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Coupled Analysis of Maxwell - Schrödinger Equations by the FDTD method

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Abstract: New optical devices using both light and quantum effects have attracted attention with recently development of nanotechnology. To analyze such devices, we must investigate both properties of electromagnetic fields and wave functions. In this paper, we will propose a novel computational method to study coupled Maxwell and Schrödinger equations by using the length gauge.

1. Introduction

New optical devices using both light and quantum effects have attracted attention with recently development of nanotechnology. To analyze such devices, properties of electromagnetic fields and wave functions must be investigated. Therefore, it is important to develope coupled solvers of Maxwell and Schrödinger equations [1-3].

In this paper, we will propose a novel computational method for solving Maxwell - Schrödinger equations. Our method can simplify the coupled analysis by using the length gauge and computational cost can be reduced.

2. Formulation

Maxwell equations for dielectric objects can be written as

$$\nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t}, \ \nabla \times \mathbf{H} = \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J}_p, \qquad (1)$$

where $\mathbf{J}_p$ is the polarization current density. To solve Maxwell equations in time domain, we apply the popular algorithm, Finite Difference Time Domain (FDTD) method. In this procedure, the electromagnetic fields **E** and **H** are updated by using finite difference schemes in space and time [4].

The time-dependent Schrödinger equation is expressed by the following equation.

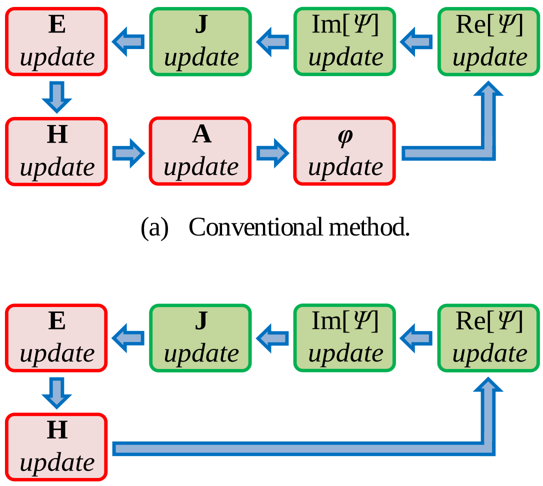
$$-\frac{\hbar}{i}\frac{\partial \psi}{\partial t} = \hat{H}\psi, \qquad (2)$$

where $\hbar$ is Dirac constant and $\hat{H}$ is the Hamiltonian. We can obtain the following equations by separating ψ into the real part ψ_{real} and imaginary part ψ_{imag} such as,

$$\frac{\partial \psi_{real}}{\partial t} = \mathrm{Re}\left[-\frac{i}{\hbar}\hat{H}\left(\psi_{real} + i\psi_{imag}\right)\right] = \frac{1}{\hbar}\hat{H}\psi_{imag}, \qquad (3)$$

$$\frac{\partial \psi_{imag}}{\partial t} = \mathrm{Im}\left[-\frac{i}{\hbar}\hat{H}\left(\psi_{real} + i\psi_{imag}\right)\right] = -\frac{1}{\hbar}\hat{H}\psi_{real}. \qquad (4)$$

To solve the Schrödinger equation in time domain, we also apply the FDTD method. Updates of functions ψ_{real} and ψ_{imag} can be performed in terms of finite difference schemes in space and time.



(a) Conventional method.

(b) Proposed method.

Figure 1. Computational algorithm for Maxwell - Schrödinger coupled equations.

The Hamiltonian in the electromagnetic field $\hat{H}_A$ can be written as

$$\hat{H}_A = \frac{1}{2m}\{-i\hbar\nabla - q\mathbf{A}\}^2 + q\varphi + V, \qquad (5)$$

where q is the charge of electron, **A** is the vector potential, φ is the scalar potential, and V is the static potential. In Figure 1 (a), the coupled algorithm is represented for the conventional method using $\hat{H}_A$. Here, red boxes indicate the part of solving the Maxwell equations in Eq. (1) and green boxes indicate the part of solving Schrödinger equation in Eqs. (3) and (4).

