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Effect of uniaxial strain on plasmon excitations in graphene

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Abstract. Uniaxial strain is known to modify significantly the electronic properties of graphene, a carbon single layer of atomic width. Here, we study the effect of applied strain on the composite excitations arising from the coupling of charge carriers and plasmons in graphene, *i.e.* the plasmarons. Specifically, we predict that the plasmaron energy dispersion, which has been recently observed experimentally in unstrained graphene, is shifted and broadened by applied uniaxial strain. Thus, strain constitutes an additional parameter which may be useful to tune graphene properties in plasmaronic devices.

Graphene is a monoatomic carbon layer with honeycomb structure. After having been considered for decades as the ideal constituent of most compounds of carbon in the sp^2 hybridization state, it has been recently obtained in the laboratory [1], thus kindling intense research activity both on the experimental and on the theoretical side. Graphene is especially characterized by a quasiparticle band structure consisting of two bands, touching at the Fermi level in a linear, cone-like fashion at the so-called Dirac points $\pm\mathbf{K}$, and a linearly vanishing density of states (DOS) at the Fermi level [2, 3]. These peculiar electronic properties, along with the reduced dimensionality, have remarkable effects on the electromagnetic properties of graphene. These include, *e.g.,* the reflectivity [4], the optical conductivity [5, 6, 7, 8, 9], the plasmon dispersion relation [10, 11, 12, 13], as well as a newly predicted transverse electromagnetic mode [14], which is characteristic of a 2D system with a double band structure, such as graphene.

The composite elementary excitations arising from the coupling of charge carriers and plasmons, the so-called plasmarons, have been considered in a general context earlier on by Lundqvist [15, 16]. Recently, plasmarons have been experimentally observed in graphene by means of angular resolved photoemission spectroscopy (ARPES) [17], and their dispersion relation described theoretically within an improved version of the random phase approximation (G_0W-RPA) [18].

In n doped graphene, a plasmaron mode with momentum $\mathbf{k}$ results from the relatively strong coupling of a quasihole with momentum $\mathbf{k}+\mathbf{q}$, and a plasmon with momentum $-\mathbf{q}$, the quasihole-plasmon coupling being stronger when the two excitations have the same group velocity [18].

At $\mathbf{k} = 0$, the plasmaron relative momentum modulus turns out to be

$$q = \frac{e^2}{8\pi\epsilon}\frac{\mu}{(\hbar v_{\rm F})^2}, \tag{1}$$

where μ is the chemical potential, $v_{\rm F}$ the Fermi velocity, $\epsilon = \epsilon_0\epsilon_r$ the dielectric constant. Therefore, the plasmaron binding energy with respect to the Fermi energy can be estimated, in first approximation, as the sum of the energies of the bare quasihole and plasmon, both having momentum modulus q, *viz.*

$$E_P = -\mu - \alpha\frac{c}{v_{\rm F}}\frac{\mu}{2\epsilon_r}, \tag{2}$$

where α is the fine structure constant. In the realistic case of graphene on a SiO_2 substrate, Eq. (2) yields $E_P \simeq -1.25\mu$. A more accurate estimate, including the contribution of the quasihole-plasmon interaction at the G_0W-RPA level [18], yields $E_P \simeq -1.3\mu$, in better agreement with the experimental results [17].

We now consider the effect of uniaxial strain on the graphene sheet. It has been shown that this amounts to a shift of the Dirac points in reciprocal space, and to an anisotropic deformation of the Dirac cone centred at those points [19], with elliptic sections at constant energy. Such a strain-induced angular dependence may also be nonuniform, as in the case of coordinate-dependent strain [20]. The effect of applied uniaxial strain on the plasmon dispersion relation of graphene has been studied in Refs. [12, 13]. Besides, is has been shown [19] that strain may significantly modify the dispersion relation of a transverse plasmon mode, which has been recently predicted to occur in graphene [14]. Therefore, it can be expected, on general grounds, that strain affects the energy dispersion of the plasmaronic modes.

