Carrier Transport in 3D Dirac Semimetals

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A theory is developed for the density and temperature dependent carrier conductivity in doped three-dimensional (3D) Dirac materials focusing on resistive scattering from screened Coulomb disorder due to random charged impurities (e.g., dopant ions and unintentional background impurities). The theory applies both in the undoped intrinsic ("high-temperature", $T \gg T_F$) and the doped extrinsic ("low-temperature", $T \ll T_F$) limit with analytical scaling properties for the carrier conductivity obtained in both regimes. The scaling properties can be used to establish the Dirac nature of 3D systems through transport measurements.

Following the very extensive research activity in graphene over the last 10 years \cite{1-6}, a great deal of interest in condensed matter physics (and beyond \cite{5}) has focused on other 2D and 3D Dirac materials where the elementary low-energy noninteracting electronic energy dispersion is linear and can be written in the continuum long wavelength limit as: $E(k) = \pm \hbar v_F |k|$ where $v_F$ is the (Dirac) Fermi velocity and the $+/−$ signs denote electron/hole (conduction/valence) bands, respectively, meeting at the so-called Dirac point $k = 0$ in our notation (where the conduction/valence bands meet making the system a gapless semiconductor or a semimetal). This linear gapless massless chiral Dirac band dispersion defines a solid state Dirac material, and exciting new materials and experimental developments \cite{6,7} have led to the laboratory realization of 3D Dirac materials (i.e., essentially the 3D generalization of 2D graphene) by several groups. In the current work, we explore the transport properties of 3D Dirac systems theoretically, obtaining the dc conductivity as a function of both carrier density ($n$) and temperature ($T$) considering both the undoped (intrinsic semimetal with the chemical potential precisely at the Dirac point) and the doped (extrinsic semiconductor with the chemical potential in the conduction band at a Fermi energy $E_F$ determined by the doping density). Similar transport theory results coupled with corresponding experimental conductivity measurements \cite{2-4,8,9} led to considerable fundamental understanding and progress in graphene physics, and the expectation is that the same should happen in 3D Dirac materials when appropriate transport measurements are carried out and compared with the theoretical results presented in the current work.

The theoretical approach we develop is physically motivated and based on the firm (and remarkably successful) conceptual framework of carrier transport theories in bulk semiconductors and semimetals as well as in 2D semiconductor systems \cite{10,11} and graphene \cite{12}. We use the semiclassical Boltzmann transport theory within the relaxation time approximation for solving the Boltzmann integral equation. We only take into account resistive scattering by long-range and short-range impurity scattering. The long-range disorder arises from random quenched charged impurities in the environment, which are invariably present either as dopant ions to produce free carriers in the system or as unintentional background impurities. The short-range disorder arises from atomic point defects which may be present. The Coulomb disorder arising from the charged impurities is screened by the random phase approximation (RPA) screening due to the Dirac electrons themselves.

For a system with a chiral linear energy dispersion, $E_k = \hbar v_F |k|$, the energy dependent transport scattering time within the Born approximation is given by

$$\frac{1}{\tau} = \frac{2\pi n_i}{\hbar} \int \frac{d^3k'}{(2\pi)^3} \frac{|\langle V(k,k') \rangle|}{(2 - (1 - \cos^2 \theta)/2) \delta(E_k - E_{k'})},$$

where $n_i$ is the impurity density, $\theta$ is the scattering angle between $k$ and $k'$, and $\langle V(k,k') \rangle$ is the scattering amplitude. For screened Coulomb disorder we have

$$\langle V(k,k') \rangle = \frac{4\pi e^2}{\kappa} \frac{1}{q^2 + q_s^2},$$

where $\kappa$ is the background lattice dielectric constant of the material, $q = |k - k'|$, and $q_s$ is the screening wave vector. We can rewrite Eq. (1) as

$$\frac{1}{\tau} = \frac{n_i}{2\pi} \frac{k^2}{\hbar^2 v_F} \int_0^\pi d\theta |V(q)|^2 \sin \theta (1 - \cos^2 \theta)/2,$$

where $q = 2k \sin (\theta/2)$.

