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Abstract. We study the wake effect in a supported graphene layer induced by external charged particles 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 explore the effects of a substrate assuming that graphene is supported by an insulating substrate, such as SiO_2, and a strongly polar substrate, such as SiC, under the gating conditions. Strong effects are observed in the wake pattern in the induced density of charge carriers in supported graphene 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. We find that the excitation of surface phonons in the substrate may exert quite strong influences on the wake effect in the total electrostatic potential in the graphene plane at low particle speeds.

1. Introduction

Graphene is a flat monolayer of carbon atoms tightly packed into a two-dimensional (2D) honeycomb lattice [1]. It is a basic building block for graphitic materials of all other dimensionalities: highly oriented pyrolytic graphite (HOPG, a stack of graphene layers), carbon nanotubes (rolled-up cylinders of graphene), and fullerene molecules (consisting of wrapped graphene by the introduction of pentagons on the hexagonal lattice) [2, 3].

The ability to screen an external electric field is an important property of any nanostructured material, including graphene. 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 [4]. 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 almost sixty years [5], its current significance encompasses diverse new areas, such as dust-crystal formation in complex plasmas [6], Coulomb explosion of large clusters, such as C_{60}, in thin solid foils [7] and plasmas [8], channelling of fast ions through nano-capillaries in solids [9] and carbon nanotubes [4, 10], as well as interactions of charged particles with 1D electron gas (1DEG) [11], one [12] and two [13, 14] layers of a 2D quantum electron gas (2DQEG), supported thin metal films [15], nanosphere [16], and with magnetized two-component plasmas [17, 18].

We have studied, in our previous publications [19, 20], the wake effect due to fast charged particles that move at speeds in excess of the Bohr's speed over a supported 2DEG characterized by a single energy band with parabolic dispersion. We have used a one-fluid hydrodynamic model with the parameters characteristic of graphene [19], which treats all four carbon's valence electrons as a single 2DEG, to present the oscillatory wake effect which develops in the induced number density when the particle speed exceeds a threshold value for the collective excitations in a 2DEG corresponding to the four valence electrons in graphene. We have also used a two-fluid hydrodynamic model with the parameters characteristic of graphene [20], which makes distinction between the contributions of carbon's σ and π electrons, to calculate the induced number density per unit area of electrons in the 2DEG and compare it with the induced number density in the one-fluid model. 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 electrostatic 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 [4, 21], whereby other charged particles may be captured in a potential well, or their state manipulated in the presence of the wake potential induced by a fast external charge.

In order to study the wake effect due to slow charged particles moving parallel to a graphene layer under the gating conditions, the dielectric-response theory for surfaces and layered structures [22] is a convenient way to proceed, given that the dielectric function for graphene is available within the random phase approximation (RPA) based on a linear approximation for the π electron bands [23, 24, 25]. As regards the applicability of the latter approximation in describing the elementary excitations in the wavenumber-frequency, (k,ω), domain pertinent to graphene, we note that conditions $k < 2k_c$ and $\omega < 2\varepsilon_c/\hbar$ should be satisfied, where $k_c \approx a^{-1}$ is a high-momentum cutoff (with $a \approx 2.46\,\text{Å}$ being the lattice constant), and $\varepsilon_c \approx 1\,\text{eV}$ is a high-frequency cutoff [2, 23, 25]. For particles moving parallel to graphene at a fixed distance z_0 and constant speed v, the former condition will be satisfied for distances $z_0 > a$ (thereby neglecting the size of the π electron orbitals in graphene). The latter condition can be transformed into a restriction on the particle speed by invoking the Bohr's adiabatic criterion and requiring that $v < 2z_0\varepsilon_c/\hbar$. When the projectile speed is normalized by the Fermi speed of graphene, v_F ($v_F \approx c/300$, where c is the speed of light in free space), the latter condition amounts to $v/v_F \leq 0.3z_0$ with z_0 expressed in angstroms.

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 single-particle excitations (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 [26, 27] 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 [28] or by introducing finite relaxation time, or decay (damping) rate, γ, using Mermin's procedure [29, 30, 31, 32].

We present the oscillatory wake effect in the charged carrier density and in the total electrostatic potential in the graphene plane in a supported graphene layer, induced by a slowly moving charged projectile. We study the effects of a substrate assuming that graphene is supported by an insulating substrate, such as SiO_2, and a strongly polar substrate, such as SiC, under the gating conditions, 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, $E_F = \hbar k_F v_F$.

