Critical Transport in Weakly Disordered Semiconductors and Semimetals

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Critical transport in weakly disordered semiconductors and semimetals

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Motivated by Weyl semimetals and weakly doped semiconductors, we study transport in a weakly disordered semiconductor with a power-law quasiparticle dispersion $\xi_{\mathbf{k}} \propto k^{\alpha}$. We show, that in 2α dimensions short-correlated disorder experiences logarithmic renormalisation from all energies in the band. We study the case of a general dimension d using a renormalisation group, controlled by an $\varepsilon = 2\alpha - d$-expansion. Above the critical dimensions, conduction exhibits a localisation-delocalisation phase transition or a sharp crossover (depending on the symmetries of the Hamiltonian) as a function of disorder strength. We utilise this analysis to compute the low-temperature conductivity in Weyl semimetals and weakly doped semiconductors near and below the critical disorder point.

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Low-temperature conductivity in weakly disordered metals is usually dominated by elastic scattering processes within a narrow shell of momentum states $\mathbf{k}$ near the Fermi surface, $|E_{\mathbf{k}} - E_F| \ll \tau^{-1}$, where τ is the elastic scattering time. It is usually believed that scattering into the states outside of this shell is either negligible or may only renormalise the quasiparticle parameters near the Fermi surface, not leading to qualitatively new effects.

However, it is well-known that Dirac-type quasiparticles in two dimensions (2D) experience logarithmic renormalisation from elastic scattering into *all* states corresponding to the linear spectrum, as it has been shown long ago in the context of Ising models[1], degenerate semiconductors[2, 3], integer Hall effect[4], d-wave superconductors[5], and topological insulators[6]. Recently, a similar renormalisation group (RG) description for transport in graphene has been developed in Ref. 7 and further discussed in Ref. 8, predicting a logarithmic dependence of physical observables on electrostatically tunable charge carrier concentration.

In this paper we show that in a broad class of systems the transport of particles with kinetic energy E experiences strong renormalisation from elastic scattering between all states in the band provided the bandwidth is sufficiently large, $W \gg E$, which typically occurs in semiconductors and semimetals.

We study transport in a weakly disordered semiconductor or a semimetal with a power-law spectrum $\xi_{\mathbf{k}} \propto k^{\alpha}$ in a d-dimensional space. Our conclusions, regarding the critical behaviour of a variety of systems, are summarised in Fig. 1. In the critical dimension $d_c = 2\alpha$, as examplified by graphene[7, 8] ($d = 2, \alpha = 1$), the disorder strength is subject to logarithmic renormalisations, qualitatively distinct from the weak-localisation corrections. Transport in materials just below or above the critical dimension is accessible to a rigorous RG treatment, supplemented by an ε expansion, where

$$\varepsilon = 2\alpha - d. \tag{1}$$

In the dimensions below critical, $d < d_c$, the renormalised

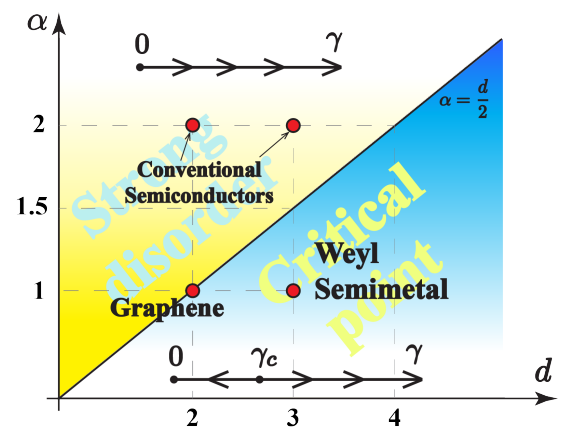

FIG. 1: (Colour online) Critical behaviour of disorder in materials with a power-low quasiparticle dispersion $\xi_{\mathbf{k}} \propto k^{\alpha}$ in d dimensions. *Above* the $\alpha = d/2$ line the effects of disorder grow at low energies (the strong-disorder regime). Materials *below* the line exhibit a critical point between the weak-disorder and strong-disorder regimes.

disorder strength increases at low energies. Above critical dimensions, the disorder strength increases if its bare value exceeds a critical value, and flows to zero otherwise. As a result, the conductivity $\sigma(\gamma)$ displays a transition[26] as a function of the bare disorder strength, as summarised, for example, for Weyl semimetal (WSM) in Fig. 2. Our conclusions persist even for quasiparticle Hamiltonians with non-trivial sublattice or valley structures, as, for example, in graphene or WSM.

