RK-HO-FDTD Scheme for Solving Time-dependent Schrodinger Equation

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***Abstract*—** The Runge-Kutta high-order finite-difference time-domain (RK-HO-FDTD) method is adopted to solve the time-dependent Schrodinger equation. The update equations of the RK-HO-FDTD method have been presented for wave function. The simulation results of the 1D potential well strongly confirm the advantages of the RK-HO-FDTD scheme over the conventional FDTD.

***Index Terms* —** Dispersion, potential well, RK-HO-FDTD, stability, the Schrodinger equation.

I. INTRODUCTION

Recently, more and more numerical solutions are employed to solve the Schrodinger equation [1]. The finite-difference time-domain (FDTD) [2] method also has been played an important role in quantum computational fields. The first attempt to use the FDTD algorithm for the Schrodinger equation was Goldberg et al. in 1967 [3], but it didn't get a lot of attention. 1990 years later, the topic began to cause greater attention [4-6], which is based on the Crank-Nicholson scheme. Soriano et al. rigorously formulated an efficient FDTD-Q algorithm and distinguished its application for quantum systems [7]. FDTD-Q method is one of the commonly adopted methods to solve the time-dependent eigenvalue problem of the Schrodinger equation, but it suffers from large dispersion errors in a long erm simulation [8-9]. The symplectic algorithm has been proposed to solve the Maxwell–Schrodinger (M-S) system for investigating light-matter interaction [11], but it suffers from intolerable dispersion errors in a long-term simulation.

The RK-HO-FDTD are proposed in [10] and has the better dispersion error and convergence. In this paper, the RK-HO-FDTD [10] scheme is used to solve the Schrodinger equation for one dimensional (1D) potential well problem. The paper is organized as follows. First, the basic theory and algorithm are introduced in Section II. The dispersion and stability for different methods are shown in Section III. Numerical example is given in Section IV. The simulation results show better numerical dispersion than the traditional FDTD and the HO-FDTD approach.

II. THEORY AND ALGORITHM

The time-dependent Schrodinger equation is written as follows:

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

where ψ is wave function of a particle related to position and time t, m is the mass of the particle, $-\frac{\hbar^2}{2m}\nabla^2$ is the kinetic energy operator, $\mathrm{V}(\vec{r})$ is the time-independent potential energy, and $-\frac{\hbar^2}{2m}\nabla^2+\mathrm{V}$ is the Hamiltonian operator. The variable $\psi(\vec{\mathrm{r}},t)$ is a complex number that can be written as:

$$\psi(\vec{\mathrm{r}},t)=\psi_R(\vec{\mathrm{r}},t)+i\psi_I(\vec{\mathrm{r}},t). \tag{2}$$

Substituting (2) into (1), the equations can be obtained as:

$$\frac{\partial\psi_R(\vec{r},t)}{\partial t}=-\frac{\hbar}{2m}\frac{\partial^2\psi_I(\vec{r},t)}{\partial x}+\frac{1}{\hbar}\mathrm{V}(\vec{r})\psi_I(\vec{r},t), \tag{3}$$

$$\frac{\partial\psi_I(\vec{r},t)}{\partial t}=\frac{\hbar}{2m}\frac{\partial^2\psi_R(\vec{r},t)}{\partial x}-\frac{1}{\hbar}\mathrm{V}(\vec{r})\psi_R(\vec{r},t), \tag{4}$$

where ψ_R is the real part of wave function ψ, ψ_I is the imaginary part of wave function ψ.

The equation can be rewritten as:

$$\frac{\partial}{\partial t}\begin{pmatrix}\psi_R\\ \psi_I\end{pmatrix}=A\begin{pmatrix}\psi_R\\ \psi_I\end{pmatrix}, \tag{5}$$

$$\frac{\partial}{\partial t}F=AF, \tag{6}$$

where $A=\begin{pmatrix}0 & \kappa\\ -\kappa & 0\end{pmatrix}$, $\kappa=-\frac{\hbar}{2m}(\nabla^2)+\frac{\mathrm{V}}{\hbar}$, $F=\begin{pmatrix}\psi_R\\ \psi_I\end{pmatrix}$.

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According to [10], we use the *p*th-order *p* stage SSP-RK scheme to discretized the temporal system in equation (5).

