Nonlocal hydrodynamic Drude resonances of nano-plasmonic scatterers: Modeling and simulations

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***Abstract*—As the plasmonic scatterers get much smaller than the wavelength of the incident light, local material models like the Drude model and the Lorentz model become inadequate to describe accurately the light-matter interactions. To overcome this, a sophisticated nonlocal hydrodynamic Drude model is investigated. In practice, it is further simplified and simulated with the curl-free approximation, which generates spurious resonances. In this work we discuss a weak formulation based rigorous numerical investigations of the nonlocal hydrodynamic Drude model. This approach does not use the curl-free approximation, and thus avoids spurious resonances. The simulated results agree good with Mie results, and the method is capable of handling arbitrarily shaped scatterers.**

I. Introduction

The dispersive material properties of plasmonic structures are usually described by the Drude model and the Lorentz model. These material models take into account spatially *purely local* interactions between electrons and the light. Recent investigations have shown that these local models are inadequate as the size of the plasmonic scatterers become much smaller than the wavelength of the incident light [1], [2]. To overcome this, a sophisticated *nonlocal* material model is required, such as the hydrodynamic model of the electron gas [3].

The hydrodynamic model is formulated by coupling macroscopic Maxwell's equations with the equations of motion of the electron gas. This gives rise to a hydrodynamic polarization current. Considering only the kinetic energy of the free electrons, it yields the nonlocal hydrodynamic Drude model, which is given in frequency domain by a coupled system of equations

$$\nabla\times\mu_0^{-1}(\nabla\times\vec{E}) - \omega^2\varepsilon_0\varepsilon_{\mathrm{loc}}\vec{E} = i\omega\vec{J}_{\mathrm{HD}}, \quad (1)$$

$$\beta^2\nabla(\nabla\cdot\vec{J}_{\mathrm{HD}}) + \omega(\omega+i\gamma)\vec{J}_{\mathrm{HD}} = i\omega\omega_{\mathrm{p}}^2\varepsilon_0\vec{E}, \quad (2)$$

where $\vec{E}$ is the electric field, $\vec{J}_{\mathrm{HD}}$ is the hydrodynamic current, $\varepsilon_{\mathrm{loc}}$ is the relative permittivity due to the local-response, β^2 is a term proportional to the Fermi velocity, γ is the damping constant, and $\omega_{\mathrm{p}}^2 = \frac{e^2 n_0}{\varepsilon_0 m_{\mathrm{e}}}$ is the plasma frequency of the free electron gas.

II. Curl-free approximation: Spurious resonances

Recently the nonlocal hydrodynamic Drude model has been simulated with the finite difference time domain (FDTD) method, but with the curl-free approximation $\nabla\times\vec{J}_{\mathrm{HD}} = 0$ [4]. As a consequence of this approximation, the tensorial grad-div operator $(\nabla(\nabla\cdot\vec{J}_{\mathrm{HD}}))$ appearing in the governing equation for the hydrodynamic current simplifies to vectorial linear Laplacian operator $(\nabla^2\vec{J}_{\mathrm{HD}})$. This was needed to render the system into a form suitable for the standard FDTD framework. However the comparison with the analytical Mie theory [1] showed that this approach produces spurious plasmonic resonances below the plasma frequency $(\omega/\omega_p < 1)$ [5].

III. Weak formulation

Here we outline a weak formulation based rigorous numerical approach for simulation of the nonlocal hydrodynamic Drude model. Details can be found in [6]. We start with (1) for the electric field. An appropriate ansatz space for the electric field is the Sobolev space $H(\mathrm{curl},\Omega) = \{\vec{E}\in(L^2(\Omega))^3\,|\,\nabla\times\vec{E}\in(L^2(\Omega))^3\}$, which contains fields with weakly defined curl-operator defined on the domain Ω [7, Sec. 3.5].

Multiply (1) with a trial function $\varphi\in H(\mathrm{curl},\Omega)$, and integrate over Ω. Then partial integration yields

$$\int_\Omega\left((\nabla\times\varphi)\cdot(\mu_0^{-1}\nabla\times\vec{E}) - \omega^2\varphi\cdot\varepsilon_{\mathrm{loc}}\vec{E}\right)dV \; + \int_{\partial\Omega}\varphi\cdot(\vec{n}\times(\mu_0^{-1}\nabla\times\vec{E}))\,dA = i\omega\int_\Omega\varphi\cdot\vec{J}_{\mathrm{HD}}\,dV, \quad (3)$$

with the outer normal $\vec{n}$. Here we need to define boundary conditions of the electric field on $\partial\Omega$, which is formulated by the Dirichlet to Neumann (DtN) operator. Using total-field/scattered-field formulation, one gets

$$\int_\Omega((\nabla\times\varphi)\cdot(\mu_0^{-1}\nabla\times\vec{E}) - \omega^2\varphi\cdot\varepsilon_{\mathrm{loc}}\vec{E} - i\omega\varphi\cdot\vec{J}_{\mathrm{HD}})\,dV + \int_{\partial\Omega}\varphi\cdot\mathrm{DtN}(\vec{E})\,dA = -\int_{\partial\Omega}\varphi\cdot(\vec{n}\times(\mu_0^{-1}\nabla\times\vec{E}_{\mathrm{inc}}))\,dA + \int_{\partial\Omega}\varphi\cdot\mathrm{DtN}(\vec{E}_{\mathrm{inc}})\,dA,\ \forall\ \varphi\in H(\mathrm{curl},\Omega), \quad (4)$$

where $\vec{E}_{\mathrm{inc}}$ is the exciting field.

