Quantum transport in three-dimensional Weyl electron system

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Quantum transport in three-dimensional Weyl (massless Dirac) electron system with long-range Gaussian impurities is studied theoretically using a self-consistent Born approximation (SCBA). We find that the conductivity significantly changes its behavior at a certain critical disorder strength which separates the weak and strong disorder regimes. In the weak disorder regime, the SCBA conductivity mostly agrees with the Boltzmann conductivity, except for the Weyl point (the band touching point) at which the SCBA conductivity exhibits a sharp dip. In the strong disorder regime, the Boltzmann theory fails in all the energy region and the conductivity becomes larger in increasing the disorder potential, contrary to the usual metallic behavior. At the Weyl point, the conductivity and the density of states are exponentially small in the weak disorder regime, and they abruptly rise at the critical disorder strength. The qualitative behavior near the zero energy is well described by an approximate analytic solution of the SCBA equation. The theory applies to three dimensional gapless band structures including Weyl semimetals.

I. INTRODUCTION

In recent condensed matter physics, enormous attention has been focused on gapless electronic systems where the conduction band and valence bands touch at some isolated points in the wave space. There the electronic band structure is described by the Weyl equation (the massless Dirac equation), which leads to unusual physical properties not observed in conventional metals and semiconductors. The two-dimensional (2D) version of Weyl electron has been extensively investigated in graphene,

for three dimensions (3D), there are a number of theoretical proposals for bulk materials with a gapless band structure including Weyl semimetals.

In this paper, we study the electronic transport in non-interacting 3D Weyl electron in the presence of disorder potential. In the gapless spectrum, generally, it is a non-trivial task to determine the conductivity near the Weyl point (band touching point), where the Boltzmann transport theory fails and we need to appropriately incorporate the finite level broadening effect. For 2D Weyl electron, the transport problem was closely studied, and the conductivity at the Weyl point was found to be of the order of \( e^2/h \) independently of the disorder strength.\(^\text{17–23} \)

The disorder effect on 3D Weyl electron was studied in several theoretical works.\(^\text{23–30} \)

Here we calculate the DC conductivity of 3D Weyl electron using a self-consistent Born approximation (SCBA), which is one of the theoretical methods to properly treat the finite level broadening, and investigate the dependence of the conductivity on the Fermi energy and the disorder strength. In 3D Weyl electron, a short-range disorder potential leads to a practical difficulty in which the self-energy diverges linearly to the cut-off energy. To avoid this, we assume long-ranged Gaussian impurities and achieve the self-consistency, and also study the dependence of the conductivity on the characteristic length scale of the impurity potential.

We show that the scattering strength is characterized by a dimensionless parameter \( W \) depending on the scattering amplitude and the impurity length scale, and we find that there is a certain critical disorder strength \( W_c \) separating the weak and strong disorder regimes. In the weak disorder regime \((W < W_c)\), the SCBA conductivity mostly agrees with the Boltzmann conductivity except at the Weyl point, where the conductivity exhibits a sharp dip. In the strong disorder regime \((W > W_c)\), the Boltzmann theory fails in all the energy region and the conductivity becomes larger in increasing the disorder potential, contrary to the usual metallic behavior. At the Weyl point, the conductivity and the density of states are exponentially small in the weak disorder regime, and they abruptly rise at \( W = W_c \). We also show that the qualitative behavior near the Weyl point is described by an approximate analytical solution of the SCBA equation, where the decay of the impurity matrix element in a large wave number is approximated by a wave space cut-off.

The paper is organized as follows. In Sec. II we introduce the model Hamiltonian, and present the formalism to calculate the Boltzmann conductivity and the SCBA conductivity. In Sec. III we derive an approximate solution of SCBA equation near zero energy, and in Sec. IV we present the numerical results for the SCBA equation, and closely argue the behavior of the conductivity and the density of states. A brief summary and discussion are given in Sec. V.

