Physics Letters A 375 (2011) 3720–3725

Contents lists available at SciVerse ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Wake effect in doped graphene due to moving external charge

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ARTICLE INFO

Article history:
Received 25 June 2011
Received in revised form 24 August 2011
Accepted 27 August 2011
Available online 2 September 2011
Communicated by R. Wu

Keywords:
Graphene
Wake effect
Dielectric function

ABSTRACT

We use the dielectric-response formalism to evaluate the induced density of charge carriers in supported graphene due to an external moving charged particle in terms of its velocity and distance from graphene for several equilibrium charge carrier densities due to graphene doping. We show that, when the particle speed exceeds a threshold value, an oscillatory wake effect develops in the induced charge density trailing the particle. Strong effects are observed in the wake pattern due to finite size of the graphene–substrate gap, as well as due to strong coupling effects, and plasmon damping of graphene's π electrons.

1. Introduction

Interactions of energetic charged particles with graphene-based materials have been studied extensively for some time, e.g., in investigations of the directional effects in ion and molecule implantation into highly oriented pyrolytic graphite (HOPG) [1,2], ion channelling through HOPG [3], and secondary electron emission from HOPG induced by fast ions [4] and clusters [5], as well as in ion channelling through carbon nanotubes [6–9], and in the excitation of plasmons in a single-walled carbon nanotube by a fast point charge moving near its surface at an arbitrary angle of incidence [10].

On the other hand, interactions of electrons with graphene have been recently studied both at high electron energies in the context of electron energy loss spectroscopy (EELS) in scanning transmission electron microscope (STEM) [11,12] and at low electron energies within the high-resolution reflection EELS (HREELS) studies of epitaxial graphene [13–16]. HREELS is particularly suitable for probing the low-energy excitations in graphene, which are dominated by the linear energy dispersions of its π-electron conduction and valence bands that meet at the so-called Dirac point, giving rise to the picture of "massless" Dirac fermions (MDF) [17]. Depending on the level of doping of graphene with charge carriers, which determines the position of its Fermi level relative to the Dirac point, both intra-band and inter-band single-particle excitations (SPEs) can play significant roles, in addition to plasmon excitations in graphene.

The ability to screen an external electric field is an important property of any nanostructured material. Depending on the speed of the external charge, the screening mechanism changes its character dramatically, going from a Debye-like screened potential of a static charge to a dynamic regime characterized by an oscillatory potential contained in a cone trailing a moving charge, which is commonly known as the wake effect [18]. It is characterized by the onset of oscillations in the polarization of the medium, which arise from resonances due to excitations of collective modes in the medium and often provide an effective mechanism of energy loss for an external charge. While the wake effect in three-dimensional (3D) plasmas has been known for more than fifty years [19], its current significance encompasses diverse new areas, such as dust-crystal formation in complex plasmas [20], Coulomb explosion of large clusters, such as C_{60}, in thin solid foils [21], channelling of fast ions through nano-capillaries in solids [22] and carbon nanotubes [6,18], as well as interactions of charged particles with one [23] and two [24] layers of a 2D quantum electron gas (2DQEG), supported thin metal films [25], and with magnetized two-component plasmas [26,27].

In our previous publications [28,29], we have used a hydrodynamic model to study the wake effect due to *fast* charged particles that move at speeds in excess of the Bohr's speed over a supported 2D electron gas (2DEG) characterized by a single energy band with parabolic dispersion. Our results showed that, when the particle speed matches the phase velocity of the quasi-acoustic π plasmon, the induced number density shows the usual wake oscillations. In addition, we have presented calculations of the total electric potential in the 2DEG plane, induced by a fast point charge moving parallel to it. Those results indicated a possibility of realizing the so-called wake riding effect in 2D [18,30], whereby other charged particles may be captured in a potential well, or their state

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0375-9601/$ – see front matter
doi:10.1016/j.physleta.2011.08.053

manipulated in the presence of the wake potential induced by a fast external charge.

In this work, we focus on the wake effect in a supported single-layer graphene under the gating conditions due to *slow* charged particles that move parallel to graphene. This configuration may be of interest for grazing scattering of slow ions from graphene [31], or for HREELS studies of graphene that involve reflection of electrons with energies on the order of several tens of eVs [13–16]. Since such interactions are expected to be dominated by the low-energy excitations of graphene's π electrons, it is convenient to use the dielectric-response theory for surfaces and layered structures [32], incorporating the polarization function for graphene that is available within the random phase approximation (RPA) based on a linear approximation for the π electron bands [33–35]. We have discussed the applicability of the latter approximation in Ref. [36], where we showed that it should work well for particles moving at sufficiently large distances and at speeds on the order of Bohr's speed, or less.

