Magnetoresistance in 3D Weyl Semimetals

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We theoretically investigate the transport and magnetotransport properties of three-dimensional Weyl semimetals. Using the RPA-Boltzmann transport scattering theory for electrons scattering off randomly distributed charged impurities, together with an effective medium theory to average over the resulting spatially inhomogeneous carrier density, we smoothly connect our results for the minimum conductivity near the Weyl point with known results for the conductivity at high carrier density. In the presence of a non-quantizing magnetic field, we predict that for both high and low carrier densities, Weyl semimetals show a transition from quadratic magnetoresistance (MR) at low magnetic fields to linear MR at high magnetic fields, and that the magnitude of the $MR \gtrsim 10$ for realistic parameters. Our results are in quantitative agreement with recent unexpected experimental observations on the mixed-chalcogenide compound TlBiSSe.

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Introduction — Electronic band structures that have protected gapless points — where the conductance and valence bands are guaranteed to meet — have been of significant theoretical and experimental interest in recent years. The two dimensional manifestation of such band structures have been extensively studied in graphene [1], where the gapless nature is protected by sublattice symmetry [2], and in 3D topological insulators [3], where the crossing point is protected by topology [4, 5]. More recently, attention has focused on the three dimensional analogues of these compounds, called Weyl semimetals [6–8]. Compounds such as Cd₃As₂ [9–11] and TlBiSSe [12, 13] have been shown to have Weyl points in their band structure [14] (see Ref. [15] for a recent review on the various candidate materials for semimetals with 3D relativistic electronic dispersions).

Theoretical efforts towards characterizing the electronic properties of Weyl semimetals are in the nascent stage and include the scattering properties of different impurity potentials [16], localization and delocalization [17, 18], thermoelectric properties [19], screening [20, 21] and temperature dependence [22], quantized magnetic field dependence [23], diffusive transport [24] and the effects of electron-electron interactions [25]. Inspired by unexpected observations in recent transport [11, 26] and scanning probe [27] experiments, we study theoretically the transport and magnetotransport properties of 3D Weyl semimetals in the presence of Coulomb impurities that are distributed randomly in the bulk. We use a random phase approximation (RPA) method to calculate the Boltzmann conductivity of the system, and then utilize an effective medium theory (EMT) to average over the spatially inhomogeneous carrier density. This formalism has been remarkably successful in providing a quantitative understanding of the transport properties close to the Dirac point in graphene [1], the 2D cousin of these Weyl semimetals. Our results allow us to make some quantitative comparisons with experiment while also yielding many qualitative insights into the behavior of Weyl semimetals under various experimental conditions.

Transport at High Carrier Density — The Hamiltonian for a Weyl semimetal is given by

$$H = \pm \hbar v_F \sigma \cdot \partial_x - \mu + \sum_j U(r - R_j),$$

(1)

where $\sigma$ is a vector of Pauli matrices, $\mu$ is the chemical potential, and $v_F$ is the Fermi velocity. The density of states is $D(E) = g/E^2/2\pi v_F^2$, where the degeneracy $g = 2$ for 3D Weyl fermions. In Eq. 1, $U(r - R_j)$ is the total potential seen by an electron at position $r$ due to charged impurities at positions $R_j$. In this work, we consider Coulomb impurities with momentum space screened potential

$$U(\mathbf{q}) = \frac{4\pi e^2}{\epsilon(\mathbf{q})|\mathbf{q}|^2},$$

(2)

where $e$ is the electronic charge and $\epsilon(\mathbf{q})$ is the dielectric function. Here $\mathbf{k}$ and $\mathbf{k}'$ are the incoming and outgoing momenta of the scattered electron and $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ is the transferred momentum. For a given concentration of impurities, $n_{\text{imp}}$, the ensemble averaged transport scattering time within the Boltzmann approximation is given by

$$\tau = \frac{2\pi n_{\text{imp}}}{\hbar} \int \frac{d^3k'c}{(2\pi)^3} [U(\mathbf{k} - \mathbf{k}')]^{1/2} \frac{1}{2} \partial_\mathbf{\theta} \delta(E_k - E_{k'}).$$

(3)

