A Volume Integral Equation Solver for Quantum-Corrected Transient Analysis of Scattering from Plasmonic Nanostructures

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Abstract—Quantum tunneling is observed between two nanostructures that are separated by a sub-nanometer gap. Electrons “jumping” from one structure to another create an additional current path. An auxiliary tunnel is introduced between the two structures as a support for this so that a classical electromagnetic solver can account for the effects of quantum tunneling. The dispersive permittivity of the tunnel is represented by a Drude model, whose parameters are obtained from the electron tunneling probability. The transient scattering from the connected nanostructures (i.e., nanostructures plus auxiliary tunnel) is analyzed using a time domain volume integral equation solver. Numerical results demonstrating the effect of quantum correction on the scattered fields are provided.

I. INTRODUCTION

Recent advances in the fabrication of nanoparticles have paved the way to miniature electromagnetic devices to nanoscale. To accurately analyze electromagnetic scattering from such devices, quantum tunneling effects be accounted for. Quantum tunneling is observed between two structures when the gap between them is less than a nanometer. Electrons tunneled from one structure to the other one generate an additional current path that cannot be modeled by classical electromagnetic solvers. This results in errors in scattered field computations. In such cases, one could use a “full” quantum mechanical solver to obtain accurate results, but computational requirements of this solver would be prohibitively high. To alleviate this problem, one can use a (one dimensional) quantum mechanical solver for only the gap and obtain an effective permittivity for an auxiliary tunnel supporting the current generated by tunneled electrons [1]. Then, one can use a classical electromagnetic solver to compute scattered fields from the combined structure (nanostructures plus auxiliary tunnel).

Among several types of classical electromagnetic solvers, time domain volume integral equation (TD-VIE) solvers offer several advantages over their differential equation counterparts [2]. In this work, a time domain-electric field volume integral equation (TD-EFVIE) is developed for transient quantum-corrected analysis of scattering from plasmonic nanostructures. The dispersive permittivity of the auxiliary tunnel, which is introduced to support the currents generated

by tunneled electrons, is represented by a Drude model whose parameters are computed from electron tunneling probability as described in [1]. The unknown electric flux density, field intensity and polarization density induced inside the nanostructures and the auxiliary tunnel are expanded in terms of full and half Schaubert-Wilton-Glisson (SWG) functions in space [3], [4] and approximate prolate spherical wave (APSW) functions [5] in time. These expansions are inserted into the TD-EFVIE and the constitutive relation (obtained by inverse Fourier transforming the Drude model) and the resulting coupled system of equations is Galerkin-tested in space. The final semi-discrete matrix system is cast in the form of an ordinary differential equation and integrated in time using a PE(CE)^m type linear multistep scheme [6] to yield the coefficients of the unknown expansions.

II. FORMULATION

Let V denote the volume of the combined structure (the plasmonic nanostructures plus the auxiliary tunnel) residing in an unbounded background medium with permittivity ε_0 and permeability μ_0 . The combined structure is excited by a band-limited electric field $\mathbf{E}^{\text{inc}}(\mathbf{r}, t)$. Upon excitation, flux density $\mathbf{D}(\mathbf{r}, t)$ and field intensity $\mathbf{E}(\mathbf{r}, t)$ induced in V satisfy

$$\mathbf{D}(\mathbf{r}, t) = \varepsilon_0 \varepsilon_\infty(\mathbf{r}) \mathbf{E}(\mathbf{r}, t) + \mathbf{P}(\mathbf{r}, t), \quad (1)$$

$$\partial_t \mathbf{E}^{\text{inc}}(\mathbf{r}, t) = \partial_t \mathbf{E}(\mathbf{r}, t) + \mathcal{L}\{\mathbf{E}(\mathbf{r}, t)\} - \mathcal{L}\{\varepsilon_0^{-1} \mathbf{D}(\mathbf{r}, t)\} \quad (2)$$

for $\mathbf{r} \in V$. Here, the $\varepsilon_\infty(\mathbf{r})$ is the relative permittivity at infinite frequency, $\mathbf{P}(\mathbf{r}, t)$ is the polarization, and the integral operator $\mathcal{L}\{\cdot\}$ is