The SSP-RK scheme is written as follows:

$$F_{n+1}=\sum_{l=0}^{p}\alpha_{p,l}F^{(l)}, \tag{7}$$

where $F_n=F(t_n)$, and the coefficients $\alpha_{p,l}$ [12] are given by:

$$\alpha_{p,p}=\frac{1}{p!}, \quad l=p,$$

$$\alpha_{p,l}=\frac{1}{l}\alpha_{p-1,l-1}, \quad l=1,2,\ldots p-1, \quad p\geq 2,$$

$$\alpha_{p,0}=1-\sum_{l=1}^{p}\alpha_{p,l}, \quad l=0.$$

Based on the Staggered difference, the wave function ψ can be written as:

$$\psi^{n+l/p}(i,j,k)=\psi_I^{n+l/p}(i\Delta x, j\Delta y, k\Delta x). \tag{8}$$

Using the fourth order staggered difference to replace the spatial derivative in *x*-axis as follows:

$$\frac{\partial\psi^{n+l/p}(i)}{\partial x^2}=\frac{-\psi^{n+l/p}(i-2)+16\psi^{n+l/p}(i-1)-30\psi^{n+l/p}(i)}{12\Delta x^2}+\frac{+16\psi^{n+l/p}(i+1)-\psi^{n+l/p}(i+2)}{12\Delta x^2}. \tag{9}$$

Employing the SSP-RK algorithm to substitute time derivates and the Taylor series to replace spatial derivates, the update equations for the real part of the RK-HO-FDTD method can be derived as follows:

$$\begin{aligned}
\psi_R^{n+l/p}(i,j,k)&=\psi_R^{n+(l-1)/p}(i,j,k)+\frac{\Delta t}{\hbar}\mathrm{V}(i,j,k)\psi_I^{n+l/p}(i,j,k)\\
&-\alpha_{x1}\frac{\Delta t}{\Delta x^2}\frac{\hbar}{2m}\left[\psi_I^{n+l/p}(i+1,j,k)-2\psi_I^{n+l/p}(i,j,k)+\psi_I^{n+l/p}(i-1,j,k)\right]\\
&-\alpha_{x2}\frac{\Delta t}{\Delta x^2}\frac{\hbar}{2m}\left[\psi_I^{n+l/p}(i+2,j,k)-2\psi_I^{n+l/p}(i,j,k)+\psi_I^{n+l/p}(i-2,j,k)\right]\\
&-\alpha_{y1}\frac{\Delta t}{\Delta y^2}\frac{\hbar}{2m}\left[\psi_I^{n+l/p}(i,j+1,k)-2\psi_I^{n+l/p}(i,j,k)+\psi_I^{n+l/p}(i,j-1,k)\right]\\
&-\alpha_{y2}\frac{\Delta t}{\Delta y^2}\frac{\hbar}{2m}\left[\psi_I^{n+l/p}(i,j+2,k)-2\psi_I^{n+l/p}(i,j,k)+\psi_I^{n+l/p}(i,j-2,k)\right]\\
&-\alpha_{z1}\frac{\Delta t}{\Delta z^2}\frac{\hbar}{2m}\left[\psi_I^{n+l/p}(i,j,k+1)-2\psi_I^{n+l/p}(i,j,k)+\psi_I^{n+l/p}(i,j,k-1)\right]\\
&-\alpha_{z2}\frac{\Delta t}{\Delta z^2}\frac{\hbar}{2m}\left[\psi_I^{n+l/p}(i,j,k+2)-2\psi_I^{n+l/p}(i,j,k)+\psi_I^{n+l/p}(i,j,k-2)\right],
\end{aligned} \tag{10}$$

where Δx, Δy, Δz is the cell size and *i*, *j*, *k* is the spatial grid index in *x*, *y*, *z* direction, respectively, and Δt is the time step size, α_{x1}, α_{x2}, α_{y1}, α_{y2}, α_{z1} and α_{z2} are the coefficients of the HO-FDTD and $\alpha_{x1}=\alpha_{y1}=\alpha_{z1}=a(1)$, $\alpha_{x2}=\alpha_{y2}=\alpha_{z2}=a(2)$ as given in Table 1.