Considering Thomas-Fermi (TF) screening we have the scattering time for long range Coulomb disorder at $T = 0$

$$\frac{1}{\tau} = \frac{4\pi n_i a^2 v_F}{k_F} I(q_0)$$

where $a = e^2/\kappa \hbar v_F$ is the effective coupling (i.e., fine structure) constant and $q_0 = q_{TF}/2k_F$ with $q_{TF} = $
\[ \sqrt{12\pi^2 n / E_F} = \sqrt{2g\alpha / \pi k_F} \] being the TF screening wave vector \((g = g_s g_v)\) is the total degeneracy with \(g_s\) and \(g_v\) being the spin and valley degeneracy, respectively. In Eq. 4 \(I(q_0)\) is given by

\[ I(q_0) = \left( q_0^2 + \frac{1}{2} \right) \log \left( 1 + \frac{1}{q_0^2} \right) - 1. \tag{5} \]

The asymptotic behaviors of \(I(q_0)\) are given by

\[ I(q_0) \sim -1 - \log(q_0) + q_0^2/2 - 2q_0^2 \log(q_0), \quad \text{for } q_0 \ll 1 \]
\[ I(q_0) \sim \frac{1}{12q_0^2} (1 - \frac{1}{q_0}), \quad \text{for } q_0 \gg 1. \tag{6} \]

Note that \(q_0 = q_{TF}/2k_F = \sqrt{g\alpha / 2\pi}\) is a function of the coupling constant \(\alpha\) and is independent of density. Since \(n = gk_F^2 / 6\pi^2\), the density dependent scattering time is given by

\[ \frac{1}{\tau} \propto \frac{n_i}{n^{2/3}}. \tag{7} \]

For the Dirac materials the zero temperature conductivity \(\sigma\) can then be expressed as

\[ \sigma = \frac{e^2 \nu_F^2}{3} D_F \tau = \frac{e^2 g \nu_F^2}{h} \frac{k_F^2}{\pi} \tau, \tag{8} \]

where \(D_F = gE_F^2 / (2\pi^2 (\hbar v_F)^3)\) is the density of states at the Fermi level. With Eq. (4) we have

\[ \sigma = \frac{e^2 g}{h} \frac{k_F^2}{12\pi^2 n_i \alpha^2} \frac{1}{I(q_0)}. \tag{9} \]

Thus, for \(q_0 \ll 1\)

\[ \sigma = \frac{e^2 g}{h} \left( \frac{3\pi^2}{4g} \right)^{1/3} \frac{n_i^{1/3}}{1} \frac{1}{\alpha^2 n_i \log(1/q_0) - 1}, \tag{10} \]

and for \(q_0 \gg 1\)

\[ \sigma = \frac{e^2 g}{h} \left( \frac{3g^2}{4\pi} \right)^{1/3} \frac{n_i^{4/3}}{n_i}. \tag{11} \]

For \(q_0 = \sqrt{g\alpha / 2\pi} \gg 1\), the conductivity is independent of the coupling constant \(\alpha\). This result also corresponds to the complete screening of the Coulomb disorder, i.e.,

\[ \langle V(k,k') \rangle = \frac{4\pi e^2}{\kappa} \frac{1}{q_s^2}. \tag{12} \]

With the completely screened Coulomb disorder the scattering time becomes

\[ \frac{1}{\tau} = \frac{4\pi^3 n_i \nu_F^2}{3g^2 k_F^6}. \tag{13} \]

Substituting this result into Eq. (4) we have the same result as Eq. (11).

![FIG. 1.](image) The density dependent conductivity calculated with the full RPA screening function for various temperatures. Here \(\alpha = 1.2\) and a fixed impurity density \(n_i = 10^{18} \text{cm}^{-3}\) are used.

For the short range disorder with \(\langle V(k,k') \rangle = V_0\) we have

\[ \frac{1}{\tau} = \frac{n_i V_0^2 k_F^2}{3\pi \hbar^2 v_F}, \tag{14} \]

and the conductivity becomes

\[ \sigma = \frac{e^2 g (\hbar v_F)^2}{h} \frac{n_i V_0^2}{n_i}. \tag{15} \]

For the short range disorder the conductivity is independent of the carrier density whereas the long-range disorder gives \(\sigma \propto n^{4/3}\) (see Fig. 1).

In the Boltzmann transport theory the temperature dependence of the conductivity arises from two contributions \[\text{[4, 13]}, \text{i.e., the temperature dependent screening and energy averaging of the energy dependent scattering time. Within the RPA the screening function (static dielectric function) is given by} \]

\[ \epsilon(q, T) = 1 - V(q)\Pi(q, T), \tag{16} \]

where \(V(q) = 4\pi e^2 / kq^2\) is the 3D Fourier transform of the Coulomb potential \(e^2 / kr\) and \(\Pi(q, T)\) is the static polarizability which is given by

\[ \Pi(q, T) = \frac{D_F}{6} \frac{q^2}{k_F^2} \ln \frac{k_c}{q} + \Pi^{(+)}(q, T) + \Pi^{(-)}(q, T), \tag{17} \]