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 single-layer graphene is located in the plane $z = 0$, where $\vec{R} = \{x, y\}$ is position in the plane and z distance from it. A semi-infinite substrate is assumed to occupy the region $z \le -h < 0$ underneath graphene, whereas the region $z > -h$ is assumed to be vacuum or air. It can be shown that, for a point charge Ze moving parallel to graphene along the x axis with speed v at a fixed distance $z_0 > 0$, the induced number density per unit area of electrons in graphene and the total electrostatic potential in the graphene plane are given by, respectively

$$n_{gr}(x,y,t) = \frac{Z}{\pi^2}\int_0^\infty\int_0^\infty e^{-kz_0}\,\mathrm{Re}\left\{\left[1-\frac{\varepsilon_{bg}(k,k_x v)}{\varepsilon(k,k_x v)}\right]e^{i[k_x(x-vt)+k_y y]}\right\}dk_x dk_y\,, \tag{1}$$

$$\Phi_{tot}(x,y,z,t)\big|_{z=0} = \frac{2Ze}{\pi}\int_0^\infty\int_0^\infty \frac{e^{-kz_0}}{k}\,\mathrm{Re}\left\{\frac{e^{i[k_x(x-vt)+k_y y]}}{\varepsilon(k,k_x v)}\right\}dk_x dk_y\,, \tag{2}$$

where we have used the symmetry properties of the real and imaginary parts of the dielectric function of the combined graphene-substrate system

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

with $\chi(k,\omega)$ being the polarization function of non-interacting π electrons in free graphene [23, 24, 25], and

$$\varepsilon_{bg}(k,\omega) = \frac{\varepsilon_s(\omega)+1}{2}\,\frac{1+\coth(kh)}{\varepsilon_s(\omega)+\coth(kh)}\,, \tag{4}$$

is the background dielectric function which quantifies the effects of substrate on the response of graphene [33, 34]. Note that $\varepsilon_{bg}(k,\omega)$ takes the values in the range between 1 and $[\varepsilon_s(\omega)+1]/2$, 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.

In equation (4), $\varepsilon_s(\omega)$ is the bulk dielectric function of the substrate, which is given in the local approximation for a material supporting only one transverse optical (TO) phonon of frequency ω_{TO} by

$$\varepsilon_s(\omega) = \varepsilon_\infty + (\varepsilon_0 - \varepsilon_\infty)\frac{\omega_{TO}^2}{\omega_{TO}^2 - \omega(\omega + i\gamma_{TO})}\,, \tag{5}$$

where ε_∞ and ε_0 are the dielectric constants at high and low frequencies, respectively, and γ_{TO} is the damping rate of the TO phonon. Note that, when substrate phonons are ignored in graphene studies, it is customary to take the static limit of the dielectric function in equation (5), $\varepsilon_s(0) = \varepsilon_0$ [2].

In order to estimate the effects of strong coupling, we go beyond the RPA regime by using the aproach outlined in reference [35] for interactions of slow charged particles with 2DEG, whence the RPA polarization function $\chi(k,\omega)$ is to be replaced with

$$\chi_{LFE}(k,\omega)=\frac{\chi(k,\omega)}{1-G(k)V(k)\chi(k,\omega)}, \tag{6}$$

where $V(k)=2\pi e^2/k$ is the Coulomb interaction in 2D.

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 $G(k)=(1/4)k(k^2+k_F^2)^{-1/2}$ [28, 36]. 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 [29, 30, 31, 32], whereby one replaces $\chi(k,\omega)$ with

$$\chi_M(k,\omega,\gamma)=\frac{\chi(k,\omega+i\gamma)}{1-\frac{i\gamma}{\omega+i\gamma}\left[1-\frac{\chi(k,\omega+i\gamma)}{\chi_s(k)}\right]}, \tag{7}$$

where the static limit of the RPA polarization, $\chi_s(k)=\lim_{\omega\to 0}\chi(k,\omega)$, is given elsewhere [23, 24, 29].

3. Results and discussion

We choose the external particle to be proton ($Z=1$) moving along the x axis with speed v at a fixed distance $z_0=20$ Å above graphene with the equilibrium charge carrier density n.

