The effect of sublattice symmetry breaking on the
electronic properties of doped graphene

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Abstract. Motivated by a number of recent experimental studies, we have
carried out the microscopic calculation of the quasi-particle (QP) self-energy and
spectral function in doped graphene when symmetry breaking of the sublattices
occurs. Our systematic study is based on the many-body G$_0$W approach that is
established on the random phase approximation and on graphene’s massive Dirac
equation continuum model. We report extensive calculations of both the real
and imaginary parts of the QP self-energy in the presence of a gap opening. We
also present results for spectral function, renormalized Fermi velocity and band
gap renormalization of massive Dirac fermions over a broad range of electron
densities. We further show that mass generating in graphene washes out the
plasmaron peak in the spectral weight.

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1. Introduction

Graphene is a single atomic layer of crystalline carbon on a honeycomb lattice, consisting of two interpenetrating triangular sublattices A and B, and has opened up a new field for fundamental studies and applications [1]–[4]. The peculiar electronic properties of graphene give rise to the possibility of overcoming silicon-based electronics limitations [5]. The single-particle energy spectrum in graphene contains two zero energies at $K^+$ and $K^-$ points of the Brillouin zone, which are called valleys or Dirac points. Due to the presence of two carbon atoms per unit cell, the quasi-particle (QP) needs to be described by a two-component wavefunction.

The charge carriers in pristine graphene show a linear and isotropic energy dispersion relation and massless chiral behavior for energy scales up to 1 eV. Recently, graphene has revealed a variety of unusual transport phenomena characteristics of two-dimensional (2D) Dirac fermions such as an anomalous integer quantum Hall effect at room temperature, minimum quantum conductivity, the Klein tunneling paradox, weak and anti-localization, the absence of Wigner crystallization phase and Shubnikov–de Haas oscillations that exhibit a phase shift of $\pi$ due to Berry’s phase [6]–[12]. One important difference between a conventional electron gas and a Dirac fermion particle is that the contribution of exchange and correlation to the chemical potential is an increasing rather than a decreasing function of carrier density. This property implies that exchange and correlation increase the effectiveness of screening, in contrast to the usual case in which exchange and correlation weaken screening. This unusual property follows from the difference in sublattice pseudospin chirality between the Dirac model’s negative energy valence band states and its conduction band states.

The massless Dirac-like carriers in graphene have almost semi-ballistic transport behavior with small resistance due to suppression of the back-scattering process, and moreover graphene is a good thermal conductor [13]. The mobility of carriers in graphene is quite high [14]–[17], much higher than the electron mobility revealed on semiconductor heterostructures [18, 19]. On the other hand, by measuring the stiffness of materials it is shown that graphene is the strongest material with a 2D structure [20, 21]. These properties as well as the capability to control the type and density of charge carriers by gate voltage or chemical doping [22]–[25] make graphene an ideal candidate for superior nano-electronic devices operating at high frequencies.

Most electronic applications are based on the presence of a gap between the valence and conduction bands in conventional semiconductors. Band gap is a measure of the threshold voltage and on–off ratio of field effect transistors (FETs) [26, 27]. Therefore, for integrating graphene into semiconductor technology, it is crucial to induce a band gap in Dirac points in order to control the transport of carriers. Consequently, band gap engineering in graphene is a hot topic with fundamental and applied significance [28]. In the literature, several methods have been proposed and applied to induce and control a gap in graphene. One of them is using quantum-confined geometries such as quantum dots and nanoribbons [29]–[33]. It is shown that the gap values increase by decreasing the nanoribbon width. Another method is spin–orbit coupling, whose origin is due to both intrinsic spin–orbit interactions and Rashba interaction [34]–[37]. Another method of generating a gap in graphene sheets is inversion symmetry breaking of sublattices when the number of electrons on A and B atoms is different [38]–[41], or Kekulé [42] distortion, e.g. graphene on proper substrates [24, 25],...
or adsorption of some molecules such as water, ammonia \cite{51, 52} and CrO$_3$ \cite{53} or an alkali-metal sub-monolayer on graphene sheets.

Recently, angle-resolved photoemission spectroscopy (ARPES) experiments on graphene epitaxially grown on SiC and \textit{ab initio} simulations reported a gap opening in the band structure of graphene placed on proper substrates, and suggested that interactions between the graphene sheet and the substrate lead to symmetry breaking of the A and B sublattices with the consequence of inducing a gap in the band structure. Experimenters \cite{24, 25, 43, 44, 54} observed a gap of 260 meV in the band structure of epitaxial graphene on a SiC substrate due to interaction with the substrate. In addition, Zhou \textit{et al} \cite{24} found a reversible metal–insulator transition and a fine tuning of carriers from electrons to holes by molecular doping in gapped graphene. A density functional theory (DFT) calculation confirmed substrate-induced symmetry breaking \cite{55}. Their results showed a gap in the band spectra of graphene of about 200 meV, which is in agreement with recent experimental observations. Their calculation determined that there is a 140 meV on-site energy difference between the two sublattices. In addition, a band gap is observed in the spectra of graphene on a Ni(111) substrate \cite{45, 46} as well as a gap of about 10 meV in suspended graphene above a graphite substrate \cite{47} due to the sublattice symmetry breaking mechanism. Moreover, based on the \textit{ab initio} calculations, it is suggested that a boron nitride substrate induced a gap of 53 meV \cite{48}. Note that the gap value calculated within DFT in general underestimates the true band gap value.

