A Novel Hamiltonian Approach for Solving Maxwell-Schrödinger Equations

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Numerical solution of the coupled Maxwell-Schrödinger system has attracted much attention recently. Several methods have been successfully proposed in the modeling of electronic/electromagnetic response of nano-devices or dynamics of electron confined in an electrostatic potential well subjected to pulsed laser fields.

In this paper, a novel Hamiltonian solution to Maxwell-Schrödinger equations is developed for modeling the interaction between classical electromagnetic (EM) fields and particles in a resonant nano-cavity. A unified Maxwell-Schrödinger system is derived based on Hamiltonian and the variational principle. To mitigate the multiscale problem caused by the disparity of wavelengths, a reduced eigenmode expansion technique is applied to represent the wave function of the particle. Consequently, a set of ordinary differential equations (ODEs) governing the time evolution of the slowly-varying expansion coefficients can be derived based on Galerkin test. To be consistent with quantum theory, the classical EM formulation in terms of fields are replaced by the vector potential with a Coulomb gauge. Finally, the coupled system is solved self-consistently with the conventional finite-difference time-domain (FDTD) method. The proposed system is shown to be well-posed and symplectic, which guarantees energy conservation during the time evolution.

In the numerical examples, the Rabi oscillations, the transition dynamics of a particle due to the perturbation of an external EM field, are characterized by this Hamiltonian approach. The proposed method is validated by the Rabi model and rotating wave approximation model. It is found that in certain cases a rigorous self-consistent numerical approach is needed. This work is helpful for the EM simulation of emerging nanodevices or next-generation quantum electrodynamic systems.