Firstly, we use equation (1) to calculate the induced number density for free-standing graphene ($h\to\infty$), without the LFE, and with vanishing damping rate ($\gamma\to 0$). Our calculations of the induced number density for $y=0$ show that the wake effect generally takes place for particle speeds satisfying $v>v_F$, and is manifested as oscillations trailing the proton ($x-vt<0$). In figure 1, we explore the spatial dependence of wake oscillations in the induced number density n_{gr} (multiplied by z_0^2) as a function of both $x-vt$ and y (both normalized by z_0), for a proton moving along the x axis with a speed $v=4v_F$ at a distance $z_0=20$ Å above graphene with an equilibrium charge carrier density of $n=10^{13}$cm^{-2}. One can observe that the V shape wake-field appears apparently behind the particle, along with multiple oscillatory lateral wakes. One notices, away from the symmetry axis $y=0$, that the amplitudes of the lateral wakes are damped which is a consequence of plasmon damping due to the inter-band SPEs.

Next, we calculate the induced number density for graphene supported by a SiO_2 substrate in the static mode ($\varepsilon_0=3.9$), without the LFE, and with vanishing damping rate ($\gamma\to 0$). We explore the effects of a variable gap height and consider the gap heights: $h=0$ for the zero gap commonly considered in the literature, $h=4$ Å for a realistic value [37] and $h\to\infty$ for free graphene. In figure 2, we compare the spatial distribution of the induced number density n_{gr} (normalized by n) as a function of $x-vt$ (multiplied by $k_F=\sqrt{\pi n}$) with $y=0$, for a proton moving at a distance $z_0=20$ Å above graphene, for several gap heights and densities, with vanishing damping ($\gamma\to 0$), at two speeds: (a) $v=2v_F$ and (b) $v=4v_F$. One can observe in figure 2(a) that the oscillation period of the induced number density decreases when the size of the gap increases, as was also shown in our previous publication [19] in the case of the wake effect in interactions of fast ions with a supported 2DEG. This effect of the gap size on the oscillation periods seems to be weaker at higher particle speeds, as shown in figure 2(b) for $v=4v_F$, but the amplitude of these oscillations in the normalized number density n_{gr}/n appears to be suppressed by the close proximity of a substrate. Such a strong

influence of the size of the graphene-substrate gap on the wake effect is in accord with the conclusions found in our previous publications [29, 30, 38] about the importance of the gap size on the stopping and image forces on external charges moving near graphene.