In this paper, we consider the sublattice symmetry breaking mechanism for a gap opening in a pristine doped graphene sheet and study the impact of the gap on some electronic properties of QPs. To investigate the influence of the gap on the many-body properties of QP in graphene, we use the random phase approximation (RPA) and the $G_0W$ approximation. It should be noted that detailed analysis providing a framework for the microscopic evaluation of QP–QP interaction in \textit{gapless graphene} by means of the RPA was carried out by us \cite{49}. To begin, we review briefly the results of the ground state thermodynamic properties that we have already presented elsewhere \cite{50}. Our new results are based on QP self-energy properties in the presence of a gap opening in the electronic spectrum. From the self-energy, we then obtain QP energies, renormalized Fermi velocity, a spectral function that can be compared with ARPES spectra and finally the band gap renormalization (BGR) of massive Dirac fermions in doped graphene. We have shown that mass generating in graphene washes out a satellite band in the spectral function, in agreement with recent experimental observations \cite{43}.

This paper is organized as follows. In section 2, we introduce our model Hamiltonian and then review some ground state properties of gapped graphene. In section 3, we focus on the properties of the imaginary and real parts of the self-energy for gapped graphene and then calculate the QP spectral function, renormalized Fermi velocity and BGR. Finally, we conclude in section 4.

2. Ground state thermodynamic properties

We consider the sublattice symmetry breaking mechanism in which the densities of particles associated with on-site energy $\mu_{a(b)}$, for the A(B) sublattice, are different. The electronic structure of graphene can be reasonably well described using a rather simple tight-binding Hamiltonian, leading to analytical solutions for their energy dispersion and related eigenstates.
The non-interacting tight-binding Hamiltonian for \( \pi \) band electrons is determined by [38]–[41]

\[
\hat{H}_0 = t \sum_i (a_i^\dagger b_i + \text{c.c.}) + \mu_a \sum_i a_i^\dagger a_i + \mu_b \sum_i b_i^\dagger b_i
\]

\[
= t \sum_i (a_i^\dagger b_i + \text{c.c.}) + \frac{\mu_a - \mu_b}{2} \sum_i (a_i^\dagger a_i - b_i^\dagger b_i) + \frac{\mu_a + \mu_b}{2} \sum_i (a_i^\dagger a_i + b_i^\dagger b_i),
\]

(1)

where the sums run over unit cells, \( t \approx 2.7 \text{ eV} \) denotes the nearest-neighbor hopping parameter and \( a_i (b_i) \) is the Fermi annihilation operator acting on the A(B) sublattice. The second term in the non-interacting Hamiltonian breaks the inversion symmetry and causes a band gap with a value of \( 2\Delta = |\mu_a - \mu_b| \) at the Dirac points. The last term is a constant and we leave it out. The effective Hamiltonian at low excited energies leads to a 2D massive Dirac Hamiltonian, \( \hat{H}_0 = \hbar v_F \vec{\sigma} \cdot \vec{k} + \Delta \sigma_3 \), where \( \vec{\sigma} \) are Pauli matrices and \( v_F = 3ta/2h \approx 10^6 \text{ m s}^{-1} \) is the Fermi velocity where \( a \approx 1.42 \text{ Å} \) is the carbon–carbon distance in the honeycomb lattice. The two eigenvalues of the non-interacting Hamiltonian are given by \( E_k = \pm \sqrt{(\hbar v_F k)^2 + \Delta^2} \) for the conduction band (+) and the valence band (−), which is fully occupied. In addition, the model Hamiltonian can be used as an approximate model for describing a graphene antidot lattice in the vicinity of a band gap with a small effective mass value [56], or used as an effective Hamiltonian for intrinsic spin–orbit interaction in graphene, where \( \Delta = \Delta_{SO} \) is the strength of the spin–orbit interaction [34]–[37]. If \( \mu_a = \mu_b \), the Hamiltonian reduces to a massless Dirac Hamiltonian with two chiral eigenstates having conical band structures \( \varepsilon \Delta = \pm \hbar v_F k \).

We consider long-range Coulomb electron–electron interaction. We leave out intervalley scattering and use the two-component Dirac fermion model. Accordingly, the total interacting Hamiltonian in a continuum model at the K \( ^{\prime} \) point is expressed as [57, 58]

\[
\hat{H} = \sum_{k, \sigma} \Psi_{k, \sigma}^\dagger \hat{H}_0 \Psi_{k, \sigma} + \frac{1}{2S} \sum_{q \neq 0} V_q (\hat{n}_q \hat{n}_{-q} - \hat{N}),
\]

(2)

where \( \Psi_{k, \sigma} = (\psi_{+, \sigma}^a (k), \psi_{+, \sigma}^b (k)) \) represents two-component pseudospinors of the non-interacting Hamiltonian, \( S \) is the sample area, \( \hat{N} \) is the total number of operators and \( V_q = 2\pi e^2/\epsilon q \) is the bare Coulomb interaction, where \( \epsilon \) is an average dielectric constant of the surrounding medium. The coupling constant in graphene is \( \alpha_{el} = g_s g_v e^2/\epsilon \hbar v_F \), with \( g_s = g_v = 2 \) being spin and valley degeneracy, respectively. The coupling constant in graphene depends only on the substrate dielectric constant while in the conventional 2D electron systems it is density dependent. The typical value of the dimensionless coupling constant is 1 or 2 for graphene supported on a substrate such as SiC or SiO2.