The model for semiconductors. Let us first consider critical behaviour in a d-dimensional semiconductor with the band gap 2Δ, an isotropic spectrum $\xi_{\mathbf{k}} = ak^{\alpha}$ in the conduction band, and a trivial valley and sublattice structure. For simplicity, we consider a model, in which the conductivity is dominated by the electrons in the conduction band, e.g., due to a large value of the gap Δ that exceeds the bandwidth or the scale $ar_0^{-\alpha}$, with r_0 being the characteristic disorder correlation length, which then determines the effective ultraviolet cutoff $K_0 = r_0^{-1}$ of

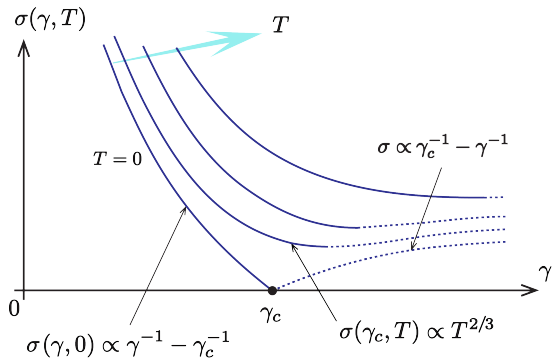

FIG. 2: (Colour online) Conductivity of Weyl semimetal at small finite doping μ as a function of the disorder strength and temperature. The dashed parts of the $\sigma(\gamma, T)$ curves correspond to the strong-disorder regime and may be affected by the interference effects at large length scales not studied here[26].

the theory[9].

We take the disorder potential $U(\mathbf{r})$ to be weak, with zero-mean and short-range correlated Gaussian statistics, $\langle U(\mathbf{r})U(\mathbf{r}')\rangle_{dis} = \gamma_0 K_0^{\varepsilon}\delta(\mathbf{r}-\mathbf{r}')$, characterised by the strength γ_0. The short-scale (ultraviolet momentum) cutoff K_0 is set by the width of the conduction band.

The dc conductivity for zero temperature and Fermi energy E is given by the Kubo-Greenwood formula

$$\sigma_{ij}^{E} = \int d\mathbf{r}' \ \mathrm{Tr}\left\langle \hat{v}_{i\mathbf{r}} G^{A}(E,\mathbf{r},\mathbf{r}')\hat{v}_{j\mathbf{r}'} G^{R}(E,\mathbf{r}',\mathbf{r})\right\rangle_{dis}, \quad (2)$$

where $\hat{\mathbf{v}}_{\mathbf{r}} = \alpha a(-i\boldsymbol{\nabla}_{\mathbf{r}})^{\alpha-1}$ is the velocity operator, $\hbar = e = 1$, and the trace is taken with respect to (wrt) the discrete degrees of freedom (spins, valleys, sublattices). All the energies E are counted from the middle of the forbidden band, where the chemical potential is located in an intrinsic semiconductor at $T = 0$. Conductivity at arbitrary temperature and doping level can be obtained from Eq. (2) as $\sigma_{ij} = -\int dE\, n_F'(E)\, \sigma_{ij}^{E}$, where $n_F(E)$ is the Fermi distribution function.

The product of the advanced G^A and retarded G^R Green's functions in Eq. (2), averaged with respect to disorder, can be written conveniently in the supersymmetric representation[10] as

$$\langle \ldots \rangle_{dis} = \int \mathcal{D}\overline{\Psi}\mathcal{D}\Psi \ldots \exp\left[-(\mathcal{L}_0 + \mathcal{L}_{int})\right], \quad (3)$$

$$\mathcal{L}_0 = i\int \overline{\Psi}\left[\lambda\left(E-\Delta\right) - \xi_{\hat{\mathbf{p}}} - i\Lambda\cdot 0\right]\Psi d\mathbf{r}, \quad (4)$$

$$\mathcal{L}_{int} = \frac{1}{2}\gamma K^{\varepsilon}\int (\overline{\Psi}\Psi)^2 d\mathbf{r}, \quad (5)$$