To make connection with existing results in the literature [22, 28] we first consider the simpler case of evaluating Eq. 3 in the Thomas-Fermi (TF) approximation, where the scattering potential can be taken as...
$U(q) = 4\pi\epsilon^2/(\kappa(q^2 + q_0^2))$. Here $\kappa$ is the dielectric constant of the material and $q_0 = \sqrt{\epsilon^2 D(E_F)/\kappa}$ is the inverse of the Thomas-Fermi screening length. Introducing the effective fine structure constant $\alpha = e^2/hv_F\kappa$ (where $\alpha \approx 0.07$ for Cd$_3$As$_2$ and $\alpha \approx 0.7$ for TIBiSSe$_3$), we have [22]

$$\sigma_{TF} = \frac{e^2 v_F^2 T}{3} D = \frac{e^2}{\hbar} \frac{g}{12\pi^2} \frac{k_F^4}{n_{imp} \alpha^2} \frac{1}{H(\sqrt{\frac{2}{\pi}})}, \quad (4)$$

where $H(z) = (z^2 + 1/2) \log(1 + z^2) - 1$. In both non-chiral two dimensional electron gases and in graphene, the accidental coincidence at zero temperature between the polarization function for $q \leq 2k_F$ and the density of states implies that the Thomas-Fermi approximation gives identical results to the RPA. However, we should emphasize that this is no longer true close to the Dirac point, or at finite temperature or in other 2D materials like bilayer graphene [1]. As we discuss below, for Weyl semimetals the Thomas-Fermi and RPA give qualitatively different results, and in what follows, we use the RPA approximation with

$$g_\alpha(q) = \left[ \frac{\alpha}{2} D(E) \tilde{\Pi}(q/2k_F) \right]^{1/2}.$$ 

Here, $\tilde{\Pi}(x)$ is the ratio of the RPA polarization function and the density of states, and is given by the sum of two components: a vacuum part $\tilde{\Pi}_V(x)$ and a finite density part $\tilde{\Pi}_M(x)$ [20]

$$\tilde{\Pi}_M = \frac{2}{3} \left[ 1 + \frac{1}{4x} (1 - x^2) \log \left| \frac{1 + x}{1 - x} - \frac{x^2}{2} \log \left| \frac{1 - x^2}{x^2} \right| \right] \right],$$

$$\tilde{\Pi}_V = \frac{2x^2}{3} \log \left| \frac{\lambda}{x} \right|. \quad (5)$$

Note that unlike the case of one and two dimensions, for Weyl fermions in $d = 3$ the vacuum polarization function is divergent and needs an ultraviolet momentum cutoff $\Lambda$, where in Eq 5, $\lambda = \Lambda/2k_F$. In principle, the transport coefficients calculated within the RPA approximation could depend on the choice of the cutoff $\Lambda$, although in practice we verified that such dependence is weak for realistic values of $\Lambda$. In this work we fix $\Lambda$ by considering the momentum value for which the band structure deviates from the linear regime in Cd$_3$As$_2$ as reported experimentally [27].

Our results for the high density transport at $B = 0$, are shown in Fig. 1. We find that far away from the Weyl point, $\sigma \sim n^{4/3}/n_{imp}$, and as seen in the figure, our results agree with calculations recently reported in Ref. [22].

**Transport at Low Carrier Density** – Randomly distributed charged impurities create an inhomogeneous carrier density landscape. When the carrier density $n$ is much larger than the fluctuations in carrier density $n_{rms}$ the homogeneous transport theory discussed above can be used. However, when $n < n_{rms}$, one needs to average over the large spatial fluctuations in carrier density using an effective medium theory (EMT). This calculation proceeds in two steps: First, the screened inhomogeneous potential needs to be calculated self-consistently giving $n_{rms}(n_{imp}, \alpha)$, and second, one needs to construct effective medium theory equations [29] which, in the presence of a magnetic field, are $2 \times 2$ ma-