$$\begin{aligned} \mathcal{L}\{\mathbf{X}(\mathbf{r}, t)\} = & -\frac{\varepsilon_0 \mu_0}{4\pi} \int_V \frac{1}{R} \partial_{t'}^3 \mathbf{X}(\mathbf{r}', t') \big|_{t'=t-R/c_0} d\mathbf{r}' \\ & + \frac{1}{4\pi} \nabla \int_V \frac{1}{R} [\nabla' \cdot \partial_{t'} \mathbf{X}(\mathbf{r}', t')] \big|_{t'=t-R/c_0} d\mathbf{r}' \end{aligned} \quad (3)$$

where $R = |\mathbf{r} - \mathbf{r}'|$ is the distance between source and observation points, $\mathbf{r}'$ and $\mathbf{r}$, and $c_0 = 1/\sqrt{\varepsilon_0 \mu_0}$ is the speed of light in the background medium. When the permittivity in

V is represented using a Drude model [1], the $\mathbf{P}(\mathbf{r}, t)$ satisfies

$$\begin{aligned}\partial_t \mathbf{P}(\mathbf{r}, t) &= \hat{\mathbf{P}}(\mathbf{r}, t) \\ \partial_t \hat{\mathbf{P}}(\mathbf{r}, t) &= -\gamma_p(\mathbf{r})\mathbf{P}(\mathbf{r}, t) + \varepsilon_0(\omega_p(\mathbf{r}))^2 \mathbf{E}(\mathbf{r}, t)\end{aligned}\quad (4)$$

where $\hat{\mathbf{P}}(\mathbf{r}, t)$ is an intermediate variable, $\gamma_p(\mathbf{r})$ is the damping factor, and $\omega_p(\mathbf{r})$ is the plasmon frequency. To numerically solve the coupled equations (1), (2), (3), and (4), V is discretized into tetrahedrons and unknowns $\mathbf{D}(\mathbf{r}, t)$, $\mathbf{E}(\mathbf{r}, t)$, $\mathbf{P}(\mathbf{r}, t)$, and $\hat{\mathbf{P}}(\mathbf{r}, t)$ are expanded

$$\begin{aligned}\mathbf{D}(\mathbf{r}, t) &= \sum_{i=0}^{N_t} \sum_{n=1}^{N_F} I_{n,i}^D T_i(t) \mathbf{f}_n^F(\mathbf{r}), \\ \mathbf{U}(\mathbf{r}, t) &= \sum_{i=0}^{N_t} \sum_{n=1}^{N_H} I_{n,i}^U T_i(t) \mathbf{f}_n^H(\mathbf{r}), \mathbf{U} \in \{\mathbf{E}, \mathbf{P}, \hat{\mathbf{P}}\}.\end{aligned}\quad (5)$$

Here, $\{\mathbf{f}_n^F(\mathbf{r}), \mathbf{f}_n^H(\mathbf{r})\}$ are the full and half SWG functions respectively [3], [4], $T_i(t) = T(t - i\Delta t)$, where $T(t)$ is the APSW functions [5] and Δt is the time step, and $I_{n,i}^K$, $K \in \{\mathbf{E}, \mathbf{D}, \mathbf{P}, \hat{\mathbf{P}}\}$ are unknown expansion coefficients. Inserting (5) into (1) and spatially testing the resulting equation with $\mathbf{f}_n^F(\mathbf{r})$, $m = 1 : N_F$, yields a matrix system at time step j

$$\mathbf{G}^{FF} \mathbf{T}^{\dagger} \mathbf{I}_j^D = \mathbf{G}^{FH} (\varepsilon_0 \varepsilon_{\infty} \mathbf{I}_j^E + \mathbf{I}_j^P). \quad (6)$$