For (2) an appropriate ansatz space is the Sobolev space $H_0(\mathrm{div},\Omega_{\mathrm{s}}) = \{\vec{J}_{\mathrm{HD}}\in(L^2(\Omega_{\mathrm{s}}))^3\,|\,\nabla\cdot\vec{J}_{\mathrm{HD}}\in(L^2(\Omega_{\mathrm{s}}))^3,\ \vec{n}\cdot\vec{J}_{\mathrm{HD}} =$

0 on $\partial\Omega_s\}$. This restricts the hydrodynamic current to the plasmonic scatterer, and imposes zero normal component on the boundary of the scatterer.

Then the variational form of (2) reads as

$$-\int_{\Omega_s} \beta^2(\nabla\cdot\psi)(\nabla\cdot\vec{J}_{\mathrm{HD}})\,dV + \omega(\omega+i\gamma)\int_{\Omega_s}\psi\cdot\vec{J}_{\mathrm{HD}}\,dV$$
$$-i\omega\omega_p^2\int_{\Omega_s}\psi\cdot\varepsilon_0\vec{E}\,dV = 0, \forall\ \psi\in H_0(\mathrm{div},\Omega_s). \qquad (5)$$

After the problem is formulated in the Sobolev space $H(\mathrm{curl},\Omega)\times H_0(\mathrm{div},\Omega_s)$ for $(\vec{E},\vec{J}_{\mathrm{HD}})$, one can use Nédélec finite element spaces, which lead to a consistent discretization of the problem, fulfilling the required boundary and material interface conditions [7, Ch. 5]. We solving the resultant discrete coupled system of with a sparse LU decomposition.

IV. Numerical Examples

A. Cylindrical plasmonic nanowires

We validate the present approach by simulating a test case of cylindrical nanowire in [1], for which analytical solution based on Mie theory is available. When this setting was simulated with the curl-free hydrodynamic current approximation as in [4], spurious (model induced) resonances were produced, which has been discussed in detail in [5].

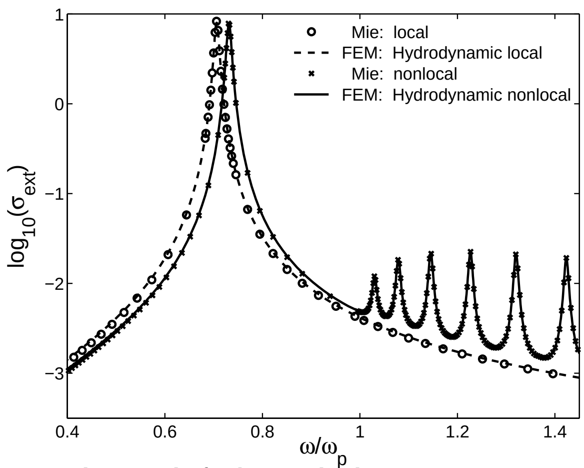

Fig. 1. Simulation results for the normalized scattering cross section σ_{ext} of the cylindrical nanowire in [1]. The curves show comparison of the finite element numerical solutions for the nonlocal and the local hydrodynamic model with the corresponding analytical solutions based on the Mie theory.

Consistent with the observations in [1], peaks due to nonlocal interactions are present *only* beyond the bulk plasma frequency. The positions of the surface plasmon resonance and the nonlocal hydrodynamic Drude resonances agree very good with the analytical Mie results.

B. V groove channel plasmon-polariton waveguides

To demonstrate capability of the method to handle an arbitrary shaped geometry, we simulate a channel plasmon-polariton (CPP) waveguide with a V groove.

We consider a V groove configuration as shown in clip of Fig. 2. First we simulated it for the local Drude model. As seen from the dashed curve in Fig. 2, several resonance modes are excited. When this setting is simulated for the nonlocal Drude model, the mode spectrum changes significantly (the solid-line curve). Some of the local Drude model modes such as at $\omega/\omega_p = 0.306332$ and $\omega/\omega_p = 0.80262$ experience small shifts towards high frequency, whereas the others like at $\omega/\omega_p = 0.466485$ and $\omega/\omega_p = 0.605087$ undergo noticeable shifts towards high frequency. As in the case of the cylindrical nanowires, also for the V groove waveguide a completely new set of resonances appear at the frequencies beyond the plasma frequency. For the present simulation setting, some of these hydrodynamic resonance modes are more prominent than the higher order waveguide resonance modes. It gives the indication with the inclusion of nonlocal effect, the modal properties of the CPP waveguides change significantly.

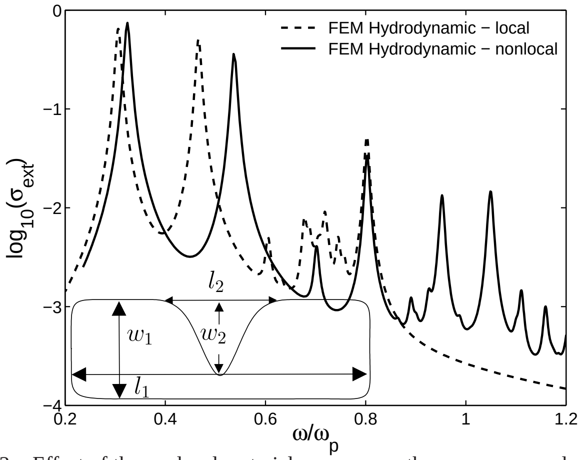

Fig. 2. Effect of the nonlocal material response on the resonance modes of V groove CPP waveguide. The waveguide parameters are as: $l_1 = 7$ nm, $w_1 = 1$ nm, a groove of length $l_2 = 0.7$ nm, width $w_2 = 0.7$ nm is placed in the center. The material and the hydrodynamic parameters are taken as in the case of cylindrical nanowires in [1]. The sharp corners of the waveguide are rounded with corner radius of 0.1 nm. Resonances are excited by a unit amplitude, x-polarized plane wave propagating in the direction of minus y-axis.

Acknowledgments

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