Coulomb screening of 2D massive Dirac fermions

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Abstract
A model of 2D massive Dirac fermions, interacting with instantaneous $1/r$ Coulomb interaction, is presented in order to mimic the physics of gapped graphene. The static polarization function is calculated explicitly to analyze the screening effect at finite temperature and density. The results are compared with the massless case. We also show that various results in other works can be reproduced with our model in a straightforward and unified manner.

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1. Introduction
Over the past several years, the physics of graphene has attracted considerable interest, both theoretically and experimentally [1]. Graphene, because of its two-dimensional (2D) hexagonal lattice structure, has a unique linear energy spectrum near the Dirac points of the Brillouin zone. Because of the unusual energy band dispersion, many electronic properties of graphene exhibit significantly different behavior from conventional 2D systems, for example the half-integer quantum Hall effect [2]. In graphene, although the motion of electrons is fixed in the 2D plane, their interactions still obey the 3D Coulomb’s law, for the electric field lines cannot be confined in 2D. While most of the early works were based on the massless Dirac fermion model, a recent work has shown that the massive case can also be created [2].

For massive fermions, this discovery is equivalent to the opening of a gap in the electronic spectrum in condensed matter physics. So the similarity between graphene and (2 + 1)-dimensional quantum electrodynamics (QED$_{2+1}$) is obvious, and a lot of results were obtained by exploring this correspondence [3]. The main difference is that graphene lacks Lorenz invariance because of its nearly instantaneous Coulomb interaction.

In addition, it should be noted that there have been many papers [4–7] on the Coulomb interaction in gapless graphene: the papers [4, 5] gave the polarization function for zero-temperature gapless graphene at finite density; [6] dealt with 2D Coulomb-interacting massless Dirac fermions and calculated the specific heat at finite temperature; whereas [7] generalized it to the finite density case. Regarding the massive Dirac fermions, there are also many works on it. However, most of them (gapless or gapped graphene) were highly succinct, used different models and did not give the calculations of the polarization function in detail.

In this paper, we consider a model of two-component Dirac fermions interacting through a 3D instantaneous Coulomb interaction and calculate the polarization functions at finite temperature and finite density using finite temperature field techniques [8]. In fact, quantum field theory at finite temperature or density is usually applied in cosmology and astrophysics. But its 2D spatial case has not been observed in nature. So graphene provides a wonderful platform for establishing QED$_{2+1}$.

2. Model
Our starting point is a model of (2 + 1)-dimensional two-component Dirac fermions mediated by 3D Coulomb interaction at temperature $T$. The action of the system $S$ is given by ($\hbar = 1$)

$$S(\bar{\psi}, \psi, \phi) = \int_0^\beta dt \left\{ \int d^3 x \frac{1}{8\pi} |\partial_\tau \phi(x, \tau)|^2 + \int d^2 x \sum_{s=1}^N (\bar{\psi}_s(x, \tau) \{ \partial_\tau + v \mathbf{\sigma} \cdot \mathbf{p} + m \sigma_3 \\
- \mu + i e \phi(x, \tau) \} \psi_s(x, \tau)) \right\}. \quad (1)$$
Here, $\beta = 1/T$ and $\mu$ is the chemical potential. The fields $\psi_s$ are two-component fermion fields, and the subscript $s$ stands for different species of fermions with $N = 4$ due to spin, valley degeneracies in graphene. The vector $\sigma = (\sigma_1, \sigma_2)$ and $\sigma_i$, $i = 1, 2, 3$, are Pauli matrices; $\sigma_0 = I$ is the $2 \times 2$ identity matrix (omitted for simplicity). $\varphi$ is the field that mediates the Coulomb interaction: the time component of the electromagnetic field. The 3D space integral of the action describes the kinetic term of the scalar field, while the remaining terms describe the kinetic term for the fermion fields and their interaction with the scalar field. In addition, we put $v = 1$ below and only restore it when necessary.

