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Spectral properties of Dirac electron system

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ABSTRACT

We present the extension of our previous G_0W_0 approach to the two-dimensional system of massless Dirac electrons interacting via the long-range Coulomb interaction. We determine the one-particle spectral function taking into account only a partially filled linear band above the Dirac point. The electron self-energy is calculated, paying particular attention to the contribution coming from the collective plasmon mode through the dynamically screened Coulomb electron–electron interaction. The obtained results show a dispersing feature in the spectral function and a low energy quasi-particle with the renormalized spectral weight. We expect the results obtained to be qualitatively in agreement with spectral properties of monolayer of MoS_2 which has the large direct band gap between the valence and conduction bands. We also discuss the influence of the underlying substrate on the obtained results.

1. Introduction

Models of two-dimensional Dirac electron systems are of increasing interest because of their applicability to realistic systems. In recent years Dirac fermions have been applied to study unusual properties of a variety of novel materials, including graphene and newly discovered three-dimensional topological insulators, for review see [1,2]. Other recent examples of Dirac electron systems include monolayer of molybdenum disulfide (ML-MDS) [3] and silicene [4]. Comparing with graphene, the biggest difference in three-dimensional topological insulators, monolayer MoS_2 and silicene is gapped Dirac electrons found in these materials. Such Dirac electrons can also be found by placing graphene on silicon carbide [5], boron nitride [6] and iridium [7], or they can appear due to intrinsic spin–orbit coupling [8–10]. Interesting is also recently fabricated two-dimensional semiconductor phosphorene [11,12]. Unlike graphene, phosphorene in its natural form exhibits the large direct band gap as monolayer MoS_2. However, anisotropic band dispersion around band gap distinguishes it from isotropic two-dimensional MoS_2.

Two-dimensional Dirac electron systems have been investigated by angle-resolved photoemission spectroscopy (ARPES) measurements that provide a direct probe of the electron spectral function which takes into account electronic correlations and comprises collective modes. The present study addresses the role of collective plasmon mode in the calculation of the spectral function within the G_0W_0 approximation related to ARPES measurements in graphene [13–15] and monolayer of MoS_2 [16]. Our earlier G_0W_0 approach to spectral properties of quasi-one-dimensional conductors introduced a wide features into the spectral function originating from the anisotropic collective modes due to the finite electron–electron Coulomb interaction [17–19]. Also,the early G_0W_0 approach to the three-dimensional "jellium" model [20,21] resulted in the spectral function showing the low energy quasi-particle peaks and additional so-called plasmaron peaks and features due to the plasmon mode. Analog results were reported for graphene [22,23] indicating the importance of electronic correlations in this material. The G_0W_0 approximation gives the dynamical electron self-energy through a product of the non-interacting Green's function G_0 and the dynamically screened Coulomb interaction W_0 obtained in the random phase approximation (RPA) [24]. In this work we present the extension of our previous G_0W_0 approach [17–19] to the two-dimensional system of massless Dirac electrons with the long-range Coulomb interaction. More precisely,we determine the one-particle spectral function for a partially filled linear band above the Dirac point with the electron self-energy calculated paying particular attention to the contribution coming from the plasmon excitations through the dynamically screened Coulomb electron–electron interaction. These excitations were analyzed earlier in [25] where it was shown that they have a gapless acoustic dispersion in the long-wavelength limit. Due to this dispersion the obtained results show a wide structure in the spectral function with a pronounced weight indicating the renormalized free-electron band profile. This behavior is in accordance with earlier results for graphene [13–15,22,23] and recent results for a monolayer of MoS_2 [16] at low energies.

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2. Green's function

We begin by considering the two-dimensional system of massless Dirac electrons with a partially filled linear band $E(\mathbf{k}) = v_F(k - k_F)$ above the Dirac point, where $\mathbf{k}$ is a wave vector, k_F is the Fermi wave number, v_F is the Fermi velocity and the energy is measured from the Fermi energy $E_F = v_F k_F$, and the long-range Coulomb electron–electron interaction V. We determine first the dynamically screened electron–electron Coulomb interaction in the long-wavelength limit within the random phase approximation (RPA). The Dyson equation for the screened Coulomb electron–electron interaction $\bar{V}$ shown in Fig. 1 reads [26]

$$\bar{V}(\mathbf{q}, \omega) = V(\mathbf{q}) + V(\mathbf{q})\Pi(\mathbf{q}, \omega)\bar{V}(\mathbf{q}, \omega), \tag{1}$$

where $V(\mathbf{q}) = 2\pi e^2/\varepsilon q$ is the bare long-range interaction with ε being the background dielectric constant equal to the average $\varepsilon = (\varepsilon_1 + \varepsilon_2)/2$ between the dielectric constant of a vacuum ε_1 and that of the underlying substrate ε_2. It comprises the bare bubble polarization diagram

$$\Pi(\mathbf{q}, \omega) = -\frac{i}{\pi}\int\frac{d^2k}{(2\pi)^2}\int d\omega' G_0(\mathbf{k}, \omega + \omega')G_0(\mathbf{k} + \mathbf{q}, \omega') \tag{2}$$

with the noninteracting electron Green's function

$$G_0(\mathbf{k}, \omega) = \frac{1 - n(\mathbf{k})}{\omega - E(\mathbf{k}) + i\eta} + \frac{n(\mathbf{k})}{\omega - E(\mathbf{k}) - i\eta}, \tag{3}$$

where $n(\mathbf{k})$ is the occupation function at zero temperature and η denotes a positive infinitesimal. The final result for the bubble polarization diagram in the long-wavelength limit reduces to a well-known expression [25]:

$$\Pi(\mathbf{q}, \omega) = \frac{v_F k_F}{\pi}\frac{q^2}{(\omega + i\eta\ \mathrm{sign}\ \omega)^2}. \tag{4}$$

