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Spectral function of the two-dimensional system of massless Dirac electrons

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HIGHLIGHTS

- We determine the spectral function for the two-dimensional system of massless Dirac electrons within the G_0W_0 approximation.
- We taking into account only a partially filled band above the Dirac point and pay particular attention to the contribution coming from the plasmon mode.
- The spectral function shows a wide structure with a pronounced weight just below the Dirac point and a renormalized quasi-particle δ-peak at the chemical potential.

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ABSTRACT

We determine the one-particle spectral function for the two-dimensional system of massless Dirac electrons interacting via the long-range Coulomb interaction. The electron self-energy is calculated within the G_0W_0 approximation, paying particular attention to the contribution coming from the collective plasmon mode. We find that, due to the acoustic plasmon dispersion, the spectral function has a renormalized quasi-particle δ-peak at the chemical potential along with a side band for the Fermi wave vector together with a wide structure with a pronounced spectral weight near the Dirac point. The present approach is appropriate for the wide range of energy scales given by the plasmon energy which may be probed in angle-resolved photoemission spectroscopy (ARPES) experiments.

1. Introduction

In condensed matter physics Dirac fermions have been applied to study a variety of novel materials, including graphene with band energy that contains two Dirac cones [1–5] and recently discovered topological insulators with the surface states that contain a single Dirac cone [6–11]. Furthermore, both systems have been investigated in numerous measurements by angle-resolved photoemission spectroscopy (ARPES) which provides a direct probe of the electronic structure giving energy and momentum information [6,7,9–14], and its data can be related to the one-electron spectral function that can be theoretically determined. However, in order to understand the spectral properties of real materials one has to take into account the electron–electron Coulomb interaction while calculating the spectral function. The consequence of electronic correlations is collective modes that influence the spectral function. In particular, in one dimension, eigenstates of a system of Dirac fermions have been calculated exactly within the Luttinger liquid model [15,16]. They are the long-range charge and spin acoustic collective modes. Moreover, the Luttinger liquid approach enables the analysis of the spectral properties of quasi-one-dimensional metals that do not show the essential property of Fermi liquids, namely the low-energy quasi-particle peaks in their spectra [17,18]. This approach, formulated at low energies, is complementary to the G_0W_0 approximation [19] for the electron self-energy for the square lattice of parallel chains coupled through the three-dimensional electron–electron Coulomb interaction that introduced a wide feature into the spectral function originating from the anisotropic plasmon dispersion [20–22]. Namely, the self-energy in the G_0W_0 approximation is the product of Green's function G_0 of non-interacting electrons and the screened W_0 interaction calculated within the random phase approximation (RPA) [19] which comprises collective modes. The early G_0W_0 approach to the three-dimensional "jellium" model[19,23,24] resulted in the spectral function showing low energy quasi-particle peaks and additional

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features due to the plasmon mode. Plasmons diminish the electron spectral weight. Electrons can interact with the plasmon mode to form the so-called plasmaron. Analog results were obtained for the two-dimensional graphene theoretically [25–30] and in ARPES measurements [12,13]. Also, plasmarons in this system could be seen in near field optics [31] as described in Ref. [32].

In this work we extend our earlier G_0W_0 approach [20–22] to the two-dimensional system of massless Dirac electrons interacting via the long-range Coulomb interaction. We take into account only a partially filled electron band above the Dirac point. Our aim is to determine the electron spectral function starting from the dynamically screened Coulomb interaction W_0 in the long-wavelength limit calculated within the random phase approximation (RPA). The main approximation comes from the neglect of the electron–hole continuum of single-particle excitations as we concentrate on the effects induced by the collective mode. After taking into account the linear band dispersion of Dirac electrons, the dynamically screened Coulomb interaction W_0 shows an acoustic plasmon with a square-root dispersion in the long-wavelength limit [33]. We note that much work has been done on the subject of screening in graphene showing the same behavior of the plasmon dispersion in this limit [27,34–36]. We also refer to work [37–41] devoted to the dielectric response of graphene under various conditions which is characterized by low-energy plasmon mode. Proceeding as in Ref. [20] we determine the dressed Dirac electron Green's function and the corresponding spectral function with a two-dimensional Coulomb electron–electron interaction screened by the plasmon mode. The obtained results show a wide structure with a quasi-particle-like feature in the spectral function just below the Dirac point and a quasi-particle δ-peak with reduced weight at the chemical potential for Fermi wave vector together with a side band due to coupling to the plasmon mode. The long-wavelength limit plasmon dispersion renormalizes the spectral function, redistributing the spectral weight towards higher energies. It is important to note that the long-wavelength limit plasmon dispersion has a dominant effect on the dressed Dirac electron propagator near the chemical potential, diminishing the weight of quasi-particle peak.