Correspondingly, the Green’s function for the free Dirac fermions is

$$G_0(k) = \frac{k_0 + \mathbf{k} \cdot \mathbf{\sigma} + m\mathbf{\sigma}_3}{k_0^2 - \mathbf{k}^2 - m^2}. \quad (2)$$

Using more symmetric three-momentum notation, $(q_0, \mathbf{q}) = (i\omega_n, \mathbf{q})$, $\mathbf{k} = (\omega_n + \mu, \mathbf{k})$, $k^2 = \omega_n^2 - k^2$, $\omega_n = (2n + 1)\pi/\beta$, $\omega_0 = 2\pi/\beta$, etc., then the polarization function in the random-phase approximation (RPA) [9] is

$$\Pi(q) = \frac{4}{\beta} \sum_n \int \frac{d^2k}{(2\pi)^2} \text{Tr}(G(k)G(\tilde{k} + \tilde{q})) = \frac{8}{\beta} \sum_n \int \frac{d^2k}{(2\pi)^2} \frac{k_0(q_0 + q_0) + \mathbf{k}(\mathbf{k} + \mathbf{q}) + m^2}{(k_0^2 - \mathbf{k}^2 - m^2)[(k + \tilde{q})^2 - m^2]} \quad (3)$$

where $v(q) = 2\pi e^2/|q|$ is the 2D Fourier transform of the 3D Coulomb interaction. Following a similar consideration given in [10], we can divide $\Pi$ into two contributions, the vacuum part and the matter part, such that

$$\Pi = \Pi_{\text{vac}} + \Pi_{\text{matter}}, \quad \lim_{T \to 0, \mu \to 0} \Pi = \Pi_{\text{vac}}. \quad (4)$$

The vacuum polarization function, both for massless and massive cases, can be calculated by the dimensional regularization approach as in [3, 12]. Here, we can reproduce their results within our model:

$$\Pi_{\text{vac}}(q) = -\frac{|q|^2}{\pi} \left\{ \frac{m}{q^2} + \frac{1}{2q} \left( 1 - \frac{4m^2}{q^2} \right) \arctan \left( \frac{q}{2m} \right) \right\}. \quad (6)$$

### 3. The polarization function for massive Dirac fermions

The sum of fermion Matsubara frequencies can be given in a standard manner [11]:

$$\frac{1}{\beta} \sum_n \frac{k_0(q_0 + q_0) + \mathbf{k} \cdot \mathbf{q} + m^2}{(q_0 - \mathbf{k}^2 + E_{k+q})} = \frac{1}{2\pi i} \int dz h(z) \frac{1}{2} \tanh(\beta z/2) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} dz h(z) \frac{1}{2} \tanh(\beta z/2)$$

with

$$h(z) = \frac{(z + \mu)(z + \mu + q_0) + \mathbf{k} \cdot (\mathbf{k} + \mathbf{q}) + m^2}{\left( (z + \mu)^2 - E_k^2 \right) \left( (z + \mu + q_0) - E_{k+q} \right)}, \quad g(z) = \frac{\beta}{2} \tanh(\beta z/2), \quad E_k = \sqrt{k^2 + m^2}.$$  

For the function $g(z)$, which has simple poles at $z = i\omega_n$, the sum emerges as the integration of the product $hg$ along a suitable path in the complex plane of $z$. We can divide the above expressions into two parts, $\pi_{\text{vac}}$ and $\pi_{\text{matter}}$, which describe the contribution of the vacuum and matter, respectively, such that

$$\pi_{\text{vac}} = \frac{1}{2\pi i} \int_{-\infty}^{\infty} dz [h(z) + h(-z)]/2, \quad (8)$$

$$\pi_{\text{matter}} = -\frac{1}{2\pi i} \int_{-\infty}^{\infty} dz h(z) \frac{1}{\epsilon^{\beta z} + 1} + \frac{1}{2\pi i} \int_{-\infty}^{\infty} dz h(z) \frac{1}{\epsilon^{-\beta z} + 1}$$

where

$$\frac{1}{2\pi i} \int_{-\infty}^{\infty} dz \frac{h(z)}{\epsilon^{\beta z} + 1} = \frac{1}{2E_k} \frac{E_k(E_k - q_0) + \mathbf{k}(\mathbf{k} + \mathbf{q}) + m^2}{(E_k - q_0)^2 - E_{k+q}^2} \frac{1}{\epsilon^{\beta(E_k - q_0)} + 1}$$

$$+ \frac{1}{2E_k} \frac{E_k(E_k - q_0) + \mathbf{k}(\mathbf{k} + \mathbf{q}) + m^2}{(E_k - q_0)^2 - E_{k+q}^2} \frac{1}{\epsilon^{\beta(E_k - q_0)} + 1}$$

$$+ \frac{1}{2E_{k+q}} \frac{E_{k+q}(E_{k+q} - q_0) + \mathbf{k}(\mathbf{k} + \mathbf{q}) + m^2}{(E_{k+q} - q_0)^2 - E_k^2} \frac{1}{\epsilon^{\beta(E_k - q_0)} + 1}$$

