Hybrid Simulation of Maxwell-Schrödinger Equations for Electromagnetic Fields Interacted with Electrons Confined in Electrostatic Potentials

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The progresses of nano-technology in last some decades have enabled us to develop many attractive devices effectively utilizing cooperative effects between light and electrons. One of typical examples is plasmonic devices in which an enormous amount of electrons in matter simultaneously oscillates by incident fields and locally generates enhanced fields. In order to numerically design and analyze the plasmonic devices, some theoretical models based on the classical physics, namely Newton's equation of motion for the electrons, have been often employed such as Drude or Lorentz-Drude models. Recent experimental works, however, have revealed that those conventional models cannot coincide with actual phenomena particularly for very small objects in sub-nano meter scale because of lack of consideration for quantum-mechanical effects. Therefore, very recently, some new ways taking into account the quantum-mechanical effects have been actively studied and proposed, for example hydrodynamic Drude model and combination of electromagnetic analysis and time-dependent density functional method.

In this paper, hybrid simulation of Maxwell-Schrödinger equations which also can compute the quantum-mechanical effects, precisely, is employed to investigate the interaction between electromagnetic fields and electrons confined in the electrostatic potentials, where we focus on the structure of the constraining potentials and make a comparison with conventional, namely classical, simulation results. The observed trends by the hybrid and conventional simulations clearly show the relationship between the influence of the quantum-mechanical effects and the potential structures.