

# Time-dependent Schrödinger Equation based on HO-FDTD Schemes

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**Abstract** — A high order finite-different time-domain methods using Taylor series expansion for solving time-dependent Schrödinger equation has been systematically discussed in this paper. Numerical characteristics have been investigated of the schemes for the Schrödinger equation. Compared with the standard Yee FDTD scheme, the numerical dispersion has been decreased and the convergence has been improved. The general update equations of the methods have been presented for wave function. Numerical results of potential well in one-dimension show that the application of the schemes is more effective than the Yee's FDTD method and the higher order has the better numerical dispersion characteristics.

**Index Terms** — HO-FDTD, numerical dispersion, stability, the Schrödinger equation.

## I. INTRODUCTION

With the devices size shrinks, quantum effects can not to be ignored in the nano-scale material and semiconductor in equipment system. In some certain circumstances, like in a quantum-dot structure, the quantum effects are remarkable and the problem requires new mathematical method to investigate. The Maxwell's equations are the basic theory for researching the electromagnetic phenomenon in macroscopic scale. The Schrödinger equations are employed to solve the nano-scale components in microscopic scale electromagnetic domain. There are many numerical methods are used to solve the Schrödinger equations [1]. The Yee's FDTD [2] algorithm is conservative and limitation with the second-order accuracy both in time and space. The numerical dispersion and computational memory of the FDTD are the dominant restriction to the application in the electronically large electromagnetic targets. The FDTD [3-5] scheme has been chosen to deal with the quantum problem for its convenient and simple. The absorbing boundary conditions for the FDTD method of the time-dependent one-dimensional Schrödinger equation are proposed in [6]. The absorbing boundary conditions are considered by using a rational-function approximation for the one- and two-dimensional

Schrodinger equations on a finite interval [7]. A new FDTD simulation scheme for coupled Maxwell-Schrödinger system is presented in [8] and the computation has been made more efficient.

The dimensional time domain which using the FDTD method to describe the simulation of the quantum magnetic susceptibility for a quantum toroid [9].

In recent years, the high order finite-difference time-domain (HO-FDTD) [10] method and multiresolution time-domain (MRTD) [11] scheme are outstanding technique in the quantum computational field. The HO-FDTD schemes is a little more complicate than the FDTD but is less complex than the MRTD method.

In this paper, we give HO-FDTD methods to deal with the time-dependent Schrödinger equation. The simulation results of the method are testified by one dimensional potential well problem. The paper is organized as follows. The basic theory of the method for the time-dependent Schrödinger equation is stated in Section II. The numerical characteristics including the dispersion and stability are discussed in Section III. Numerical simulation is given in Section IV. Consequently, the HO-FDTD algorithms is more accuracy but more computational time than that of FDTD method.

## II. THEORY AND ALGORITHM

### A. The Schrödinger equation

The time-dependent Schrödinger equation is the governing equation for system's quantum effects can be written as follows:

$$i\hbar \frac{\partial \psi(\vec{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}, t) + V(\vec{r})\psi(\vec{r}, t), \quad (1)$$

where  $\psi$  is a particle's wave function, the mass of the electron  $m$  is  $9.109 \times 10^{-31} \text{kg}$ , the Planck constant  $\hbar$  is  $1.0546 \times 10^{-34} \text{J} \cdot \text{s}$ , the imaginary unit "i" is the square root of minus one,  $V(\vec{r})$  is the potential energy,  $-\frac{\hbar^2}{2m} \nabla^2$  is the kinetic energy operator, and  $-\frac{\hbar^2}{2m} \nabla^2 + V$  is the Hamiltonian operator. The wave function  $\psi(\vec{r}, t)$  is a complex which can be written as follows:

$$\psi(\vec{r}, t) = \psi_{re}(\vec{r}, t) + i\psi_{im}(\vec{r}, t), \quad (2)$$

where  $\psi_{re}$  and  $\psi_{im}$  is the real part and imaginary part of wave function  $\psi$ .

