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Wake effect in the interaction of slow correlated charges with supported graphene due to plasmon–phonon hybridization

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ABSTRACT

We study correlated motion of two ions resulting from a dissociative grazing scattering of a slow diatomic molecular ion on supported graphene. A low-frequency collective mode resulting from hybridization of graphene's Dirac plasmon and the optical phonon modes in the insulating substrate may be excited by matching its phase velocity with the ion speed lower than the graphene Fermi speed. The resulting wake effect gives rise to the strongly directional, oscillatory patterns in both the inter-particle interaction potential and the total stopping power for the two ions, which may be detectable in their angular and the energy loss spectra.

1. Introduction

Recent developments in the area of graphene-based nanoplasmonics are concerned with hybridization of the Dirac plasmon (also known as the two-dimensional, or sheet plasmon) in a heavily doped graphene layer with the optical phonon modes in a polar, insulating substrate, such as SiC [1,2] and SiO_2 [3–6]. These low-energy collective modes in supported graphene may be efficiently probed by the incident charged particles, e.g., by using low-energy electrons in the Reflection Electron Energy Loss Spectroscopy (REELS) [1,7]. On the other hand, it was shown that the energy loss during grazing scattering of low-energy ions [8,9] and diatomic molecules [10] from a bare LiF surface may also be used to probe the excitation of optical phonons in insulating surfaces.

The interaction of moving charged particles with the bulk and surface regions of various materials is characterized by the wake effect, which arises when the particle speed matches the phase velocity of a collective mode in the target [11,12]. The resulting anisotropic wake potential may be considered as a signature of the excitations of collective modes in the surface of a target material by externally moving charges. Taking the gradient of that potential at the instantaneous location of a point charge gives rise to a stopping force on that charge, related to its energy loss rate or the stopping power [11,12]. At large distances, the wake potential of a single point charge may give rise to the wake riding bound states for other moving charges in the system [11], or it may cause strong orientational effects in the Coulomb explosion patterns of molecular projectiles, after their dissociation in solids [13] and during grazing scattering from solid surfaces [14,15]. Probably the most studied manifestation of the wake effect was concerned with the orientational effects in the total stopping power for moving correlated charges in solids [16] and on surfaces [15]. It is interesting that the wake effect may also arise due to static charged impurities in the presence of drifting charge carriers in doped semiconductors [17], or in a two-dimensional (2D) electron gas driven by an external microwave field [18]. While all those studies were concerned with the wake effect due to the plasmon excitation in targets containing (quasi-)free charge carriers, we note that a pure optical phonon wake was never observed in polar solids but rather in a strongly-coupled, 2D dusty plasma crystal [19].

The wake effect was also recently studied in graphene for individual charged particles [20,21], spatially correlated multiple charged particles [22], and point dipoles [22,23] moving parallel to a free graphene. It was found that the wake effect in graphene only arises if the speed v of the incident particle exceeds the Fermi speed $v_F \approx c/300$ (where c is the speed of light in vacuum) of graphene's π electron bands in the Dirac cone approximation [24]. The existence of such a threshold speed v_F for the occurrence of the wake effect in a single-layer graphene is interpreted as a signature of the excitation of its Dirac plasmon by an externally moving charge [20]. It was further shown that the Dirac plasmon wake in graphene gives rise to oscillatory patterns in both the interaction potential energy and the total stopping power as functions

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of the distance between two separated point charges that move at equal velocities $\mathbf{v}$ parallel to a free graphene layer when their speed $v \equiv \|\mathbf{v}\|$ exceeds v_F [22].

