Polarization function and plasmons in graphene with a finite gap in the quasiparticle spectrum

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Abstract. The one-loop polarization function of graphene with a finite gap in the spectrum of Dirac quasiparticles has been calculated analytically at arbitrary wave vector, frequency and chemical potential. The result, which is given in terms of elementary functions, has been employed to obtain the plasmon dispersion within the random phase approximation and to explore its behavior at different gap values.

1. Introduction
Charge carriers in graphene at small energies are described by a relativistic (2 + 1)-dimensional Dirac equation, where the Fermi velocity \( v_F \approx 10^6 \text{m/s} \) plays the role of the speed of light (see [1] for a review). The present study deals with the case when Dirac quasiparticles are massive, and their spectrum \( E_{\pm}(k) = \mp (v_F k^2 + \Delta^2)^{1/2} \) is gapped (\( \hbar = 1 \) is used throughout this paper). Physically, this gap can be induced if the sublattice symmetry of graphene is broken due to the interaction with the substrate of the certain type, which has been observed in recent experiments [2, 3]. The objects under consideration are the polarization function of graphene and the collective electron modes which are determined by it. The dynamical polarization function has been calculated previously for the usual gapless spectrum in [4, 5] and the results have been used there to find the dispersion of plasmons. On the other hand, numerical results for the plasmon spectrum in the gapped case have been obtained in [6]. The present work examines the influence of the fermionic gap on the plasmon dispersion at zero temperature in more detail.

2. Polarization function
The polarization function of graphene is proportional to the time component of the vacuum polarization tensor in a three-dimensional quantum electrodynamics (QED$_3$). The one-loop expression reads

\[
\Pi(i\omega_m, k) = \frac{2\pi e^2 T N_f}{\epsilon_0} \sum_{n=-\infty}^{+\infty} \int \frac{d^2 q}{(2\pi)^2} \text{tr} \left[ \gamma_0 S(i\omega_m + i\Omega_n, k + q) \gamma_0 S(i\Omega_n, q) \right],
\]

(1)

where \( \omega_m = 2\pi n T \), \( \Omega_n = (2n + 1)\pi T \) are Matsubara frequencies, \( N_f \) is a number of fermion species (here \( N_f = 2 \) because of two spin projections) and the fermionic propagator has the form

\[
S(i\Omega_n, q) = \frac{i}{(i\Omega_n - \mu) + v_F q + \Delta},
\]

(2)
where $\mu$ is a chemical potential, $\gamma^i$ are $4 \times 4$ gamma matrices and $\Delta$ is a usual Dirac mass. The retarded polarization function is given by the analytic continuation $\Pi^R(\omega, k) = \Pi(i\omega_m \to \omega + i0, k)$. The final result for $T = 0$, $\Delta > \mu$ is a well-known expression [7] from QED$_3$,

$$\Pi^R(\omega, k) = \frac{e^2 N_f k^2}{2\varepsilon_0 (v_F^2 k^2 - \omega^2)} \left( 2\Delta + \frac{v_F^2 k^2 - \omega^2 - 4\Delta^2}{\sqrt{v_F^2 k^2 - \omega^2}} \arcsin \sqrt{\frac{v_F^2 k^2 - (\omega + i0)^2}{v_F^2 k^2 - (\omega + i0)^2 + 4\Delta^2}} \right),$$

(3)

At $T = 0$ and $\Delta < \mu$ the final result can be written in the next form

$$\text{Re} \Pi^R(\omega, k) = -f(\omega, k) \times \begin{cases} 0, & 1A \\ G_<(\frac{(2\mu - \omega)}{v_F k}), & 2A \\ G_<(\frac{(2\mu + \omega)}{v_F k}) + G_<(\frac{(2\mu - \omega)}{v_F k}), & 3A \\ G_<(\frac{(2\mu - \omega)}{v_F k}) - G_<(\frac{(2\mu + \omega)}{v_F k}), & 4A \\ G_>(\frac{(2\mu - \omega)}{v_F k}) - G_>(\frac{(2\mu + \omega)}{v_F k}), & 1B \\ G_>(\frac{(2\mu + \omega)}{v_F k}), & 2B \\ G_>(\frac{(2\mu + \omega)}{v_F k}) - G_>(\frac{(2\mu - \omega)}{v_F k}), & 3B \\ G_>(\frac{(2\mu - \omega)}{v_F k}) + G_>(\frac{(2\mu + \omega)}{v_F k}), & 4B \\ G_0(\frac{(2\mu + \omega)}{v_F k}) - G_0(\frac{(2\mu - \omega)}{v_F k}), & 5B \end{cases}$$

$$\text{Im} \Pi^R(\omega, k) = f(\omega, k) \times \begin{cases} G_>(\frac{(2\mu + \omega)}{v_F k}) - G_>(\frac{(2\mu - \omega)}{v_F k}), & 1A \\ G_>(\frac{(2\mu + \omega)}{v_F k}), & 2A \\ 0, & 3A, 4A, 1B, 5B \\ -G_<(\frac{(2\mu - \omega)}{v_F k}), & 2B \\ \pi(2 - x_0^2), & 3B, 4B \end{cases}$$

(4)

