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Computational Modeling of Optical Response from Excitons in a Nano Optical Medium†

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Abstract. Consider a time-harmonic electromagnetic plane wave incident on a microscopic semiconductor. Inside the medium, at any given frequency ω, more than one polariton mode can arise with the same frequency but different wavenumbers due to the presence of excitons. Besides Maxwell's boundary conditions, additional boundary conditions are required to handle the multi-mode polariton. In order to model the confinement effect of excitons in the microscopic semiconductor, Maxwell's equations and the Schrödinger equation are coupled to characterize the polarization in terms of the quantum description. In the weak confinement regime, we derive a perturbed dispersive dielectric constant by taking the exciton effect into account. We also analyze and compute the optical linear response of the exciton in both one-dimensional and two-dimensional confinements. For the one-dimensional case, the existence and uniqueness of the analytical solution are established in the resonance region. A finite difference method is developed to compute the two dimensional confinement.

AMS subject classifications: 78A45, 78M20, 81V10

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1 Introduction

The electric and optical properties of microscopic semiconductor structures are of great interest in the design and potential device applications of such structures. The most widely studied systems of this type are the quantum well, quantum wire, and quantum

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dot, which have interesting electric and optical properties [20, 25, 26, 34]. Applications include diode lasers, amplifiers, biological sensors, detection of tumor in fluorescence spectroscopy, and making better displays (quantum dot-LED displays). An emerging research direction of nanotechnologies is to understand and study the electrodynamics of the above mentioned nano optical media.

In macroscopic electromagnetic theory of bulk media, all the variables (fields, polarization, charge and current densities$\cdots$) are averaged quantities. However, when the size of medium reduces to microscopic, it is essential to consider the microscopic fields which are created by atomic electric charges in motion. In this case, the quantum mechanical description of the matter system must be studied. The motion of EM fields is described by Maxwell's equations and the motion of charged particles is governed by the Schrödinger equation. From this prospective, a great deal of research has been devoted to the study of optical responses of microscopic media. To fully characterize the interaction of atoms and photons, the quantum theory of light [10] and quantum electrodynamics (QED) must be employed. In this setting, the EM fields as well as the medium are quantized and a many-body Schrödinger equation needs to be solved in QED, hence the computation of QED seems to be a formidable task without any approximation. So far, QED has been widely used in atomic physics and quantum optics [31] where the size is smaller than microscopic. Although QED provides accurate characterizations of the fields and media of interest, the required extremely intense computation prohibits QED from many practical applications. In order to overcome the high computational cost of QED, for the microscopic medium of our interest, we present a semiclassical approach which combines the classical treatment of the EM fields and the quantum mechanical treatment of the medium. The semiclassical approach has been widely used with much success in nano optics modeling. Both Cho's microscopic nonlocal response approach [9] and Keller's local field theory [21] are semiclassical methods. In Cho's theory, the induced polarization is calculated in a nonlocal way which means the applied field $\mathbf{E}(\mathbf{r})$ at a point $\mathbf{r}$ induces polarization $\mathbf{P}(\mathbf{r})$ not only at the same position, but also at other positions within the extent of relevant wave functions" [9]. Keller's method is similar to Cho's in building two integral equations for the EM fields and the current density. However, in Cho's approach, the transverse component of the EM fields and full Coulomb interaction among particles are included in the matter Hamiltonian while the full Coulomb interaction is not included in Keller's free Hamiltonian. Another semiclassical method is called the coherent wave approach proposed by Stahl [28]. The idea is to use interband transition amplitudes to set up the constitutive equation between the current density and electric field. It should be pointed out that a common limitation of these similar semiclassical approaches is that there are many quantum effects cannot be described by the above methods: for example, the Raman scattering and luminescence. By introducing the notion of transition polarizability, Born and Huang [7] showed one can describe the Raman scattering semiclassically, which cannot be treated by all above approaches.

In this paper, we start from Cho's nonlocal response theory. However, a different Hamiltonian is used for the Schrödinger equation. For the matter Hamiltonian (unper-