Finite Difference Schemes for the Unsteady State Schrödinger Equation in Three Dimensions with Complex Variables

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Abstract:

In this paper we introduce three finite difference schemes to solve the three dimensions unsteady Schrödinger equation. The finite difference scheme developed for this purpose are based on the (1, 7) fully explicit scheme, the (7, 7) Crank-Nicolson technique and fourth order compact scheme. The computational accuracy is demonstrated by comparing the results of these schemes. The results show that the compact fourth order finite difference scheme is more accurate than the other schemes.

Keyword: compact finite difference, three dimension 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 [2, 5] and has received considerable attention because of its usefulness as a model that describes several important physical and chemical phenomena [3] .

The three dimensions unsteady Schrödinger equation with the potentialv(x, y, z) is written by

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

…(1)

where $i=\sqrt{-1}$

The initial conditions are

$$\Box(x,y,z,0)=\Box_0(x,y,z)$$

…(2)

The boundary condition

$$\Box(0,y,z,t)=\Box_1(y,z,t), \qquad \Box(x,0,z,t)=\Box_2(x,z,t),$$

$$\Box(1,y,z,t)=\Box_3(y,z,t), \qquad \Box(x,1,z,t)=\Box_4(x,z,t),$$

$$\Box(x,y,0,t)=\Box_5(x,y,t), \qquad \Box(x,y,1,t)=\Box_6(x,y,t)$$

…(3)

Numerical solution of Schrödinger equation has been considered by a few authors. Dia [4] solve the one dimension Schrödinger equation with variable coefficients by using three level explicit difference scheme. Subasi in [3] presents three different finite difference schemes to solve the two dimension Schrödinger equation using three schemes, all these schemes are of second order for space. Recently, Shatha A. Mahdi [1] presents a fourth order accurate finite difference scheme for solving the 2D Schrödinger equation.

The aim of this paper is to get the fourth order accuracy in space and second order in time for 3D Schrödinger equation. The organization of the paper is as follows. In the sections 2.1, 2.2 and 2.3 we introduce the explicit, Crank-Nicolson and fourth order finite difference schemes respectively. In section 3 we detailed comparisons of our schemes. In section 4 we discuss the conclusions.

2. The numerical techniques

Let us consider a cubic domain = [0,1]×[0,1]×[0,1]. We discretize 2 with uniform mesh sizes Ax Ay and Az respectively in the x, y and z coordinate directions. Define Nx =1/Ax, Ny =1/Ay and Nz =1/Az the numbers of uniform subintervals along the x, y and z coordinate directions, respectively. The mesh points are (x,y,z) where x = i Ax y_1 = j Дy, Zk = k Az, 0 ≤ i ≤ Nx, 0 ≤ j ≤ Ny, 0 ≤ k ≤ Nz. In the sequel, we may also use the index (i,j,k) to represent the mesh point (x,y,z). In this paper we take_Δx = Δy = Δz = h, and Nx = Ny =Nz = N. Also, we discretize the time interval with uniform mesh sizesΔt.

The standard second order central difference operators defined at grid point (i, j, k) can be written as

$$\left.\begin{aligned}
\delta_x^2\psi_{ijk}^n &= \frac{\psi_{i+1jk}^n - 2\psi_{ijk}^n + \psi_{i-1jk}^n}{h^2} \\
\delta_y^2\psi_{ijk}^n &= \frac{\psi_{ij+1k}^n - 2\psi_{ijk}^n + \psi_{ij-1k}^n}{h^2} \\
\delta_z^2\psi_{ijk}^n &= \frac{\psi_{ijk+1}^n - 2\psi_{ijk}^n + \psi_{ijk-1}^n}{h^2} \\
\delta_t\psi_{ijk}^n &= \frac{\psi_{ijk}^{n+1} - \psi_{ijk}^n}{\Delta t}
\end{aligned}\right\} \qquad \ldots(4)$$

The derivatives in Eq.(1) can be approximated to second order accuracy as

$$\left.\begin{aligned}
\left.\frac{\partial^2\psi}{\partial x^2}\right|_{ijk}^n &= \left[\delta_x^2\psi - \frac{h^2}{12}\frac{\partial^4\psi}{\partial x^4}\right]_{ijk}^n + O(h^4) \\
\left.\frac{\partial^2\psi}{\partial y^2}\right|_{ijk}^n &= \left[\delta_y^2\psi - \frac{h^2}{12}\frac{\partial^4\psi}{\partial y^4}\right]_{ijk}^n + O(h^4) \\
\left.\frac{\partial^2\psi}{\partial z^2}\right|_{ijk}^n &= \left[\delta_z^2\psi - \frac{h^2}{12}\frac{\partial^4\psi}{\partial z^4}\right]_{ijk}^n + O(h^4) \\
\left.\frac{\partial\psi}{\partial t}\right|_{ijk}^n &= \left[\delta_t\psi - \frac{\Delta t}{2}\frac{\partial^2\psi}{\partial t^2}\right]_{ij}^n + O(\Delta t^2)
\end{aligned}\right\} \qquad \ldots(5)$$