A central quantity in many-body techniques is the non-interacting dynamical polarizability function \( \chi^{(0)}(q, i\omega, \mu) \), where \( \mu \) is the chemical potential. The problem of linear density response is set up by considering a fluid described by the Hamiltonian, \( \hat{H} \), which is subject to an external potential. The external potential must be sufficiently weak for low-order perturbation theory to suffice. The induced density change has a linear relation to the external potential through the non-interacting dynamical polarizability function. This function has been recently
calculated along the imaginary frequency axis and is given by [50]

\[
\chi^{(0)}(q, \omega, \mu \geq \Delta) = -\frac{g_s g_v}{2\pi \hbar^2 v_F^2} \left\{ \mu - \Delta + \frac{\epsilon_q^2}{2} \left( \frac{\Delta}{\alpha^2} + \frac{x^2}{2y} \tanh \left( \frac{y}{2\Delta} \right) \right) \right.
\]

\[
-\frac{\epsilon_q^2}{4y} \Im \left[ \chi^2 \left( \frac{\sin^{-1} \left( z(\mu) \right)}{x_+} - \sin^{-1} \left( \frac{z(\Delta)}{x_+} \right) \right) \right]
\]

\[
+\frac{\epsilon_q^2}{4y} \Re \left[ \frac{z(\mu)\sqrt{x_+^2 - z^2(\mu)} - z(\Delta)\sqrt{x_+^2 - z^2(\Delta)}}{x_+^2} \right] \}
\]

(3)

where \( x_+ = \sqrt{1 \pm 4\Delta^2/\epsilon_q^2 + \hbar^2 \omega^2}, \; y = \sqrt{\epsilon_q^2 + \hbar^2 \omega^2}\) and \( z(x) = (2x + i\hbar \omega)/\epsilon_q\). The Fermi energy of a 2D massive Dirac fermion system is given by \( E_F = \mu = \sqrt{(\hbar v_F k_F)^2 + \Delta^2}\) and the Fermi wavevector is \( k_F = \sqrt{4\pi n/g_s g_v}\), where \( n\) is the density of carriers. The non-interacting density of states (DOS) is determined by \( D(E) = g_s g_v |E|/2\pi \hbar^2 v_F^2 \Theta(E^2 - \Delta^2)\), which is density dependent at the Fermi surface. It should be noticed that \( D(E_F)\) equals \( m/2\pi \hbar^2\) in the conventional 2D electron gas system. Here, \( \Theta(x)\) is the Heaviside step function.

We now present our first numerical results, which are based on the non-interacting polarization function. The static polarization function as a function of wavevector for various gap values is shown in figure 1(a). The static polarization function in the gapless case is a smooth function whereas a kink at \( q = 2k_F\) occurs for gapped graphene, and thus the derivatives of \( \chi^{(0)}(q, 0, \Delta \neq 0)\) have a singular feature. The singular behavior is the source of several phenomena such as Friedel oscillations and moreover the Ruderman–Kittel–Kasuya–Yoshida (RKKY) interaction, which is absent in gapless graphene. In figures 1(b) and (c), we plotted the dynamic polarization function as a function of frequency for wavevectors smaller and larger than \( q = 2k_F\), respectively. \( \chi^{(0)}(q, i\omega)\) tends to zero like \( \omega^{-1}\) in the large-frequency region.

The polarization function along the real \( \omega\) axis can be obtained by performing analytical continuation of equation (3) [50, 59, 60]. In figure 2, we present the real and imaginary parts of the non-interacting polarization function as a function of frequency. Sharp cutoffs in the imaginary part of \( \chi^{(0)}(q, \omega)\) are related to the rapid swing in the real part of \( \chi^{(0)}(q, \omega)\). These behaviors are a result of the fact that the real and imaginary parts of the polarization function are related through the Kramers–Krönig relations. Importantly, the sign change of the real part from negative to positive shows a sweep across the electron–hole continuum. At very large gap values, the polarization function of massive Dirac fermions can be reduced to the polarization function (Lindhard’s function) of conventional 2D electron gas systems, as determined in figures 1 and 2. Consequently, we can describe a range of band structures from Dirac’s cone (gapless graphene) to parabolic (conventional semiconductors) band structure behavior by tuning the gap values from zero to a large value, respectively. We limited our calculations to the intermediate values of \( \Delta\) and thus expect a wide range of particular properties related to the unique behavior of the polarization function.