The equation (1) can be rewritten as:

$$\frac{\partial \psi_{re}(\vec{r}, t)}{\partial t} = -\frac{\hbar}{2m} \frac{\partial^2 \psi_{im}(\vec{r}, t)}{\partial x} + \frac{1}{\hbar} \mathbf{V}(\vec{r}) \psi_{im}(\vec{r}, t), \quad (3)$$

$$\frac{\partial \psi_{im}(\vec{r}, t)}{\partial t} = \frac{\hbar}{2m} \frac{\partial^2 \psi_{re}(\vec{r}, t)}{\partial x} - \frac{1}{\hbar} \mathbf{V}(\vec{r}) \psi_{re}(\vec{r}, t). \quad (4)$$

## B. The HO-FDTD for Schrödinger equation

The wave function  $\psi$  can be written as follows:

$$\psi^{n+1/p}(i, j, k) = \psi^{n+1/p}(i\Delta x, j\Delta y, k\Delta z). \quad (5)$$

The wave function relevant in (5) is expand in a Taylor series of basis function, the update equations of the HO-FDTD(2,2n) methods for the real part of the method can be written as follows:

$$\begin{aligned} \psi_{re}^{n+1}(i, j, k) &= \psi_{re}^n(i, j, k) + \frac{\Delta t}{\hbar} \mathbf{V}(i, j, k) \psi_{im}^n(i, j, k) \\ &- \sum_{v=1}^{\infty} a(v) \frac{\Delta t}{\Delta x^2} \frac{\hbar}{2m} \left[ \psi_{im}^n(i+v, j, k) - 2\psi_{im}^n(i, j, k) + \psi_{im}^n(i-v, j, k) \right] \\ &- \sum_{v=1}^{\infty} a(v) \frac{\Delta t}{\Delta y^2} \frac{\hbar}{2m} \left[ \psi_{im}^n(i, j+v, k) - 2\psi_{im}^n(i, j, k) + \psi_{im}^n(i, j-v, k) \right], \\ &- \sum_{v=1}^{\infty} a(v) \frac{\Delta t}{\Delta z^2} \frac{\hbar}{2m} \left[ \psi_{im}^n(i, j, k+v) - 2\psi_{im}^n(i, j, k) + \psi_{im}^n(i, j, k-v) \right] \end{aligned} \quad (6)$$

where  $\Delta x, \Delta y, \Delta z$  is the cell size and  $i, j, k$  is the spatial grid index in  $x, y, z$  direction, respectively,  $\Delta t$  is the time step size,  $a(v)$  are the coefficients as shown in Table 1.

Table 1: Coefficients of spatial difference

(2, 2p)	a(1)	a(2)	a(3)	a(4)	a(5)
FDTD	1				
(2,6)	97/84	-1/84	-1/84		
(2,8)	353/324	-1/324	-1/324	-1/324	
(2,10)	489/462	-1/924	-1/924	-1/924	-1/924

## III. NUMERICAL CHARACTERISTICS

### A. Stability condition of the HO-FDTD method for the Schrödinger equation

On the basis of the von Neumann stability, the solution of the wave function can be written as superpositions of the plane wave [19] as:

$$\psi(x, y, z, t) = A \exp(-i(i\Delta_x k_x + j\Delta_y k_y + k\Delta_z k_z - \omega n \Delta t)), \quad (7)$$

where  $k_x = k_0 \sin \theta \cos \varphi$ ,  $k_y = k_0 \sin \theta \sin \varphi$ ,  $k_z = k_0 \cos \theta$ ,  $k_0$  is the wave number,  $k_0 = p_m / \hbar$ ,  $p_m$  is the momentum,  $(\theta, \varphi)$  is the wave propagation angle in spherical coordinate,  $n$  is the quantity of the time steps,  $\omega$  is the frequency of the incident wave.

In one dimension and  $V = 0$  for simplicity, the general stability condition of the HO-FDTD methods for the Schrödinger equation [12]-[18] can be given as:

$$\Delta t \leq \frac{m\Delta^2}{\hbar\sqrt{d} \sum_{v=1}^{\infty} |a(v)|} = s_{\max} \frac{m\Delta^2}{\hbar}, \quad (8)$$

$$s_{\max} = \frac{1}{\sqrt{d} \sum_{v=1}^{\infty} |a(v)|}, \quad (9)$$

where  $\Delta x = \Delta y = \Delta z = \Delta$ ,  $d$  is the number of spatial dimensions, 1, 2 or 3, the Courant-Friedrichs-Lewy (CFL) stability condition is in equation (8),  $s_{\max}$  is the maximum CFL stability factor that is shown in Table 2. The investigations are that the HO-FDTD methods have the more stricter stability condition than FDTD. From the comparisons among the HO-FDTD, it is obvious that the higher order has the looser stability condition.