where Ψ is a vector in $AR \otimes PH \otimes FB$ space; AR, PH, and FB being, respectively, the advanced-retarded, particle-hole, and fermion-boson subspaces; $\Lambda = \hat{\sigma}_z^{AR} \otimes \mathbb{1}^{PH} \otimes \mathbb{1}^{FB}$, and $\overline{\Psi} = \Psi^{\dagger}\Lambda \equiv (\mathbb{C}\Psi)^T$, where $\mathbb{C} = \hat{\sigma}_z^{AR} \otimes (\hat{\sigma}_-^{PH} \otimes \mathbb{1}^{FB} - \hat{\sigma}_+^{PH} \otimes \hat{\sigma}_z^{FB})/2$ and $\hat{\mathbf{p}} = -i\boldsymbol{\nabla}_{\mathbf{r}}$. The parameters λ, γ and others will be found to flow upon renormalisation, with the initial values $\lambda(0) = 1$, $\gamma(0) = \gamma_0$, and K being the running momentum cutoff, which starts at $K = K_0$. In a Fermi liquid λ would correspond to the inverse Z-factor, the quasiparticle weight.

RG analysis. Perturbative treatment of disorder leads to divergent contributions (with vanishing particle energy E) to physical observables (conductivity, density of states, etc.). These can be analysed using an RG approach, which consists in integrating out the modes with the largest momenta $\mathbf{k}$: $K' < |\mathbf{k}| < K$. The action is reproduced with a new momentum cutoff K', renormalised gap $\Delta(l)$, and the parameters $\lambda(l)$ and $\gamma(l)$ running according to

$$\partial_l \lambda = C_d \frac{\gamma}{a^2}\lambda, \quad (6)$$

$$\partial_l \gamma = \varepsilon\,\gamma + \frac{4C_d}{a^2}\gamma^2, \quad (7)$$

where $l = \ln(K/K')$, $C_d = S_d/(2\pi)^d$, S_d is the area of a unit sphere in a d-dimensional space.

Eqs. (6)-(7) are the one-loop perturbative RG equations controlled by the dimensionless measure of disorder $\gamma a^{-2} \ll 1$ and, therefore, break down when this parameter flows to a value of order unity. The RG flow is terminated if the ultraviolet cutoff K reaches $1/L$, L being the characteristic size of the sample, or the value K_m, at which the energy scale $aK_m^{\alpha}/\lambda(K_m)$ is of the order the energy E.

If $\varepsilon > 0$, γ flows towards larger values in accordance with Eq. (7). However, for $\varepsilon < 0$, γ flows to larger values if initially $\gamma > \gamma_c$, and flows to zero if $\gamma < \gamma_c$, where

$$\gamma_c = -\varepsilon(4C_d)^{-1}a^2 \quad (8)$$

is the critical fixed point at which γ does not flow. We expect, as is common in the study of critical phenomena, that such a critical point exists even if ε is not small.

We note, that in addition to the random potential, considered here, there exist other types of disorder, which we do not consider and which lead to an RG equation similar to Eq. (7), but with a negative coefficient before the γ^2-term (for example, 2D Dirac fermions with random-mass disorder). In that case, the disorder strength flows towards smaller values above the critical dimensions ($\varepsilon < 0$) and has an attractive fixed point otherwise[1, 4].

Qualitative interpretation. Effectively the RG coarse-grains over the random disorder potential on the scale of a wavelength k^{-1}, interpreting a complex of underlying impurities on smaller scale as an effective impurity generating a renormalized random potential. The structure of the linear (in γ) term in the beta-function in Eq. (7) and the existence of the critical dimension can be understood qualitatively by comparing the typical value $\gamma_0^{\frac{1}{2}} K_0^{\frac{\varepsilon}{2}} k^{\frac{d}{2}}$ of the average disorder potential in

volume k^{-d}, with the kinetic energy ak^α for momentum k. If $d < 2\alpha$, the relative strength of disorder grows as $k \to 0$. In contrast, for $d > 2\alpha$ the typical potential decreases at low momenta relative to the kinetic energy. Carrying this coarse-graining procedure to higher (e.g., second) orders[7] in the disorder strength (e.g., by replacing a pair of impurities, separated by $\lesssim k^{-1}$, by an effective impurity) one arrives at the γ^2 and higher-order terms in the RG flow equation for the disorder strength.

Solutions. To analyse the low-energy behaviour of the conductivity, we solve Eqs. (6) and (7) with the result

$$\gamma(K)K^\varepsilon = \frac{\gamma_0 K_0^\varepsilon}{1-\gamma_0/\gamma_c + (\gamma_0/\gamma_c)(K_0/K)^\varepsilon}, \tag{9}$$

$$\lambda(K) = [\gamma(K)K^\varepsilon]^{1/4}(\gamma_0 K_0^\varepsilon)^{-1/4}. \tag{10}$$

At $K = K_m$, when the RG stops, one arrives at an effective low-energy theory with a renormalised action, which can be used further to evaluate physical observables (conductivity, heat capacitance, magnetic susceptibility, etc.), e.g., in the usual Fermi-liquid approximation.