II. FORMULATION

A. Hamiltonian

We consider a three-dimensional, single-node Weyl electron system described by a Hamiltonian,

\[
\mathcal{H} = \hbar \mathbf{v} \cdot \mathbf{k} + \sum_j U(\mathbf{r} - \mathbf{r}_j),
\]  

(1)
where \( \bm{\sigma} = (\sigma_x, \sigma_y, \sigma_z) \) is the Pauli matrices, \( \bm{k} \) is a wave vector, \( v \) is a constant velocity. The second term is the disorder potential, where \( r_j \) is the positions of randomly distributed scatterers. For each single scatterers, we assume a long-ranged Gaussian potential,

\[
U(r) = \frac{\pm u_0}{(\sqrt{\pi}d_0)^3} \exp \left( -\frac{r^2}{d_0^2} \right),
\]

where \( d_0 \) is the characteristic length scale, and scatterers of \( \pm u_0 \) are randomly distributed with equal probability. This is Fourier transformed as \( U(r) = \int dq u(q) e^{i\mathbf{q} \cdot \mathbf{r}}/(2\pi)^3 \)

\[
u(q) = \pm u_0 \exp \left( -\frac{q^2}{d_0^2} \right),
\]

and \( q_0 = 2/d_0 \). We introduce an energy scale associated with the potential length scale,

\[
\varepsilon_0 = \hbar v q_0,
\]

and define a dimensionless parameter characterizing the scattering strength,

\[
W = \frac{1}{4\pi} \frac{n_i u_0^2 q_0}{\hbar^2 e^2},
\]

where \( n_i \) is the number of scatterers per unit volume.

**B. Boltzmann transport theory**

The Boltzmann transport equation for the distribution function \( f_{sk} \) is given by

\[
-\mathbf{e} \mathbf{E} \cdot \mathbf{v}_{sk} \frac{\partial f_{sk}}{\partial \varepsilon_{sk}} = \sum_{s'} \int \frac{d\mathbf{k}'}{(2\pi)^3} (f_{s'k'} - f_{sk}) W_{s's'k',sk},
\]

where \( s = \pm 1 \) is a label for conduction and valence bands, and \( W_{s's'k',sk} \) is the scattering probability,

\[
W_{s's'k',sk} = \frac{2\pi}{\hbar} n_i \langle s'k'\mid U \mid sk \rangle^2 \delta(\varepsilon_{s'k'} - \varepsilon_{sk}).
\]

The conductivity is obtained by solving Eq. (6). As usual manner, the transport relaxation time \( \tau_{tr} \) is defined by

\[
\frac{1}{\tau_{tr}(\varepsilon_{sk})} = \int \frac{d\mathbf{k}'}{(2\pi)^3} (1 - \cos \theta_{kk'}) W_{sk',sk},
\]

where \( \theta_{kk'} \) is the angle between \( \bm{k} \) and \( \bm{k'} \). For the isotropic scatterers, i.e., \( u(q) \) depending only on \( q = |\bm{q}| \), it is straightforward to show that \( \tau_{tr}(\varepsilon_{sk}) \) solely depends on the energy \( \varepsilon \) and written as

\[
\frac{1}{\tau_{tr}(\varepsilon)} = \frac{\pi}{\hbar} n_i D_0(\varepsilon) \int_{-1}^{1} d(\cos \theta) u^2[2k \sin(\theta/2)]
\times (1 - \cos \theta) \frac{1 + \cos \theta}{2},
\]

where \( k = \varepsilon/\hbar v \) and \( D_0(\varepsilon) \) is the density of states in the ideal Weyl electron,

\[
D_0(\varepsilon) = \frac{\varepsilon^2}{2\pi^2(\hbar v)^3}.
\]

The conductivity at \( T = 0 \) is written as

\[
\sigma_B(\varepsilon) = e^2 v^2 \frac{1}{3} D_0(\varepsilon) \tau_{tr}(\varepsilon),
\]

For the Gaussian scatter, Eq. (2), the relaxation time and conductivity are explicitly written as

\[
\tau_{tr}(\varepsilon) = \frac{\hbar}{2\varepsilon_0} \frac{1}{\hbar} \left( \frac{\varepsilon}{\varepsilon_0} \right),
\]

\[
\sigma_B(\varepsilon) = \frac{1}{12\pi^2} \frac{\varepsilon}{\hbar} \frac{1}{W} \left( \frac{\varepsilon}{\varepsilon_0} \right)^2 \frac{2}{\pi} \left( \frac{\varepsilon}{\varepsilon_0} \right),
\]

where

\[
\hbar(x) = \frac{64x^4}{4x^2 - 1 + (4x^2 + 1) \exp(-8x^2)}.
\]

