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Wake effect in interactions of dipolar molecules with doped graphene

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ABSTRACT

We study the wake effect in the charge carrier density in free graphene induced by an electric dipole moving parallel to it by using the dynamic polarization function of graphene within the random phase approximation for its π electrons described as Dirac's fermions. We show that, while the equilibrium doping density of graphene sets a length scale for the period of the wake via graphene's Fermi wavenumber, qualitative properties of the wake are strongly affected by the speed of the dipole, its distance from graphene, and the dipole moment orientation.

1. Introduction

The passage of a fast charged particle through a target that contains quasi-free charge carriers has been known to induce oscillatory pattern called wake in the polarization charge density that trails the particle, both in three-dimensional (3D) plasmas [1] and for ion channeling through nanocapillaries [2]. The wake is intimately related to the stopping force on the incident particle, and the appearance of the wake often requires that the particle speed exceeds a threshold such that its energy loss is dominated by the collective excitations of charge carriers, or plasma oscillations in the target. The wake was recently shown to play important roles in dusty plasmas [3], cluster propagation through thin foils [4] and plasmas [5], channeling through carbon nanotubes [6,7], as well as in interactions of charged particles with 1D electron gas (1DEG) [8], one [9] and two [10] layers of a 2D quantum electron gas (2DQEG), supported thin metal films [11], nanosphere [12] and with magnetized two-component plasmas [13,14].

We have studied previously the wake effect due to fast charged particles moving parallel to a supported 2DEG that represents graphene by using a one-fluid hydrodynamic model for all four valence electrons [15], as well as a two-fluid hydrodynamic model, which makes distinction between the contributions of carbon's σ and π electrons [16]. Our results showed that the wake in the induced charge density occurs when the particle speed matches the phase velocity of the quasi-acoustic π plasmon. In addition, our previous calculations of the total electric potential in the 2DEG plane due to passage of a fast charged particle showed the possibility of realizing the so-called wake riding effect in 2DEG by other charged particles [6,17].

In order to study the wake effect due to low-energy excitations of graphene's π electrons induced by a charged particle moving parallel to a graphene, we use the polarization function within the random phase approximation (RPA) [18], which is based on a linear approximation for the π electron bands [19–22]. A detailed discussion of the applicability of such approach to dynamic polarization of graphene is given in Ref. [23].

In our previous publications we have studied the wake effect due to ions moving parallel to graphene supported by an insulating [24] and a strongly polar substrate [25]. Our results showed that, when the projectile speed exceeds a threshold value on the order of graphene's Fermi speed v_F ($v_F \approx c/300$, where c is the speed of light in free space), the oscillatory wake effect develops both in the induced number density [24] and in the total electrostatic potential in the plane of graphene [25] trailing the particle. It was shown that the potential for graphene on a substrate that supports a phonon mode also exhibits spatial oscillations at sub-threshold speeds, $v < v_F$ [25]. In our recent publication [26], in passing, we showed that the wake effect in the induced charge density due to a moving dipole with the dipole moment parallel to graphene and perpendicular to the direction of motion is asymmetric with respect to the direction of motion.

In this Letter, we focus on the wake effect in a free-standing graphene under the gating conditions due to dipoles that move parallel to graphene at the speeds in excess of its Fermi speed v_F. This configuration may be of interest for grazing scattering of the

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molecular projectiles from graphene [26]. We analyze for the first time the oscillatory wake effect in the spatial distribution of fluctuations in the charged carrier density in free graphene, induced by a moving dipole, taking into account the influence of variations in: the equilibrium charge carrier density n due to doping of graphene, the distance z_0 and the speed v of the projectile, as well as the dipole moment orientation.

