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Modeling and Computation of Nano-Optics

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Abstract. This work is devoted to a review of our recent studies in the modeling and computation of nano optical devices. Motivated by technological advances at nano scale, to quantitatively understand the mechanism and improve the designing, we make an effort to model nano optical systems involving multiple physical processes across different time and space scales, and develop multiscale and adaptive numerical methods for simulation. Challenges on rigorous analysis of the models and algorithms are also discussed.

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1 Introduction

Recent advances in nano optical technology have been made in a variety of fields such as molecular imaging, optical-mechanical systems, negative-index metamaterials, etc. The study of efficient and accurate numerical methods for multiphysical models of nano scale optical devices has become more important than ever [1]. When size of optical structures reaches sub-micro scale, the energy level for the electron excitation becomes comparable to the wavelength of the incident light. In this case, to faithfully capture light-matter interactions, it is imperative to consider microscopic fields generated by electronic charges in motion. As a complete characterization of the microscopic interaction of light and charged particles, the Quantum Electrodynamics Theory (QED) [2] has been widely used

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with much success in atomic modeling of optical phenomena. However, the fact that QED requires extremely intense computation prohibits it from many applications at meso and nano scales. To avoid the complexity of QED while keeping essential physics, semiclassical models have been recently developed in the form of a nonlocal response theory [3–5], in which the evolution of electromagnetic (EM) field is described continuously using classical Maxwell's equations, and the motion of electrons is treated quantum mechanically by the Schrödinger equation. Compared with QED, the semiclassical model only takes into account averaged quantities, such as certain amplitude and phase, instead of detailed properties, of the statistical ensemble of photons in each mode.

Although the semiclassical approach reduces the computational cost that would otherwise be tremendous in QED, a time dependent many body Schrödinger equation is still involved, for which numerical solutions are prohibitively expensive in many practical situations. A recent effort by the authors [6–12] is to adopt the Time Dependent Current Density Functional Theory (TD-CDFT) [14] to further simplify the semiclassical model and its computation. In the Density Functional Theory (DFT), a one-to-one correspondence (up to an arbitrary constant) between the external potential and the ground state electron density has been proved in the seminal work of Hohenberg and Kohn [15]. Hence, the wavefunction can be obtained as a functional of the electron density, which allows evaluation of all observables of the system. Similar results have been extended to the case of time evolutionary electronic structures in the form of Time Dependent Density Functional Theory (TD-DFT) by Runge and Gross [16]; and later to the situation of external electric and magnetic fields with arbitrary time dependence by Ghosh and Dhara [14] in the form of TD-CDFT, where the current density is introduced as the fundamental variable. A synthetic noninteracting many body system under an effective external potential, referred as the Kohn-Sham (KS) system [17], is designed to calculate electron and current densities, which greatly simplifies the computation by reducing dimension of the problem. In the KS system, many body effects are included via so called exchange-correlation (xc) potentials.

The incorporation of TD-CDFT into the framework of the semiclassical optical response theory leads to a system formulated as coupled Maxwell-Kohn-Sham (MKS) equations (also see [18–20] for similar systems). Challenges still remain in numerically solving the MKS system when applied to nano optical applications of interest. First of all, the MKS system has a multiscale nature due to space and time scale separations between electrodynamics and electronic motions, for the fact that the EM field spreads the whole medium domain while electrons are confined in nano scale structures. It is recently observed that at nano scale, the speed of photon excited electrons is about 375 times slower than the speed of light [21]. Direct and uniform space and time discretizations of the MKS system will result in very large and ill-conditioned equations. The situation becomes more subtle when it comes to non-adiabatic coupling of different physical processes, e.g., light driven molecular motions and transitions under strong external fields, where the dynamics can be highly nonlinear and a large number of degrees of freedom is needed to resolve details across all scales.