By using the length gauge with a unitary transform, $\hat{H}_A$ can be replaced by $\hat{H}_L$ such as[5].

$$\hat{H}_L = -\frac{\hbar^2}{2m}\Delta - q\mathbf{E}\cdot\mathbf{r} + V. \qquad (6)$$

Figure 1 (b) shows our new algorithm using $\hat{H}_L$. Compared with the conventional method, the proposed algorithm can

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reduce the computational procedure, since update of $\mathbf{A}$ and φ are not required.

3. Numerical results

We assume a two-dimensional dielectric plate which has nanoscale thickness as in Figure 2. The incident wave propagates to the positive x - direction and impinges perpendicular to the surface.

Figure 3 shows the comparison of computational results by using $\hat{H}_A$ and $\hat{H}_L$. Figure 3 (a) shows the polarization current $\mathbf{J}_p$ at t = 60 fs. The solid line indicates the result for $\hat{H}_A$ and circles indicate that for $\hat{H}_L$. Here, the horizontal axis indicates the position along the y axis. We confirm that both results are in good agreements. Figure 3 (b) plots the wavepacket $|\psi|^2$ at the same time. Both results are in good agreements for all the positions, as well. In addition, we have confirmed that space integration for $|\psi|^2$ becomes 1 and computational cost of our method is almost half compared with the conventional method.

4. Conclusions

The coupled solver of Maxwell and Schrödinger equations has been proposed. In our novel algorithm using the length gauge computational process can be simplified. Compared with conventional method, computational cost can be reduced by almost half and the same computational accuracy is achieved.

5. Acknowledgements

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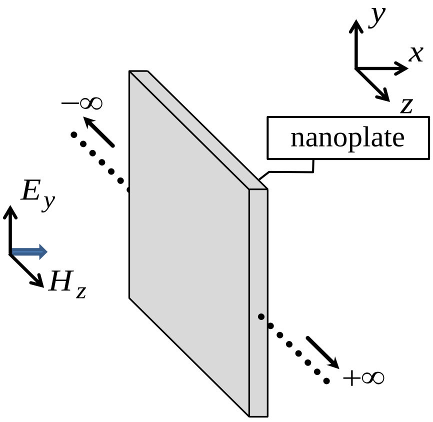
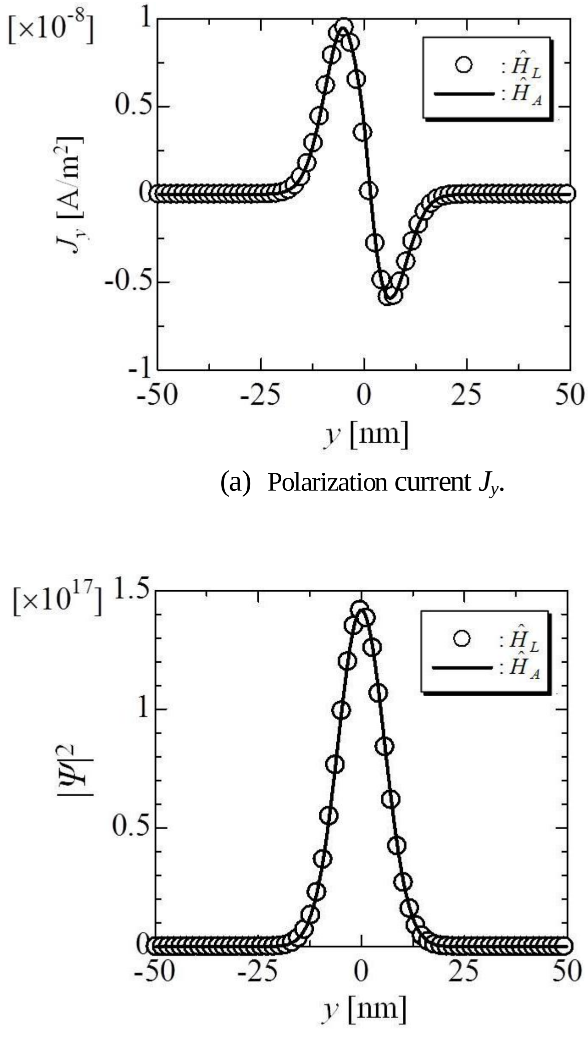


Figure 2. Coordinate systems of the nanoplate.



(a) Polarization current J_y.

(b) Wavepacket $|\psi|^2$.

Figure 3. Comparison of two coupled algoritms.