$$+ \frac{1}{2E_{k+q}} \frac{E_{k+q}(E_{k+q} - q_0) + \mathbf{k}(\mathbf{k} + \mathbf{q}) + m^2}{(E_{k+q} - q_0)^2 - E_k^2} \frac{1}{\epsilon^{\beta(E_k - q_0)} + 1}$$

$$\frac{1}{2E_k} \left[ f(q_0) + f(-q_0) \right] N_F(E_k), \quad (9)$$

where we have defined

$$f(q_0) = \frac{E_k(E_k - q_0) + \mathbf{k}(\mathbf{k} + \mathbf{q}) + m^2}{(E_k - q_0)^2 - E_{k+q}^2}, \quad N_F(E_k) = \frac{1}{\epsilon^{\beta(E_k - q_0)} + 1} + \frac{1}{\epsilon^{\beta(E_k + q_0)} + 1}. $$

For the vacuum part we obtained in the last section, this describes the intrinsic graphene, in which the conduction band is empty while the valence band is fully occupied at zero temperature. As $m \to 0$, graphene varies from an insulator to the zero-gap semiconductor system. If we take into account the finite density effect, the Fermi energy could lie either in
the valence band ($\mu < 0$) or in the conduction band ($\mu > 0$):

$$\Pi_{\text{matter}} = 8 \int \frac{d^2 k}{(2\pi)^2} \frac{1}{2E_k} \left[ f(q_0) + f(-q_0) \right] \Theta(E_k - \mu)$$

$$= \frac{1}{\pi^2} \text{Re} \int_0^{k_F} \frac{d k k}{E_k} \int_{-1}^1 d x \frac{1}{\sqrt{1-x^2}}$$

$$\times \left( \frac{4E_k^2 - 4q_0E_k + q_0^2 - q^2}{q_0^2 - 2q_0E_k - q^2 - 2kqx} - 1 \right). \quad (10)$$

The retarded polarization function of the free fermions is

$$\text{Im} \Pi_{\text{matter}}^\text{ret} = \frac{1}{\pi} \int_0^{k_F} \frac{d k k}{E_k} \int_{-1}^1 d x \frac{4E_k^2 - 4q_0E_k + q_0^2 - q^2}{\sqrt{1-x^2}}$$

$$\times \delta(q_0^2 - 2q_0E_k - q^2 - 2kqx) \quad (11)$$

and in the above equations, we have defined

$$\text{Re} f(q_0) = [f(q_0) + f(-q_0)]/2,$$

$$\text{Re} \delta(f(q_0)) = [\delta(f(q_0)) - \delta(f(-q_0))] / 2.$$ If we set $m = 0$, calculating explicitly we find that they just coincide with [4, 5], and their finite-temperature counterparts were discussed in [6, 7]; we emphasize that within our model we do not need the overlapping factor used in their work and the results come out more naturally:

$$\text{Im} \Pi_{\text{matter}}^\text{ret} = \frac{1}{\pi} \text{Re} \int_0^{k_F} d k k \int_{-1}^1 d x \frac{4k^2 - 4kq_0 + q_0^2 - q^2}{\sqrt{1-x^2}}$$

$$\times \delta(q_0^2 - 2q_0E_k - q^2 - 2kqx), \quad (12)$$

$$\text{Im} \Pi_{\text{matter}}^\text{ret} = \frac{1}{\pi} \int_0^{k_F} d k k \left[ \frac{(q_0 - 2k)^2 - q^2}{q^2 - q_0^2} \right]^{1/2}$$

$$\times \left\{ \Theta(q - q_0) \Theta \left[ k - \frac{q + q_0}{2} \right] + \Theta(q_0 - q) \right\}$$

$$\times \left\{ \Theta \left( \frac{q_0 + q}{2} - k \right) - \Theta \left( q_0 - \frac{q}{2} - k \right) \right\}$$

$$= \frac{1}{\pi} \int_0^{k_F} d k k \left[ \frac{(q_0 + 2k)^2 - q^2}{q^2 - q_0^2} \right]^{1/2}$$

$$\times \Theta(q - q_0) \Theta \left( k - \frac{q - q_0}{2} \right), \quad (13)$$

$$\Pi_{\text{matter}} = \Theta(q_0 - q) \Pi_1^\text{ret} + \Theta(q - q_0) \Pi_2^\text{ret}, \quad (14)$$

