

Simulation of Behavior of Electrons Constrained in Electrostatic Potential by Using Maxwell-Newton and Maxwell-Schrödinger Schemes

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Abstract: A media in the high frequency electromagnetic fields have frequency dispersion. To solve the electromagnetic scattering problems of such media, the Maxwell-Newton and Maxwell-Schrödinger schemes have been developed. In this paper, we compare behavior of electrons in a nanoplate by using the two schemes and clarify that they give the same results when the electrostatic potential in the nanoplate is a single-well structure.

1. Introduction

A media in the high frequency electromagnetic fields have the frequency dispersion. To solve the electromagnetic scattering problems of such media, the Maxwell-Newton^[1] and Maxwell-Schrödinger^[2, 3] schemes have been developed. However, the applicable range of two schemes have not been clear.

In this paper, we compare behavior of electrons in a nanoplate by using the Maxwell-Newton and Maxwell-Schrödinger schemes and clarify that the two schemes give the same results when the electrostatic potential in the nanoplate is a single-well structure.

2. Formulation

Maxwell's equations with the polarization current density \mathbf{J} can be written as

$$\nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t}, \quad (1)$$

$$\nabla \times \mathbf{H} = \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J}. \quad (2)$$

We simulate Maxwell's equations by applying the Finite Difference Time Domain(: FDTD) method^[4].

The one of numerical methods to treat a dispersive medium is given by evaluating the polarization current density obtained from behavior of electrons in the medium: An electron in the electromagnetic fields is governed by the following Newton's equation in the classical theory:

$$m \frac{d^2 \mathbf{r}}{dt^2} = q\mathbf{E} + \mathbf{F}_V, \quad (3)$$

$$\mathbf{F}_V = -\nabla V, \quad (4)$$

where we assume that an electron does not feel any frictional forces and is constrained by the electrostatic potential V .

The polarization vector and polarization current density in the Maxwell-Newton scheme^[1] are defined by

$$\mathbf{P} = qN\mathbf{r}, \quad (5)$$

$$\mathbf{J} = \frac{\partial \mathbf{P}}{\partial t}. \quad (6)$$

We can simulate Eqs. (5) and (6) by applying the finite difference formula^[1]. The Maxwell-Newton scheme can be realized by simulating Eqs. (1), (2) and Eqs. (5), (6).

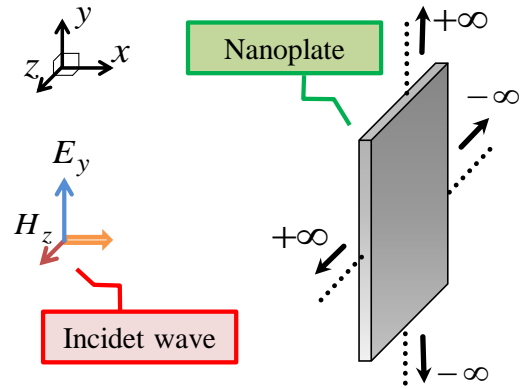


Figure 1. Coordinate systems of the nanoplate.

An electron in the electromagnetic fields is governed by the following Schrödinger's equation in the quantum theory:

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}_L \psi, \quad (7)$$

$$\hat{H}_L = -\frac{\hbar^2}{2m} \Delta - q\mathbf{E} \cdot \mathbf{r} + V, \quad (8)$$

where we have applied the length gauge^[5]. We simulate the wave function in Eq. (7) by applying the FDTD method^[6].

The polarization vector and polarization current density in the Maxwell-Schrödinger scheme^[3] are defined by

$$\mathbf{P} = \int_{-\infty}^{\infty} \psi^* \mathbf{r} \psi dv, \quad (9)$$

$$\mathbf{J} = \int_{-\infty}^{\infty} \psi^* \frac{\hbar}{i} \nabla \psi dv. \quad (10)$$

We can simulate Eqs. (9), (10) by applying the finite difference formula and quadrature^[3]. The Maxwell-Schrödinger scheme can be realized by simulating Eqs. (1), (2), and (10).

