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Many-body exchange-correlation effects in graphene

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Abstract

We calculate, within the leading-order dynamical-screening approximation, the electron self-energy and spectral function at zero temperature for extrinsic (or gated/doped) graphene. We also calculate hot carrier inelastic scattering due to electron–electron interactions in graphene. We obtain the inelastic quasiparticle lifetimes and associated mean free paths from the calculated self-energy. The linear dispersion and chiral property of graphene give energy dependent lifetimes that are qualitatively different from those of parabolic-band semiconductors.
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1. Introduction

Recent developments in techniques for fabricating conducting graphene layers [1] have provided the physics community with a unique opportunity to study an interacting two-dimensional (2D) massless Dirac fermion system. This has led to considerable experimental and theoretical activity in this field [2,3]. The band structure of graphene, by dint of its honeycomb lattice, has linear dispersions near the K and K′ points of the Brillouin zone [4]. The corresponding kinetic energy of graphene for 2D wave vector $\mathbf{k}$ is given by $\varepsilon_{\mathbf{k}s} = s\gamma|\mathbf{k}|$, where $s = \pm 1$ indicate the conduction (+1) and valence (−1) bands, respectively, and γ is a band parameter (and Fermi velocity of graphene is given by $v_F = \gamma/\hbar$). The corresponding density of states (DOS) is given by $D(\varepsilon) = g_s g_v |\varepsilon|/(2\pi\gamma^2)$, where $g_s = 2$, $g_v = 2$ are the spin and valley degeneracies, respectively. The Fermi momentum (k_F) and the Fermi energy (E_F) of 2D graphene are given by $k_F = (4\pi n/g_s g_v)^{1/2}$ and $E_F = \gamma k_F$ where n is the 2D carrier (electron or hole) density.

Many electronic properties of a system are strongly influenced by the presence of electron–electron interaction.

In this paper, we investigate theoretically the electron–electron interaction induced exchange-correlation effects in 2D graphene layer. We calculate, within the leading-order dynamical-screening approximation, the electron self-energy for extrinsic graphene at zero temperature. The self-energy is the central quantity that determines the other Fermi liquid parameters. We obtain the single-particle spectral function and the inelastic quasiparticle lifetimes and associated mean free paths from the calculated electron self-energy.

In the G_0W approximation [5], the self-energy is given by

$$\Sigma_s(\mathbf{k}, i\omega_n) = -\frac{1}{\beta} \sum_{s'} \sum_{\mathbf{q}, iv_n} G_{0,s'}(\mathbf{k} + \mathbf{q}, i\omega_n + iv_n)$$
$$\times \frac{V_c(q)}{\varepsilon(\mathbf{q}, iv_n)} F_{ss'}(\mathbf{k}, \mathbf{k} + \mathbf{q}), \qquad (1)$$

where $\beta = 1/k_B T$, $s, s' = \pm 1$ denote the band indices, $G_{0,s}(\mathbf{k}, i\omega_n) = 1/(i\omega_n - \xi_{\mathbf{k}s})$ is the unperturbed Green's function ($\xi_{\mathbf{k}s} = \varepsilon_{\mathbf{k}s} - \mu$ where μ is the chemical potential), $V_c(q) = 2\pi e^2/\kappa q$ is the bare Coulomb potential (with background dielectric constant κ), $\varepsilon(q, \omega)$ is the dynamical-screening function (dielectric function) given by $\varepsilon(q, \omega) = 1 - v_c(q)\Pi(q, \omega)$, where $\Pi(q, \omega)$, the 2D polarizability, is given by the bare bubble diagram [6]. In Eq. (1) $F_{ss'}(\mathbf{k}, \mathbf{k} + \mathbf{q})$ is the overlap of states, given by

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$F_{ss'}(\mathbf{k}, \mathbf{k}') = (1 + ss' \cos\theta_{\mathbf{k}\mathbf{k}'})/2$, where θ is the angle between $\mathbf{k}$ and $\mathbf{k}'$.

