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Substrate interaction effects on optical and acoustical plasmons in bi-waveguides based on graphene ☆

Cesar E.P. Villegas *, Marcos R.S. Tavares

Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, Santo André, SP 09210-170, Brazil

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ABSTRACT

We theoretically study the dynamic dielectric response function of a gas of massless Fermions embedded in a coupled double quantum wire structure based on graphene. We write the dielectric function within the random phase approximation (RPA). We approach the system using the two-dimensional (2D) Dirac-like Hamiltonian in the first place, where a parameter β, accounting for the interaction between the substrate and the graphene sheet, is considered in an *ad-hoc* manner. We study the weak tunneling regime between the two ribbons and find the energy dispersion of the acoustical and optical plasmon modes. Our results show that different choices for the parameter β in the structure should induce spatial anisotropy effects on the plasmon modes.

1. Introduction

There has been a great deal of interest in studying a single 2D layer of carbon atoms, the graphene, due to its intriguing electronic properties [1]. More recently, there has been also much experimental concern about substrate induced effects on the graphene sheets. Anisotropic effects have been observed [2] on the conductivity in such experiments. These effects were claimed to be induced by the interaction between the graphene sheet and the underlying substrate. In fact, the graphene–substrate interaction is causing important effects in solving the 2D Dirac-like Hamiltonian which describes the graphene within the low-lying energy approximation [3]. Furthermore, the improving experimental techniques of growing and controlling such samples leads to the fabrication of one-dimensional (1D) graphene nanoribbons (GNRs), which are of promising technological applications [4]. The effects induced by both the electron–electron (e–e) correlation and the screening in these doped 1D systems have been subject of intense theoretical study [5,6]. The dispersion relation of intrasubband collective excitations (plasmons) in these ribbons has been obtained. But, these results turned out to be dependent on the kind of GNR obtained in the laboratory. The band structure of the GNRs depends strongly on the kind of the edge of the ribbon (armchair or zigzag edges). Such a dependence leads to a challenging realization in a laboratory of ribbons of identical atomic structures [7].

In this paper we theoretically propose a simple model to describe two coupled quantum wires (ribbons) based on the graphene which has eventually been deposited over some sort of substrate. The graphene–substrate interaction is considered here through a phenomenological parameter which is taken into account in an *ad-hoc* manner [3]. We consider the 1D spatial confinement, which forms the coupled ribbons, as being produced by electrostatic gate potentials, so we avoid the edge effects on the sample. We then study the dynamically screening properties of a (massless) Fermion gas which is laid in the structure. We calculate the dielectric response function within the RPA, which turned out to be a good approximation describing e–e correlations in graphene even for small charge densities [8]. The roots of this function provide us with the collective excitations in the system. Our results show that the graphene–substrate interaction induced effects play an important role in obtaining the bare Coulomb potential and the dielectric function of the system. Such a role manifests itself in the dispersion relation of the optical and acoustical plasmon modes. We found that the graphene–substrate interaction might eventually increase the damping effects on these modes.

The paper is organized as follows. In Section 2 we present the theoretical formulation to the problem. In Section 3 we show our numerical results and in Section 4 we conclude our work.

2. Theoretical formalism

In order to study collective excitations in our double quantum wire system based on graphene, we should find first the spectrum of the Hamiltonian $H = H_{2D} + U(x)$, where

$$H_{2D} = \gamma \vec{\sigma}.\vec{k} + \beta\sigma_z \tag{1}$$

is the 2D Dirac-like Hamiltonian describing the low-energy band structure for a single valley (K lattice point) in graphene. Here, the wavevector $\vec{k} = (k_x, k_y \equiv k)$ and the 2D Pauli vector $\vec{\sigma} = (\sigma_x, \sigma_y)$. The parameter β models a more general diatomic system in which the

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* Corresponding author.
E-mail address: cesar.villegas@ufabc.edu.br (C.E.P. Villegas).

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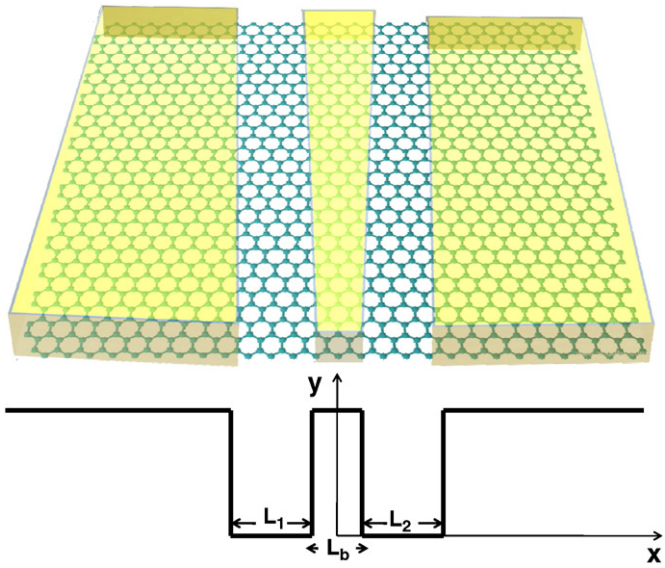

Fig. 1. Schematic representation of the potential profile forming a biwire structure based on graphene. It shows two coupled wires of widths L_1 and L_2, separated by a barrier of width L_b.

graphene lattice sites A and B might have a different number of electrons [9,10]. This is the parameter which will mimic here, in an *ad-hoc* manner, the graphene–substrate interaction strength [11]. We consider the lattice parameter $\gamma = \sqrt{3}a_0 t/2$, where $a_0 = 0.246$ nm and the hopping energy between the nearest neighbors $t \approx 2.8$ eV. The double square-well potential $U(x)$, schematically shown in Fig. 1, models our double quantum wire system. This figure shows a possible gate architecture to form two coupled quantum wires of widths L_1 and L_2 separated by a barrier of width L_b [12].