Table 2: The maximum stability factor  $s_{\max}$  for HO-FDTD methods

	FDTD	(2, 6)	(2, 8)	(2, 10)
$s_{\max}$	$1/\sqrt{d}$	$0.848/\sqrt{d}$	$0.910/\sqrt{d}$	$0.941/\sqrt{d}$

### B. Numerical dispersion of HO-FDTD methods for the Schrödinger equation

Using the 2p<sup>th</sup>-order difference to discretize the spatial derivatives as follows:

$$\frac{\partial^2 \psi}{\partial x^2} \approx \sum_{v=-p}^p C_v \frac{\psi(i+v, j, k)}{(\Delta x)^2} = \sum_{v=-p}^p C_v \frac{\exp(-j_0 v k_x \Delta x)}{(\Delta x)^2} \psi(i, j, k), \quad (10)$$

$$\frac{\partial^2 \psi}{\partial y^2} \approx \sum_{v=-p}^p C_v \frac{\psi(i, j+v, k)}{(\Delta y)^2} = \sum_{v=-p}^p C_v \frac{\exp(-j_0 v k_y \Delta y)}{(\Delta y)^2} \psi(i, j, k), \quad (11)$$

$$\frac{\partial^2 \psi}{\partial z^2} \approx \sum_{v=-p}^p C_v \frac{\psi(i, j, k+v)}{(\Delta z)^2} = \sum_{v=-p}^p C_v \frac{\exp(-j_0 v k_z \Delta z)}{(\Delta z)^2} \psi(i, j, k), \quad (12)$$

where  $C_v$  is the coefficients of 2p<sup>th</sup>-order spatial difference as shown in Table 3.

In Maxwell's equation and free space, the dispersion relation of the free electron can be written as

$$\omega = \left( \frac{\hbar}{2m} \right) |\vec{k}|^2, \quad (13)$$

where  $\vec{k}$  is the wave vector with the amplitude  $k$ ,  $c$  is velocity of the light. Similarly, the theoretic velocity of the Schrödinger equation is  $v = (\hbar/2m)$  and the numerical velocity is  $v_p = \omega/k_0^2$ . Substituting the equations (7) and

(10), (11), (12) in to the wave equation to get the relative numerical dispersion error  $\eta=20\log_{10}|v_p/v-1|$  shows

in the Fig. 1 with the stability factor  $(\hbar\Delta t/\Delta 2m) = 0.25$  and wave propagation angle  $\theta = 0^\circ$  and  $\phi = 0^\circ$ .

Table 3: Coefficients of  $2p$ th-order spatial difference

$(2,2p)$	$C_{-5}$	$C_{-4}$	$C_{-3}$	$C_{-2}$	$C_{-1}$	$C_0$	$C_1$	$C_2$	$C_3$	$C_4$	$C_5$
FDTD					1	-2	1				
(2,4)				-1/12	4/3	-5/2	4/3	-1/12			
(2,6)			-1/84	-1/84	97/84	-95/42	97/84	-1/84	-1/84		
(2,8)		-1/324	-1/324	-1/324	353/324	-175/81	353/324	-1/324	-1/324	-1/324	
(2,10)	-1/924	-1/924	-1/924	-1/924	489/462	-487/231	489/462	-1/924	-1/924	-1/924	-1/924

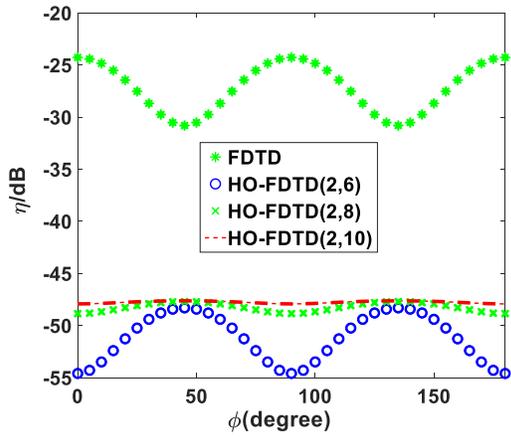


Fig. 1. Dispersion errors against  $\phi$  with the incident angle  $\theta = 30^\circ$  of different HO-FDTD methods.

