Simulation Tool for Coupled Quantum Transport and Electrodynamics

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Accurate simulation of light-matter interaction at the nanoscale requires a computational approach that combines quantum transport and electrodynamics, self-consistently and at every time step. Here we present the development of a new tool for this purpose — Quantum Transport and Electrodynamics Simulation Tool (QuTEST) — which self-consistently couples a full-wave finite-difference time-domain (FDTD) electrodynamics solver for the potentials with a density-matrix-based quantum transport solver. A schematic of the coupling is depicted in Fig. 1. The current density $\boldsymbol{J}$ and charge density ρ are calculated from the density matrix and inputted back into the FDTD; FDTD produces the vector potential $\boldsymbol{A}$ and scalar potential Φ, both of which are needed in the density-matrix equation of motion.

The non-traditional 3D FDTD formulation for the potentials is implemented by discretizing Maxwell's equations for $\boldsymbol{A}$ and Φ in the Lorentz gauge [1]. Calculations on a simple current source are depicted in Fig. 2 and show excellent agreement between analytical results and numerical calculation in our implementation. The rigorous density-matrix formalism for quantum transport is based on a Markovian master equation that preserves the positivity of the density matrix [2,3] and it employs the calculated $\boldsymbol{A}$ and Φ in the Hamiltonian. We are currently developing the coupled simulation and, at conference time, we will present the results obtained on several sample systems (e.g., the bowtie antenna).

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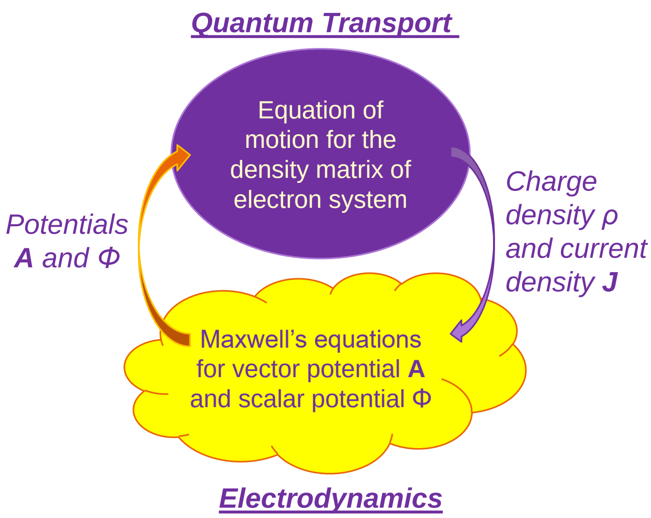

*Fig. 1: Schematic illustrating the self-consistent coupling between the full-wave electrodynamic solver for vector potential **A** and scalar potential Φ and the density-matrix based quantum transport solver, which produce current density **J** and charge density ρ for the coupled simulator.*

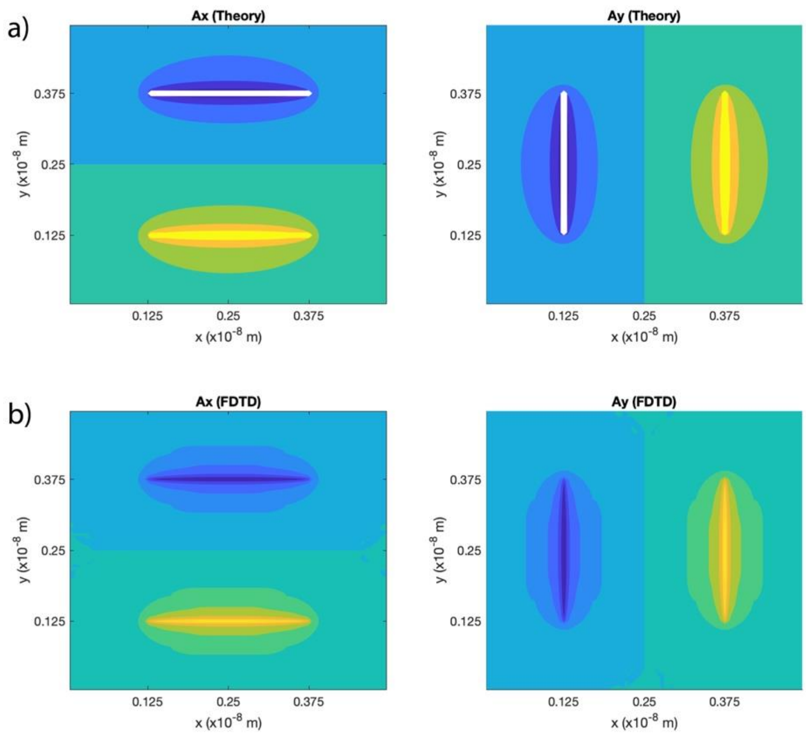

*Figure 2: Contour plot of relative magnitudes of magnetic vector potential **A** (yellow: high; blue: low) for a square wire with constant current density **J** flowing counter-clockwise around the wire, as calculated a) analytically and b) from FDTD for the potentials within the Lorentz gauge.*