The equilibrium charge carrier density n may be controlled by doping the graphene sheet with adsorbed atoms or molecules or via application of the electrostatic potential external gates. n is a particularly important parameter because it determines the Fermi wavenumber of graphene's π-electrons, $k_F = \sqrt{\pi n}$ (we assume $n > 0$ without loss of generality), which sets the typical screening length in doped graphene to be proportional to k_F^{-1}. In this work, we consider a range of equilibrium charge carrier densities defined by $10^{11}\ \text{cm}^{-2} \leqslant n \leqslant 10^{14}\ \text{cm}^{-2}$, but several comments will also be made about intrinsic, or undoped graphene with $n = 0$. In addition, we shall compare our results for the wake effect in graphene with the wake effect in a 2DEG with a parabolic energy band with the effective mass $m_* = \hbar k_F / v_F$. With this choice of m_*, the "massive" 2DEG will have the same long-wavelength limit of the plasmon dispersion relation as single-layer, given by $\omega_p(k) = \sqrt{2\pi n e^2 k/m_*} = \sqrt{2e^2 v_F k_F k/\hbar}$, so that the roles of plasmon excitations on the wake formation in the two systems would be compared on the same footing.

The Letter is organized as follows. After outlining the theoretical model in the following section, we shall present and discuss the results for the induced number density per unit area of electrons in graphene for a range of the relevant parameters. Concluding remarks will be given in the last section.

Note that we use Gaussian electrostatic units and denote the charge of a proton by $e > 0$.

2. Basic theory

We use a Cartesian coordinate system with coordinates $\{\vec{R}, z\}$ and assume that graphene is located in the plane $z = 0$, where $\vec{R} = \{x, y\}$ is position in the plane and z distance from it. Furthermore, a projectile is assumed to move parallel to the graphene in the upper half-space defined by $z > 0$. By performing the Fourier transform with respect to coordinates in the xy plane, $\vec{R} \to \vec{k}$, and time, $t \to \omega$, we can express the induced number density per unit area of electrons in graphene, n_{gr}, in terms of the local value of the total electric potential, Φ_{tot}, evaluated at $z = 0$, in the form

$$n_{gr}(\vec{k}, \omega) = e\chi(k, \omega)\Phi_{tot}(\vec{k}, z, \omega)|_{z=0} \tag{1}$$

where $\chi(k, \omega)$ is the polarization function within RPA for non-interacting π electrons in graphene with $k = \sqrt{k_x^2 + k_y^2}$. One may express $\Phi_{tot}(\vec{k}, z, \omega)|_{z=0}$ in terms of the Fourier transform of the potential $\Phi_{ext}(\vec{R}, z, t)$ due to external charge distribution as

$$\Phi_{tot}(\vec{k}, z, \omega)|_{z=0} = \frac{1}{\varepsilon(k, \omega)}\Phi_{ext}(\vec{k}, z, \omega)|_{z=0} \tag{2}$$

where $\varepsilon(k, \omega)$ is the dielectric function of free graphene, given by

$$\varepsilon(k, \omega) = 1 + \frac{2\pi e^2}{k}\chi(k, \omega). \tag{3}$$

For the dielectric response of graphene in Eq. (3), we use the polarization function for graphene's π electron excitations in the RPA, $\chi(k, \omega)$, which is described in detail in Refs. [19,20,23].

We consider a projectile represented by a rigid distribution of charge with the volume density $\hat{\rho}_{ext}(\vec{R}, z)$, which moves parallel to the graphene at constant velocity $\vec{v} = \{v_x, v_y\}$, so that its density in the laboratory frame of reference can be written as $\rho_{ext}(\vec{R}, z, t) \equiv \hat{\rho}_{ext}(\vec{R} - \vec{v}t, z)$. The Fourier transform of the external potential in the graphene plane can be expressed as

$$\Phi_{ext}(\vec{k}, z, \omega)|_{z=0} = \frac{(2\pi)^2\delta(\omega - \vec{k}\cdot\vec{v})}{k}F(\vec{k}) \tag{4}$$

with the structure factor of the external charge given by

$$F(\vec{k}) = \int \hat{\rho}_{ext}(\vec{R}, z) f(\vec{R}, z; \vec{k}) d^2\vec{R}\, dz \tag{5}$$

where we have defined $f(\vec{R}, z; \vec{k}) \equiv e^{-i\vec{k}\cdot\vec{R} - kz}$.