We now apply the above analysis of the renormalised field theory [Eqs. (3)-(5), (9), (10)] to the conductivity of a variety of systems. For a finite doping in the conduction band, corresponding to the Fermi momentum K_m, the Drude contribution[11] to the conductivity is given by

$$\sigma(K_m) = \frac{v^2(K_m)}{2\pi\gamma(K_m)K_m^\varepsilon d} = \frac{\alpha^2 a^2 K_m^{2\alpha-2}}{2\pi\gamma(K_m)K_m^\varepsilon d}, \tag{11}$$

where $v(K_m)$ is the velocity. The Drude formula neglects weak-localisation effects and accurately describes the conductivity only when they are small and the disorder is weak, $\gamma(K)a^2 \ll 1$.

Relevant disorder. Let us consider the case of lower than critical dimensions, $\varepsilon > 0$. This is realised, for example, in conventional 2D and 3D semiconductors with a quadratic dispersion ($\alpha = 2$) near the bottom of the conduction band (the top of the valence band), Fig. 1. At $\varepsilon > 0$ the disorder strength, Eq. (9), grows upon renormalisation and diverges at a finite momentum cutoff

$$K_{loc} = K_0(1-\gamma_c/\gamma_0)^{-1/\varepsilon}. \tag{12}$$

The singularity in the disorder strength in Eq. (9),

$$\gamma(K)K^\varepsilon \propto (K-K_{loc})^{-1}, \tag{13}$$

signals of the mobility threshold at the momentum (12). Strictly speaking, our calculation is not a proof of the localisation of the states with momenta $k < K_{loc}$, because the perturbative RG has to be stopped when the disorder strength becomes too large, $\gamma/a^2 \sim 1$. At momenta $k \lesssim K_{loc}$ transport and localisation have to be studied by means of other techniques, such as non-linear sigma-model[10], derived from our renormalised effective action.

For sufficiently large temperature T, the RG flow is terminated at energies $E \sim T$, while the disorder is still weak, $\gamma a^{-2} \ll 1$. The respective cutoff momentum K is determined by the condition $aK^\alpha \sim \lambda(K)T$. In this case the conductivity remains finite and sufficiently large, $\sigma[K(T)] > \sigma(K^*)$, where K^* is the value of momentum at which the perturbative RG breaks down, $\gamma(K^*)a^{-2} \sim 1$.

For small finite doping in the conduction band and a large forbidden band $\Delta \gg T$, the charge carriers are described by Boltzmann statistics with the distribution function $n_F(E) \propto T^{-d/\alpha}e^{-E/T}$. Using Eqs. (2), (10) and (11), we estimate

$$\sigma(T) \propto T^{4-d/\alpha}. \tag{14}$$

At zero doping the conductivity is exponentially small, $\sigma \propto e^{-\Delta/T}$, as the charge carriers have to get thermally excited to the conduction band in order to contribute to transport.

Critical points of the disorder strength. When the dimensionality of space is above its critical value, $\varepsilon < 0$, the flow of γ has a critical point γ_c. Near the critical point the dependency of the conductivity on $\gamma_c - \gamma_0$, T, and the chemical potential can be understood from the standard scaling arguments[12].

The characteristic wavelength ξ of the charge carriers, which dominate the conductivity at $T = 0$, scales with small $\delta\gamma = \gamma_c - \gamma_0$ as $\xi \propto |\delta\gamma|^{-\nu}$. It can be shown that the scaling of the conductivity at $T = 0$ is given by the dimensional analysis, $\sigma \propto \xi^{2-d}$. This leads to the scaling form of the conductivity

$$\sigma^E(\delta\gamma) \sim |\delta\gamma|^{\nu(d-2)} g\left[(E-\Delta)|\delta\gamma|^{-z\nu}\right], \tag{15}$$

where z is the dynamic critical exponent[12], g is a scaling function (which, in general, depends on the sign of $\delta\gamma$), and $E > \Delta$ (e.g., due to doping). The conductivity at zero doping and finite temperature can be obtained by averaging $\sigma^E(\delta\gamma)$ wrt E with the distribution function $n_F'(E)$, yielding

$$\sigma(\delta\gamma, T) \sim T^\zeta |\delta\gamma|^{\nu(d-2)} \tilde{g}\left[T|\delta\gamma|^{-z\nu}\right], \tag{16}$$

where $\tilde{g}$ is another scaling function, $\zeta = 0$ for gapless semiconductors ($\Delta \ll T$) and $\zeta = -d/\alpha$ for gapped semiconductors ($\Delta \gg T$).