Then the dynamically screened electron–electron Coulomb interaction in the long-wavelength limit reads

$$\bar{V}(\mathbf{q}, \omega) = V(\mathbf{q})\frac{(\omega + i\eta\ \mathrm{sign}\ \omega)^2}{(\omega + i\eta\ \mathrm{sign}\ \omega)^2 - \omega^2(\mathbf{q})}, \tag{5}$$

where its poles are given by the plasmon excitations [25]

$$\omega(\mathbf{q}) = \omega_0\sqrt{q}, \quad \omega_0 = \sqrt{\frac{2e^2 v_F k_F}{\varepsilon}}. \tag{6}$$

The plasmon frequency depends on the background dielectric constant. The expression (6) has been written for the massless Dirac electron model with the spin degeneracy. The degeneracy is 4 for graphene and there is no degeneracy for electron liquid on the surface of three-dimensional topological insulator. As in Lundqvist's calculation [20] the main approximation comes from the neglection of the single particle excitations in the long-wavelength limit. We note that an analog result was obtained at low energies in doped graphene [23,27–30] and for electron liquid on a surface of three-dimensional topological insulator [31], i.e. a gapless plasmon mode which disperses as $\omega_{pl}(q) \sim \sqrt{q}$. The plasmon in the latter case will merge into the particle–hole continuum at lower frequency as the dielectric constant for the topological insulator is much greater than that for graphene. Moreover, gapped Dirac electrons, as found in a monolayer of molybdenum disulfide, exhibit also a square root plasmon dispersion dependent on the background dielectric constant [32]:

$$\omega(\mathbf{q}) = \omega_0\sqrt{q}, \quad \omega_0 = \frac{2E_F}{\Delta}\sqrt{\frac{2e^2 v_F k_F}{\varepsilon}}, \tag{7}$$

where Δ is a band gap and $2E_F/\Delta \approx 1$. As their energy dispersion of the conduction band $E_c(\mathbf{k}) = \sqrt{a^2t^2k^2 + \Delta^2/4}$, where t is the effective hopping amplitude and a is the hexagonal lattice constant, can be linearized around the Fermi energy, the approach presented below for the dressed Green's function also applies to them. A similar situation is found in silicene, but with the small band gap [33,34].

Experimentally, the square-root plasmon dispersion was observed in momentum-resolved low energy electron energy-loss spectroscopy (EELS) measurements in graphene [35,36] and should be directly observable in analog measurements in a monolayer of molybdenum disulfide [37]. Moreover, two-dimensional plasmons of massless Dirac electrons were recently observed in three-dimensional topological insulator Bi_2Se_3 using infrared spectroscopy [38].

In the present work we extend the G_0W_0 method of [17] to calculate the effect of the Coulomb interaction on the spectral function of two-dimensional Dirac electron band. The Dyson equation for the dressed Green's function in the G_0W_0 approximation comprising the infinite series of the bare bubble polarization diagrams, as shown in Fig. 2, can be expressed in terms of the RPA screened Coulomb electron–electron interaction and reads [17,26]

$$G^{-1}(\mathbf{k}, \omega) = \omega - E(\mathbf{k}) - i\eta[1 - n(\mathbf{k})] - \frac{i}{2\pi}\int\frac{d^2q}{(2\pi)^2}\left\{\int d\omega' G_{0s}(\mathbf{q}, \omega')V(\mathbf{k} - \mathbf{q})e^{i\omega'\delta} + \int d\omega' G_{s0}(\mathbf{q}, \omega')[\bar{V}(\mathbf{k} - \mathbf{q}, \omega - \omega') - V(\mathbf{k} - \mathbf{q})]\right\}. \tag{8}$$

It contains the corresponding bare Green's function that comprises a shift of the chemical potential

$$G_{0s}(\mathbf{k}, \omega) = \frac{1 - n(\mathbf{k})}{\omega - E(\mathbf{k}) - \mu + i\eta} + \frac{n(\mathbf{k})}{\omega - E(\mathbf{k}) - \mu - i\eta}. \tag{9}$$

Here μ is the chemical potential of the dressed Green's function that is determined self-consistently. In Eq. (8) we separate the exchange contribution (including the phase factor with a positive infinitesimal δ) from the contribution comprising only the sum of the RPA bubble polarization diagrams. The screened Coulomb electron–electron interaction (5) comprising the collective plasmon mode, which enters into the G_0W_0 Green's function (8), will affect the noninteracting Green's function $G_0^{-1}(\mathbf{k}, \omega) = \omega - E(\mathbf{k}) - i\eta[1 - n(\mathbf{k})]$. We note that Green's function (8) can be changed by changing the dielectric environment surrounding the Dirac electron system or by changing the Fermi energy.

The integrations in (8) lead to the rather lengthy expressions for Green's function calculated in [39] which we do not reproduce

Fig. 1. The Dyson equation for the RPA screened Coulomb interaction.

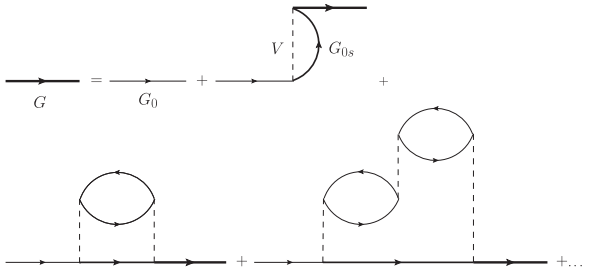

Fig. 2. The Dyson equation for the G_0W_0 Green's function.