The paper is organized in the following manner. In Section 2 we calculate the wave vector dependence of the plasmon collective mode for a two-dimensional system of massless Dirac electrons within the approach of Ref. [33]. Section 3 is devoted to the calculation of the Dirac electron Green's function within the G_0W_0 method of Ref. [20]. In Section 4 we calculate and discuss the corresponding spectral function. The concluding Section 5 summarizes the main results.

2. Dielectric function and plasmon excitation

We begin by considering two-dimensional massless Dirac plasma, a system of electrons whose energy band dispersion is linear, i.e. $E_s(\mathbf{k}) = sv_Fk$, where $\mathbf{k}$ is a two-dimensional wave vector, $s = \pm$ denotes the conduction $(+)$ and the valence $(-)$ band, and v_F is the Fermi velocity. We are interested in the long-wavelength plasmon collective mode in a conduction band. Here, we use the random phase approximation (RPA) for the dynamical dielectric function which describes the screening properties of electron system:

$$\varepsilon(\mathbf{q},\omega) = 1 - V(\mathbf{q})\Pi(\mathbf{q},\omega), \tag{1}$$

where $V(\mathbf{q}) = 2\pi e^2/q$ is the two-dimensional bare Coulomb electron–electron interaction. We take into consideration only intraband transitions very close to the Fermi level in the conduction band. The RPA polarization diagram in $(\mathbf{q}, \omega)$-space entering into expression (1) reads

$$\Pi(\mathbf{q},\omega) = 4\int \frac{d^2k}{(2\pi)^2} \frac{n(\mathbf{k})[E(\mathbf{k}+\mathbf{q}) - E(\mathbf{k})]}{(\omega + i\eta\ \mathrm{sign}\ \omega)^2 - [E(\mathbf{k}+\mathbf{q}) - E(\mathbf{k})]^2}, \tag{2}$$

where

$$n(\mathbf{k}) = \begin{cases} 1, & E(\mathbf{k}) < 0 \\ 0, & E(\mathbf{k}) > 0 \end{cases} \tag{3}$$

is the occupation function at zero temperature, the energy $E(\mathbf{k}) = E_+(\mathbf{k}) - E_F$ is measured from the Fermi energy $E_F = v_Fk_F$ with k_F being the Fermi wave number, and $\eta \to 0^+$. Note that the expression (2) is simplification in the long-wavelength limit ($\mathbf{q} \to 0$) of the polarization formulas that comprise summations over indexes which include chirality overlap factors $F_{ss'}(\mathbf{k}, \mathbf{k}+\mathbf{q}) = (1 + ss'\ \cos\ \theta_{\mathbf{k},\mathbf{k}+\mathbf{q}})/2$ with $s, s' = \pm$ denoting the conduction $(+)$ and the valence $(-)$ band [34–36]. $\theta_{\mathbf{k},\mathbf{k}+\mathbf{q}}$ is the angle between wave vectors $\mathbf{k}$ and $\mathbf{k}+\mathbf{q}$. In the long-wavelength limit, this angle is small and $\cos\ \theta_{\mathbf{k},\mathbf{k}+\mathbf{q}} \approx 1$. Thus the chirality factor $F_{++}(\mathbf{k}, \mathbf{k}+\mathbf{q}) \approx 1$ does not influence the long-wavelength limit and the interband transitions vanish due to $F_{-+}(\mathbf{k}, \mathbf{k}+\mathbf{q}) \approx 0$.

The RPA enters through the dielectric function (1) into the dynamically screened electron–electron Coulomb interaction:

$$\overline{V}(\mathbf{q},\omega) = \frac{V(\mathbf{q})}{\varepsilon(\mathbf{q},\omega)}. \tag{4}$$

The zeroes of the real part of the dielectric function (1) determine the energies of the collective excitations as a function of the wave vector in the region where its imaginary part is zero, i.e. outside of an intraband electron–hole continuum of single-particle excitations defined by the poles of the polarization diagram (2). Because of the linear band dispersion $E(\mathbf{k}) = v_F(k - k_F)$, the intraband excitations are confined to the region where $\omega < v_Fq$, above which collective modes can exist. Now, being concentrated on the long-wavelength limit $\mathbf{q} \to 0$, where $\omega \gg E(\mathbf{k}+\mathbf{q}) - E(\mathbf{k})$, the polarization diagram reduces to Ref. [42]

$$\Pi(\mathbf{q},\omega) = \frac{2}{(\omega + i\eta\ \mathrm{sign}\ \omega)^2} \int \frac{d^2k}{(2\pi)^2} n(\mathbf{k})(\mathbf{q}\cdot\nabla_{\mathbf{k}})^2 E(\mathbf{k}) \tag{5}$$

with

$$(\mathbf{q}\cdot\nabla_{\mathbf{k}})^2 E(\mathbf{k}) = \frac{q^2}{k}\frac{\partial}{\partial k}\left[k\frac{\partial E(k)}{\partial k}\right]. \tag{6}$$