In particular, at zero temperature in a gapless weakly-doped material $\sigma \propto |\gamma_c - \gamma_0|^{\nu(d-2)}$. At the critical point $\gamma = \gamma_c$, $\sigma(T) \propto T^{(d-2)/z}$ and $\sigma(T) \propto T^{(d-2)/z-d/\alpha}$ for gapless and gapped semiconductors respectively.

Dirac-type quasiparticles. The case of higher than critical dimensions, $d > 2\alpha$, may be realised in WSM (cf. Fig. 1), 3D materials with Dirac quasiparticle spectrum[13–19] (with $\alpha = 1$) $\xi_{\mathbf{k}}^{Weyl} = v\hat{\boldsymbol{\sigma}} \cdot \mathbf{k}$, where the "pseudospin" $\hat{\boldsymbol{\sigma}}$ is the vector of Pauli matrices. The quasiparticle Hamiltonian may also have a non-trivial

sublattice and valley structure, which has to be properly taken into account. For simplicity, we focus on long-scale disorder confining the analysis near a single Weyl point.

In 2D our $\varepsilon = 0$ RG flow, Eqs. (6)-(7), reduces to that of Ref. [7] for the strongest long-wavelength disorder in graphene (neglecting the other four types of disorder), cf. Fig. 1.

An equation similar to Eq. (7) for Weyl fermions has been also derived in Refs. 2 and 6. In contradiction to our findings, in Ref. 2 the conductivity has been found to vanish at weak disorder. We attribute this to the shortcoming of the large N (number of valleys) approximation, equivalent to the self-consistent Born approximation (SCBA) (also used recently in Ref. 20), which does not account properly for the renormalisation effects found here (for the criticism of the SCBA see Refs. 7 and 8).

In order to generalise our RG approach to WSM, we analyse the quasiparticle Hamiltonian of the form

$$\xi_{\mathbf{k}} = vk^{\frac{1}{2}+\frac{\varepsilon}{2}}\hat{\boldsymbol{\sigma}}\cdot\mathbf{k}. \tag{17}$$

At $\varepsilon = 0$ it corresponds to $\alpha = 3/2$, in which case $d = 3$ is the critical dimensions. At $\varepsilon = -1$ the spectrum (17) turns into that of WSM. So, in order to address conduction in 3D Weyl semimetal, we carry out the RG analysis for the dispersion (17) at small ε and then in the spirit of ε-expansion set $\varepsilon = -1$.

Repeating the above calculation with the spectrum (17), we arrive at the same RG equations (6)-(7) with the factor 4 (corresponding to the four equally-weighted diagrams in Fig. 3) in Eq. (7) replaced by 2 (corresponding to the diagrams a) and b) cancelling each other for Dirac-type quasiparticles[8]). This leads to the doubling of the critical disorder strength γ_c, Eq. (8), and the exponent, $1/4 \to 1/2$, in Eq. (10). In 3D $\gamma_c = \pi^2 v^2$.

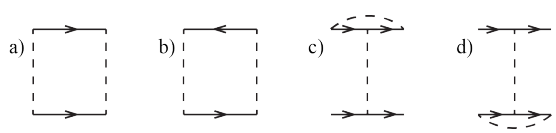

FIG. 3: Diagrams for the renormalisation of the disorder strength.

Thus, the presence of the pseudospin does not modify qualitatively the structure of the RG equations and their solutions, but only changes coefficients of order unity.

Conductivity of Weyl semimetals. The RG equations (6), (7) yield the values of the critical exponents[6]

$$\nu = -\varepsilon^{-1},\ z = 3/2. \tag{18}$$

For $\varepsilon = -1$, $\nu = 1$.

The Drude conductivity of WSM [13, 20–22] [27]

$$\sigma = \frac{v^2}{2\pi\gamma(K)K^{-1}} \tag{19}$$

with renormalised disorder strength $\gamma(K)K^{-1}$ is again suppressed for $\gamma > \gamma_c$ at low energies, and remains large for $\gamma < \gamma_c$ [26].