We can calculate the total ground state energy of gapped graphene within RPA [50, 58]. The ground state energies can be calculated using the coupling constant integration technique, which has the contributions \( \delta \epsilon_{\text{tot}} = \epsilon_{\text{kin}} + \epsilon_{\text{xc}}\). The kinetic energy per particle is given by \( \epsilon_{\text{kin}} = 2(E_F^3 - \Delta^3)/3E_F^2\).

As discussed previously [50, 58], we might subtract the vacuum energy contribution from the total energy, \( \delta \epsilon_{\text{tot}} = \epsilon_{\text{tot}}(k_F) - \epsilon_{\text{tot}}(k_F = 0)\). Because the number of states in the Brillouin...
Figure 1. (a) Static non-interacting polarization function as a function of $q$ for various $\Delta$. Dimensionless non-interacting dynamic polarization at (b) $q = 0.5k_F$ and (c) $q = 2k_F$ as a function of $\omega$ for various $\Delta$.

Figure 2. Gap dependence of the real and imaginary part of the non-interacting polarization function as a function of $\omega$ for wavevectors (a), (c) $q = 0.5k_F$ and (b), (d) $q = 2.5k_F$.

zone must be conserved, we need an ultraviolet cutoff $k_z$, which is approximated by $\pi k_z^2 \simeq (2\pi)^2/A_0$, where $A_0$ is the area of the unit cell. The dimensionless parameter $\Lambda$ is defined as $k_z/k_F \simeq (g_\alpha^2 n^{-1}\sqrt{3}/9.09)^{1/2} \times 10^3$.

In figure 3, we have shown the exchange–correlation energy in units of $\varepsilon_F = \hbar v_F k_F$ as a function of $n^{-1/2}$ in units of $10^{-6}$ cm for various $\Delta$ values. The exchange energy arising entirely...
from the antisymmetry of the many-body wavefunction on exchange of two electrons is positive while the correlation energy, the difference between the ground state energy and the sum of the kinetic energy and the exchange energy, is negative. This has important implications on the thermodynamic properties and can be calculated from the derivative of the ground state energy with respect to density. The compressibility can be calculated from its definition, \( \kappa^{-1} = n^2 \delta^2 (n \delta \epsilon_{\text{tot}}) / \partial n^2 \). Figure 3(b) shows the ratio between the non-interacting value, \( \kappa_0 = 2 / n \epsilon_F \), and the interaction value of compressibility as a function of \( n^{-1/2} \). The exchange tend to reduce the compressibility while correlations tend to enhance it. At large \( \Delta \), a minimum structure occurs at the inverse of compressibility behavior and we expect that at very large \( \Delta \), it starts at \( \kappa_0 \) and reduces by increasing \( n^{-1/2} \), behaving like the compressibility of the conventional 2D electron gas.

3. The QP self-energy and the spectral function

The generation of QPs in an electron liquid leads to two effects. First, it induces decay of a particle losing momentum via inelastic scattering, which is determined by the imaginary part of the self-energy. Second, renormalization of the dispersion relation of carriers is described by the real part of self-energy. \( \Re e \Sigma^{\text{ret}}(k, \omega) \) is defined as the difference between the measured carrier energy \( \hbar \omega \), and the energy of the free particle, \( \xi_{sk} = s E_k - E_F \). To satisfy causality, the real and imaginary parts of the self-energy are related by a Hilbert transformation. In this section, we first derive the imaginary and the real parts of QP self-energies and then calculate some important quantities such as renormalized Fermi velocity, a spectral function and BGR in the presence of a band gap value. These quantities are related to some important physical properties of both theoretical and practical applications like the band structure of ARPES, the energy dissipation rate of injected carriers and the width of the QP spectral function [61, 62].

In \( G_0 W \) approximation, the self-energy of gapped graphene is given by (\( \beta = 1 / (k_B T) \)) [63]

\[
\Sigma_s(k, i \omega_n) = -\frac{1}{\beta} \sum_{s'} \int \frac{d^2q}{(2\pi)^2} F^{ss'}(k, k + q) \sum_{m=-\infty}^{+\infty} W(q, i \Omega_m) G_s^{(0)}(k + q, i \omega_n + i \Omega_m),
\]

Figure 3. (a) Exchange–correlation energy and (b) compressibility as a function of \( n^{-1/2} \) (in units of \( 10^{-6} \) cm) for various \( \Delta \) values.
where \( W(q, i\Omega_m) = V_q / \epsilon(q, i\Omega_m) \) is the dynamical screened effective interaction and 

\[ \epsilon(q, i\Omega_m) = 1 - V_q \chi^{(0)}(q, i\Omega_m) \]

is the dynamical dielectric function in RPA. The overlap function for gapped graphene \( F^{ss'}(k, k + q) \) arises from the graphene band structure and is given by [50]

\[
F^{ss'}(k, k + q) = \frac{1}{2} \left( 1 + s s' \frac{\hbar^2 k \cdot (k + q) + \Delta^2}{E_k E_{k+q}} \right). \tag{5}
\]