$$\text{Im} \Pi_1^\text{ret} = -\frac{1}{2\pi \sqrt{q_0^2 - q^2}} \left( 2E_F - q_0 \right) \sqrt{q^2 - (2E_F - q_0)^2}$$

$$+ q^2 \arcsin \left( \frac{2k_F - q_0}{2k_F} \right) \Theta(q - |q_0 - 2k_F|)$$

$$+ \frac{\pi q^2}{2} \left[ \Theta(2k_F - q_0 - q) + \Theta(2k_F - q_0 + q) \right] \quad (15)$$

$$\text{Im} \Pi_2^\text{ret} = \frac{\Theta(2k_F + q_0 - q)}{2\pi \sqrt{q^2 - q_0^2}} - \frac{\Theta(2k_F + q_0 + q)}{2\pi \sqrt{q^2 - q_0^2}} \left( 2k_F - q_0 \right) \sqrt{q^2 - (2k_F + q_0)^2}$$

$$- q^2 \ln \left( \frac{(2k_F + q_0)(2k_F - q_0)^2 - q^2}{2k_F + q_0} \right) \quad (16)$$

$$\times \Theta(2k_F - q_0 - q) \right\}.$$ The real part can be obtained using the Kramers–Kronig relation

$$\text{Re} \Pi_{\text{matter}}^\text{ret} = \frac{1}{\pi} \int_{-\infty}^{\infty} dq_0 \frac{\text{Im} \Pi_{\text{matter}}^\text{ret}(q_0)}{q_0 - q} \quad (17)$$

For the massive case (gapped graphene), the explicit calculation of the polarization function is straightforward [13, 14], so we just consider an important static case $q_0 = 0$:

$$\Pi_{\text{matter}}(q, 0) = \frac{2}{\pi^2} \int_0^{k_F} d k k$$

$$\times \int_{-1}^1 d x \frac{1}{\sqrt{1-x^2}} \left( \frac{q^2 - 4E_k^2}{q^2 + 2kqx} - 1 \right)$$

$$= -\frac{2}{\pi} \left( \sqrt{k_F^2 + m^2 - \sqrt{m^2}} \right) + \frac{2}{\pi q} \int_0^{k_F} \frac{d k k}{\sqrt{k^2 + m^2}}$$

$$\times \left( \sqrt{\frac{q^2 - 4k^2 - 4m^2}{q^2 - 4k_F^2}} - \frac{q}{2} - k \right)$$

$$= -\frac{2}{\pi} (\mu - m) + \frac{2}{\pi q} \int_m^\mu d \epsilon \left( \sqrt{\epsilon^2 + 4m^2 - 4\epsilon^2} \right) \Theta \left( \sqrt{\epsilon^2 + 4m^2 - 2\epsilon} \right) \quad (18)$$

$$= \frac{2}{\pi q} \int_m^\mu d \epsilon \left( \sqrt{\epsilon^2 + 4m^2 - 4\epsilon^2} \right) \Theta \left( \sqrt{\epsilon^2 + 4m^2 - 2\epsilon} \right)$$

$$- \frac{2}{\pi q} \int_m^\mu d \epsilon \left( \sqrt{\epsilon^2 + 4m^2 - 4\epsilon^2} \right) \Theta \left( \sqrt{\epsilon^2 + 4m^2 - 2\epsilon} \right)$$

$$= \frac{1}{\pi q} \left\{ \left[ -mq + \frac{q_0 - 2m^2}{2} \arctan \frac{q}{2m} \right] \Theta(2k_F - q)$$

$$+ \mu \sqrt{q_2 - 4k_F^2} - m q - \frac{q_0^2 - 2m^2}{2} \arctan \frac{q}{2m} \right\} \Theta(q - 2k_F). \quad (19)$$

4. Static screening

The static screening properties of the massive Dirac fermions in the RPA are controlled by the static dielectric function
\( \varepsilon_{\text{RPA}}(q, 0) \):

\[
\varepsilon_{\text{RPA}}(q, 0) = 1 - \frac{2\pi e^2}{\kappa q} [\Pi_{\text{vac}}(q, 0) + \Pi_{\text{matter}}(q, 0)].
\]

(20)

Without the matter contribution (the polarized charge distribution has been discussed in [12]), if we take into account the matter part, things will be quite different:

For \( q \leq 2k_F \),

\[
\Pi(q, 0) = -\frac{2\mu}{\pi}.
\]

(21)