Graphene usually appears in the experimental situations as supported by a substrate [37,38]. Surprisingly, most theoretical models of graphene's dynamic response assume a zero gap between the graphene and a substrate [33,34], even though the size of such gap is expected to be on the order of the distance between graphene layers in graphite, or even larger, as documented experimentally [38]. In our previous publications we have evaluated the stopping and dynamic image forces acting on slow ions by means of a semiclassical kinetic (Vlasov) equation for graphene's π electrons [39] and by using the dielectric response formalism for graphene's π electron bands in the RPA model [36,40], and we pointed to a strong need to take into account the finite size of the graphene–substrate gap.

Although we consider the RPA dielectric function to be a basic, parameter-free model that provides an adequate description of both the inter-band and intra-band SPEs, as well as plasmon excitations, of graphene's π electrons, the model nevertheless has its shortcomings. For example, it ignores the local-field effects (LFE) due to electron–electron correlations [41,42] and assigns an infinitely long lifetime to the electron excitations. Only one of these shortcomings can be qualitatively corrected in the RPA dielectric function at a time, e.g. by using either the Hubbard approximation (HA) for the LFE in the static limit [43] or by introducing finite relaxation time, or decay (damping) rate, γ, using Mermin's procedure [36,40,44,45].

In this Letter, we present for the first time the oscillatory wake effect in the charged carrier density in a supported graphene, induced by a slowly moving charged projectile, taking into account the influence of: the equilibrium charge carrier density n due to doping of graphene, the distance z_0 and the speed v of the projectile, the size of the graphene–substrate gap h, and the damping rate γ of elementary excitations in graphene.

The equilibrium charge carrier density is a particularly important parameter because it determines the Fermi wavenumber of graphene's π-electrons, $k_F = \sqrt{\pi n}$ (we shall assume $n > 0$, i.e., graphene doped by electrons, without loss of generality), and the corresponding Fermi energy, $E_F = \hbar k_F v_F$, where $v_F \approx c/300$ is the Fermi speed of the linearized π bands, and c is the speed of light in free space. In this work, we shall consider a range of equilibrium charge carrier densities from 10^{11} cm^{-2} to 10^{13} cm^{-2}. In addition, we shall make explicit comparison of our results for the wake effect in graphene with those arising in a 2DEG with a parabolic energy band parameterized by the effective mass $m_* = \hbar k_F / v_F$. In this way, both the single-layer graphene and the "massive" 2DEG share the same form of the plasmon dispersion relation in the long wavelength limit, given by $\omega_p(k) = \sqrt{2\pi n e^2 k/m_*} = \sqrt{2e^2 v_F k_F k/\hbar}$.

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. A substrate with dielectric constant ε_s is assumed to occupy the region $z \leqslant -h$ underneath the graphene, whereas the region $z > -h$ is assumed to be vacuum or air. 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

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

where $\chi(k, \omega)$ is the polarization function within RPA for non-interacting π electrons in free graphene with $k = \sqrt{k_x^2 + k_y^2}$. Taking into account the effects of substrate, 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 with the density $\rho_{ext}(\vec{R}, z, t)$ as

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

where $\varepsilon(k, \omega)$ is the dielectric function of the combined graphene–substrate system, given by

$$\varepsilon(k, \omega) = \varepsilon_0(k) + V(k)\chi(k, \omega) \tag{3}$$

with $V(k) = 2\pi e^2/k$ being the Coulomb interaction in 2D and

$$\varepsilon_0(k) \equiv \frac{1}{1 - \frac{\varepsilon_s - 1}{\varepsilon_s + 1} e^{-2kh}} \tag{4}$$

the background dielectric function, which quantifies the effects of the substrate. Note that $\varepsilon_0(k)$ takes the values in the range between 1 and $(\varepsilon_s + 1)/2$, characterizing, respectively, the case of a free-standing graphene ($h \to \infty$) and the case of a zero gap ($h = 0$) between graphene and a substrate.

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. [33,34,36]. In order to estimate the effects of strong coupling, we go beyond the RPA regime by using the approach outlined in Ref. [46] for interactions of slow charged particles with 2DEG, whence the RPA polarization function $\chi(k, \omega)$ is to be replaced with

$$\chi_{LFE}(k, \omega) = \frac{\chi(k, \omega)}{1 - G(k)V(k)\chi(k, \omega)}. \tag{5}$$

For the sake of simplicity, we use static limit of the LFE correction function, $G(k)$, which is given in the Hubbard approximation (HA) by $G(k) = \frac{k}{4\sqrt{k^2 + k_F^2}}$ [43,47]. On the other hand, the finite lifetime of the excitation modes of charge carriers in graphene is treated by introducing a finite damping rate, γ, in the RPA polarization function through Mermin's procedure [36,40,44,45], whereby one replaces $\chi(k, \omega)$ with

$$\chi_M(k, \omega, \gamma) = \frac{\chi(k, \omega + i\gamma)}{1 - \frac{i\gamma}{\omega + i\gamma}\left[1 - \frac{\chi(k, \omega + i\gamma)}{\chi_s(k)}\right]} \tag{6}$$