It should be noted that \( F^{s=-s'}(q = 0) = 0 \). However, in gapless graphene, intraband backward scattering should not be allowed, namely \( F^{s=-s'}(q = -2k, \Delta = 0) = 0 \), as well as \( F^{s=-s'}(q = 0, \Delta = 0) = 0 \). In equation (4), \( G^{(0)}_s(k, i\omega) = 1/(i\omega - \xi_{sk}/\hbar) \) is the non-interacting Green’s function. Notice that in the typical density of carriers in graphene, namely \( n > 10^{12} \text{ cm}^{-2} \), the Fermi temperature is about \( T_F = \varepsilon_F / k_B > 10^3 \text{ K} \), and we can therefore eliminate the temperature parameter in our calculations. To evaluate the zero-temperature retarded self-energy, we perform line-residue decompositions, \( \Sigma^{\text{ret}}_s(k, \omega) = \Sigma^{\text{line}}_s(k, \omega) + \Sigma^{\text{res}}_s(k, \omega) \), where \( \Sigma^{\text{line}} \) is obtained by performing analytic continuation before summing over the Matsubara frequencies, and \( \Sigma^{\text{res}} \) is the correction that must be taken into account in the total self-energy [57]. At zero temperature we have

\[
\Sigma^{\text{line}}_s(k, \omega) = -\sum_{s'} \int \frac{d^2 q}{(2\pi)^2} V_q F^{s's'}(k, k + q) \int_{-\infty}^{\infty} \frac{d\Omega}{2\pi} \frac{1}{\epsilon(q, i\Omega)} \frac{1}{\omega + i\Omega - \xi_{s'}(k + q)/\hbar} \tag{6}
\]

and

\[
\Sigma^{\text{res}}_s(k, \omega) = \sum_{s'} \int \frac{d^2 q}{(2\pi)^2} \frac{V_q}{\epsilon(q, \omega - \xi_{s'}(k + q)/\hbar)} F^{s's'}(k, k + q) \times [\Theta(\omega - \xi_{s'}(k + q)/\hbar) - \Theta(-\xi_{s'}(k + q)/\hbar)]. \tag{7}
\]

The line contribution of the self-energy is purely real. The imaginary part of the self-energy has two contributions where \( \Im m \Sigma^{\text{ret}}_s(k, \omega) = \Im m \Sigma^{\text{line}, \text{ intra}}_s(k, \omega) + \Im m \Sigma^{\text{line}, \text{ inter}}_s(k, \omega) \), and the real part of the self-energy can be decomposed as \( \Re e \Sigma^{\text{ret}}_s(k, \omega) = \Sigma^{\text{line}}_s(k, \omega) + \Re e \Sigma^{\text{res}}_s(k, \omega) + \Re e \Sigma^{\text{line}, \text{ intra}}_s(k, \omega) \).

For \( \omega > 0 \) and fixed \( q \), the RPA decay process represents scattering of an electron from momentum \( k \) and energy \( \omega \) to \( k + q \) and \( \xi_{s'}(k + q) \), with all energies in equation (7) measured from the Fermi energy of doped graphene. Since the Pauli exclusion principle requires that the final state is unoccupied, it must lie in the conduction band, i.e. \( s' = +1 \). Furthermore since the Fermi sea is initially in its ground state, the QP must lower its energy, i.e. \( \xi_{s'} < \omega \), and electrons decay by decreasing in energy. For \( \omega < 0 \), the self-energy expresses the decay of holes inside the Fermi sea, which scatter to a final state, by exciting the Fermi sea. In this case the final state must be occupied so both band indices are allowed for \( s' \), and energy conservation requires that holes decay by increasing in energy. Since photoemission measures the properties of holes produced in the Fermi sea by photoejection, only \( \omega < 0 \) is relevant for this experimental probe.

In what follows, we calculate the intraband and interband contributions of the self-energy. We found the intraband term of the residue part of the self-energy as follows for various values

\[8\]

\[\text{http://www.njp.org/}\]
of frequency, 

\[
\Sigma_{\text{res, intra}}^{\text{res}} (k, \omega > 0) = C \int_{\max(0, k - k - \beta)}^{k + \beta} dq \int_{\min(\hbar \omega + E_F, \alpha_+)}^{\max(\hbar \omega + E_F, \alpha_-)} dy f_+ (y, q),
\]

\[
\Sigma_{\text{res, intra}}^{\text{res}} (k, \Delta - E_F < \hbar \omega < 0) = -C \int_{\max(0, k - k, \beta - k)}^{k + k} dq \int_{\max(0, \hbar \omega + E_F, \alpha_-)}^{\min(\hbar \omega + E_F, \alpha_+)} dy f_+ (y, q),
\]

\[
\Sigma_{\text{res, intra}}^{\text{res}} (k, \hbar \omega < -(\Delta + E_F)) = -C \int_{\max(0, k - k)}^{k + k} dq \int_{\max(0, \hbar \omega + E_F, \alpha_-)}^{\min(\hbar \omega + E_F, \alpha_+)} dy f_+ (y, q),
\]

where 

\[
f_+ (y, q) = \frac{\pm (y \pm E_k)^2 + q^2}{\epsilon (q, \omega + E_F \mp y) \sqrt{4k^2q^2 - (y^2 - E_k^2 - q^2)^2}},
\]

\[C = \frac{e^2}{2 \pi \epsilon E_k}, \quad \alpha_\pm = \sqrt{\hbar^2 v_F^2 (k \pm q^2) + \Delta^2} \quad \text{and} \quad \beta = \sqrt{\hbar^2 \omega^2 + \hbar^2 v_F^2 k^2 + 2 \hbar \omega E_F}.
\]