On the other hand, the effects of optical phonons in a polar substrate were recently studied for individual charged particles [2,25] and for point dipoles [22] moving parallel to an epitaxial graphene layer grown on a SiC substrate. It was shown that the stopping power of those particles is significantly increased [2,22], and the wake potential strongly modified [25] at high particle speeds, $v > v_F$, due to the plasmon–phonon hybridization in the graphene-substrate system. On the other hand, the stopping and image forces at slowly moving charges with $v < v_F$ were found to be largely unaffected by the substrate phonon in the case of a heavily doped graphene on SiC [2,25]. However, it was observed that a relatively weak wake effect may still exist in an epitaxial graphene, even at subthreshold speeds $v < v_F$, when the substrate phonon is included in the response of the graphene-SiC system [25]. This was tentatively explained by a reduced screening ability of graphene at low frequencies [25], when the substrate phonon remains the only collective mode of excitation giving rise to a phonon wake effect.

Thus, one may suspect that the remnant wake due to the substrate phonon excited at a subthreshold speed may give rise to the possibly observable orientational effects in the Coulomb explosion patterns and the energy loss spectra of slow diatomic molecular ions after their dissociation during grazing scattering from supported graphene, in a setting similar to that used for the bare LiF surface [10]. We suggest that graphene may provide more favorable conditions for observing the phonon wake via the molecular grazing scattering than the bare surface of an insulator [8–10] owing to graphene's ability to partially heal the roughness of the underlying insulator surface [26] and to provide more abundant charge exchange channels [27], which are needed for promoting a dissociative Coulomb explosion on a solid surface [10,15]. However, it remains unclear how the substrate phonon modes may survive in a graphene-substrate system where the intra-band single-particle excitations (SPEs) within the π electron bands of doped graphene should give rise to a strong Landau damping of any low-energy collective excitation modes. While this issue was recently discussed for graphene-based nanoplasmonics applications [3–6], we need to re-address it in the context of the proposed method for observing the surface phonon wake via the dissociative molecular grazing scattering. In particular, it is unclear to what extent the wake potential due to the hybridized plasmon–phonon mode(s) will affect the inter-particle interaction potential and the total stopping power for a pair of spatially correlated charges that move at a subthreshold speed over a supported graphene layer in the regime of heavy doping.

In order to explore this problem, we adopt here the dielectric formalism of Ref. [22] and consider a single-layer graphene on the technologically relevant SiO_2 substrate, where graphene is spontaneously doped with holes at a rather high density of $n \approx 2.9 \times 10^{12}$ cm^{-2} [3]. Thus, the presumably strong Landau damping in graphene's intra-band SPEs and the relatively large gap of $h \approx 4$ Å between graphene and the SiO_2 surface [28] may both diminish the role of the substrate phonon modes in the interaction between the two slow charges.

After outlining the theoretical model in the next section, we discuss the plasmon–phonon hybridization via the loss function based on the random phase approximation (RPA) for graphene on SiO_2, and we present our numerical results for the interaction energy and stopping power for two co-moving protons, followed by a brief summary. Note that we use Gaussian electrostatic units and set $\hbar = 1$, unless otherwise explicitly stated.

2. Theory

We use a Cartesian system with coordinates $\{\mathbf{r}, z\}$, where $\mathbf{r} = \{x, y\}$, and assume that graphene is placed in the $z = 0$ plane, a semi-infinite SiO_2 substrate occupies the region $z \leq -h < 0$, and the region $z > -h$ is vacuum or air. We further assume that two point particles with charges $Z_1 e$ and $Z_2 e$ (where $e > 0$ is the proton charge) move above graphene with equal velocities $\mathbf{v}_1 = \mathbf{v}_2 = \mathbf{v}$ directed parallel to graphene. With the positions of the particles in their moving frame of reference being $\{\mathbf{r}_1, z_1\}$ and $\{\mathbf{r}_2, z_2\}$, we assume that their distances $z_1 > 0$ and $z_2 > 0$ from graphene, as well as the projection of their relative distance in the plane of graphene, $\mathbf{d} = \mathbf{r}_2 - \mathbf{r}_1$, are independent of time at the time scales that characterize the dynamic polarization of the graphene-substrate system [15]. This polarization gives rise to both the conservative and the dissipative processes, which may be quantified by an electrostatic self-energy of the moving charges, $U_{\rm pol}$, and their total energy loss rate, or the stopping power $S_{\rm pol}$, respectively. By performing a 2D Fourier transform (FT) with respect to the coordinates parallel to graphene ($\mathbf{r} \to \mathbf{q}$) and a FT with respect to time ($t \to \omega$), the two quantities of interest may be written as [22]