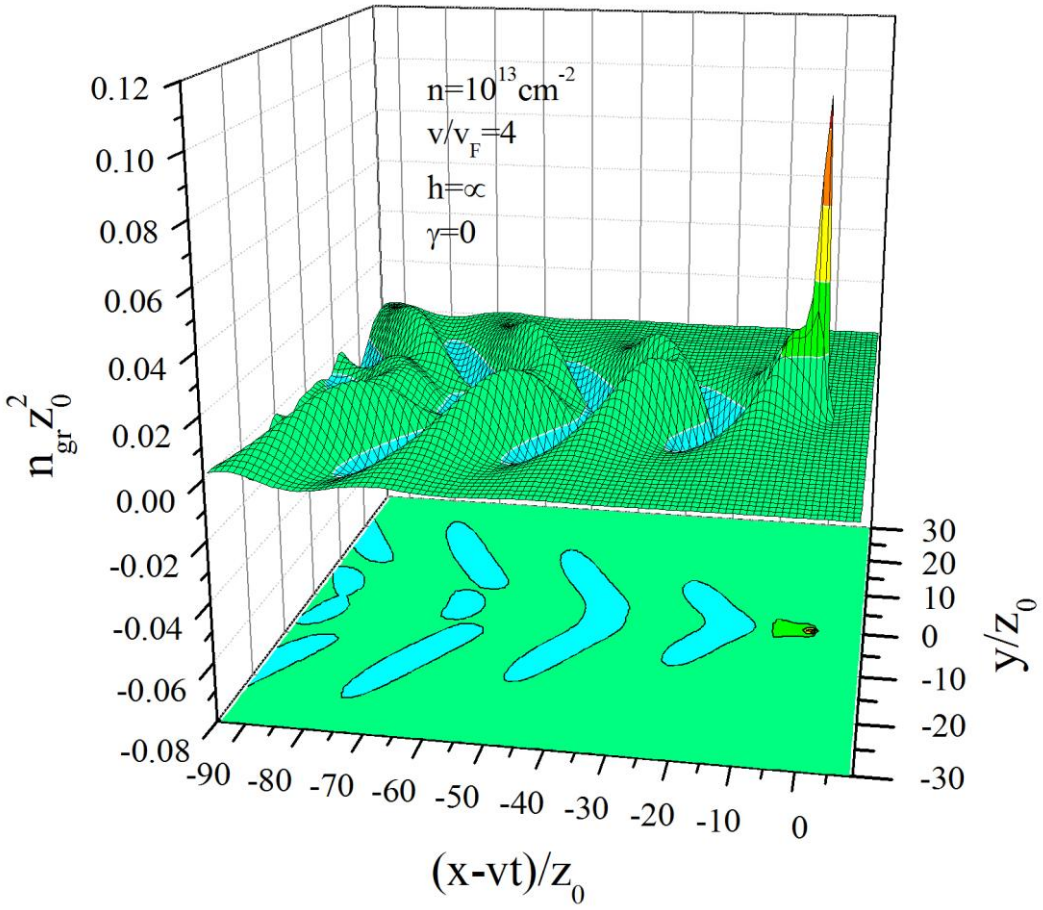

Figure 1. (Color online.) The induced number density n_{gr} (multiplied by the square of the particle distance z_0^2) as a function of $x-vt$ and y (both normalized by z_0) in the wake-field region created by a proton moving along the x axis with a speed $v=4v_F$ at a distance $z_0=20$ Å above free-standing graphene ($h\to\infty$) with an equilibrium charge carrier density of $n=10^{13}\text{cm}^{-2}$, and with vanishing damping ($\gamma\to 0$).

We also discuss the local-field effects (LFE) and the effects of finite damping rate on the induced number density. While the LFE is an inherent feature of graphene's electronic response that is particularly important at low particle speeds [35], the damping rate γ depends on graphene's environment and hence may vary quite strongly from sample to sample because γ arises from various mechanisms for charge carrier scattering, including charged impurities, local defects, and ripples in graphene [28]. For example, it was found for epitaxial graphene that a reasonable value for the damping rate γ is on the order of several hundred meV [29]. Thus, we compare in figure 3 several cases: graphene with $\gamma=0$ and $\gamma=100\,\text{meV}$ (without LFE), and graphene with the LFE included (whence $\gamma=0$). Figure 3 shows the spatial distribution of the induced number density n_{gr}

(normalized by n) as a function of $x-vt$ (multiplied by $k_F=\sqrt{\pi n}$) with $y=0$, for two equilibrium densities n of $10^{11}\,\mathrm{cm}^{-2}$ to $10^{13}\,\mathrm{cm}^{-2}$, for a proton moving at a distance $z_0=20\,\text{Å}$ above graphene on a SiO_2 substrate ($\varepsilon_0=3.9$ and $h=4\,\text{Å}$) at two speeds: (a) $v=2v_F$ and (b) $v=4v_F$. One notices that the main result of including the LFE is an increase in the period of the wake oscillations, which is similar to the effect of decreasing the graphene-substrate gap in figure 2. As expected, the LFE is seen to be more pronounced at the lower speed in figure 3 [35]. On the other hand, one notices that finite damping rate exerts quite strong influence in reducing the amplitudes of the wake oscillations at both speeds shown in figure 3. The observed suppression of the wake oscillations with increasing γ occurs due to the broadening of the plasmon resonance in the (k,ω) plane.