On the other hand, the interband contribution of the residue part of the self-energy is determined by 

\[
\Sigma_{\text{res, inter}}^{\text{res}} (k, \hbar \omega < -(\Delta + E_F)) = -C \int_{\max(0, k - k)}^{k + k} dq \int_{\max(0, \hbar \omega + E_F, \alpha_-)}^{\min(\hbar \omega + E_F, \alpha_+)} dy f_- (y, q),
\]

and eventually for the line contribution of the self-energy we have 

\[
\Sigma_{\text{line, intra}}^{\text{line}} (k, \omega) = -\frac{e^2}{4 \pi^2 \epsilon} \int_0^{k_c} dq \int_0^{2 \pi} d\phi F^{\gamma+} (q, \mathbf{q} + \mathbf{k}, \Delta) \int_{-\infty}^{+\infty} d\Omega \frac{g_+(\phi, \Omega, q)}{\epsilon (q, i\Omega)},
\]

\[
\Sigma_{\text{line, inter}}^{\text{line}} (k, \omega) = -\frac{e^2}{4 \pi^2 \epsilon} \int_0^{k_c} dq \int_0^{2 \pi} d\phi F^{\gamma-} (q, \mathbf{q} + \mathbf{k}, \Delta) \int_{-\infty}^{+\infty} d\Omega \frac{g_- (\phi, \Omega, q)}{\epsilon (q, i\Omega)},
\]

where 

\[
g_\pm (\phi, \Omega, q) = \frac{\hbar \omega + E_F \mp E_{k+q}}{(\hbar \omega + E_F \mp E_{k+q})^2 + \hbar^2 \Omega^2}.
\]

and \(\phi\) denotes an angle between \(k\) and \(q\). Note that the real part of the self-energy is \(k_c\) dependent.

Now we can calculate some important physical quantities. The QP lifetime or the single-particle relaxation time \(\tau\) is obtained by setting the frequency to the on-shell energy in the imaginary part of the self-energy, \(\tau^{-1} = \Gamma_s (k, \xi_{ik}/\hbar) = \frac{2}{\hbar} |\Im m \Sigma^{\text{ret}} (k, \xi_{ik}/\hbar)|\), where \(\Gamma_s (k, \xi_{ik}/\hbar)\) is the quantum level broadening of the momentum eigenstate \(|k\rangle\). This quantity is identical with Fermi’s golden rule expression for the sum of the scattering rate of a QP and quasi-hole at wavevector \(k\) [57]. From equations (8) and (9), one can conclude that the total contribution of the imaginary part of the retarded self-energy on the energy shell comes from the intraband term, \(\Im m \Sigma^{\text{ret}} (k, \xi_{ik}/\hbar) = \Im m \Sigma^{\text{res}} (k, \xi_{ik}/\hbar)\) [63]. In the case of gapless graphene, scattering rate is a smooth function because of the absence of both plasmon emission and interband processes [64, 65]. However, by generating a gap and increasing the amount of it,
plasmon emission causes discontinuities in the scattering time, similar to the conventional 2D electron gas [66, 67]. We thus have two mechanisms for scattering of the QPs: the excitation of electron–hole pairs, which is the dominant process at long-wavelength regions, and the excitation of plasmons in a specific wavevector. As discussed previously [63], in clean graphene sheets the inelastic mean free path reduces by increasing the gap whereas the mean free path is large enough in the range of typical gap values of 10–130 meV, and thus transport remains in the semi-ballistic regime.

The many-body interactions in graphene as a function of doping can be observed by ARPES, which plays a central role in investigating QP properties such as group velocity and lifetime of carriers on the Fermi surface. ARPES is a useful complementary tool, which is capable of measuring constant energy surfaces for all partially occupied states and the fully occupied band structure. Information on band dispersion and the Fermi surface can be elicited from those data measured in ARPES experiments. The relation of Green’s function to the single-particle excitation spectrum in the interacting fluid is expressed by its spectral function. The spectral function is related to the retarded self-energy by the following expression [57]:

\[ A_s(k, \omega) = \frac{\hbar}{\pi} \frac{|\Im m \Sigma^\text{ret}(k, \omega)|}{|\hbar \omega - \xi(k) - \Im \Re \Sigma^\text{ret}(k, \omega)|^2 + |\Im m \Sigma^\text{ret}(k, \omega)|^2}, \]

where \( \Delta \Sigma^\text{ret}(k, \omega) = \Sigma^\text{ret}(k, \omega) - \Sigma_0^\text{ret}(k, 0) \), and then ARPES intensity can be described by \( I(k, \omega) = A(k, \omega) n(\omega) \), where \( n(\omega) \) is the Fermi–Dirac distribution. The spectral function is the Lorentzian function where \( \Im \Re \Sigma \) specifies the location of the peak of the distribution, and \( |\Im m \Sigma| \) is the linewidth. The amplitude of the Lorentzian function is proportional to \( 1/|\Im m \Sigma| \). This quantity is the distribution of energies \( \hbar \omega \) in the system when a QP with momentum \( k \) is added or removed. For the non-interacting system we obtain \( A^{(0)}(k, \omega) = \delta(\omega - \xi(k)/\hbar) \). The Fermi liquid theory applies only when the spectral function at the Fermi momentum \( A^{(0)}(k = k_F, \omega) \) behaves as a delta function and has a broadened peak indicating damped QPs at \( k \neq k_F \).

