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Multiscale Computations for the Maxwell–Schrödinger System in Heterogeneous Nanostructures

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Abstract. In this paper, we study the multiscale computations for the Maxwell–Schrödinger system with rapidly oscillating coefficients under the dipole approximation that describes light-matter interaction in heterogeneous nanostructures. The multiscale asymptotic method and an associated numerical algorithm for the system are presented. We propose an alternating Crank–Nicolson finite element method for solving the homogenized Maxwell–Schödinger system and prove the existence of solutions to the discrete system. Numerical examples are given to validate the efficiency and accuracy of the algorithm.

AMS subject classifications: 35Q40, 35Q60, 65M60

Key words: Maxwell–Schrödinger system, homogenization, multiscale asymptotic method, Crank–Nicolson scheme.

1 Introduction

The macroscopic Maxwell's equations has been widely used to model the optical properties of materials since their advent. In the macroscopic electromagnetic theory, the response of materials to incident electromagnetic fields is incorporated into linear or nonlinear susceptibilities, also known as constitutive laws, and the microscopic charge and current densities are smeared out. This theory has been quite successful for the study of bulk materials irradiated by external electromagnetic fields of moderate intensity. However, as the rapid development of laser and nanofabrication technologies, the macroscopic Maxwell's equations are facing challenges in some realistic applications. On

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one hand, the constitutive laws in the macroscopic electromagnetic theory, which are built under the perturbation assumption of the incident fields, are often invalid in the studies with intense and ultrashort laser pulses. On the other hand, the macroscopic Maxwell's equations fail to capture the microscopic induced polarization in physical devices of nanoscale, which is usually crucial in nanophotonics. In view of these limitations, in the past few decades, many researchers have attempted to couple the Maxwell's equations with the Schrödinger equation describing the motion of charged particles to model complex physical processes due to light-matter interaction, such as optical responses of nanostructures [5], strong-field ionization of molecular gas [17], carrier dynamics in nano-devices [21], and the interaction of electron wave packets with optical gratings [25].

The (macroscopic) Maxwell equations can be written as

$$\begin{aligned} \nabla\times\mathbf{E}&=-\frac{\partial\mathbf{B}}{\partial t}, \qquad & \nabla\cdot\mathbf{B}&=0,\\ \nabla\times\mathbf{H}&=\frac{\partial\mathbf{D}}{\partial t}+\mathbf{J}, \qquad & \nabla\cdot\mathbf{D}&=\rho, \end{aligned} \tag{1.1}$$

where $\mathbf{E}$, $\mathbf{H}$, $\mathbf{J}$, and ρ are respectively the electric fields, the magnetic fields, the current density, and the charge density. $\mathbf{D}$ and $\mathbf{B}$ denote the electric displacement and magnetic flux density, respectively. In a linear medium, they are related to $\mathbf{E}$ and $\mathbf{H}$ by the constitutive laws

$$\mathbf{D}=\epsilon\mathbf{E}, \quad \mathbf{B}=\mu\mathbf{H}, \tag{1.2}$$

with ϵ and μ being the electric permittivity and magnetic permeability, respectively.

When interacting with the incoming electromagnetic fields, the time-dependent Schrödinger equation for an electron can be written as [13]

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t}=\Big\{\frac{1}{2m}(-\mathrm{i}\hbar\nabla-q\mathbf{A})^2+q\phi+V_c\Big\}\Psi, \tag{1.3}$$

where Ψ is the wave function, V_c is the confinement potential, $\hbar$ is the reduced Planck's constant, m and $q=-e$ respectively denote the effective mass and the charge of the electron. $\mathbf{A}$ and ϕ are respectively the vector potential and the scalar potential that satisfy

$$\mathbf{B}=\nabla\times\mathbf{A}, \quad \mathbf{E}=-\nabla\phi-\frac{\partial\mathbf{A}}{\partial t}, \tag{1.4}$$

where $\mathbf{E}$ and $\mathbf{B}$ are the electric fields and magnetic flux density, respectively. If the spatial extent of the region where the electron can move is much smaller than the wavelength of the incident fields, we can apply the dipole approximation, also known as length gauge, in which case the Schrödinger equation can be transformed as

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t}=\Big\{-\frac{\hbar^2}{2m}\nabla^2+q\mathbf{E}\cdot\mathbf{x}+V_c\Big\}\Psi. \tag{1.5}$$