2.1 The (1, 7) Explicit finite difference method

In this section, we describe explicit second order finite difference formula. This formula resulting by substituting the finite difference approximations (4) in equation (1):

$$\psi_{ijk}^{n+1} = \psi_{ijk}^n + is(\psi_{i+1jk}^n - 2\psi_{ijk}^n + \psi_{i-1jk}^n) + is(\psi_{ij+1k}^n - 2\psi_{ijk}^n + \psi_{ij-1k}^n)$$
$$+ is(\psi_{ijk+1}^n - 2\psi_{ijk}^n + \psi_{ijk-1}^n) + i\Delta t v_{ijk}\psi_{ijk}^n$$

where s = $\frac{\Delta t}{\text{h2}}$

Since this formula involves one grid point at the new time level and 7 at the old level, this procedure is referred to as the (1, 7) method.

2.2 Crank-Nicolson method.

In this method, we replace all spatial derivatives with average of their values at the n and n+1 time level and then substitute centered-difference for all derivatives:

$$\frac{\partial^2 \Box_{ijk}^{n}}{\partial x^2} = \frac{1}{2h^2}\left(\Box_{i+1,jk}^{n+1} - 2\Box_{ijk}^{n+1} + \Box_{i-1,jk}^{n+1}\right) + \frac{1}{2h^2}\left(\Box_{i+1,jk}^{n} - 2\Box_{ijk}^{n} + \Box_{i-1,jk}^{n}\right),$$

$$\frac{\partial^2 \Box_{ijk}^{n}}{\partial y^2} = \frac{1}{2h^2}\left(\Box_{ij+1k}^{n+1} - 2\Box_{ijk}^{n+1} + \Box_{ij-1k}^{n+1}\right) + \frac{1}{2h^2}\left(\Box_{ij+1k}^{n} - 2\Box_{ijk}^{n} + \Box_{ij-1k}^{n}\right),$$

$$\frac{\partial^2 \Box_{ijk}^{n}}{\partial z^2} = \frac{1}{2h^2}\left(\Box_{ijk+1}^{n+1} - 2\Box_{ijk}^{n+1} + \Box_{ijk-1}^{n+1}\right) + \frac{1}{2h^2}\left(\Box_{ijk+1}^{n} - 2\Box_{ijk}^{n} + \Box_{ijk-1}^{n}\right)$$

and

$$\frac{\partial \Box_{ijk}^{n}}{\partial t} = \frac{1}{\Delta t}\left(\Box_{ijk}^{n+1} - \Box_{ijk}^{n}\right) \qquad \ldots(7)$$

Substituting these forms in the three-dimensional Schrödinger equation give (7, 7) implicit finite difference formula as follows:

$$\begin{aligned}(2+6is-i\Delta t v_{ijk})\Box_{ijk}^{n+1} - is(\Box_{i+1,jk}^{n+1} + \Box_{i-1,jk}^{n+1}) - is(\Box_{ij+1k}^{n+1} + \Box_{ij-1k}^{n+1}) - is(\Box_{ijk+1}^{n+1} + \Box_{ijk-1}^{n+1}) = \\ (2-6is+i\Delta t v_{ijk})\Box_{ijk}^{n} + is(\Box_{i+1,jk}^{n} + \Box_{i-1,jk}^{n}) + is(\Box_{ij+1k}^{n} + \Box_{ij-1k}^{n}) + is(\Box_{ijk+1}^{n} + \Box_{ijk-1}^{n})\end{aligned} \qquad \ldots(8)$$

2.3 Fourth order compact scheme

Using the finite difference operators in (4) and (5), Eq.(1) can be discretized at a given grid point (x, y, z) as

$$i\square_t\square^n_{ijk}+\square^2_x\square^n_{ijk}+\square^2_y\square^n_{ijk}+\square^2_z\square^n_{ijk}+v_{ijk}\square^n_{ijk}-\square^n_{ijk}=0 \qquad \ldots(9)$$

where the truncation error is

$$\square^n_{ijk}=\left[\frac{\square i\Delta t}{2}\frac{\partial^2\square}{\partial t^2}+\frac{h^2}{12}\frac{\partial^4\square}{\partial x^4}+\frac{h^2}{12}\frac{\partial^4\square}{\partial y^4}+\frac{h^2}{12}\frac{\partial^4\square}{\partial z^4}\right]^n_{ijk}+O(h^4,\Delta t^2)$$

…(10)

We have include both O(h²) and O(At) term in Eq.(10) as we wish to approximate all of them in order to construct an O(h) and O(At²) scheme.