To progress to the interband single-particle excitation and plasmon effects on \( \Im m \Sigma^\text{ret} \), we must study the retarded self-energy on the off-shell frequency, which is \( \omega \neq \xi(k)/\hbar \) [49, 68]. This quantity gives the scattering rate of a QP with momentum \( k \) and kinetic energy \( \hbar \omega + E_F \). The scattering rate or the linewidth arising from electron–electron interactions is anisotropic and varies significantly via a wavevector at constant energy. The imaginary part of self-energy shows the width of the QP spectral function.

In figure 4, we have shown the absolute value of the imaginary part of the self-energy in units of \( \epsilon_F \) for various gap values. It is noticed that there is an area of frequency associated with the gap value, \( 2\Delta \), in which no QP could enter. In this case, there is a gap in the \( \Im m \Sigma \) between \( \xi_{-k=0} \) and \( \xi_{+k=0} \). We see that \( \Im m \Sigma_{\epsilon} \) vanishes as \( \omega^2 \) because \( \omega \) tends to zero, universal properties of a normal Fermi liquid. Moreover, at large frequency, \( \Im m \Sigma_{\epsilon} \) tends towards \( \omega \) linearly. Except from the Dirac point, the conduction band \( \Im m \Sigma_{\epsilon} \) peaks broaden because of the dependence on the scattering angle of \( \xi(k+q) \). For low energy, only intraband single-particle excitation contributes to \( \Im m \Sigma \) up to \( E_F \) and then the interband single-particle excitation contribution increases sharply about \( E_F \). The interband contribution increases with increasing gap values.

To evaluate the scattering rate in the interband channel, we have shown \( \Im m \Sigma_{\text{inter(intra)}} \) as a function of frequency in figure 5. The intraband contribution of the imaginary part of self-energy associated with the scattering rate of QP in the intraband contribution increases with increasing
Figure 4. Absolute value of the imaginary part of retarded self-energy (+ channel) as a function of (a) $\omega$ and (b) $k$ for the various energy gaps.

Figure 5. (a) Intraband and (b) interband contributions of the imaginary part of self-energy (+ channel) as a function of $\omega$ for the various energy gaps at $k = 0.25k_F$.

gap values while the interband contribution reduces, as physically expected. Moreover, by increasing the electrons in the conduction band the interband scattering rate reduces whereas the intraband scattering contribution increases. The gap value suppresses the scattering rate at $\omega = -\varepsilon_F$.

In figure 6, we plotted the real part of self-energy in units of $\varepsilon_F$ as a function of energy for various gap values. Note again that the real part of residue self-energy has a gap, which is associated with the feature calculated in the imaginary part of the self-energy. The line part of the self-energy is a continuous curve and then we have a jump near the boundary of the gap values in the $\Re \Sigma$ for gapped graphene. A kink around $E_F$ is associated with the interband plasmon contribution and it is broadened due to the gap value. This feature affects noticeably the interacting electron DOS.

As discussed before [49, 68] in zero-temperature and disorder-free gapless graphene, the peaks of the spectral function correspond to the neighbour solutions of Dyson’s equation in which the QP excitation energies are obtained by $E = \xi_+ + \Re \delta \Sigma^\text{ret}_+$. The intersection of
Figure 6. Real part of retarded self-energy (+ channel) as a function of (a) $\omega$ and (b) $k$ for the various energy gaps at $\Lambda = 100$. The $\Re \Sigma_+$ are measured from the interaction contribution of the chemical potential $\Re \Sigma_+(k_F, \omega = 0)$.

Figure 7. QP spectral function for the + channel as a function of (a) $\omega$ and (b) $k$ for the various energy gaps at $\Lambda = 100$.

$\Re \Sigma$ and the lines $E - \xi_r$ indicates a satellite long-wavelength plasmaron peak related to electron–plasmon excitation due to the long-range electron–electron Coulomb interaction and the Dyson equation with $\Im m \Sigma = 0$ corresponds to a QP peak related to single-particle excitation. Importantly, in the presence of gap values, the plasmaron peak is suppressed. Figures 7(a) and (b) show the energy distribution curves (EDC) and momentum distribution curves (MDC), respectively. In the presence of gap values, as shown in figure 7(a), there is only a single QP peak.

The valence band self-energy contributions are shown in figure 8. There is an area of frequencies associated with the gap value in which no QP could exist in $\Im m \Sigma_-$ exactly the same as the conduction band. The $s = +1$ and $-1$ peaks in $\Im m \Sigma_-$ in figures 4 and 8 separate at finite $k$ because of chirality factors that emphasize $k$ and $q$ in nearly parallel directions for the conduction band and $k$ and $q$ in nearly opposite directions for the valence band states. Consequently, at finite $\Delta$, the QP peak of $A_-(k, \omega)$, which is broadened, shifts toward the left in the opposite behavior of $A_+(k, \omega)$. These features have significant effects in the interacting electron DOS.