The eigenvector n of the Hamiltonian H can be written as $\psi_{nk}(x,y) \approx e^{iky}\phi_{nk}(x)$, where $\phi_{nk}(x)$ is a two-component pseudo-spinor which is obtained here in the extremely weak tunneling regime between the wires. In such a regime, the pseudo-spinor is considered to be identically zero outside both wires and, as a consequence, the subband index n should be treated as the *wire* index. Within each wire n, the pseudo-spinor assumes then the following form:

$$\phi_{nk}(x) = \begin{pmatrix} A_n sink_n^0\left[x + (-1)^{n+1}L_b/2\right] \\ B_n\left\{k_n^0 cosk_n^0\left[x + (-1)^{n+1}L_b/2\right] - ksink_n^0\left[x + (-1)^{n+1}L_b/2\right]\right\} \end{pmatrix}. \tag{2}$$

Here, the coefficients $A_n = \sqrt{2/L_n}$ and $B_n = -i\gamma A_n/[E_n + \beta]$, with $E_{n=1,2}(k) = \gamma\sqrt{k^2 + (k_n^0)^2 + (\beta\gamma^{-1})^2}$ being the eigenvalues of H, which are hyperbolic functions of k. Notice that $k_n^0 = \pi/L_n$ is the quantized wavevector corresponding to the fundamental quantum state in both wires.

Our model deals with a 1D massless Fermion gas confined along the wires, i.e., along the y-direction. Due to the 1D topology, the bare Coulomb potential between quasi-charges in the sample is a function which depends on 3 wavevectors and is given by [13]

$$\upsilon_{nnn'n'}(k,k',q) = \frac{2e^2}{\varepsilon_0}\int dx' \int dx\ \phi_{n,k}(x)\phi_{n,k+q}(x) \times K_0(q|x-x'|)\phi_{n',k'+q}(x')\phi_{n',k'}(x'), \tag{3}$$

with $n,n' = 1,2$. Here, ε_0 is the static background dielectric constant which depends on the substrate over which the graphene sheet is deposited [14], and K_0 is the zero-order modified Bessel function of the second kind. For two identical wires ($L_1 = L_2$), which case we consider here, there are only two different elements of υ, $\upsilon_{1111}(q,k,k') = \upsilon_{2222}(q,k,k') = V_A$ and $\upsilon_{1122}(q,k,k') = \upsilon_{2211}(q,k,k') = V_C$ [15]. These elements describe a scattering event in which charges always remain in their original wire after the wavevector q is transferred due to Coulomb interaction.

For the present system, the function which gives the dielectric response function $\varepsilon(q,\omega)$ is a 2×2 matrix whose elements can be written as

$$\delta_{nn'} - \sum_{kk'} \nu_{nn'n'n'}\Pi_{n'n'}. \tag{4}$$

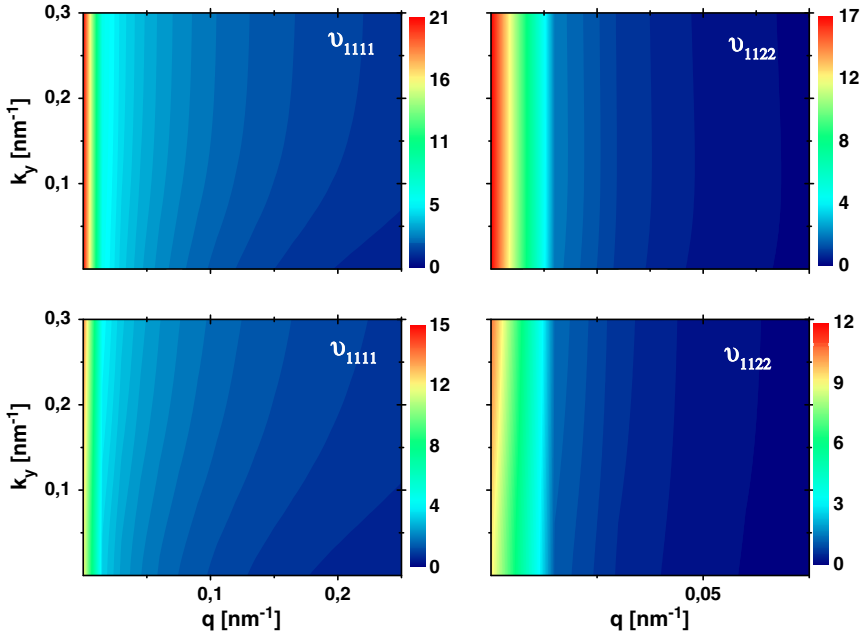

Fig. 2. The intensity of the Coulomb matrix elements $V_A(k,k',q)$ and $V_C(k,k',q)$ as a function of k and q considering two different values for the phenomenological parameter β. At the top (bottom) the parameter is $\beta = 0$ ($\beta = 30$ meV). The other parameters are $L_1 = L_2 = 20$ nm and $L_b = 10$ nm.