To obtain compact approximation to the O(h²) and O(At) terms in Eq.(10), we simply take the appropriate derivatives of Eq.(1),

$$\frac{\partial^4\square}{\partial x^4}=-i\frac{\partial^3\square}{\partial x^2\partial t}-\frac{\partial^4\square}{\partial x^2\partial y^2}-\frac{\partial^4\square}{\partial x^2\partial z^2}-v\frac{\partial^2\square}{\partial x^2}-2\frac{\partial\square}{\partial x}\frac{\partial v}{\partial x}-\square\frac{\partial^2 v}{\partial x^2}$$

$$\frac{\partial^4\square}{\partial y^4}=-i\frac{\partial^3\square}{\partial y^2\partial t}-\frac{\partial^4\square}{\partial y^2\partial x^2}-\frac{\partial^4\square}{\partial y^2\partial z^2}-v\frac{\partial^2\square}{\partial y^2}-2\frac{\partial\square}{\partial y}\frac{\partial v}{\partial y}-\square\frac{\partial^2 v}{\partial y^2}$$

$$\frac{\partial^4\square}{\partial z^4}=-i\frac{\partial^3\square}{\partial z^2\partial t}-\frac{\partial^4\square}{\partial z^2\partial x^2}-\frac{\partial^4\square}{\partial z^2\partial y^2}-v\frac{\partial^2\square}{\partial z^2}-2\frac{\partial\square}{\partial z}\frac{\partial v}{\partial z}-\square\frac{\partial^2 v}{\partial z^2}$$

$$i\frac{\partial^2\square}{\partial t^2}=-\frac{\partial^3\square}{\partial t\partial x^2}-\frac{\partial^3\square}{\partial t\partial y^2}-\frac{\partial^3\square}{\partial t\partial z^2}-v\frac{\partial\square}{\partial t}$$

…(11)

$$\square_{ij}^{n} = \left[\begin{array}{l} \frac{\Delta t}{2}\left(-\frac{\partial^3\square}{\partial t\partial x^2}-\frac{\partial^3\square}{\partial t\partial y^2}-\frac{\partial^3\square}{\partial t\partial z^2}-v\frac{\partial\square}{\partial t}\right) \\ +\frac{h^2}{12}\left(-i\frac{\partial^3\square}{\partial x^2\partial t}-\frac{\partial^4\square}{\partial x^2\partial y^2}-\frac{\partial^4\square}{\partial x^2\partial z^2}-v\frac{\partial^2\square}{\partial x^2}-2\frac{\partial\square}{\partial x}\frac{\partial v}{\partial x}-\square\frac{\partial^2 v}{\partial x^2}\right) \\ +\frac{h^2}{12}\left(-i\frac{\partial^3\square}{\partial y^2\partial t}-\frac{\partial^4\square}{\partial y^2\partial x^2}-\frac{\partial^4\square}{\partial y^2\partial z^2}-v\frac{\partial^2\square}{\partial y^2}-2\frac{\partial\square}{\partial y}\frac{\partial v}{\partial y}-\square\frac{\partial^2 v}{\partial y^2}\right) \\ +\frac{h^2}{12}\left(-i\frac{\partial^3\square}{\partial z^2\partial t}-\frac{\partial^4\square}{\partial z^2\partial x^2}-\frac{\partial^4\square}{\partial z^2\partial y^2}-v\frac{\partial^2\square}{\partial z^2}-2\frac{\partial\square}{\partial z}\frac{\partial v}{\partial z}-\square\frac{\partial^2 v}{\partial z^2}\right) \end{array}\right]_{ijk}^{n} + O(h^4,\Delta t^2)$$

…(12)

