Quantum-Corrected Transient Analysis of Plasmonic Nanostructures Using a Volume Integral Equation Solver

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Numerical schemes capable of analyzing electromagnetic wave/field interactions on plasmonic structures are indispensable in the design of nanoscale devices in a wide range of applications ranging from bio-molecular sensing to efficient solar energy conversion (de Aberasturi, et al., Adv. Opt. Mat., 3 602-617, 2015). Oftentimes, such analysis can be carried out accurately using classical electromagnetic solvers. However, if a sub-nanometer gap exists between two structures, quantum-tunneling effects become relevant. This means that the current path generated by the electrons "jumping" from one structure to the other should be accounted for in the simulation. To address this problem, a "quantum-correction" can be achieved by introducing an auxiliary tunnel between the two structures to this additional current (R. Esteban et al., Nat. Commun., 3, 825, 2012). It is assumed that the permittivity of the auxiliary tunnel follows a simple Drude model in frequency. The other parameters of the model are obtained from the tunneling probability computed by solving a one-dimensional Schrödinger equation. Once the material properties of the auxiliary tunnel are known, a classical electromagnetic solver is used for computing electromagnetic wave/field interactions on the combined structure (two structures plus the auxiliary tunnel).

In this work, this quantum correction scheme is incorporated into a time domain volume integral equation (TDVIE) solver. The TDVIE is formulated in the form of a first-order ordinary differential equation (ODE) in time (H.A. Ulku et al., IEEE Trans. Antennas Propag., 61, 4120-4131, 2013). Additionally, the constitutive relation between electric field intensity and flux density (as represented by the Drude model in the frequency domain) is easily cast in the form of a first-order ODE. The solver expands the unknown electric field intensity and flux density using full and half Schaubert-Wilton-Glisson (SWG) basis functions in space (D. H. Schaubert et al., IEEE Trans. Antennas Propag., 32, 77-85, 1984, G. Kobidze et al., IEEE Trans. Antennas Propag., 53, 1215-1226, 2005). The time-retardation in the TDVIE operator is taken into account by using a temporal interpolation function (D. S. Weile et al., IEEE Trans. Antennas Propag., 52, 283–295, 2004). The resulting coupled system of the spatially-discretized TDVIE and constitutive relation are integrated in time using an explicit $PE(CE)^m$ scheme to yield the unknown expansion coefficients of SWG functions.

Numerical examples, which show the accuracy and the applicability of the proposed solver in analyzing plasmonic structures as well as the effect of the quantum correction on the transient electromagnetic interactions, will be presented.