Table 1: Coefficients for HO-FDTD method

	$a(1)$	$a(2)$
FDTD	1	
HO-FDTD (2,4)	4/3	-1/12

III. NUMERICAL STABILITY AND DISPERSION

A. Stability of RK-HO-FDTD for the Schrodinger equation

The solution of the wave function can be represented as a superposition of plane wave on the basis of the von Neumann stability method as follows:

$$\psi(x,y,z,t)=A_m\exp(-j_0(i\Delta_x k_x+j\Delta_y k_y+k\Delta_z k_z)), \tag{11}$$

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 and $k_0=\mathrm{p}_m/\hbar$, p_m is the momentum, (θ, φ) is the wave propagation angle in spherical coordinate, j_0 is the imaginary unit.

For simplicity, we consider the Schrodinger equation in one dimension (1D) and set the potential energy zero (V=0). Using the m'th-order difference to discretize the spatial derivatives as follows:

$$\frac{\partial\psi}{\partial x^2}\approx\sum_{L=-m'/2}^{m'/2}C_L\frac{\psi(i,j,k+L)}{\Delta_x^2}=\sum_{L=-m'/2}^{m'/2}C_L\frac{\exp(-j_0Lk_x\Delta_x)}{\Delta_x^2}\psi(i,j,k)=T_x\psi, \tag{12}$$

where $T_x=\sum_{L=-m'/2}^{m'/2}C_L\frac{\exp(-j_0Lk_x\Delta_x)}{\Delta_x^2}$, $\mathrm{C_L}$ is the coefficients of *m*′th-order spatial difference which is listed in Table 2.

Table 2: Coefficients of *m*′th-order spatial difference [14-15]

Order (*m*′)	C_1	C_2	C_3	C_4	C_5
FDTD	1	-2	1		
HO-FDTD (2,4)	4/3	-1/12	-5/2	4/3	-1/12

Equation (5) can be rewritten as:

$$\frac{\partial}{\partial t}\begin{pmatrix}\psi_R\\ \psi_I\end{pmatrix}=H\begin{pmatrix}\psi_R\\ \psi_I\end{pmatrix}, \tag{13}$$

$$H=\begin{pmatrix}0 & -\frac{\hbar}{2m}T_x\\ \frac{\hbar}{2m}T_x & 0\end{pmatrix}, \tag{14}$$

where *H* is spatial growth matrix, the eigen equation of *H* is written as $|\lambda\mathrm{I}-H|=0$ which can be used to solve the eigen value, the positive sign solution of the eigen value

can be derived as follows:

$$\left|\lambda \mathrm{I}\text{-}H\right| = \lambda^2 + (\frac{\hbar}{2m}T_x)^2 = 0\,, \tag{15}$$

$$\begin{aligned}\lambda &= j_0 \frac{\hbar}{2m}T_x \\ &= j_0\lambda_j\,,\end{aligned} \tag{16}$$

where λ_j is the imaginary part of λ.

Equation (7) of the SSP-RK method can be rewritten [9], [12] as:

$$F(t_{n+1}) = \sum_{l=0}^{p}\frac{1}{l!}(\Delta t H)^l F(t_n) = GF(t_n)\,, \tag{17}$$

$$\xi = \sum_{l=0}^{p}\frac{1}{l!}(\lambda\Delta t)^l\,, \tag{18}$$

where G is the total gain factor of F, ξ is the gain factor of F when $H = \lambda$. The SSP-RK algorithm is stable and convergent under the condition of $|G| \le 1$ and $|\xi| \le 1$, and the solution of the equation (17) can be written as $\lambda_j\Delta t \le C_f$, C_f is a constant. The stability condition of the RK$_3$-HO-FDTD (2, 4) when p = 3 for the Schrodinger equation can be derived as:

$$\xi = \left|\sum_{l=0}^{3}\frac{1}{l!}(\lambda\Delta t)^l\right| = \left|\sum_{l=0}^{3}\frac{1}{l!}(j_0\lambda_j\Delta t)^l\right| \le 1\,, \tag{19}$$

$$\begin{aligned}&\left|\left(1-\frac{1}{2}(\lambda_j\Delta t)^2\right) + j_0\left(\lambda_j\Delta t - \frac{1}{6}(\lambda_j\Delta t)^3\right)\right| \le 1 \\ &\left(1-\frac{1}{2}(\lambda_j\Delta t)^2\right)^2 + \left(\lambda_j\Delta t - \frac{1}{6}(\lambda_j\Delta t)^3\right)^2 \le 1 \\ &1+\frac{1}{4}(\lambda_j\Delta t)^4 - (\lambda_j\Delta t)^2 + (\lambda_j\Delta t)^2 + \\ &\qquad \frac{1}{36}(\lambda_j\Delta t)^6 - \frac{1}{4}(\lambda_j\Delta t)^4 \le 1 \\ &\qquad \frac{1}{36}(\lambda_j\Delta t)^2 \le \frac{1}{12} \\ &\qquad \lambda_j\Delta t \le \sqrt{3}.\end{aligned} \tag{20}$$