![FIG. 1: 3D Weyl fermion conductivity as a function of carrier density using RPA-Boltzmann theory (Ref. [22], blue curve), self-consistent Thomas-Fermi (Ref. [28], green curve) and the effective medium approach discussed in the main text (red curve). The effective medium theory predicts a minimum conductivity $\sigma_{min} \approx 4.2 n^* \mu_j$ close to the Weyl point and reproduces the Boltzmann transport theory $\sigma \sim n^{4/3}/n_{imp}$ far away from the Weyl point. The EMT provides the full crossover from the inhomogeneous transport regime $n < n^*$ to the homogeneous transport regime $n > n^*$. The inset is a blow-up close to the Weyl point.](image1)

![FIG. 2: Ratio of self-consistent carrier density $n^*$ and charged impurity density $n_{imp}$, as a function of effective fine structure constant $\alpha$ using the Thomas-Fermi approximation [28] and the Random Phase Approximation. Notice that for 3D Weyl fermions in TIBiSSe$_3$ ($\alpha = 0.68$, indicated by dotted lines), the Thomas-Fermi result provides quantitatively inaccurate results, but for Cd$_3$As$_2$ ($\alpha = 0.065$, indicated by dotted lines), the Thomas-Fermi approximation and RPA agree for $n^*$, but not for conductivity (see main text). Within the RPA, $n^*/n_{imp} < 1$ for all values of $\alpha$ (e.g. within the RPA, for $n_{imp} = 10^{23} m^{-3}$, $n^* \lesssim 5$% of $n_{imp}$ for $\alpha = 2$, whereas the Thomas-Fermi gives $n^*$ comparable to $n_{imp}$).](image2)
trix equations [30]. We note that Ref. [28] used the self-consistent theory [31] developed in the context of graphene to calculate $\sigma_{\text{min}}$ for Weyl semimetals within the Thomas-Fermi approximation. This gives a minimum conductivity plateau $\sigma_{\text{min}}^{\text{TF}} = n_{\text{imp}} e \mu \sqrt{2 \pi e^2}$. In this work we use the RPA screening theory and show that the Thomas-Fermi result [28] is inadequate, e.g. significantly underestimating $\sigma_{\text{min}}$ at small $\alpha$ and overestimating $\sigma_{\text{min}}$ at large $\alpha$. To illustrate this point, in Fig 2 we show the ratio of the self-consistent carrier density $n^*$ and the impurity concentration $n_{\text{imp}}$ for both the RPA and Thomas-Fermi approximation. For the RPA, we have $n^* \ll n_{\text{imp}}$ for all experimentally relevant values of $\alpha$, while the Thomas-Fermi result yields $n^*/n_{\text{imp}} \sim 1$ for $\alpha \approx 2$. (In graphene, we have $n^*/n_{\text{rms}} \sim 1$, and this is one of the important differences between graphene and Weyl semimetals). We also note that the Thomas-Fermi approximation is also incorrect at high carrier density, and this can be clearly seen in Fig. 1. To solve the problem accurately, we proceed to construct the EMT equations generalizing a recent result developed for two dimensional materials [32] that constrains our system to conserve current at all points and ensures that the net fluctuations in local electric fields sum to zero.

$$\int dn P[n, n_0, n_{\text{rms}}] \frac{\sigma_{xx}^2 + \sigma_{xx} \sigma_{xy}^{\text{EMT}} - 2(\sigma_{xx}^{\text{EMT}})^2 + (\sigma_{xy} - \sigma_{xy}^{\text{EMT}})^2}{(\sigma_{xx} + 2\sigma_{xx}^{\text{EMT}})^2 + (\sigma_{xy} - \sigma_{xy}^{\text{EMT}})^2} = 0$$

$$\int dn P[n, n_0, n_{\text{rms}}] \frac{\sigma_{xy} \sigma_{xx}^{\text{EMT}}(\sigma_{yy} - \sigma_{yy}^{\text{EMT}})}{(\sigma_{xx} + 2\sigma_{xx}^{\text{EMT}})^2 + (\sigma_{xy} - \sigma_{xy}^{\text{EMT}})^2} = 0.$$  