For \( q > 2k_F \),

\[
\Pi(q, 0) = -\frac{2\mu}{\pi} + \frac{1}{\pi q} \Theta(q - 2k_F)
\times \left[ \mu \sqrt{q^2 - 4k_F^2} - \frac{q^2 - 4m^2}{2} \arctan \left( \frac{\sqrt{q^2 - 4k_F^2}}{2\mu} \right) + \text{semi-analytical results.} \right]
\]

(22)

Similar results have been obtained in [15]. From the above, we can deduce that the density of state at the Fermi surface is given by \( D(k_F) = 2\mu/\pi \). In the two limiting cases, the total static polarizability becomes a constant as in normal 2D electron liquid systems and 2D massless Dirac fermion systems. For the 2D electron liquid, the 2D Thomas–Fermi wave vector is given by \( q_{TF} = me^2/\hbar \). Consider an external charge density embedded in the homogeneous fermions. Even though \( V_e(x) = C \delta(x) \) is short ranged, the density response is not short ranged, which can be calculated by linear response theory [16]:

\[
\Pi(x) = C \int \frac{d^2q}{(2\pi)^2} \Pi(q, 0) e^{i q \cdot x}.
\]

(23)

It is interesting to note that like the normal 2D electron liquid, the 2D Dirac fermions also have an oscillatory term due to the non-analyticity at \( k = k_F \). Next, we take into account the finite temperature-dependent screening. The polarization function at \( T \neq 0 \) is

\[
\Pi_{\text{matter}}^\text{ret}(q, T) = -\frac{2}{\pi} \left\{ \mu - m + \frac{1}{\beta} \ln[1 + e^{-\beta(-\mu - m)}] + \frac{1}{\beta} \ln[1 + e^{-\beta\mu}] \right\}
+ \frac{2}{\pi q} \int_{-q/2}^{q/2} d\epsilon \left( 2\sqrt{\epsilon^2 - \epsilon^2 - \epsilon^2} \right)
- \frac{2m^2}{\sqrt{\epsilon^2 - \epsilon^2}} 
\times \left[ \frac{1}{1 + e^{\beta(-\mu - m)} + \frac{1}{1 + e^{\beta\mu}}} \right].
\]

(24)

At low temperature \( (T \ll T_F) \), we have the asymptotic form of the polarizability from the above equation:

\[
\Pi(q, T) \approx -\frac{2\mu(T)}{\pi}, \quad \text{for} \quad \epsilon_{q/2} < \mu.
\]

(25)

In particular, for \( q = 2k_F, m \to 0 \), we have

\[
\Pi_{\text{matter}}^\text{ret}(q, T) = -\frac{2}{\pi} \left\{ \mu - m + \frac{1}{\beta} \ln[1 + e^{-\beta\mu}] + \frac{1}{\beta} \ln[1 + e^{-\beta\mu}] \right\}
\]
\[+ \frac{4}{\pi q} \int_{-q/2}^{q/2} d\epsilon \sqrt{\epsilon^2 - \epsilon^2} \left[ \frac{1}{1 + e^{\beta(-\mu - m)} + \frac{1}{1 + e^{\beta\mu}}} \right].
\]

(26)

The total polarization function is

\[
\Pi(q, T) \approx -\frac{2}{\pi} \mu(T) - \frac{2}{\pi k_F} \left( 1 - \frac{\sqrt{2}}{2} \right) \xi \left( \frac{3}{2} \right) T^{3/2}.
\]

(27)

While for a general \( m \), analytic expressions cannot be obtained, it is quite easy to obtain numerical results from our semi-analytical results.

At high temperature \( (T \gg T_F) \)

\[
\Pi(q, T) \approx \frac{2}{\pi} \mu(T) + \frac{1}{\pi T} \left[ \frac{q^2}{12} - m^2 \right].
\]

(28)

For the chemical potential \( \mu(T) \), we can obtain its explicit form from the conservation of the total electron density. For the massless Dirac fermions, the asymptotic expression has been given in [17]. We note that for the massive case the expression is the same.

5. Conclusion

In summary, we have presented a finite-temperature field model for the 2D massive Dirac fermions and calculated the polarization functions for massive Dirac fermions. Finite temperature and finite density were taken into account to analyze the physics of gapped graphene in a more general case and connect various other group’s important work [4–7]. These results may be useful for finite-temperature screening within the RPA. Other important quantities, for example conductivity or specific heat, can be obtained from our results.

The polarization function at finite temperature can also be used to calculate the thermodynamic properties of massive Dirac fermions.

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