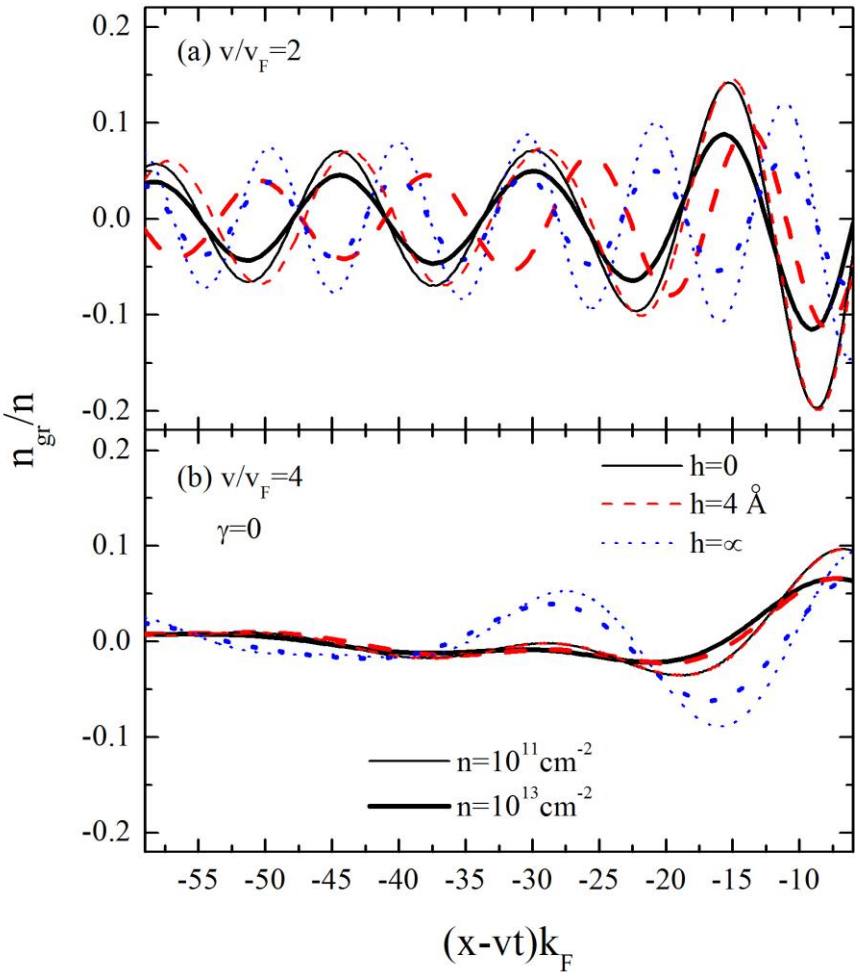

Figure 2. (Color online.) The spatial distribution of the induced number density n_{gr} (normalized by the equilibrium charge carrier density n) as a function of $x-vt$ (multiplied by the Fermi momentum $k_F=\sqrt{\pi n}$) with $y=0$, for a proton moving at a distance $z_0=20\,\text{Å}$ above graphene on a SiO_2 substrate ($\varepsilon_0=3.9$), with vanishing damping ($\gamma\to 0$), at two speeds: (a) $v=2v_F$ and (b) $v=4v_F$. Results are shown for three values of the gap heights: $h=0$ (black solid lines), $h=4\,\text{Å}$ (red dashed lines), and $h\to\infty$ (blue dotted lines). Thin and thick lines represent the cases of $n=10^{11}\,\mathrm{cm}^{-2}$ and $n=10^{13}\,\mathrm{cm}^{-2}$, respectively.