Here, $\{\mathbf{I}_j^K\}_n = I_{n,i}^K$ and the elements of the $\mathbf{G}^{AB}$, $A \in \{\mathbf{F}, \mathbf{H}\}$, $B \in \{\mathbf{F}, \mathbf{H}\}$, are

$$\{\mathbf{G}^{AB}\}_{m,n} = \int_{V_m} \mathbf{f}_m^A(\mathbf{r}) \cdot \mathbf{f}_n^B(\mathbf{r}) d\mathbf{r}. \quad (7)$$

Similarly, inserting (5) into (2), (3), and (4) and testing the resulting equations with $\mathbf{f}_n^H(\mathbf{r})$, $m = 1 : N_H$, yield three coupled matrix systems at j

$$\partial_t \mathbf{I}_j^P = \mathbf{I}_j^{\hat{P}}, \quad \partial_t \mathbf{I}_j^{\hat{P}} = -\gamma_p \mathbf{I}_j^P + \varepsilon_0 \omega_p^2 \mathbf{I}_j^E \quad (8)$$

$$\begin{aligned}\mathbf{G}^{HH} \partial_t \mathbf{I}_j^E &= \mathbf{V}_j^{\text{inc}} - \mathbf{Z}_0^{HH} \mathbf{I}_j^E - \sum_{i=0}^{j-1} \mathbf{Z}_{j-i}^{HH} \mathbf{I}_i^E + \\ &\varepsilon_0^{-1} \mathbf{Z}_0^{HF} \mathbf{I}_j^D + \varepsilon_0^{-1} \sum_{i=0}^{j-1} \mathbf{Z}_{j-i}^{HF} \mathbf{I}_i^D\end{aligned}\quad (9)$$

where $\{\mathbf{Z}_{j-i}^{AB}\}_{m,n} = \int_{V_m} \mathbf{f}_m^A(\mathbf{r}) \cdot \mathcal{L}\{\mathbf{f}_n^B(\mathbf{r}) T_i(t)\}|_{t=j\Delta t} d\mathbf{r}$. Coupled system of equations (6), (8) and (9) are integrated in time using a linear k -step PE(CE)^m scheme [6] to yield the unknown expansion coefficients $\mathbf{I}_j^K$ for $j = 1 : N_t$.

III. NUMERICAL RESULTS

The proposed solver is used for analyzing scattering from a sodium dimer consisting of spheres with radius 2.17 nm. The separation between the spheres is 0.265 nm. The auxiliary tunnel is modeled using four concentric cylinders. The outer radius of the outermost shell is 0.8 nm. The Drude model parameters for the sodium and the tunnel are same as the ones in [1]. The dimer is excited using a plane wave with $\mathbf{E}^{\text{inc}}(\mathbf{r}, t) = \hat{\mathbf{x}} \cos[2\pi f_0(t - t_0 - \mathbf{r} \cdot \hat{\mathbf{z}}/c_0)] e^{-(t-t_0-\mathbf{r} \cdot \hat{\mathbf{z}}/c_0)^2/2\sigma^2}$, where $f_0 = 1200$ THz, $\sigma = 3.6/(2\pi f_0)$, and $t_0 = 6\sigma$. Discretization parameters $N^F = 5330$, $N^H = 10196$, $\Delta t = 0.01$ fs, and $N_t = 4000$. The predictor-corrector coefficients used for the PE(CE)^m scheme are the sixth order Adams-Bashforth and backward difference formula (BDF6) coefficients. For comparison, scattering from the dimer without the auxiliary tunnel is also studied under the same excitation.

Fig. 1. $\mathbf{E}(\mathbf{r}_0, t)$ at $\mathbf{r}_0 = (2.3, 0.0, 0.0)$ nm

Fig. 2. Extinction cross section of the sodium dimer.

Fig. 1 compares $\mathbf{E}(\mathbf{r}_0, t)$ for $\mathbf{r}_0 = (2.3, 0.0, 0.0)$ nm computed for the dimers with and without the auxiliary tunnel. The result clearly shows that the solver provides stable results for both the cases. In Fig. 2 the extinction cross section of the dimers obtained by Fourier transforming the time domain solution is compared to that of obtained directly by a frequency domain VIE solver. The results agree well. The figure also shows that introducing auxiliary tunnel significantly changes the computed radiation pattern of the dimer.

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