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INTERACTIONS OF FAST IONS WITH SUPPORTED GRAPHENE: QUANTUM HYDRODYNAMIC MODEL

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Abstract. We use a quantum hydrodynamic (QHD) model to describe the high-frequency plasmon excitations of the carbon valence electrons responding to fast ions which move parallel to a single sheet of graphene supported by an insulating substrate. We calculate the stopping and the image forces on ions. Numerical results are obtained showing the effects of variation in size of the gap between graphene and the SiO_2 substrate, as well as the effects of a finite frictional coefficient, on these quantities.

1. INTRODUCTION

Graphene is a single sheet of carbon atoms forming hexagonal lattice (Novoselov et al. 2004). Besides being the fundamental building block of highly oriented pyrolytic graphite (HOPG), carbon nanotubes and fullerene molecules, graphene is currently attracting a great deal of interest on its own right owing to its fascinating physical properties (Castro Neto et al. 2009).

In the present paper, we use a quantum hydrodynamic (QHD) model to explore the effects of dynamic-polarization forces on fast charges incident upon a single sheet of graphene supported by an insulating substrate. Specifically, we calculate the dissipative or stopping force on fast ions moving parallel to the graphene and the perpendicularly oriented conservative force on such ions due to the dynamic image interaction.

Atomic units (a.u.) will be used throughout unless indicated otherwise.

2. BASIC THEORY

We use a Cartesian coordinate system with coordinates $(\vec{R}, z)$, where $\vec{R} = (x, y)$ is position in the graphene plane and z distance from it. A substrate with dielectric constant ε_s is assumed to occupy the region $z \leq -h$ underneath the graphene, whereas the region $z > -h$ is assumed to be vacuum or air. Furthermore, we consider the ion to be a point charge Q, moving parallel to the graphene in the upper half-space defined by $z > 0$, with a constant velocity v, at a fixed distance z_0. Denoting the electric potentials due to charge polarization on graphene and the induced surface charge on the substrate, respectively, by Φ_{gr} and Φ_s, the total electric potential in the system, Φ_{tot}, can be written as the sum $\Phi_{tot} = \Phi_{ext} + \Phi_{gr} + \Phi_s$, where Φ_{ext} is the external perturbing potential. Next, we consider the graphene's valence electrons as a uniformly distributed free-electron gas with the surface density (density per unit area) of $n_0 = 0.428$. The perturbations of its density $n(\vec{R},t)$ and its velocity field $\vec{u}(\vec{R},t)$ satisfy the linearized continuity equation:

$$\frac{\partial n(\vec{R},t)}{\partial t} + n_0 \nabla_{\parallel} \cdot \vec{u}(\vec{R},t) = 0 \tag{1}$$

and the linearized momentum-balance equation:

$$\frac{\partial \vec{u}(\vec{R},t)}{\partial t} = \nabla_{\parallel} \Phi_{tot}(\vec{R},z,t)\big|_{z=0} - \frac{\alpha}{n_0} \nabla_{\parallel} n(\vec{R},t) + \frac{1}{4n_0} \nabla_{\parallel}[\nabla_{\parallel}^2 n(\vec{R},t)] - \gamma \vec{u}(\vec{R},t) \tag{2}$$

Note that, in Eqs. (1) and (2), $\nabla_{\parallel} = \partial / \partial \vec{R}$ is the component of the full gradient operator which differentiates in directions parallel to the sheet. The first term in the right side of Eq. (2) is the tangential force on an electron due to the total electric field at $z = 0$. The second term represents the internal interactions in the electron fluid based on the Thomas-Fermi model, giving $\alpha = \pi n_0$. The third term describes the quantum diffraction effects coming from the quantum pressure. The last term in Eq. (2) describes the frictional force on an electron due to scattering on the positive charge background, where γ is the frictional coefficient.

By eliminating the velocity field $\vec{u}(\vec{R},t)$ from Eqs. (1) and (2), followed by performing the Fourier transformation in the xy plane and in time ($\vec{R} \to \vec{k}$ and $t \to \omega$), one can use the expression for the total potential Φ_{tot} to obtain an expression for $\Phi_{ind}(\vec{k},z,\omega)$. Finally, by performing the inverse Fourier transformation ($\vec{k} \to \vec{R}$ and $\omega \to t$), we obtain the expression for the induced potential as follows:

$$\Phi_{ind}(\vec{R},z,t) = -\frac{Q}{2\pi} \int \frac{e^{-k(z+z_0)}}{k} \left[1 - \frac{1}{\varepsilon(k, \vec{k} \cdot \vec{v})} \right] e^{i\vec{k}\cdot(\vec{R}-\vec{v}t)} d^2\vec{k} \tag{3}$$

where $\varepsilon(k,\omega) = \varepsilon_0(k) + \frac{2\pi}{k} \chi(k,\omega)$ is the dielectric function of supported graphene, with $\varepsilon_0(k) = \frac{\varepsilon_s + 1}{2} \frac{1 + \coth(kh)}{\varepsilon_s + \coth(kh)}$ being the background dielectric function which quantifies the effects of substrate on the response of graphene and the polarization function of graphene is given by $\chi(k,\omega)=\dfrac{n_0 k^2}{(1/4)k^4+\alpha k^2-\omega^2-i\gamma\omega}$.