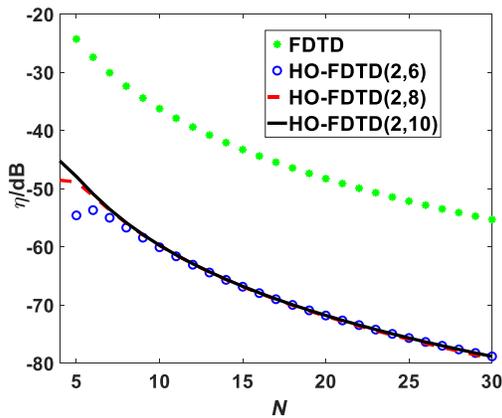


Fig. 2. Numerical dispersion against  $N$  of different HO-FDTD methods.

Figure 1 shows that HO-FDTD methods present the better numerical dispersion than FDTD. The higher order of the methods the more accuracy, but the HO-FDTD (2, 6) performs better. The relative numerical dispersion error  $\eta$  versus the number of cells per wavelength  $N$  for different HO-FDTD methods are illustrated in Fig. 2. The comparisons show that the HO-FDTD methods have the lower numerical dispersion and

the higher order allows coarser cells per wavelength and less memory required.

#### IV. NUMERICAL SIMULATION

A particle trapped in an infinite potential well in one dimension are discussed as follows:

$$V(x) = \begin{cases} 0, & 0 < x < l \\ \infty, & \text{otherwise} \end{cases}, \quad (14)$$

where the length of the well  $l$  is  $0 < l < 1nm$ ,  $x$  is the position of the particle in axis. The cell size  $\Delta x$  is  $0.015nm$ . The total time step is 3000. The expression of energy for level  $L$  of the quantum well is quantized as:

$$E_L = \frac{1}{2m} \left( \frac{\hbar\pi L}{l} \right)^2, \quad L = 1, 2, 3... \quad (15)$$

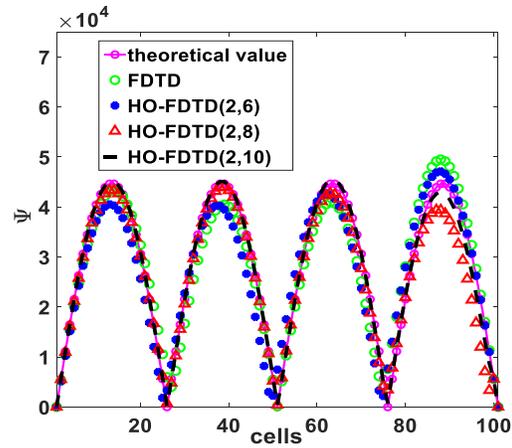


Fig. 3. The comparisons of simulations for the wavefunction with different methods and theoretical value in one dimensional infinite well.

Figure 3 shows the simulation of the FDTD and HO-FDTD algorithms for wavefunction with the energy level  $L = 4$ . The results show that the HO-FDTD more similar to the theoretical value than FDTD method and the HO-FDTD (2, 10) is the more closely to the theoretical value among other HO-FDTD methods. The time step size, spatial cell size, time steps, computational domain and CPU time consumption are listed in table 4.

It shows that the CPU time consumption of the HO-FDTD methods are more than FDTD. It is clear that the more complicated algorithm affords the better dispersion but need more computational time with the same computational condition.

Table 4: Computational parameters different methods

Methods	FDTD	(2,6)	(2,8)	(2,10)
$\Delta x$ (nm)	0.015nm	0.015nm	0.015nm	0.015nm
$\Delta t$ (s)	$4.3188 \times 10^{-21}$	$4.3188 \times 10^{-21}$	$4.3188 \times 10^{-21}$	$4.3188 \times 10^{-21}$
Spatial cells	150	150	150	150
Time steps	3000	3000	3000	3000
CPU time(s)	6.8750	8.6378	9.2674	9.5683

## V. CONCLUSIONS

Different order of the HO-FDTD methods for solving time-dependent Schrödinger equation has been investigated in this paper. The simulation of the wave function for a particle in one dimensional infinite potential well are used to validate the accuracy of the HO-FDTD and FDTD methods. The results show that the HO-FDTD schemes afford the better numerical dispersion under the same computational condition and the higher order the more accuracy.

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