(5)

where the $(k, \omega)$ plane is divided into the 9 regions

1A: $\omega < \mu - \sqrt{v_F^2 (k - k_F)^2 + \Delta^2}$,

2A: $\pm \mu \mp \sqrt{v_F^2 (k - k_F)^2 + \Delta^2} < \omega < -\mu + \sqrt{v_F^2 (k + k_F)^2 + \Delta^2}$,

3A: $\omega < -\mu + \sqrt{v_F^2 (k - k_F)^2 + \Delta^2}$,

4A: $-\mu + \sqrt{v_F^2 (k + k_F)^2 + \Delta^2} < \omega < v_F k$,

1B: $\sqrt{v_F^2 k^2 + 4\Delta^2} < \omega < \mu + \sqrt{v_F^2 (k - k_F)^2 + \Delta^2}$, $k < 2k_F$,

2B: $\mu + \sqrt{v_F^2 (k - k_F)^2 + \Delta^2} < \omega < \mu + \sqrt{v_F^2 (k + k_F)^2 + \Delta^2}$,

3B: $\omega > \mu + \sqrt{v_F^2 (k + k_F)^2 + \Delta^2}$,

4B: $\sqrt{v_F^2 k^2 + 4\Delta^2} < \omega < \mu + \sqrt{v_F^2 (k - k_F)^2 + \Delta^2}$, $k > 2k_F$,

5B: $v_F k < \omega < \sqrt{v_F^2 k^2 + 4\Delta^2}$,

(6)

with $k_F = \sqrt{\mu^2 - \Delta^2}/v_F$, and the following notations were introduced

$$f(\omega, k) = \frac{e^2 N_f k^2}{4\varepsilon_0 \sqrt{v_F^2 k^2 - \omega^2}}$$

$$x_0 = \sqrt{1 + \frac{4\Delta^2}{v_F^2 k^2 - \omega^2}}$$

(7)

$$G_<(x) = x\sqrt{x^2_0 - x^2} - (2 - x_0^2) \arccos(x/x_0)$$

$$G_>(x) = x\sqrt{x^2 - x_0^2} - (2 - x_0^2) \arccosh(x/x_0)$$

$$G_0(x) = x\sqrt{x^2 - x_0^2} - (2 - x_0^2) \arcsinh(x/\sqrt{-x_0^2})$$
Figure 1. Plasmon dispersion: (a) $\Delta/\mu = 0$; (b) $\Delta/\mu = 0.2$; (c) $\Delta/\mu = 0.3$; (d) $\Delta/\mu = 0.9$. Shaded area denotes the regions of single-particle excitations in which plasmons damp (the damped plasmon mode is shown by the dotted line).

3. Plasmon dispersion

The spectrum of plasmons is obtained by finding zeros of the dielectric function $\varepsilon(\omega, k) \equiv 1 + \Pi^R(\omega, k)/k$, i.e. by solving the equation

$$\Pi^R(\omega_p, k) + k = 0.$$  \hfill (8)

It can be easily shown that the equation (8) has no solutions with $\Pi^R(\omega, k)$ defined at (3), thus plasmons are absent at $\Delta > \mu$.

For $\Delta < \mu$ at small wave vectors and frequencies the equation (8) can be solved analytically,

$$\omega_p(k) = \sqrt{\frac{e^2 N_f k \mu}{\varepsilon_0} \left(1 - \frac{\Delta^2}{\mu^2}\right)},$$  \hfill (9)

which differs from the spectrum in the gapless case [4, 5] only by the factor $\sqrt{1 - \Delta^2/\mu^2}$. 


For arbitrary \( k \) and \( \omega \) the dispersion equation (8) with \( \Pi^R(\omega, k) \) defined at (4), (5) is solved numerically, using parameters \( v_F = 10^6 \text{m/s} \), \( \varepsilon_0 = 2.5 \). The shape of plasmon spectrum for different gap values are shown at Fig. 1. The results are in agreement with [6], where a graph, similar to Fig. 1c has been obtained numerically for the case of zero temperature. In the regions of single particle excitations, where \( \Im \Pi^R(\omega, k) \neq 0 \), the equation

\[
\Pi^R(\omega_p - i\gamma, k) + k = 0,
\]

is solved, finding both the dispersion \( \omega_p(k) \) (Fig. 1a-b) and the decay rate \( \gamma(k) \) (Fig. 2) of plasmons.

The effect of the gap value on the plasmon spectrum is illustrated at Fig. 3. At zero gap there exists one plasmon mode (Fig. 1a). When \( \Delta \) becomes different from zero but still small compared to chemical potential, a new undamped mode arises in the gap which opens between two regions of single-particle excitations (Fig. 1b). At \( \Delta/\mu \approx 0.22 \), these two modes merge (Fig. 1c). With the further growth of \( \Delta \) this resulting undamped mode shortens (Fig. 1d) and vanishes at \( \Delta/\mu = 1 \).

4. Conclusions

The analytic expression for the polarization function has been obtained and used to find the spectrum of plasmons in gapped graphene. Plasmons exist only at \( \mu > \Delta \) and their dispersion shows the usual for the 2D electron systems square root behavior at long wavelengths.

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