In equation (20) $C_f = \sqrt{3}$ and C_f is dependent on the order of the time discretization, then C_f of the RKp-HO-FDTD (2, 2m') can be deduced in the same way. From the equation (16), it can be found that the spatial stability condition is dependent on λ_j correspond to the spatial discretization order m. To sum up, the stability condition of the RK-HO-FDTD method for the Schrodinger equation is decided by equation (16) and (20), then the general form of stability condition for the RKp-HO-FDTD (2, 2m') [11] can be given as:

$$\Delta t \le C_f \frac{m\Delta^2}{\hbar\sqrt{d}\sum_{\mathrm{L'}=1}^{m'}|a(m')|} = \beta\frac{m\Delta^2}{\hbar}\,, \tag{21}$$

$$\beta = \frac{C_f}{\sqrt{d}\sum_{L'=1}^{m'}|a(m')|}\,, \tag{22}$$

where $\Delta x = \Delta y = \Delta x = \Delta$, L' is the number of the coefficients in Table 1, d is the spatial dimension, equation (21) is the Courant-Friedrichs-Lewy (CFL) stability condition, β is the CFL stability factor which is shown in Table 3. The investigation is that the RK$_3$-HO-FDTD (2, 4) has the looser stability condition than other methods and the SSP-RK method can increase the algorithm stability.

Table 3: Stability factor for different methods

	FDTD	HO-FDTD (2, 4)	RK$_3$-HO-FDTD (2, 4)	RK$_4$-HO-FDTD (2, 4)
β	$1/\sqrt{d}$	$0.7059/\sqrt{d}$	$1.2226/\sqrt{d}$	$1.9965/\sqrt{d}$

B. Dispersion of RK-HO-FDTD for the Schrodinger equation

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

$$\omega = \left(\frac{\hbar}{2m}\right)\left|\vec{k}\right|^2\,, \tag{23}$$

where c is velocity of light, $\vec{k}$ is the wave vector with the amplitude k, and $k_x = k\sin\theta\cos\phi$, $k_y = k\sin\theta\sin\phi$, $k_z = k\cos\theta$, (θ, ϕ) is the wave propagation angle in spherical coordinate. Similarly, the theoretic velocity of the Schrodinger equation is $v = \left(\frac{\hbar}{2m}\right)$ and the numerical velocity is $v_p = \frac{\omega}{k_0^2}$. The dispersion relation can be derived from the expansion of the plane wave and the SSP-RK theory [13] as follows:

$$\omega\Delta t = \mathrm{Arg}(\xi)\,. \tag{24}$$

According to the CFL stability condition, defining the stability factor $S = (\hbar\Delta t/\Delta 2m) = 0.25$, and with the wave propagation angle $\theta = 0°$ and $\phi = 0°$.

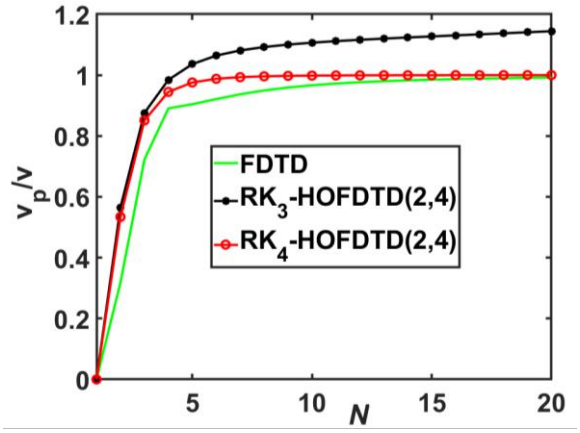

Fig. 1. Dispersion errors against N of the FDTD and RK-HO-FDTD method.