$$U_{\rm pol} = \frac{1}{2}\int \frac{d^2\mathbf{q}}{(2\pi)^2} V_{\rm C}(q)\left|\mathcal{F}(\mathbf{q})\right|^2 \Re\left[\frac{1}{\epsilon(q, \mathbf{q}\cdot\mathbf{v})} - 1\right], \tag{1}$$

$$S_{\rm pol} = \frac{1}{v}\int \frac{d^2\mathbf{q}}{(2\pi)^2} V_{\rm C}(q)\left|\mathcal{F}(\mathbf{q})\right|^2 (\mathbf{q}\cdot\mathbf{v}) \Im\left[\frac{-1}{\epsilon(q, \mathbf{q}\cdot\mathbf{v})}\right], \tag{2}$$

where $V_{\rm C}(q) = 2\pi e^2/q$ is a 2DFT of the bare Coulomb interaction between unit charges in the plane of graphene and

$$\mathcal{F}(\mathbf{q}) = \sum_{j=1}^{2} Z_j e^{-i\mathbf{q}\cdot\mathbf{r}_j - qz_j} \tag{3}$$

is a form factor of the external charges in their moving frame of reference. In the above expressions we have defined an effective dielectric function for the graphene-substrate system as $\epsilon(q, \omega) = \epsilon_{\rm bg}(q, \omega) + V_{\rm C}(q)\Pi(q, \omega)$, where $\Pi(q, \omega)$ is the RPA polarization function of the non-interacting π electrons in a free graphene layer [29–31] and

$$\epsilon_{\rm bg}(q, \omega) = \left[1 - \frac{\epsilon_{\rm s}(\omega) - 1}{\epsilon_{\rm s}(\omega) + 1} e^{-2qh}\right]^{-1} \tag{4}$$

is a background dielectric function due to the substrate described by a frequency-dependent dielectric function $\epsilon_{\rm s}(\omega)$. For an SiO_2 substrate, there are two well-defined, non-dispersing transverse optical (TO) phonon modes at the frequencies $\omega_{\rm TO1} = 55.6$ meV and $\omega_{\rm TO2} = 138.1$ meV with the corresponding damping rates $\gamma_{\rm TO1} = 5.37$ meV and $\gamma_{\rm TO2} = 8.95$ meV, giving rise to a dielectric function of the form [32]

$$\epsilon_{\rm s}(\omega) = \epsilon_\infty + \frac{(\epsilon_i - \epsilon_\infty)\omega_{\rm TO2}^2}{\omega_{\rm TO2}^2 - \omega(\omega + i\gamma_{\rm TO2})} + \frac{(\epsilon_0 - \epsilon_i)\omega_{\rm TO1}^2}{\omega_{\rm TO1}^2 - \omega(\omega + i\gamma_{\rm TO1})}, \tag{5}$$

where $\epsilon_0 = 3.9$, $\epsilon_i = 3.05$, and $\epsilon_\infty = 2.5$ are the values of the dielectric constant for SiO_2 at the zero, intermediate, and very large frequencies.

The electrostatic self-energy of the two moving charges in Eq. (1) may be partitioned as

$$U_{\rm pol} = Z_1 Z_2 V_{\rm int}(\mathbf{d}, \bar{z}) + \sum_{j=1}^{2} Z_j^2 V_{\rm image}(z_j), \tag{6}$$

where $V_{\rm int}(\mathbf{d}, \bar{z})$ describes the interaction potential between two unit point charges mediated by the graphene-substrate system,