Note that all term on the right hand side of Eq.(12) have compact O(h², Δt, Ath²) approximations at noted ijk, and the approximation of these terms has the following forms:

$$\left.\frac{\partial\square}{\partial x}\right|_{ijk}^{n} = \square_x\square_{ijk}^{n} = \frac{\square_{i+1,jk}^{n}-\square_{i-1,jk}^{n}}{2h}+O(h^2)$$

$$\left.\frac{\partial\square}{\partial y}\right|_{ijk}^{n} = \square_y\square_{ijk}^{n} = \frac{\square_{ij+1k}^{n}-\square_{ij-1k}^{n}}{2h}+O(h^2)$$

$$\left.\frac{\partial\square}{\partial y}\right|_{ijk}^{n} = \square_z\square_{ijk}^{n} = \frac{\square_{ijk+1}^{n}-\square_{ijk-1}^{n}}{2h}+O(h^2)$$

$$\left.\frac{\partial^4 \square}{\partial x^2 \partial y^2}\right|_{ijk}^{n} = \square_x^2 \square_y^2 \square_{ijk}^n = \frac{1}{h^4}\left(4\square_{ijk}^n - 2\left(\square_{i-1jk}^n + \square_{i+1jk}^n + \square_{ij-1k}^n + \square_{ij+1k}^n\right) + \square_{i-1j-1k}^n + \square_{i+1j-1k}^n + \square_{i-1j+1k}^n + \square_{i+1j+1k}^n\right) + O(h^2)$$

$$\left.\frac{\partial^4 \square}{\partial x^2 \partial z^2}\right|_{ijk}^{n} = \square_x^2 \square_z^2 \square_{ijk}^n = \frac{1}{h^4}\left(4\square_{ij}^n - 2\left(\square_{i-1jk}^n + \square_{i+1jk}^n + \square_{ijk-1}^n + \square_{ijk+1}^n\right) + \square_{i-1jk-1}^n + \square_{i+1jk-1}^n + \square_{i-1jk+1}^n + \square_{i+1jk+1}^n\right) + O(h^2)$$

$$\left.\frac{\partial^4 \square}{\partial y^2 \partial z^2}\right|_{ijk}^{n} = \square_y^2 \square_z^2 \square_{ijk}^n = \frac{1}{h^4}\left(4\square_{ijk}^n - 2\left(\square_{ijk-1}^n + \square_{ijk+1}^n + \square_{ij-1k}^n + \square_{ij+1k}^n\right) + \square_{ij-1k-1}^n + \square_{ij-1k+1}^n + \square_{ij+1k-1}^n + \square_{ij+1k+1}^n\right) + O(h^2)$$

$$\left.\frac{\partial^3 \square}{\partial x^2 \partial t}\right|_{ijk}^{n} = \square_x^2 \square_t \square_{ijk}^n = \frac{1}{\Delta t\, h^2}\left[\square_{i-1jk}^{n+1} - 2\square_{ijk}^{n+1} + \square_{i+1jk}^{n+1} - \left(\square_{i-1jk}^n - 2\square_{ijk}^n + \square_{i+1jk}^n\right)\right] + O(h^2, \Delta t)$$

$$\left.\frac{\partial^3 \square}{\partial y^2 \partial t}\right|_{ijk}^{n} = \square_y^2 \square_t \square_{ijk}^n = \frac{1}{\Delta t\, h^2}\left[\square_{ij-1k}^{n+1} - 2\square_{ijk}^{n+1} + \square_{ij+1k}^{n+1} - \left(\square_{ij-1k}^n - 2\square_{ijk}^n + \square_{ij+1k}^n\right)\right] + O(h^2, \Delta t)$$

$$\left.\frac{\partial^3 \square}{\partial z^2 \partial t}\right|_{ijk}^{n} = \square_z^2 \square_t \square_{ijk}^n = \frac{1}{\Delta t\, h^2}\left[\square_{ijk-1}^{n+1} - 2\square_{ijk}^{n+1} + \square_{ijk+1}^{n+1} - \left(\square_{ijk-1}^n - 2\square_{ijk}^n + \square_{ijk+1}^n\right)\right] + O(h^2, \Delta t)$$

…(13)