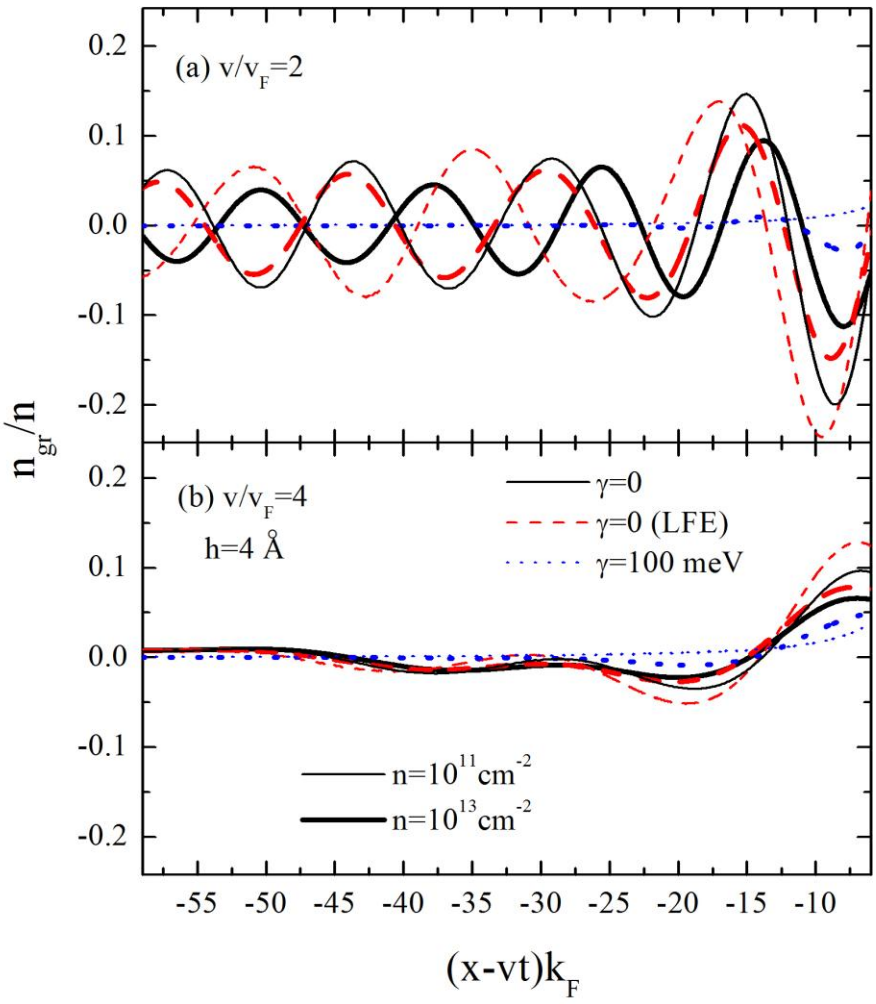

Figure 3. (Color online.) The spatial distribution of the induced number density n_{gr} (normalized by the equilibrium charge carrier density n) as a function of $x-vt$ (multiplied by the Fermi momentum $k_F=\sqrt{\pi n}$) with $y=0$, for a proton moving at a distance $z_0=20\,\text{Å}$ above graphene on a SiO_2 substrate ($\varepsilon_0=3.9$ and $h=4\,\text{Å}$), at two speeds: (a) $v=2v_F$ and (b) $v=4v_F$. Results are shown for three values of the damping rates γ: $\gamma=0$ (black solid lines), $\gamma=0$ with the LFE (red dashed lines), and $\gamma=100\,\text{meV}$ (blue dotted lines). Thin and thick lines represent the cases of $n=10^{11}\,\text{cm}^{-2}$ and $n=10^{13}\,\text{cm}^{-2}$, respectively.

Finally, we use equation (2) to calculate the total electrostatic potential in the plane of graphene with an equilibrium charge carrier density of $n=10^{13}\,\text{cm}^{-2}$, without the LFE, and with vanishing damping rate ($\gamma\to 0$). We explore the effects of a strongly polar substrate, such as SiC. Note that we use the following values in equation (5): $\varepsilon_\infty\approx 6.7$, $\varepsilon_0\approx 9.7$, $\omega_{TO}\approx 97\,\text{meV}$, and $\gamma_{TO}\approx 10\,\text{meV}$ [30]. For the sake of simplicity, we set $h=0$ noting that the effects of finite h are considered in figure 2. In figure 4, we show the total electrostatic potential in the plane of graphene Φ_{tot} (normalized by $\Phi_0=Ze/z_0$) as a function of $x-vt$ (normalized by z_0) with $y=0$, for four model systems: graphene on a substrate with phonon (g-SiC-phonon), graphene on a substrate in the static

mode (g-SiC-static), bare substrate with phonon (SiC-phonon), and free graphene (g-free). Since the wake effect is critically dependent on the particle speed, we consider three cases: $v/v_F = 0.5$, 1 and 2, in the panels (a), (b) and (c) of figure 4, respectively. Numerical results show that, when the projectile speed exceeds a threshold value on the order of graphene's Fermi speed v_F, the oscillatory wake effect develops in the total electrostatic potential in the graphene plane trailing the particle, as shown in figure 4(c) for the speed $v = 2v_F$. However, the potential for graphene on a substrate that supports a phonon mode also exhibits spatial oscillations at sub-threshold speeds, $v \le v_F$, as shown in figure 4(a) for $v = 0.5v_F$ and in figure 4(b) for the speed $v = v_F$. This may be due to hybridization of the plasmon in graphene and the substrate phonon.