After the standard procedure of analytical continuation, the self-energy can be separated into the exchange and correlation parts $\Sigma_s(\mathbf{k}, \omega) = \Sigma_s^{\text{ex}}(\mathbf{k}) + \Sigma_s^{\text{cor}}(\mathbf{k}, \omega)$. The exchange part is given by

$$\Sigma_s^{\text{ex}}(\mathbf{k}) = -\sum_{s'\mathbf{q}} n_F(\xi_{\mathbf{k}+\mathbf{q},s'}) V_c(\mathbf{q}) F_{ss'}(\mathbf{k}, \mathbf{k}+\mathbf{q}), \tag{2}$$

where $n_F(\xi_{\mathbf{k}s}) = \theta(\xi_{\mathbf{k}s})$ is the Fermi function at $T = 0$. The correlation part, $\Sigma_s^{\text{cor}}(\mathbf{k}, \omega)$, is defined to be the part of $\Sigma_s(\mathbf{k}, \omega)$ not included in Σ_s^{ex}. Since the exchange part of self-energy $\Sigma_s^{\text{ex}}(\mathbf{k}, \omega)$ is studied in Ref. [7] we provide in this paper the results of correlation part. In the GW approximation, the $\Sigma_s^{\text{cor}}(\mathbf{k}, \omega)$ can be written in the line and pole decomposition $\Sigma_s^{\text{cor}} = \Sigma_s^{\text{line}} + \Sigma_s^{\text{pole}}$, where

$$\Sigma_s^{\text{line}}(\mathbf{k}, \omega) = -\sum_{s'\mathbf{q}} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{V_c(\mathbf{q}) F_{ss'}(\mathbf{k}, \mathbf{k}+\mathbf{q})}{\xi_{\mathbf{k}+\mathbf{q},s'} - \omega - i\omega'}$$
$$\times \left[\frac{1}{\varepsilon(q, i\omega')} - 1 \right], \tag{3}$$

$$\Sigma_s^{\text{pole}}(\mathbf{k}, \omega) = \sum_{s'\mathbf{q}} [\theta(\omega - \xi_{\mathbf{k}+\mathbf{q},s'}) - \theta(-\xi_{\mathbf{k}+\mathbf{q},s'})]$$
$$\times V_c(\mathbf{q}) F_{ss'}(\mathbf{k}, \mathbf{k}+\mathbf{q}) \left[\frac{1}{\varepsilon(q, \xi_{\mathbf{k}+\mathbf{q},s'})} - 1 \right]. \tag{4}$$

The Σ_{line} is completely real because $\varepsilon(q, i\omega)$ is real. Thus, $\text{Im}[\Sigma_{\text{pole}}]$ gives the total contribution to the imaginary part of the self-energy. In this calculation we use the cut-off at the wave vector k_c with respect to the Dirac point; i.e., the integral is cut off at $k = k_c$. From the calculated self-energy $\Sigma(k, \omega)$, we can obtain the single-particle spectral function given by

$$A(k, \omega) = \frac{2\,\text{Im}[\Sigma(k, \omega)]}{\{\omega - \xi_k - \text{Re}[\Sigma(k, \omega)]\}^2 + \{\text{Im}[\Sigma(k, \omega)]\}^2}. \tag{5}$$

The spectral function $A(k, \omega)$ satisfies the sum rule

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A(k, \omega) = 1, \tag{6}$$

which is generally satisfied to within less than a percent in our numerical calculations.

2. Results

In this section we show the real and the imaginary parts of the self-energy and spectral function for $k = 0$ (the Dirac point) and $k = k_F$ (Fermi surface). Throughout this paper we use the following parameters: dielectric constant $\kappa = 2.5$ which corresponds to graphene on SiO$_2$ substrate, Fermi velocity $v_F = \gamma/\hbar = 10^8$ cm/s, and cut-off momentum $k_c = 1/a$, where $a = 2.46$ Å is the lattice constant of graphene.