In particular, the conductivity at the Weyl point is

\[
\sigma_B(0) = \frac{1}{8\pi^2} \frac{e^2 q_0}{\hbar} \frac{1}{W} = \frac{1}{2\pi} \frac{e^2 v^2 h}{n_i u_0^2},
\]

which is independent of \( q_0 \). Fig. 1 shows the Boltzmann conductivity Eq. (12) as a function of the Fermi energy.
C. Self-consistent Born approximation

We introduce the self-consistent Born approximation (SCBA) for 3D Weyl electron in a similar manner to the 2D version in Ref. 22. The following formulation does not depend on the specific form of the single impurity potential $U(r)$, as long as it is isotropic. We define the averaged Green’s function as

$$
\hat{G}(k, \varepsilon) = \left\langle \frac{1}{\varepsilon - \hat{H}} \right\rangle = \frac{1}{\varepsilon - \hbar v \sigma \cdot k - \Sigma(k, \varepsilon)},
$$

(15)

where $\langle \cdots \rangle$ represents the average over the configuration of the impurity position. $\hat{\Sigma}(k, \varepsilon)$ is the self-energy matrix, which is approximated in SCBA as

$$
\hat{\Sigma}(k, \varepsilon) = \int \frac{dk'}{(2\pi)^3} n_1 |u(k - k')|^2 \hat{G}(k', \varepsilon).
$$

(16)

Eqs. (15) and (16) are a set of equations to be solved self-consistently. From the symmetry of the present system, the self-energy matrix can be expressed as

$$
\hat{\Sigma}(k, \varepsilon) = \Sigma_1(k, \varepsilon) + \Sigma_2(k, \varepsilon)(\sigma \cdot n),
$$

(17)

where $k = |k|$ and $n = k/k$. By defining $X(k, \varepsilon)$ and $Y(k, \varepsilon)$ as

$$
X(k, \varepsilon) = \varepsilon - \Sigma_1(k, \varepsilon),
$$

(18)

$$
Y(k, \varepsilon) = \hbar v k + \Sigma_2(k, \varepsilon),
$$

(19)

Eqs. (16) and (16) are written as

$$
\hat{G}(k, \varepsilon) = \frac{1}{X(k, \varepsilon) - Y(k, \varepsilon)(\sigma \cdot n)},
$$

(20)

and

$$
\hat{\Sigma}(k, \varepsilon) = \int \frac{dk'}{(2\pi)^3} n_1 |u(k - k')|^2 \frac{X' + Y' \sigma \cdot n'}{X'^2 - Y'^2},
$$

(21)

where $X' = X(k', \varepsilon)$, $Y' = Y(k', \varepsilon)$, and $n' = k'/k'$. Now, we divide $n'$ as

$$
n' = n'_\parallel + n'_\perp.
$$

(22)

where $n'_\parallel = (n \cdot n')n$ is the component of parallel to $n$, and $n'_\perp$ is the perpendicular part. Then Eq. (21) becomes

$$
\hat{\Sigma}(k, \varepsilon) = \int \frac{dk'}{(2\pi)^3} n_1 |u(k - k')|^2 \frac{X'}{X'^2 - Y'^2}
+ \int \frac{dk'}{(2\pi)^3} n_1 |u(k - k')|^2 \frac{Y'}{X'^2 - Y'^2}(\sigma \cdot n'_\parallel)
+ \int \frac{dk'}{(2\pi)^3} n_1 |u(k - k')|^2 \frac{Y'}{X'^2 - Y'^2}(\sigma \cdot n'_\perp).
$$

(23)

The third term vanishes after the integration over the $k'$ direction, giving

$$
\hat{\Sigma}(k, \varepsilon) = \int \frac{dk'}{(2\pi)^3} n_1 V_0^2(k, k') \frac{X'}{X'^2 - Y'^2}
+ (\sigma \cdot n) \int \frac{dk'}{(2\pi)^3} n_1 V_1^2(k, k') \frac{Y'}{X'^2 - Y'^2},
$$

