Multi-Quantum State Control of Nano-tube by the Maxwell-Schrödinger Hybrid Method

Z. D. Yang, L. Zhang, H. Zeng, D.Z. Ding and R.S. Chen
Department of Communication Engineering
Nanjing University of Science and Technology, Nanjing, 210094, China
eerschen@njust.edu.cn

***Abstract*—In this paper, the Maxwell-Schrödinger hybrid method is used to analyze the quantum state control problem in the one-dimensional nano-tube structure. The coupling equations of the three-dimensional Maxwell equation and the one-dimensional Schrödinger equation with the control equation of quantum state are employed and solved by the Finite Difference Time-Domain (FDTD) numerical algorithm. In the numerical examples, the accuracy of the Maxwell-Schrödinger hybrid method is validated by the comparison with [1]. Finally, the multi-quantum state control of nano-tube is realized by the Maxwell-Schrödinger hybrid method.**

Keywords—Maxwell-Schrödinger Hybrid Method, Quantum State Control Equation, FDTD.

I. INTRODUCTION

Although existing all conventional computers so far, that is, “classical computers”, have employed a certain operating system to the elementary component determining only 0 or 1, a quantum computer utilizes the superposition of discrete quantum levels of a particle, namely q-bits, such as an electron, an atom, and a molecule. Recent researches in the quantum states control of atoms, molecules, and nanoscale objects have been attracted great attention [2-5]. The quantum states transition process of electrons from the ground state to the excited state is controlled by external light pulses.

In this paper, The Maxwell-Schrödinger hybrid equations and the quantum state control equation are simultaneously solved by the FDTD method. The quantum effect of nano-tube is calculated by the one-dimensional Schrödinger equation and the electromagnetic field distribution of the free space and the nano-tube domains is obtained by the three-dimensional Maxwell equation. The feedback from the electrons to the electromagnetic field is incorporated by adding to Maxwell’s equations a polarization current density that is obtained from the time-dependent wave function of the electrons.

II. THEORY

A. Control Equation of Quantum States

The control equation of quantum states can be given as follows:

$$E_z^i = -2\frac{E_0}{m_0}\operatorname{Im}\langle\psi|Wez|\psi\rangle \tag{1}$$

$$E_0 = A\exp\left\{-\frac{t-\tau}{\gamma}u(t-\tau)\right\} \tag{2}$$

Here, $A = 0.5\text{GV/m}$, $\tau = 15\text{fs}$, $\gamma = 3\text{fs}$. $u(t)$ is the step function. $W = |\psi_1\rangle\langle\psi_1|$ denotes the projection operator to the objective state ψ_1. ψ is the current state wave function. m_0 is electron effective mass. E_z^i is the incident electromagnetic pulse.

B. Maxwell-Schrödinger Hybrid Method

The Maxwell equation and quantum Schrödinger equation are presented in (3) and (4), respectively:

$$\begin{cases} \nabla\times\boldsymbol{E} = -\mu_0\dfrac{\partial \boldsymbol{H}}{\partial t} \\ \nabla\times\boldsymbol{H} = \varepsilon_0\dfrac{\partial \boldsymbol{E}}{\partial t} + \boldsymbol{J} \\ \dfrac{\partial \boldsymbol{A}}{\partial t} = -\boldsymbol{E} - \nabla\varphi \\ \dfrac{\partial \varphi}{\partial t} = -c_0^2\nabla\cdot\boldsymbol{A} \end{cases} \tag{3}$$

$$i\hbar\frac{\partial}{\partial t}\psi = \begin{bmatrix} -\dfrac{\hbar^2}{2m_0}\nabla^2 + \dfrac{ie\hbar}{m_0}\boldsymbol{A}\cdot\nabla + \\ \dfrac{ie\hbar}{2m_0}(\nabla\cdot\boldsymbol{A}) + \dfrac{e^2}{2m_0}\boldsymbol{A}^2 + e\varphi \end{bmatrix}\psi \tag{4}$$

Here, $\boldsymbol{E}$ and $\boldsymbol{H}$ are the electrical field and magnetic field, respectively. ε_0 and μ_0 represent the dielectric constant and permeability of vacuum, respectively. $\boldsymbol{A}$ and φ denote the magnetic vector potential and electrical scalar potential of electromagnetic field. $\hbar = h/2\pi$, h is the Planck constant, ψ is the wave function where $|\psi|^2$ represents the probability density function of the particle.