For $k = 0$ (Fig. 1) we find a strong peak in $\text{Im}[\Sigma(k, \omega)]$ (associated with a finite step in $\text{Re}[\Sigma(k, \omega)]$) due to plasmon emission. Since $\text{Im}[\Sigma]$ is non-zero for all energies except
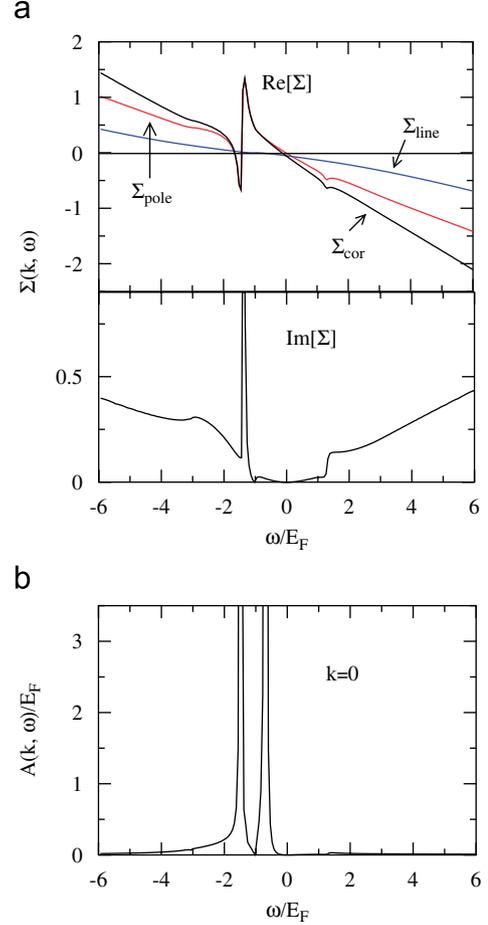

Fig. 1. (a) Real (top panel) and imaginary (bottom panel) parts of the self-energy $\Sigma(k, \omega)$ and (b) spectral function $A(k, \omega)$ as a function of the energy ω for $k = 0$ (the Dirac point).

$\omega = 0$ we expect a finite damping in the spectral function. In spectral function we find two peaks. The first peak (from $\omega = 0$) in $A(k, \omega)$ corresponds to the usual quasiparticle (i.e. a bare particle surrounded by a cloud of virtual plasmons and particle–hole excitations), and the second peak corresponds to a plasmaron, which is interpreted as a hole coupled to a cloud of real plasmons [8].

In Fig. 2 we show the self-energy and spectral function for the Fermi wave vector ($k = k_F$). In particular, the behavior of the self-energy and spectral function at $k = k_F$ determines the low-energy properties of the system. For $k = k_F$ there is only one peak in $A(k, \omega)$ at $\omega = 0$, which is a δ-function peak because $\text{Im}\,\Sigma(k_F, \omega) \propto \omega^2 \ln|\omega|$ as $\omega \to 0$ [9]. Thus, the doped (or gated) graphene is a Fermi liquid because it possesses a Fermi surface (or a discontinuity in momentum distribution function) whose presence is indicated by a δ-function in $A(k_F, \omega)$ at $\omega = 0$ (or, equivalently, non-zero many-body renormalization factor).