(24)

where

$$
V_0^2(k, k') = 2\pi \int_{-1}^{1} d(cos \theta_{kk'}) |u(k - k')|^2 \cos^n \theta_{kk'}.
$$

(25)

Eq. (24) immediately leads to the self-consistent equation,

$$
X(k, \varepsilon) = \varepsilon - \int \frac{dk'}{(2\pi)^3} n_1 V_0^2(k, k') \frac{X'}{X'^2 - Y'^2},
$$

(26)

$$
Y(k, \varepsilon) = \hbar v k + \int \frac{dk'}{(2\pi)^3} n_1 V_1^2(k, k') \frac{Y'}{X'^2 - Y'^2},
$$

(26)

which are to be solved numerically. From the obtained Green’s function, the density of states per unit area is calculated as

$$
D(\varepsilon) = -\frac{1}{\pi} \text{Im} \int \frac{dk}{(2\pi)^3} \text{Tr}[\hat{G}(k, \varepsilon + i0)].
$$

(27)

The Kubo formula for the conductivity is given by

$$
\sigma(\varepsilon) = -\frac{\hbar e^2 v^2}{4\pi} \sum_{s,s' = \pm 1} \int \frac{dk'}{(2\pi)^3} \text{Tr}
\left[ \sigma_x \hat{G}(k', \varepsilon + i0) \right.
\times \hat{J}_x(k', \varepsilon + i0) \bigg[ \hat{G}(k', \varepsilon + is') \bigg] \bigg].
$$

(28)

where $\hat{J}_x$ is current vertex-part satisfying the Bethe-Salpeter equation

$$
\hat{J}_x(k, \varepsilon, \varepsilon') = \sigma_x \int \frac{dk'}{(2\pi)^3} n_1 |u(k - k')|^2 \hat{G}(k', \varepsilon)
\times \hat{J}_x(k', \varepsilon, \varepsilon') \hat{G}(k', \varepsilon').
$$

(29)

To calculate this, we consider an integral

$$
I(k) = \int \frac{dk'}{(2\pi)^3} |u(k - k')|^2 F(k')(\sigma \cdot n') \sigma_x (\sigma \cdot n'),
$$

(30)

where $F(k)$ is an arbitrary function. After some algebra, we have

$$
I(k) = \sigma_x \int \frac{k' d3}{(2\pi)^3} F(k') \left( \frac{1}{2} V_0^2(k, k') + \frac{1}{2} V_1^2(k, k') \right)
+ (\sigma \cdot n) \sigma_x (\sigma \cdot n) \int \frac{k' d3}{(2\pi)^3} F(k') \left( \frac{1}{2} V_0^2(k, k') + \frac{3}{2} V_2^2(k, k') \right).
$$

(31)
In a similar way as for the self-energy, we obtain
\[
\int \frac{dk'}{(2\pi)^3} |u(k-k')|^2 F(k')(\sigma \cdot n') \sigma_x \\
= (\sigma \cdot n) \sigma_x \int \frac{k'^2 dk'}{(2\pi)^3} F(k') V_1^2(k, k'),
\]
\[
\int \frac{dk'}{(2\pi)^3} |u(k-k')|^2 F(k') \sigma_z (\sigma \cdot n') \\
= \sigma_z (\sigma \cdot n) \int \frac{k'^2 dk'}{(2\pi)^3} F(k') V_1^2(k, k').
\]