Denoting by ε the modulus of applied strain, θ its direction (with $\theta = 0$ and $\theta = \pi/6$ referring to strain along the zig zag and armchair directions, respectively), and ν the Poisson's ratio of graphene ($\nu = 0.14$ [21], to be compared with the known experimental value $\nu = 0.165$ for graphite [22], and with $\nu = -1$, corresponding to the hydrostatic limit), following Ref. [19], the quasiparticle dispersion relation, to linear order in ε, reads

$$\epsilon_{\mathbf{q}} = \pm\hbar v_{\rm F} q[(1-\kappa(1-\nu)\varepsilon) - \kappa(1+\nu)\varepsilon\cos(2\theta+2\varphi)], \tag{3}$$

where the $+$ $(-)$ sign refers to the conduction (valence) band, and while the plasmon dispersion relation under strain becomes

$$\hbar\omega_{\rm pl} = \sqrt{\frac{e^2}{2\pi\epsilon}\mu}\,[1-\kappa(1+\nu)\varepsilon\cos(2\theta-2\varphi)]\,\sqrt{q}. \tag{4}$$

Deriving the corresponding group velocities from the above Eqs. (3) and (4), Eqs. (1) and (2) for the plasmaron momentum and energy, respectively, get modified into

$$q = [1+2\kappa(1-\nu)\varepsilon]\frac{e^2}{8\pi\epsilon}\frac{\mu}{(\hbar v_{\rm F})^2}, \tag{5a}$$

$$E_P(\varphi) = -\mu - \alpha\frac{c}{v_{\rm F}}\frac{\mu}{2\epsilon_r}[1+\kappa(1-\nu)\varepsilon - \kappa(1+\nu)\varepsilon\cos(2\theta-2\varphi)], \tag{5b}$$

to linear order in the strain modulus ε. Here, $\kappa = (a/2t)|\partial t/\partial a| - \frac{1}{2} \approx 1.1$ is related to the logarithmic derivative of the nearest-neighbor hopping t at $\varepsilon = 0$, a is the carbon–carbon distance, and θ is the direction of the stress.

Eq. (5b) shows that, in the presence of applied uniaxial strain, the plasmaronic energy at $\mathbf{k} = 0$ acquires an explicit dependence on the angle φ of the quasihole momentum $\mathbf{q}$. This is

due to the anisotropy of both the electronic and the plasmon spectrum. Correspondingly, the plasmaron energy is characterized by a central value

$$E_P^{\rm c} = -\mu - \alpha \frac{c}{v_{\rm F}} \frac{\mu}{2\epsilon_r} [1 + \kappa(1-\nu)\varepsilon], \tag{6}$$

and a strain-induced energy spread

$$\Delta E_P = \alpha \frac{c}{v_F} \frac{\mu}{\epsilon_r} \kappa(1+\nu)\varepsilon. \tag{7}$$

Considering again the realistic case of graphene on a SiO_2 substrate, one can estimate the central plasmaron energy in the unstrained case as $E_P^{\rm c}(\varepsilon = 0) = -1.25\mu = -125$ meV, for $\mu = 100meV$, with zero energy spread. Correspondingly, in the case of an applied strain $\varepsilon = 10$ %, one finds a central plasmaron energy of $E_P^{\rm c}(\varepsilon = 10\ \%) = -127.4$ meV, with an energy spread $\Delta E_P(\varepsilon = 10\ \%) = 6.27$ meV.

In conclusion, the effect of applied uniaxial strain on graphene is therefore that of shifting and broadening the plasmaron energy, proportionally to the strain modulus. Therefore, by suitably applying uniaxial strain, one gains further control on the energy of the plasmaronic excitation, besides the possibility of tuning the relative dielectric constant ϵ_r [23]. This may be instrumental for the realization of 'plasmaronic' devices.

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