In Fig. 3 we show a quasiparticle lifetime due to electron–electron interactions, which is given by $1/\tau(k) = 2\,\text{Im}[\Sigma(k, \xi_k)]$. Since the velocity of the quasiparticles close the Dirac points is approximately a constant, the inelastic mean free path ℓ is obtained by $\ell(\xi) = v_F \tau(\xi)$. In inset of
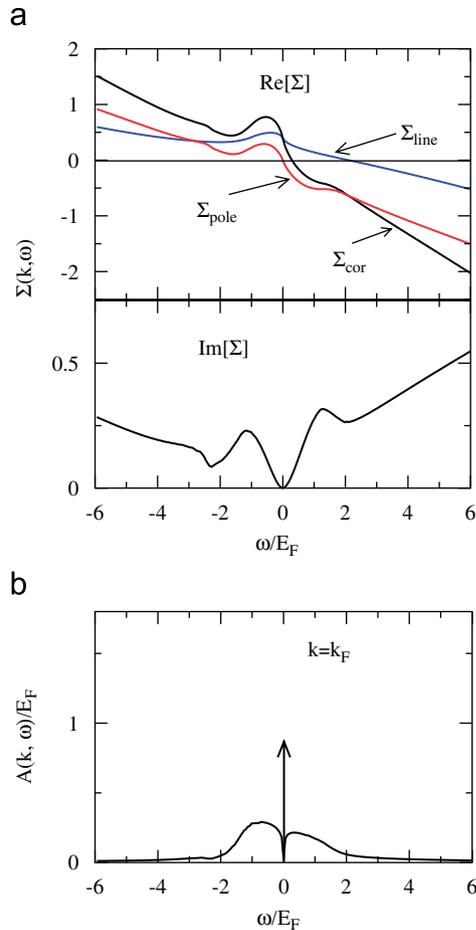
a

b

Fig. 2. (a) Real (top panel) and imaginary (bottom panel) parts of the self-energy $\Sigma(k, \omega)$ and (b) spectral function $A(k, \omega)$ as a function of the energy ω for $k = k_F$ (at the Fermi surface). The vertical arrow in (b) denotes δ-function in the spectral function of weight $(2\pi \times 0.9)$ at $\omega = 0$.

Fig. 3. Inelastic quasiparticle lifetime, $1/\tau = 2 \operatorname{Im}\Sigma(k, \xi_k)$, in graphene due to dynamically screened electron–electron interactions, as a function of energy at $T = 0$ for different densities. Inset shows the corresponding quasiparticle mean free path for $n = 10^{13}\,\mathrm{cm}^{-2}$.

within the leading-order dynamical-screening approximation. Our calculated spectral function indicates that the extrinsic graphene (i.e. $E_F \neq 0$) is a Fermi liquid. We also calculate hot carrier inelastic scattering due to electron–electron interactions. The linear dispersion and chiral property of graphene give lifetime energy dependences that are qualitatively different from those of parabolic-band semiconductors. We can apply our calculated self-energy to obtain other quasiparticle properties of graphene.

Fig. 3, we provide the corresponding ℓ, which shows that at $n = 10^{13}\,\mathrm{cm}^{-2}$ a hot electron injected with an energy of 1 eV above E_F has an ℓ due to electron–electron interactions that is on the order of 20 nm. This will have implications for designing any hot electron transistor type graphene devices [10]. Note that in the calculated scattering time both plasmon emission and interband processes are absent because conservation of energy and momentum restricts electron–electron scattering [11]. In parabolic-band semiconductors [8] plasmon emission and interband collision thresholds cause discontinuities in the scattering time.

3. Summary

In summary, we calculate the electron–electron interaction induced quasiparticle self-energy in graphene layer
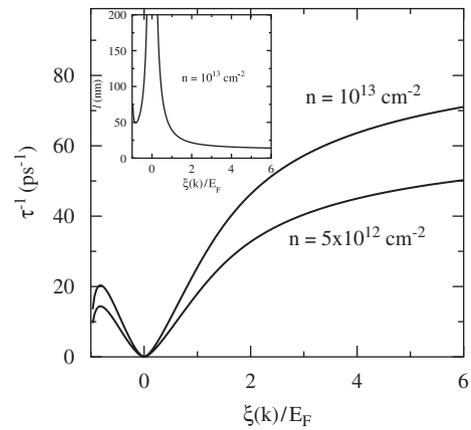
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