Here, $P[n, n_0, n_{\text{rms}}]$ is the density distribution of the carrier concentration, with local carrier concentration $n$, average carrier concentration $n_0$ and distribution width $n_{\text{rms}}$. In this analysis, we use a Gaussian distribution although, in principle, Eq. 6 is valid for an arbitrary density distribution. In order to obtain $n_{\text{rms}}$, one proceeds as follows: first the inhomogeneous self-consistent carrier density is computed by equating the effective band energy with the disorder averaged fluctuations in the impurity potential, $U_{\text{rms}} = \langle U(r - \mathbf{R}_i)U(r - \mathbf{R}_j) \rangle$, where the average is taken over the impurity distribution, yielding

$$n^* = \frac{g}{6\pi^2} \left[ \frac{1}{\hbar v_F} \sqrt{n_{\text{imp}}} \int \frac{d^3q}{(2\pi)^3} U^2(q, n^*) \right]^3.$$  

Similar to the two-dimensional case, once $n^*$ has been obtained, one can calculate all moments of potential distribution. In particular, we are interested in $n_{\text{rms}} \sim [U^3]_{\text{rms}} \approx \sqrt{15} n^*$, and once the fluctuations in carrier density are known, we can solve the EMT equations and find $\sigma_{\text{EMT}}(0) = 4.2 n^*e\mu$. (This is again different from graphene, where solving the EMT equations gives $\sigma_{\text{min}} = n^*e\mu$).

**Crossover Between Homogenous and Inhomogeneous Regimes** – In Figure 1, we show the conductivity at zero magnetic field as a function of carrier density using $\alpha = 1.2$, $g = 2$ and $n_{\text{imp}} = 10^{12} \text{cm}^{-3}$. These values are chosen to make the comparison correctly with Ref. [22]. Notice that for large carrier density, our results reproduce those of Ref. [22]. At zero carrier density, and in the inhomogeneous regime, our results differ significantly from the conductivity calculated in Ref. [28]. This is a result of a more accurate value of $n^*$ and the Boltzmann conductivity by the RPA approximation over the Thomas-Fermi approximation as well as the use of the EMT theory. The transport theory for Weyl fermions shown in Fig. 1 represents the full crossover from the inhomogeneous regime close to the Weyl point to the homogeneous regime far away from the Weyl point.

Next, we proceed to apply our theory to address a recent experimental puzzle in TIBiSSe. Reference [26] noticed an increase in mobility with decreasing carrier density. In order to make connection with the experimental data, one identifies the experimental mobility $\mu_{\text{exp}}$ and carrier density $n_{\text{exp}}$ from experimentally determined parameters [33]

$$\mu_{\text{exp}} = \frac{\sigma_{yy}(B \rightarrow 0)}{B \sigma_{xx}(B \rightarrow 0)}, n_{\text{exp}} = \frac{\sigma_{xx}(B = 0)}{\mu_{\text{exp}}}.$$  

The observation in Ref. [26] of decreasing mobility with increasing carrier density is prima facie surprising in light of the results already discussed in Fig. 1 above, where for fixed $n_{\text{imp}}$, the mobility clearly increases with carrier density. This is shown as the blue curve in Fig. 3 along with the experimental data that shows the opposite trend. However, we now argue that there are two other possibilities that are consistent with our theory that correctly explain these observations (and as we discuss below, it is not possible to determine from this data alone, which of these two scenarios correspond to the experimental situation).

In the first case, we consider the experiment to be in the homogeneous regime, but that the charged impurities are also dopants that shift the chemical potential. The average induced carrier density is then estimated
After some discussion, it is determined that the mobility $\mu_{\exp}$ decreases as a function of the measured carrier density $n_{\exp}$, whereas the Boltzmann theory (blue curve) would predict the opposite trend. In the main text, we explain two possible scenarios compatible with our theory. The red curve assumes that the experiments are in the inhomogeneous regime with $n_{\exp} = n^* << n_{imp}$, but assuming correlated charged impurities. Alternatively, the green curve assumes that the experiments are in the homogeneous regime $n >> n^*$, but where the charged impurities are also responsible for doping the material where as discussed in the text, $n_{exp} = n_0 \approx 5 \times 10^{-22}$ by

$$
n_0 \approx \frac{g}{6\pi^2} \left[ \frac{1}{h v_{F}} n_{imp} U(q, n^*) \right]^3. \quad (9)
$$

Solving this equation gives $n_0 \approx 5 \times 10^{-22}$ in the density regime of interest. The green curve in Fig. 3 uses $n_{exp} = n_0 = 5 \times 10^{-22}$ and shows good agreement with the experimental data. Therefore, a plausible resolution of this experimental mystery is that the charged impurities that are responsible for scattering carriers are also responsible for doping these samples.

