Multiscale modeling of electrodynamic radiation from quantum monopole antenna

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The AC non-equilibrium Green function (NEGF) formalism provides a powerful tool to model the dynamic behavior of electrons in nanoscale devices [2]. Here, we present a novel simulation technique that couples the AC NEGF formulation with the full so- lution of Maxwell's equations to capture the electrodynamic coupling that is necessary to characterize the high-frequency operation of electron devices. We demonstrate the efficacy of the technique by simulating a quantum wire monopole antenna.

The total retarded Green function, that is, the impulse response of the system Hamilto- nian, at energy E can be expressed as

$$G^r(E) = G_o^r(E) + G_w^r(E), \tag{1}$$

where $G_0^r(E)$ is the DC retarded Green func- tion and $G_w^r(E)$ is first-order response due to an AC perturbation. The DC component is calculated via standard NEGF formalism [1].

The AC bias is introduced perturbatively resulting in a small-signal retarded AC Green function $G_w^r(E)$ at frequency ω that is expressed as a product of DC Green functions at energies E and $E^+ = E + \hbar\omega$ [2]:

$$G_w^r(E) = G_0^R(E^+)\,[-eV + \Sigma_\omega^R(E)]\,G_0^r(E) \tag{2}$$

Here V is the AC potential profile and Σ_ω^R is the AC contact self-energy, which is given by

$$\Sigma_\omega^\gamma(E) = \frac{e\pi VAC}{\hbar\omega}[\Sigma_0^\gamma(E) - \Sigma_0^\gamma(E^+)], \tag{3}$$

where e is the electron charge, $\gamma = r, <, VAC$ is the bias amplitude and Σ_0^r is the typical DC self-energy.

The retarded Green function must be con- volved with the lesser self-energy $\Sigma < (E)$ to account for the application of the bias and the occupancy of the leads. The resulting AC lesser Green function is written as

$$\begin{aligned} G_\omega^<(E) = G_0^r(E^+)\Sigma_0^<(E^+)G_\omega^r(E)\dagger \\ +G_0^r(E^+)\Sigma_\omega^<(E)G_0^r(E)\dagger \\ +G_\omega^r(E)\Sigma_0^<(E)G_0^r(E)\dagger \end{aligned} \tag{4}$$

The AC charge and current density is calculated in a similar fashion to DC NEGF by substituting the AC lesser Green function $G_\omega^<(E)$ for the DC version $G_0^<(E)$.

The output charge density, ρ, and current density, **J**, from AC NEGF is then input into the electrodynamics simulation. We solve di- rectly for the scalar potential, V, and vector potential, **A**, in the frequency domain using the Lorenz gauge, resulting in the following governing equations:

$$\left(\nabla^2 + \frac{\omega^2}{C^2}\right)V = -\frac{\rho}{\varepsilon} \tag{5}$$

$$\left(\nabla^2 + \frac{\omega^2}{C^2}\right)\boldsymbol{A} = -\mu\boldsymbol{J} \tag{6}$$

Here, c is the speed of light, ε is the electric permittivity, μ is the magnetic permeability. Figure 1 illustrates the staggered Yee cell that the fields are solved on using the finite- difference frequency-domain (FDFD) formula- tion with absorbing boundary conditions [3]. The output scalar potential and vector poten- tial are then reinserted into the Hamiltonian via an on-site energy and a Peierl's phase, respectively. Equations (2)-(6) are iterated in the process described by Fig. 2 until the change in V on successive iterations is less than 1 μV, our criterion for self-consistency.

Figure 3 illustrates the quarter-wave monopole antenna system we simulate. The antenna is modeled using a 1D metal tight- binding Hamiltonian with hopping energy $t0$ = 1.5 eV placed on a perfect conductor in a larger 3D FDFD simulation domain. After self-consistency is achieved, the far-field radiation pattern is calculated using a near- to-far-field transformation. Figure 4 shows the far-field radiation pattern of the antenna operating at 100 GHz, which agrees well with typical quarter wave monopole radiation. The ability of this technique to capture the dynamic radiative fields of an antenna demonstrates its promise to model more complex dynamic light-matter interactions where the quasi-static approximation fails.

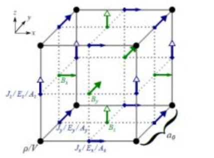

Fig. 1. The FDFD electromagnetic equations are solved on a Yee cell to solve directly for the scalar potential, V, and the vector potential components, A_i, generated by the charge density, ρ, and current density components, J_i, extracted from AC NEGF. The electric field compo- nents, E_i, and magnetic field components, B_i, are then computed from the potentials. The side length of the cell is the lattice constant $a_0 = 37.5\,\mu$m of the Hamiltonian. This placement guarantees that the currents and charge density from NEGF align exactly with the Yee grid of the FDFD simulation.

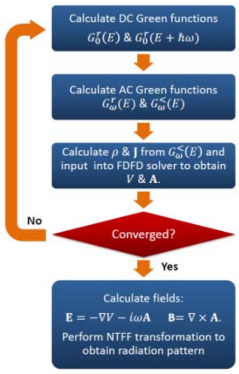

Fig. 2. Solution procedure to achieve self-consistent electrodynamic fields with AC NEGF.

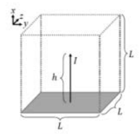

Fig. 3. Monopole radiation is simulated by using AC NEGF to simulate transport in a 1D metal wire with length $h = 750\,\mu$m in an FDFD simulation of side length $L = 1.73$ mm. Perfect electrical conductor electromag- netic boundary conditions are applied on $y - z$ plane, shown as the solid gray cube face, while absorbing boundary conditions are applied to all other faces, il- lustrated as transparent faces with dashed edges.

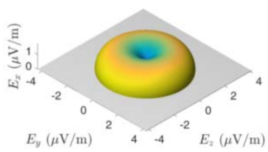

Fig. 4. The far-field radiation pattern at a distance $r = 1$ cm obtained by performing a near-to-far-field transformation of the electric and magnetic fields out- side the wire. We see that the antenna radiates as a quarter-wave monopole thereby demonstrating the ability of this method to capture radiative electrodynamic phenomena.

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