where \(D_F = gE_F^2 / (2\pi^2 (\hbar v_F)^3)\) is the density of states at the Fermi level, \(k_c\) is the ultraviolet cutoff arising from the linear band dispersion \((k_c \sim a^{-1})\) where \(a\) is the lattice constant) and \(\Pi^{(\pm)}\) are given by

\[ \Pi^{(\pm)}(q, T) = \frac{D_F}{k_F} \int_0^\infty dk f^{(\pm)}_k \left[ k - \frac{q^2 + 4k^2}{4q} \ln \left| \frac{q + 2k}{q - 2k} \right| \right], \tag{18} \]
where $f^{(±)}_k = \frac{1}{\sqrt{\pi}} \exp \left( -\frac{x^2}{2} \right)$, where $\varepsilon_k = \hbar v_F k$ and $\mu$ is the finite temperature chemical potential which is determined by the conservation of the total electron density. At zero temperature $\mu(T) = E_F$, and $\Pi^{-1}(q) = 0$ and

$$\Pi^{(+)}(q) = \frac{2D_F}{3} \left[ 1 + \frac{k_F}{2q} \left( 1 - \frac{3q^2}{4k_F^2} \right) \ln \left| \frac{2k_F + q}{2k_F - q} \right| - \frac{q^2}{8k_F^2} \ln \frac{4k_F^2 - q^2}{q^2} \right].$$  \hspace{1cm} \text{(19)}

In the low temperature limit ($T < T_F$) the asymptotic forms of the polarizability become at $q = 0$

$$\tilde{\Pi}(0, T) = 1 - \frac{\pi^2}{3} \left( \frac{T}{T_F} \right)^2,$$  \hspace{1cm} \text{(20)}

and at $q = 2k_F$

$$\tilde{\Pi}(2k_F, T) = \tilde{\Pi}(2k_F, 0) - \frac{\pi^2}{6} \left[ 1 + \ln \frac{\pi^2}{12} + \ln \left( \frac{T}{T_F} \right)^2 \right].$$  \hspace{1cm} \text{(21)}

where $\tilde{\Pi} = \Pi/D_F$, and $\tilde{\Pi}(2k_F, 0) = \frac{2\pi}{3} [1 + \ln(k_c/2k_F)]$. At high temperatures ($T > T_F$) we have

$$\tilde{\Pi}(0, T) = \frac{\pi^2}{3} \left( \frac{T}{T_F} \right)^2 + \frac{1}{\pi^4} \left( \frac{T}{T_F} \right)^4.$$  \hspace{1cm} \text{(22)}

Before considering the full RPA screening effect we first consider TF screening which is defined as the $q = 0$ limit of RPA. The temperature dependent TF wave vector can be calculated at low temperatures ($T/T_F < 1$)

$$q_{TF}(T) = q_{TF}(0) \left[ 1 - \frac{\pi^2}{6} \left( \frac{T}{T_F} \right)^2 \right],$$  \hspace{1cm} \text{(23)}

and at high temperatures ($T/T_F > 1$)

$$q_{TF}(T) = q_{TF}(0) \frac{\pi}{\sqrt{3}} \left( \frac{T}{T_F} \right) \left[ 1 + \frac{3}{2\pi^2} \left( \frac{T}{T_F} \right)^6 \right].$$  \hspace{1cm} \text{(24)}

where $q_{TF}(0) = \sqrt{2\alpha_0/\pi k_F}$ is the zero temperature TF wave vector.

Since the energy dependence of the scattering time for the long range Coulomb disorder is given by $\tau(E) \propto E^2$ we have the energy averaged scattering time at low temperatures

$$\langle \tau(T) \rangle = \tau(0) \left[ 1 + \frac{\pi^2}{3} \left( \frac{T}{T_F} \right)^4 \right],$$  \hspace{1cm} \text{(25)}

and at high temperatures

$$\langle \tau(T) \rangle = \tau(0) \frac{7\pi^4}{30} \left( \frac{T}{T_F} \right)^4,$$  \hspace{1cm} \text{(26)}

where $\tau(0)$ is the zero temperature scattering time given in Eq. (41). Thus, combining the temperature dependent scattering time with the energy averaged terms we have the total temperature dependent conductivity. For the long range disorder the temperature dependent screening wave vector gives rise to the addition temperature dependence in the conductivity. Thus, the $\tau(0)$ in Eqs. (25) and (26) can be considered temperature dependent scattering time arising from temperature dependent screening.