We can easily get an $O(h^1, At^2)$ method by substituting difference expressions for the $O(h^2, At, Ath^2)$ term in Eq.(12) and including these in the finite difference approximation (9). The resulting higher-order scheme follows from

$$\frac{i}{\Delta t}\psi^{n+1}_{ijk}+\frac{1}{2}(\delta_x^2+\delta_y^2+\delta_z^2)\psi^{n+1}_{ijk}+\frac{1}{2}v_{ijk}\psi^{n+1}_{ijk}+\frac{i}{12\Delta t}(\delta_x^2+\delta_y^2+\delta_z^2)\psi^{n+1}_{ijk}=\frac{i}{\Delta t}\psi^{n}_{ijk}+$$
$$(\frac{i}{12\Delta t}-\frac{1}{2}-\frac{h^2}{12}v_{ijk})(\delta_x^2+\delta_y^2+\delta_z^2)\psi^{n}_{ijk}-\frac{h^2}{6}(\delta_x^2\delta_y^2+\delta_x^2\delta_z^2+\delta_y^2\delta_z^2)\psi^{n}_{ijk}-\frac{1}{2}v_{ijk}\psi^{n}_{ijk}$$
$$-\frac{h^2}{6}(\delta_x\psi^{n}_{ijk}\delta_x v_{ijk}+\delta_y\psi^{n}_{ijk}\delta_y v_{ijk}+\delta_z\psi^{n}_{ijk}\delta_z v_{ijk})-\frac{h^2}{12}\psi^{n}_{ijk}(\delta_x^2+\delta_y^2+\delta_z^2)v_{ijk}$$
$$\ldots(14)$$

Equation (14) is called a high order compact difference scheme of order 4 (HOC-4). Equations (6), (8) and (14) can be separated to two equations real and imaginary. The linear systems generating is solved iteratively by using Gauss-Seidel iterative method.

3. Numerical Results

Now we consider two test problems to compare the accuracy for the schemes which used in this paper.

Test problem 1: The exact solution of this test problem

(x, y, z,t) = x^2y^2ze''. The initial and boundary conditions are directly taken from this solution. The potential v(x, y, z) =1 --2 2 2 x^2 y^2 22 2 z

The results obtained for at T =1.0, computed for k h=0.1 and s = 0.01 using the (1, 7) explicit method, the Crack-Nicholson (7, 7) implicit method and fourth order compact finite difference scheme are listed in Table I, according to real and imaginary parts of (x, y, z, t). When the same problem is solved with values h = 0.1 s = 0.007, s = 0.005, s = 0.001 given in Table II, Table III and Table IV respectively. We note that the explicit scheme has very large error when s = 0.01, s = 0.007 and its accuracy increases with the value of s. Also, we observe the following:

1- In this example the accuracy of the Crank-Nicholson scheme and fourth order scheme do not change with decrease the value of s.

2- The Crank-Nicholson scheme has accuracy of order $O(h^2, At^2)$ and fourth order scheme has accuracy of order $O(h, Ar^2)$ but we notes that the error of Crank-

Nicholson is small less the fourth order.

This is accruing because the value of the function is very small such that the error already becomes very small. The high computation of fourth order scheme "compare with the Crank-Nicholson" must be generated some expected errors in evaluation process.

4. Conclusions

In this paper, we introduce three finite difference scheme the (1, 7) fully explicit scheme, the Crank-Nicholson scheme and the fourth order compact finite difference schemes to solve the three dimensions unsteady Schrödinger equation subject to initial and boundary conditions. We used two problems to test the accuracy of this with others. We note that the accuracy of the fourth order scheme is very high compare with the other schemes. The linear system resulted from these scheme is solved iteratively by using the Gauss-Seidel iterative method.

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أساليب الفروقات المحددة لحل معادلة شرودنكر ثلاثية البعد غير المستقرة مع الزمن ذات المتغيرات العقدية

عقيل جاسم حرفش

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الخلاصة:

في هذا البحث استخدمنا ثلاث أسليب للفروقات المحددة لحل معادلة شرودنكر غير المستقرة مع الزمن بصيغتها النهائية بصيغتها الثلاثية البعد عددياً ، الأسلوب الأول المستخدم للحل هو اسلوب الفروقات المحددة الصريح (١،٧) والاسلوب الثاني هو الضمني (٧٧) (كرانك نيكولسون) ، وفي الاسلوب الثالث تمكنا من تطبيق الفروقات المحددة المضغوطة من الرتبة الرابعة مع طريقة كرانك نيكولسون للحصول على دقة من الرتبة الرابعة بالنسبة للحيز وثنائية بالنسبة للزمن ، أما النظام الخطي الناتج من صيغة الفروقات المحددة فقمنا بحله باستخدام طريقة كاوس سايدل التكرارية ، وقد قمنا بتطبيق هذه الأساليب على مثالين اختباريين لقياس الدقة ، فوجدنات ان دقة الاسلوب الثالث عالية جدا مقارنة بالاسلوب الآخرين.