3. RESULTS AND DISCUSSION

The stopping and image forces are defined by (Radović and Borka 2010): $F_s=-Q(\vec{v}/v)\cdot\nabla_{\|}\Phi_{ind}(\vec{R},z,t)\Big|_{\vec{R}=\vec{v}t,z=z_0}$ and $F_{im}=-Q(\partial\Phi_{ind}(\vec{R},z,t)/\partial z)\Big|_{\vec{R}=\vec{v}t,z=z_0}$, with the derivatives $\nabla_{\|}\Phi_{ind}(\vec{R},z,t)$ and $\partial\Phi_{ind}(\vec{R},z,t)/\partial z$ taken at the ion position $(\vec{R}=\vec{v}t, z=z_0)$. For an ion of charge Q moving along the x axis with speed v at a fixed distance $z_0>0$ above graphene, the stopping and the image forces are given by, respectively:

$$F_s=\frac{2Q^2}{\pi}\int_0^\infty\int_0^\infty\frac{k_x e^{-2kz_0}}{k}\,\mathrm{Im}\left[\frac{1}{\varepsilon(k,k_x v)}\right]dk_x dk_y \tag{4}$$

$$F_{im}=-\frac{2Q^2}{\pi}\int_0^\infty\int_0^\infty e^{-2kz_0}\,\mathrm{Re}\left[1-\frac{1}{\varepsilon(k,k_x v)}\right]dk_x dk_y \tag{5}$$

where we have used the symmetry properties of the real and imaginary parts of the dielectric function $\varepsilon(k,\omega)$.

In Fig. 1, we display the velocity dependencies of the (a) stopping and (b) image forces on proton ($Q=1$) for three values of the gap h between graphene and a SiO_2 substrate (with $\varepsilon_s=3.9$) at fixed distance $z_0=3\,a.u.$ with zero damping $\gamma=0$. The most remarkable features shown in Fig. 1 are the very strong dependencies of both forces on values of the graphene-substrate gap.

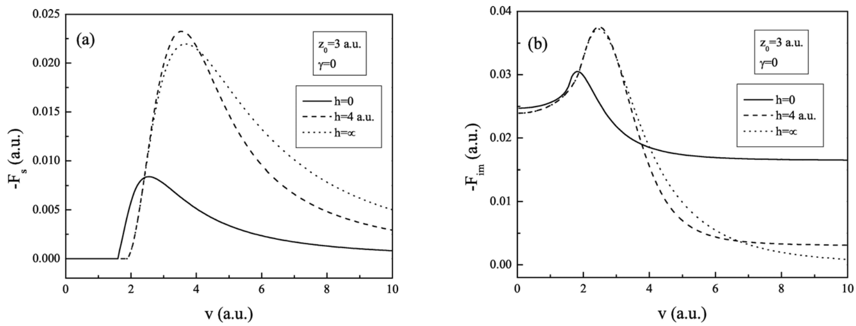

Figure 1: The dependencies on speed v (in $a.u.$) of (a) stopping and (b) image forces (in $a.u.$) on proton moving at distance $z_0=3\,a.u.$ above graphene for three values of the gap between graphene and a SiO_2 substrate (with $\varepsilon_s=3.9$), $h=0$ (solid lines), $4\,a.u.$ (dashed lines) and ∞ (dotted lines), with zero damping $\gamma=0$.

In Fig. 2, we illustrate the effects of a finite frictional coefficient γ on the velocity dependencies of the (a) stopping and (b) image forces at fixed proton-graphene distance $z_0 = 3\, a.u.$, and for the value of the gap $h = 4\, a.u.$, which is probably close to a typical experimental situation (Ishigami et al. 2007). One notices the effect of smoothing out the resonant features in both forces around the speed $v = 2\, a.u.$, with little influences on their high-speed behaviours and on the low-speed behaviour of the image force. However, the low-speed values of the stopping force are noticeably dependent on γ, indicating that a threshold for energy loss to the plasmon excitations moves to lower speeds with increasing frictional coefficient.

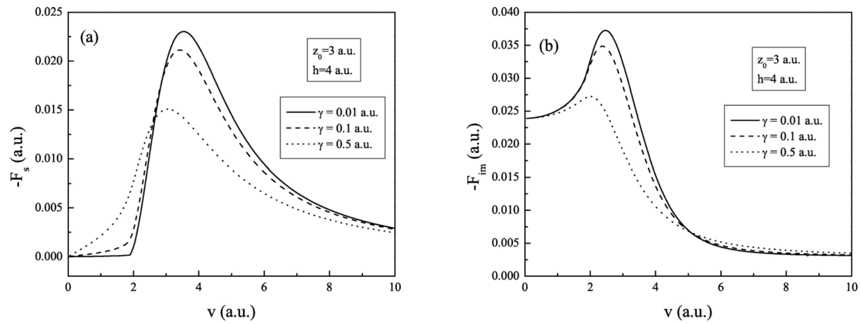

Figure 2: The dependencies on speed v (in $a.u.$) of (a) stopping and (b) image forces (in $a.u.$) on proton moving at distance $z_0 = 3\, a.u.$ above graphene with SiO_2 substrate (with $\varepsilon_S = 3.9$ and $h = 4\, a.u.$), for three values of damping, $\gamma = 0.01\, a.u.$ (solid lines), $0.1\, a.u.$ (dashed lines) and $0.5\, a.u.$ (dotted lines).

Acknowledgements

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