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3. Numerical results

A nanoplate shown in Figure 1 is investigated. We assume that the nanoplate is uniform along the y - z plane. All electrons in the nanoplate are constrained by a harmonic oscillator and can only move along the y -direction. The electrostatic potential V is given by the following expression in this case:

$$V = V_s = \frac{m\omega_s y^2}{2}. \quad (11)$$

The potential V_s is the single-well structure as shown in Figure 2. The electromagnetic fields have only E_y and H_z components and the incident wave is given by the narrow gaussian pluse shown in Figure 3.

Figure 4 shows a comparison of the time response of the polarization vector. The circles and the solid line indicate the results obtained by the Maxwell-Newton and Maxwell-Schrödinger schemes, respectively. It is shown that both results are in an excellent agreement. In addition, we have confirmed that two schemes give the same results for the polarization current density and electric field in this case.

4. Conclusions

We have compared the behavior of electrons in a nanoplate by using the Maxwell-Schrödinger and Maxwell-Newton schemes based on the FDTD method. It has been clarified that two schemes give the same results when the electrostatic potential in the nanoplate is the single-well structure.

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6. References

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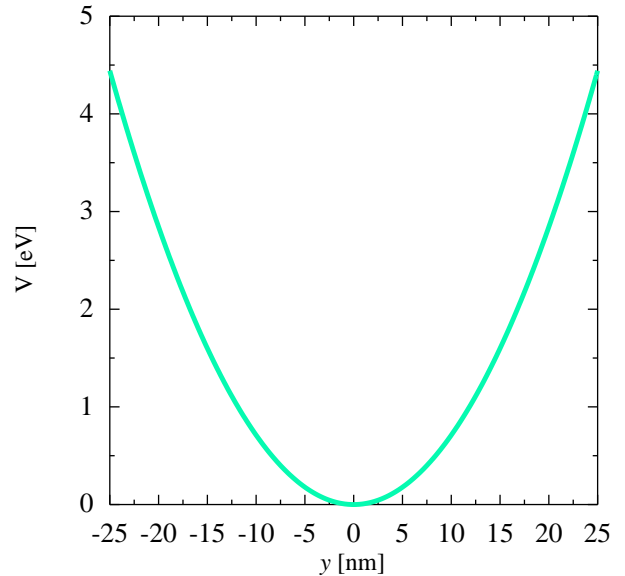


Figure 2. Electrostatic potential V_s .

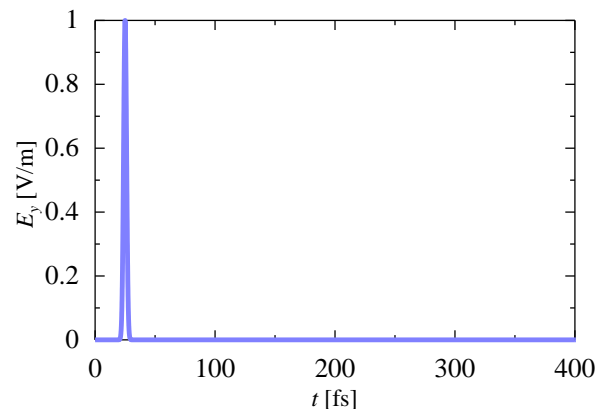


Figure 3. Incident wave in time domain.

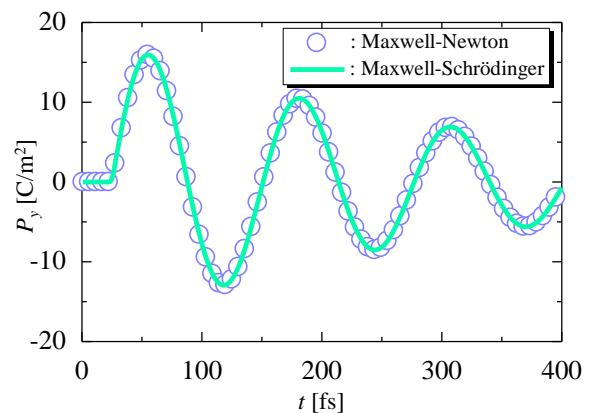


Figure 4. Comparison of the time response of the polarization vector.