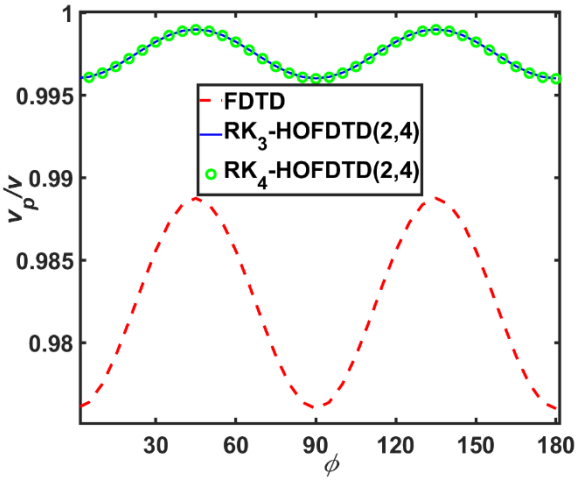

Fig. 2. Dispersion errors against ϕ with the incident angle $\theta = 30°$ of the FDTD and RK-HO-FDTD method.

Figure 1 shows the dispersion errors v_p / v versus the number of cells per wavelength N for the FDTD, RK_3-HO-FDTD(2, 4) and RK_4-HO-FDTD(2, 4) methods. The results show that the RK-HO-FDTD methods have the lower numerical dispersion and the higher order allows coarser cells within a given accuracy. The dispersion characteristic of the RK_3-HO-FDTD is not good, the reason maybe the temporal order 3 is not matching with the spatial order 4. There is no difference between RK_4-HO-FDTD (2, 4) and FDTD when N is greater than 20. Figure 2 demonstrates that RK-HO-FDTD method present the better dispersion error.

IV. NUMERICAL SIMULATION

In order to demonstrate the efficiency of the RK-HO-FDTD methods for 1D infinite potential well simulation is presented. Considering a particle trapped in an infinite potential well as:

$$V(x) = \begin{cases} 0, & 0 < x < d \\ \infty, & \text{otherwise} \end{cases}, \tag{25}$$

where d is the length of the well and x is the position of the particle in axis.

Without loss of generality, the size of the d is $0<d<10^{-9}$m and the cell size Δx is 10^{-11}m. The total time step is 2000. The eigenenergies of the quantum well are quantized as:

$$E_n = \frac{h^2\pi^2}{2ma^2}n^2, \quad n = 1, 2, 3... \tag{26}$$

The wavefunction calculated with the FDTD and RK-HO-FDTD schemes are drawn in Fig. 3. It shows that the RK-HO-FDTD schemes accord closely with the theoretical predictions than FDTD method. Table 4 gives the temporal discretization, spatial discretization, total computational domain, total time steps and CPU time. From the data, we know that the CPU times of the HO-FDTD (2,4) is more than the FDTD. The conclusion is the better dispersion need more computational time with the same computational condition.

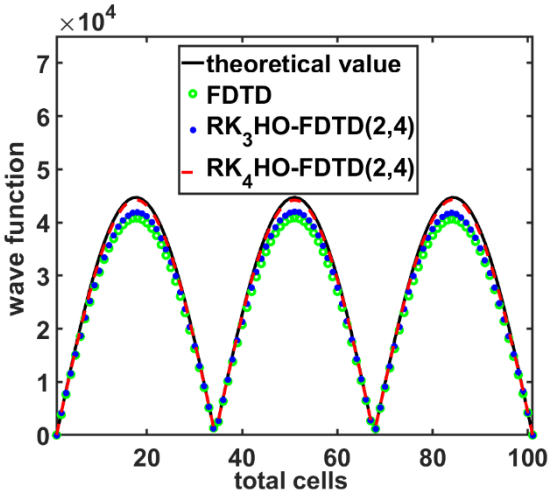

Fig. 3. The comparisons of the wavefunction calculated in different methods and theoretical value in 1D infinite well.

Table 4: Computational time for FDTD and RK-HO-FDTD method

Methods	FDTD	RK3-HO-FDTD (2,4)	RK4-HO-FDTD (2,4)
Δx (m)	10^{-11}	10^{-11}	10^{-11}
Δt	6.5039×10^{-19}	6.5039×10^{-19}	6.5039×10^{-19}
Total cells	100	100	100
Total time	2000	2000	2000
CPU time(s)	5.995	13.296	18.873

V. CONCLUSIONS

The characteristics of the RK-HO-FDTD methods have been discussed in this paper for solving the Schrodinger equation. The RK-HO-FDTD and FDTD method are implemented to mode the wave function of a particle in 1D infinite potential well. The results show that the scheme can increase the accuracy of wavefunction simulation.

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