Then the polarization current density $\boldsymbol{J}$ in (3) can be written as follows:

$$\boldsymbol{J} = \frac{-ie\hbar}{2m_0}\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right] - \frac{e^2}{m_0}\psi^*\boldsymbol{A}\psi \tag{5}$$

In order to solve the above equations (1)-(5), the FDTD method is utilized to solve the unknowns $\boldsymbol{E}$, $\boldsymbol{H}$, $\boldsymbol{A}$, φ , ψ and $\boldsymbol{J}$. The absorbing boundary conditions and PML of

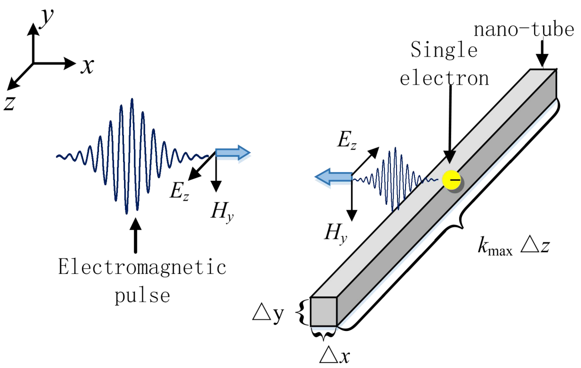

Fig. 1. Interaction between the incident control pulse and nano-tube

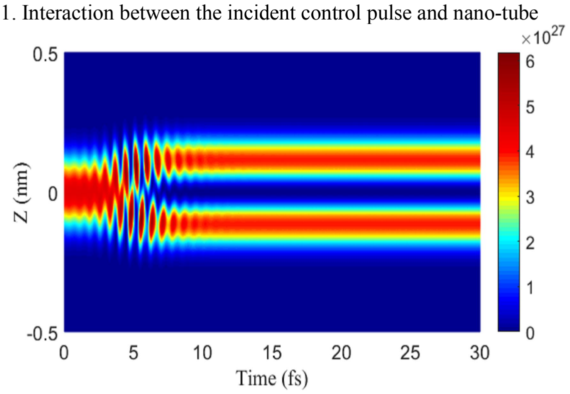

Fig. 2. Probability distribution of electrons in the nano-tube.

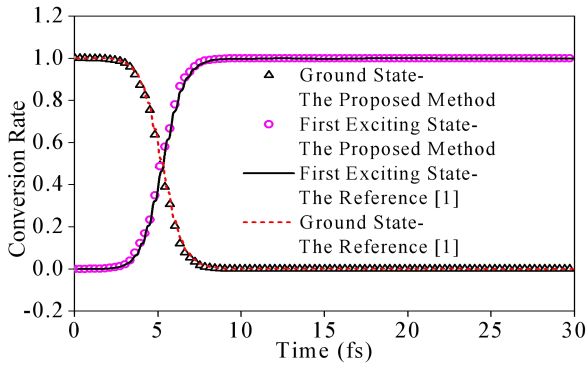

Fig. 3. Ground state and first excited state conversion rate.

electromagnetic field and the Dirichlet boundary conditions of wave function are employed here.

III. Numerical Results

The interaction between the incident electromagnetic pulse and the one-dimensional nano-tube is described in Fig.1. The cross-sectional size of the nano-tube is $\Delta x \times \Delta y = 1\text{nm} \times 1\text{nm}$, the calculated electromagnetic space is $30\Delta x \times 30\Delta y \times 200\Delta z$. Here, $\Delta z = 0.01\text{nm}$. The time step size and time step number are $\Delta t = 3\times 10^{-5}\text{fs}$ and 1000000, respectively. Then the conversion process and rate of ground state and first excited state are given in Fig.2 and Fig. 3. The accuracy of the method can be validated by the comparison with the reference [1]. Then, the multi-quantum state control of nano-tube is shown in Fig. 4 and the conversion rate of electronic states in the nano-tube is calculated in the Fig. 5.

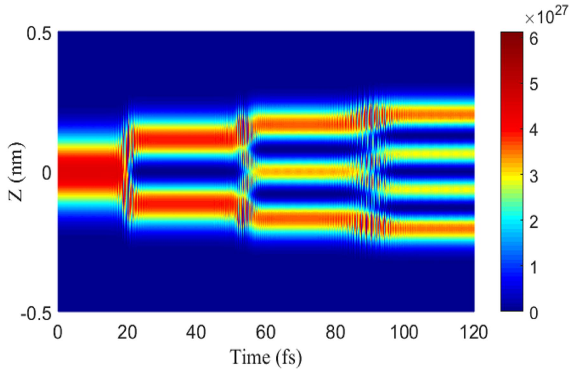

Fig. 4. Probability distribution of electrons in the nano-tube.

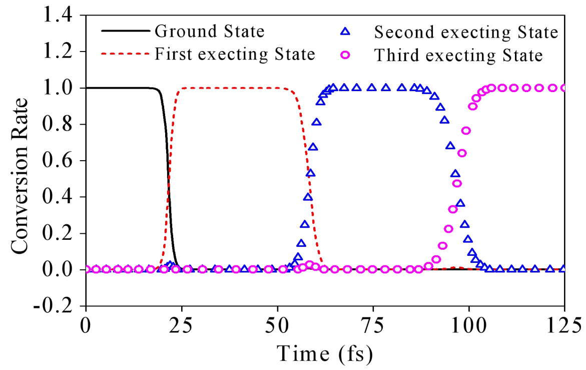

Fig. 5. Conversion rate of electronic states in the nano-tube

IV. Conclusion

The Maxwell-Schrödinger hybrid method and the control equation of quantum state are utilized to analyze the multi-quantum state control of nano-tube. The coupling equations are solved by the FDTD method. The accuracy of the simulation results is validated and the multi-quantum state control is realized by the Maxwell-Schrödinger hybrid method.

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