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shows renormalized Fermi velocity in units of bare Fermi velocity as a function of 

eigenvalues. In the gapless case, we have obtained an induced band gap or kink 

the electron density, and in the small energy gap values it is less density dependent with respect 

the BGR for various gap values as a function of electron density. BGR decreases by increasing 

energy is also changed. The QP energy measured from the chemical potential of the interacting 

renormalization from the backflow of fluid around a moving particle. The DOS at the Fermi 

feature: for example, plasmon damping, disorder effects, electron interactions with the buffer 

graphene has not been seen in experiments. There are several effects that could wash out this 

one bit of important information that can be extracted from ARPES spectra is 

the renormalized Fermi velocity \( v^* \). A consequence of the interaction is Fermi velocity 

renormalization from the backflow of fluid around a moving particle. The DOS at the Fermi 

energy is also changed. The QP energy measured from the chemical potential of the interacting 

system, \( \delta E_{QK} \), can be calculated by solving self-consistently the Dyson equation 

\( \delta \Sigma^e_{\text{ret}}(k, \omega) = \frac{\Im \Sigma^e_{\text{ret}}(k, \omega)}{\epsilon_k(k_F)} \). In isotropic systems, the QP energy depends on the magnitude of 

k. Expanding \( \delta E_{QK} \) to first order in \( k - k_F \), we can write 

\( \delta E_{QK} \approx \hbar v^*_s(k - k_F) \), which effectively defines the renormalized velocity as 

\( \hbar v^*_s = d\delta E_{QK} / d(k|k_F) \). From the Dyson equation, we can calculate the renormalized Fermi velocity as [63, 69, 70] 

\[
\frac{v_s^*}{v_s} = \frac{\epsilon_F E_F^{-1} + (\hbar v_s)^{-1} \partial_k \Re[\delta \Sigma^e_{\text{ret}}(k, \omega)]|_{\omega=0,k=k_F}}{1 - \hbar^{-1} \partial_k \Re[\delta \Sigma^e_{\text{ret}}(k, \omega)]|_{\omega=0,k=k_F}},
\]

where \( v_s = s v_F \). It has been found previously [63], [69]–[72] that electron–electron interaction 

increases the renormalized Fermi velocity in gapless graphene sheets. This behavior is in contrast to the conventional 2D electron gas [66, 73].

Figure 9 shows renormalized Fermi velocity in units of bare Fermi velocity as a function of 

band gap for various carrier densities. The renormalized Fermi velocity decreases on increasing 

the gap value. \( v^* \) is density independent after \( \Delta = 0.8\epsilon_F \), which is in good agreement with recent experimental observations [24, 25].

Finally, we calculated BGR [74]–[77]. BGR for the conductance band is given by the QP 

self-energy at the band edge, namely 

\( \text{BGR} = \Re \Sigma^e_{\text{ret}}(k = 0, \omega = (\Delta - E_F)/\hbar) \). Figure 10 shows the 

BGR for various gap values as a function of electron density. BGR decreases by increasing 

the electron density, and in the small energy gap values it is less density dependent with respect 

to large energy gap values. In the gapless case, we have obtained an induced band gap or kink

\[ \lambda = \Re \Sigma_{-}(k_F, \omega = 0) \]. QP spectral function as a function of \( \omega \) (c) for the various 

energy gaps at \( \Lambda = 100 \).
due to many-body electron–electron interactions and it tends to a constant on increasing the electron density [49, 68, 71, 72]. This feature is in agreement with the results obtained within ab initio DFT calculation [71].

**Figure 9.** Renormalized velocity (+ channel) as a function of energy gap for various densities at $\alpha_{gr} = 1$.

**Figure 10.** BGR as a function of electron density for various energy gaps at $\alpha_{gr} = 1$. 

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4. Summary and conclusion

We have revisited the problem of the microscopic calculation of QP self-energy and many-body effective velocity suppression in gapped graphene when the conduction band is partially occupied. We have performed a systematic study based on the many-body $G_0W$ approach that is established upon the RPA and on graphene’s massive Dirac equation continuum model. We have carried out extensive calculations of both the real and the imaginary parts of the QP self-energy and discussed the interband and intraband contributions in the scattering process in the presence of gap values. We have also presented results for the effective velocity and for the BGR over a wide range of coupling strengths. Accordingly, we have critically examined the merits of gap values in dynamical QP properties.

Most features of mass generating in graphene represent the washing out of the plasmaron peak in the spectral weight. Increasing the gap value makes the renormalized Fermi velocity behave independently of density. We have shown that BGR in gapped graphene decreases by increasing the carrier density at large $\Delta$. This is in contrast to the gapless case in which many-body electron–plasmon interactions induce a very small gap in band structure. These distinct features of massive Dirac fermions are related to mixing the chiralities and reduce the interband transitions in graphene sheets.

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