The elastic scattering time at momentum K

$$\tau(K) = \frac{1}{\pi\nu(K)\gamma(K)K^{-1}} = \frac{2\pi v}{K^2\left[\gamma(K)K^{-1}\right]} \tag{20}$$

diverges $\propto K^{-2}$ at small momenta $K \to 0$, as the disorder strength $\gamma(K)K^{-1}$ saturates at a constant value for $\gamma_0 < \gamma_c$, (9). The divergent scattering time $\tau(K)$ ensures a finite conductivity $\sigma \sim v^2\nu(K)\tau(K)$ at low energies, despite the vanishing density of states $\nu(K)$. We note, that at very small momenta $K < K_{rare}$ the conductivity may be dominated by non-perturbative effects from exponentially rare spatial regions[23].

Eq. (20) implies that the parameter $Kv\tau(K)$ remains large under the RG for $\gamma < \gamma_c$ if it was so in the bare system. Then one may neglect diagrams with crossed impurity lines[11] in the system with renormalised parameters, and the weak-localisation corrections to the Drude conductivity of a 3D material are small.

Thus, at weak disorder, the Drude conductivity in terms of the renormalised parameters, Eq. (19), accurately describes the full conductivity of WSM. Moreover, since $\gamma(K)K^{-1}$ saturates at a constant for low energies, Eq. (19) also describes the conductivity at zero doping and finite temperature, $T \gg \tau^{-1}, vK_{rare}$.

To compute the conductivity at $\gamma_0 < \gamma_c$, we use Eq. (19) with the renormalised disorder strength $\gamma(K_m)K_m^{-1}$, given by Eqs. (9), (10) [with the aforementioned $1/4 \to 1/2$ replacement], and the flow terminated by the cutoff K_m, set by $vK_m \sim \lambda(K_m)T$.

We find

$$\sigma_0(T) = \frac{v^2K_0}{2\pi\gamma_0}\left(1 - \frac{\gamma_0}{\gamma_c} + \frac{\gamma_0}{\gamma_c}\frac{T}{W}\right) \tag{21}$$

for $T \ll W$, where W is a constant of the order of $K_0 v(1-\gamma_0/\gamma_c)^{1/2}$. Eq. (21) is consistent with the scaling theory, Eq. (16), with the scaling exponents (18).

For $\gamma_0 > \gamma_c$, the system flows to the strong disorder regime. As discussed above, the RG may be terminated by sufficiently high temperature, also ensuring that the weak-localisation corrections remain small. Similarly to Eq. (14), we find $\sigma(T) \sim \gamma_0^{-1}K_0(T/K_{loc})^2 \propto T^2\delta\gamma^{-2}$. Close to the critical point Eq. (16) yields $\sigma(T) \propto T^{2/3}$.

At low temperatures, zero doping, and $\gamma > \gamma_c$ the RG breaks down when the disorder becomes strong, $\gamma \sim v^2$, equivalent to the criterion when weak-localisation corrections become important. At the breakdown point the system has no small parameters and is characterised by momentum scale K^*. Although the conductivity is strongly suppressed, *single*-node Weyl fermions are topologically protected from localisation[14, 24].

Assuming a finite conductivity σ in this regime, we estimate, using Eq. (9),

$$\sigma^* \sim K_0\left(\kappa v^{-2} - \gamma_c^{-1}\right)^{-1}\left(\gamma_0^{-1} - \gamma_c^{-1}\right), \tag{22}$$

where κ is a constant of order unity. The linear dependency of the conductivity on the disorder strength, $\sigma^* \propto \gamma_0 - \gamma_c$ near the critical point is consistent with the predictions of the scaling theory, Eqs. (16) and (18).

Experimental implications. Recently, Dirac (Weyl) quasiparticle dispersion has been reported[15–19] in Cd_3As_2 and Na_3Bi, which possibly present a platform for observing the conductivity dependency $\sigma(\gamma, T)$, Eqs. (21)-(22) and Fig. 2, which we predict. Our results apply to Weyl materials with short-range-correlated disorder (e.g., neutral impurities or vacancies) slightly doped away from the Weyl point or at finite temperatures.

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Note added. While this work was under review in Physical Review Letters, another paper, Ref. [25], was submitted and published, numerically addressing conductivity of WSM at zero doping. We present a detailed comparison of our results for WSM with those of Ref. [25] in the Supplemental Material.

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[26] Depending on the symmetries of the Hamiltonian, this can be Anderson localisation transition or a sharp crossover. The details of the transition very close to the critical point are determined by the interference effects on sufficiently large length scales [weak-(anti)localisation effects], which have to be studied for particular materials by other techniques, such as non-linear sigma-model[10].
[27] See Supplemental Material [url].