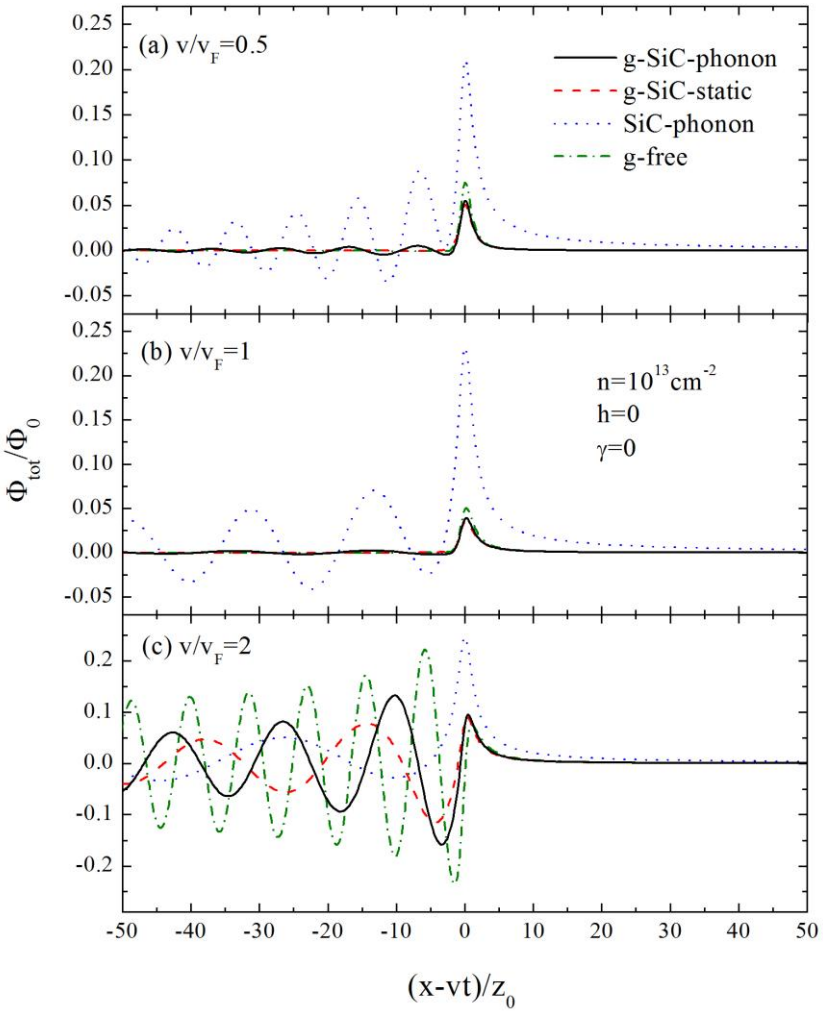

Figure 4. (Color online.) The spatial distribution of the total electrostatic potential in the plane of graphene Φ_{tot} (normalized by $\Phi_0 = Ze/z_0$) as a function of $x - vt$ (normalized by z_0) with $y = 0$, for a proton ($Z = 1$) moving at a distance $z_0 = 20$ Å above graphene with an equilibrium charge carrier density $n = 10^{13}$cm^{-2}, with vanishing damping ($\gamma \to 0$), at three speeds: (a) $v = 0.5v_F$, (b) $v = v_F$, and (c) $v = 2v_F$. Results are shown for four model systems: graphene on a substrate with phonon (g-SiC-phonon), graphene on a substrate in the static mode (g-SiC-static), bare substrate with phonon (SiC-phonon), and free graphene (g-free).

4. Conclusions

We have presented the wake effect in interactions of moving external charges with supported graphene under the gating conditions. Calculations of the induced number density per unit area of electrons in graphene, as well as of the total electrostatic potential in the graphene plane as functions of the speed of the projectile moving parallel to graphene and the particle distance, were performed within the random phase approximation (RPA) based on a linear approximation for the π electron bands.

We have found that the presence of a substrate can exert strong influence on the wake effect as well, e.g., via the dependence of the oscillation period of the induced number density trailing the charged particle on the size of the graphene-substrate gap (the oscillation period decreases when the size of the graphene-substrate gap increases). Similarly, strong influence was also observed at lower particle speeds when local-field effects were included in graphene's electronic response. In addition, we have found that the amplitudes of oscillations are heavily suppressed by increasing the damping rates of plasmons in graphene.

The total electrostatic potential in the plane of graphene exhibits the usual wake effect in both free graphene and graphene on a substrate in the static limit, showing spatial oscillations that lag the particle, which moves at a speed v exceeding the threshold value of v_F, the Fermi speed in graphene. Surprisingly, the potential for graphene on a substrate that supports a phonon mode also exhibits spatial oscillations at sub-threshold speeds, $v \leq v_F$, that trail a moving charge. While this may be due to hybridization of the plasmon in graphene and the substrate phonon, such an unusual manifestation of the wake effect warrants further investigation.

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