821	10.3494604	7.26E-06	5.86E-04	8.98E-08
0.7	0.7	3.4123331	4.64818651	4.53E-06	4.16E-04	8.22E-08
0.8	0.8	4.1678331	1.41092889	2.45E-06	2.44E-04	4.25E-08
0.9	0.9	5.0906029	2.59E-01	8.31E-07	9.47E-05	3.79E-08

The errors in the tables are all absolute errors between the numerical and exact solution. As can be seen in the tables, the method developed by Subasi[4] achieves second order and much less accurate than using the method of the fourth order for real and imaginary parts.
We note that for two test problem the error of the three methods described by Subasi[4] increases when s decreases (s=0.007).
Also we note that the HOC-4 gives the best and highest accuracy, converges for any values of s.

4. Conclusions

In this paper, the fourth order compact finite difference schemes are derived to solve the two dimensions unsteady Schrödinger equation subject to initial and boundary conditions. We use two problems to test the accuracy of this method with others. The computational is simple and easy to implement, the HOC-4 is presented, analyzed, and successfully applied in the approximation of

Schrödinger equation . The linear system resulted from this scheme is solved iteratively by using the Gauss-Seidel iterative method. We note that the fourth order scheme is much better and very high accuracy of compare with the lower order existing schemes. The fourth order compact finite difference schemes offers compromise between the computed accuracy of the solution and the cost of computing the solution.

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