We can now obtain the overall temperature dependence of the conductivity by combining the energy averaging and temperature dependent screening. For $q_0 < 1$ Eqs. (14) and (20) give the low temperature conductivity as

$$\sigma(T) = \sigma(0) \left[ 1 + \frac{\pi^2}{3} \left( \frac{2 + \frac{1}{1 + \ln q_0}}{T_F} \right)^2 \right],$$  \hspace{1cm} \text{(27)}

and Eqs. (14) and (20) give the high temperature conductivity for $q_0 T/T_F < 1$

$$\sigma(T) = \sigma(0) \frac{7\pi^4}{30} \left( \frac{T}{T_F} \right)^4 \left[ 1 + \frac{1 + \ln q_0}{1 + \ln(\pi q_0/\sqrt{3}) + \ln(T/T_F)} \right],$$  \hspace{1cm} \text{(28)}

and for $q_0 T/T_F > 1$ we have

$$\sigma(T) = \sigma(0) \frac{7\pi^8}{90} \left( \frac{T}{T_F} \right)^8.$$  \hspace{1cm} \text{(29)}

Thus, for $q_0 < 1$ there is a crossover in the temperature dependence from an exponent 4 to 8 in the high temperature conductivity. For $q_0 > 1$ we have the low temperature conductivity

$$\sigma(T) = \sigma(0) \left[ 1 + \mathcal{O}(T/T_F)^4 \right]$$  \hspace{1cm} \text{(30)}

and the high temperature conductivity

$$\sigma(T) = \sigma(0) \frac{7\pi^8}{90} \left( \frac{T}{T_F} \right)^8.$$  \hspace{1cm} \text{(31)}

Due to the cancelation between the screening effect and the energy averaging, the low temperature conductivity is almost temperature independent. The $T^8$ dependence of conductivity in the high $q_0 T/T_F$ limit is completely artificial, arising from the independent considerations of the screening and energy averaging. As shown in Figs. 2 and 3 the energy dependence of the screening gives $T^4$ behavior in the high temperature limit even for the TF screening.

For the short range disorder we have the energy averaged scattering time at low temperatures

$$\langle \tau(T) \rangle = \tau(0) \left[ 1 - e^{-T_F/T} \right],$$  \hspace{1cm} \text{(32)}

and at high temperatures

$$\langle \tau(T) \rangle = \tau(0) \left[ \frac{1}{2} + \frac{1}{4\pi^2} \left( \frac{T_F}{T} \right)^3 \right],$$  \hspace{1cm} \text{(33)}
where $\tau(0)$ is given in Eq. (14). For the short range disorder the temperature dependent conductivity comes from the energy averaging of the scattering time because there is no screening effect.

In Figs. 1–3 we show our full numerically calculated RPA screened (i.e., full wave vector, temperature, and density dependent static screening) transport results for 3D Dirac systems, emphasizing that the asymptotic low- and high-temperature results agree well with our analytical theories. A particularly noteworthy and unexpected feature is that, except for a small window of temperature around $T/T_F \sim 0.5$ where the conductivity decreases with increasing temperature, the impurity-induced transport behavior in 3D Dirac materials is ‘insulating’ at all temperatures with the conductivity increasing with increasing temperature.

For comparison with experimental results (when they become available), it is important to emphasize that, unlike in graphene where the Fermi level and the carrier density can be tuned by externally applied gate voltages, the only way to obtain a finite carrier density in a 3D Dirac system is through doping by impurities in which case $n \leq n_i$ will apply generically, leading to the $T = 0$ conductivity $\sigma \sim n^{4/3}/n_i \sim n^{1/3}$ in general, assuming $n = n_i$. Such an $n^{1/3}$ (or equivalently $n_i^{1/3}$) scaling dependence of the low-temperature ($T \ll T_F$) conductivity with doping density should be the hallmark of a 3D doped Dirac system. Since such variable doping samples are not easy to use in controlled experimental studies (e.g., the unintentional background impurities could vary from sample to sample in an unknown manner), we believe that the study of temperature scaling of conductivity may be the ideal way of establishing the Dirac nature of a candidate 3D Dirac system. In particular, the intrinsic undoped semimetallic behavior should manifest in the high-temperature limit ($T/T_F \gg 1$), where $\sigma(T) \sim T^4$ if
Coulomb disorder prevails (as is likely to be the case in the presence of charged dopants or impurities). At low temperatures \((T \ll T_F)\), the extrinsic doped behavior of the conductivity would lead to basically a temperature independent conductivity.

In summary, we have provided a theory for impurity-scattering limited transport properties of 3D Dirac systems, both in undoped and doped situations and both for high and low temperatures. Our predicted temperature dependent scaling behavior of the conductivity should distinguish a Dirac system from an ordinary semiconductor.

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