A second possibility is that the samples are in the inhomogeneous regime where $n_0 \ll n_{imp}$. The red curve in Fig. 3 considers samples with varying disorder ($n_{imp}$ varying from $2 \times 10^{23} m^{-3}$ to around $6 \times 10^{24} m^{-3}$) and we identify $n_{exp}$ with $n^*$ and use the EMT equations discussed above in the limit $B \to 0$ and $n_0 \to 0$ to determine the following scaling law: $\mu_{exp} \approx C(n_{exp})^{-4/5}$ where we take $C$ to be a fit parameter. This scenario shows good agreement between the scaling law and the experimental data. However, we note that the value of $C$ that gives the best fit is somewhat lower than that calculated within the Boltzmann theory. This could arise if the scatterers had some degree of correlation (quantified by a structure factor, $S(q, r_0)$) which would increase the mobility without changing the carrier density fluctuations [34, 35]. Generalizing this idea to 3D Weyl semimetals, we find that in the inhomogeneous regime with $n_{imp} = 10^{24} m^{-3}$, the structure factor $S(q \to 0, r_0) = 1 - (4/3) n_{imp} \pi r_0^3 \approx 6.4 \times 10^{-3}$ for a reasonable correlation length of $r_0 \approx 6 \text{ nm}$ and this gives the correct experimental value of $C$.

While both the homogeneous and inhomogeneous scenarios are generally consistent with the power law decrease of $\mu_{exp}$ with $n_{exp}$, below we argue that within the semiclassical theory considered here, these two cases give very different scales for the magnetoresistance.

**Magnetoresistance** - To calculate the magnetotransport of Weyl semimetals, we assume that locally one can define a conductivity matrix with

$$
\sigma_{xx} = \sigma_B(r) \frac{1}{1 + \mu^2 B^2}, \quad \sigma_{xy} = \sigma_B(r) \frac{\mu B}{1 + \mu^2 B^2}, \quad (10)
$$

where $\sigma_B(r) = \sigma(n(r))$ is the RPA-Boltzmann conductivity discussed earlier.

The above set of equations constitute the input for the EMT model. The solution of the EMT equations contains both the magnetoresistance caused by having two types of carriers (electrons and holes) [36] and the disorder-induced magnetoresistance discussed in the context of silver chalcogenides [37, 38] and other two dimensional systems [32]. Here MR $\equiv (\rho_{xx}(B) - \rho_{xx}(B = 0))/\rho_{xx}(B = 0)$. In Fig. 4 we show our results for $n_0 = 3.8 \times 10^{23} m^{-3}$ and $n_{imp} = 7.6 \times 10^{22} m^{-3}$ (homogeneous regime), and for $n_0 \to 0$, $n_{imp} = 7.6 \times 10^{21} m^{-3}$ (inhomogeneous regime). These values were chosen so that...
they correspond to very similar $\mu_{\text{exp}}$ and therefore they cannot be distinguished from mobility alone. The results in Fig. 4 demonstrate convincingly that within the semi-classical theory presented here, the magnetoresistance in the inhomogeneous regime is much larger than that of the homogeneous regime. We also note that in the inhomogeneous regime MR is of the same order of magnitude as seen by Ref. [26] for matching parameters. For Weyl semimetals in general, our theory predicts that the MR should be quadratic at low magnetic fields (see inset) and linear at high magnetic fields (main panel). Within this model, having MR > 10 is easily achievable in the inhomogeneous regime for moderate values of B, but it is more than an order of magnitude weaker in the homogeneous regime. This suggests a clear way to experimentally distinguish between these two regimes. Moreover, an order of magnitude weaker in the homogeneous regime for moderate values of B, but it is more than an order of magnitude weaker in the homogeneous regime. This suggests a clear way to experimentally distinguish between these two regimes. Moreover, an easy way to increase MR for technological applications is to make the sample dirtier, a counterintuitive, yet easily achievable, experimental goal.

Note added: After completion of this work, experiments in TaAs, a new Weyl semimetal, show results [39] consistent with our predictions.

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