Substituting Eq. (4) via Eq. (2) into Eq. (1) and using Eq. (3), it is easy to obtain the Fourier transform of the induced number density per unit area of charge carriers in graphene as

$$n_{gr}(\vec{k}, \omega) = \frac{2\pi}{e}\delta(\omega - \vec{k}\cdot\vec{v})\left[1 - \frac{1}{\varepsilon(k, \omega)}\right]F(\vec{k}). \tag{6}$$

By performing the inverse Fourier transformation in the xy plane and in time, one obtains an expression for the induced number density as follows

$$n_{gr}(\vec{R}, t) = \frac{1}{(2\pi)^2 e}\int F(\vec{k})\left[1 - \frac{1}{\varepsilon(k, \vec{k}\cdot\vec{v})}\right]e^{i\vec{k}\cdot(\vec{R} - \vec{v}t)}d^2\vec{k}. \tag{7}$$

In order to approximate the structure factor $F(\vec{k})$, we assume that the external charge density $\hat{\rho}_{ext}(\vec{R}, z)$ is both highly peaked and appreciable only around point $\{\vec{R}_0, z_0\}$ in the moving frame of reference. By using the Taylor expansion of $f(\vec{R}, z; \vec{k})$ about $\{\vec{R}_0, z_0\}$, so that

$$f(\vec{R}, z; \vec{k}) \approx f(\vec{R}_0, z_0; \vec{k}) + (\vec{R} - \vec{R}_0)\cdot\frac{\partial}{\partial\vec{R}}f(\vec{R}, z; \vec{k})\Big|_{\vec{R}=\vec{R}_0,\, z=z_0} + (z - z_0)\frac{\partial}{\partial z}f(\vec{R}, z; \vec{k})\Big|_{\vec{R}=\vec{R}_0,\, z=z_0} \tag{8}$$

and replacing Eq. (8) into Eq. (5) one obtains

$$F(\vec{k}) = (Q - i\vec{k}\cdot\vec{\mu}_\parallel - k\mu_z)f(\vec{R}_0, z_0; \vec{k}) \tag{9}$$

where $Q = \int \hat{\rho}_{ext}(\vec{R}, z) d^2\vec{R}\, dz$ is the total charge and $\vec{\mu} = \{\vec{\mu}_\parallel, \mu_z\}$ is the dipole moment. Note that $\vec{\mu}_\parallel = \int \hat{\rho}_{ext}(\vec{R}, z)(\vec{R} - \vec{R}_0)\, d^2\vec{R}\, dz$ and $\mu_z = \int \hat{\rho}_{ext}(\vec{R}, z)(z - z_0)\, d^2\vec{R}\, dz$ are the components of dipole moment parallel and perpendicular to graphene, respectively. We also note that by setting $Q \neq 0$ and $\vec{\mu} = 0$ one obtains the point-charge model for ions, whereas taking $Q = 0$ along with $\vec{\mu} \neq 0$ gives the point-dipole model.

For a point dipole moving along the x axis with speed v at the distance $z_0 > 0$ above graphene, we shall use the angles from spherical coordinates to describe the orientation of its moment of magnitude μ, $\vec{\mu} = \{\mu_x, \mu_y, \mu_z\} \equiv \mu\{\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta\}$, with the polar angle θ taken relative to the z axis and the azimuthal angle φ relative to the x axis (i.e., the direction of the dipole motion parallel to graphene). By setting $Q = 0$ and $\vec{R}_0 = \vec{0}$ one obtains from Eq. (9) that the structure factor is given by

$$F(\vec{k}) = -\mu\left[i\sin\theta(k_x\cos\varphi + k_y\sin\varphi) + k\cos\theta\right]e^{-kz_0}. \tag{10}$$

Finally, substituting Eq. (10) into Eq. (7) one obtains, for a point dipole moving along the x axis with speed v, an expression for the induced number density as follows

$$n_{gr}(x, y, t) = \frac{\mu}{\pi^2 e}\int_0^\infty\int_0^\infty e^{-kz_0}k_x\sin\theta\cos\varphi\cos(k_y y) \times\left\{\text{Re}\left[1 - \frac{1}{\varepsilon(k, k_x v)}\right]\sin\left[k_x(x - vt)\right]\right.$$