Using these, the vertex part $\hat{J}$ is written as
\[
\hat{J}(k, \epsilon, \epsilon') = \sigma_x J_0(k, \epsilon, \epsilon') + (\sigma \cdot n) \sigma_x (\sigma \cdot n) J_1(k, \epsilon, \epsilon') \\
+ (\sigma \cdot n) \sigma_x J_2(k, \epsilon, \epsilon') + \sigma_x (\sigma \cdot n) J_3(k, \epsilon, \epsilon'),
\]
and the Bethe-Salpeter equation becomes
\[
\begin{pmatrix}
J_0 \\
J_1 \\
J_2 \\
J_3
\end{pmatrix} = 
\begin{pmatrix} 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix} + 
\int_0^\infty \frac{k'^2 dk'}{(2\pi)^3} \frac{n_i}{(X^2 - Y^2)(X'^2 - Y'^2)} \\
\times \begin{pmatrix}
V_0^2 - (V_0^2 - V_2^2)/2 & 0 & 0 & 0 \\
0 & -(V_0^2 - 3V_2^2)/2 & 0 & 0 \\
0 & 0 & V_0^2 & 0 \\
0 & 0 & 0 & V_2^2
\end{pmatrix} \\
\times \begin{pmatrix}
XX' & YY' & XY' & X'Y' \\
YX' & XY' & XX' & Y'X' \\
XY' & YY' & XX' & X'Y' \\
Y'X' & X'Y' & XX' & Y'X'
\end{pmatrix}
\begin{pmatrix}
J_0' \\
J_1' \\
J_2' \\
J_3'
\end{pmatrix},
\]
where $X = X(k', \epsilon)$, $X' = X(k', \epsilon')$, $J_0 = J_0(k, \epsilon, \epsilon')$, $J_0' = J_0(k', \epsilon, \epsilon')$, etc. Finally, the conductivity is written as
\[
\sigma(\epsilon) = \frac{4\pi e^2 v_f^2}{3} \int_0^\infty \frac{k'^2 dk}{(2\pi)^3} \\
\times \text{Re} \left[ \frac{1}{|X^2 - Y^2|^2} \right. \\
\times \left\{ (3|X|^2 - |Y|^2) J_0^{++} + (3|Y|^2 - |X|^2) J_0^{--} + (3XY^* - XY^*) J_0^{+-} + (3XY^* - XY^*) J_0^{-+} \right. \right. \\
- \left. \left. \frac{1}{|X^2 - Y^2|^2} \right. \\
\times \left\{ (3X^2 - Y^2) J_0'^{++} + (3Y^2 - X^2) J_0'^{--} + 2XY J_0'^{+-} + 2X'Y' J_0'^{-+} \right. \right. \right],
\]
where $X = X(k, \epsilon + i0)$, $J_0^{\epsilon\epsilon'} = J_0(k, \epsilon + i0, \epsilon + i\epsilon')$, etc.

The SCBA is a valid approximation when the disorder scattering is relatively weak so that $k_Fl \gg 1$, where $k_F$ is the Fermi wave length, and $l = v_F/\tau$ is the mean free path given by the Fermi velocity $v_F$ and the relaxation time $\tau$. In the 3D Weyl electron, $v_F$ is the constant band velocity, and in the case of Gaussian impurities, $\tau$ is roughly estimated by $\tau_0', \tau_0''$, and in the case of Gaussian impurities, $\tau_0'$.

Near zero energy $\epsilon \ll \epsilon_0$, in particular, $h(\epsilon/\epsilon_0^2)$ is approximated by $(3/2)(\epsilon/\epsilon_0)^{-2}$ and the condition reduces to $(4/3)\epsilon/\epsilon_0 \ll 1/W$, i.e., the approximation is better for smaller energy. In higher energy region $\epsilon > \epsilon_0$, the function $h(\epsilon/\epsilon_0)$ approximates $16(\epsilon/\epsilon_0)^2$, and the condition becomes $8(\epsilon/\epsilon_0)^3 \gg W$, i.e., the approximation is valid also in the higher energy region.

III. APPROXIMATE ANALYTICAL SOLUTION NEAR ZERO ENERGY

Near $\epsilon = 0$, we can derive an approximate analytical solution of the SCBA equation in the previous section, as long as the level broadening $\Gamma(\epsilon)$ is much smaller than $\epsilon_0$. There we replace $u(q)$ with the constant $u_0$ (i.e., short-ranged impurity), but, instead, introduce a cutoff $k_c \sim 0$ in the $k$-space interval to simulate the exponential decay of $u(q)$ in a large $q$. The approximation is rather crude, while it effectively explains the qualitative behavior peculiar to the 3D Weyl electron as shown in the following section.

In this simplified system (short-range impurities with cutoff), the self-energy equation Eq. (16) is approximately solved in $\epsilon \ll \epsilon_c$ and $\Gamma \ll \epsilon_c$ as
\[
\hat{\Sigma}(k, \epsilon) \approx (1 - \alpha)\epsilon - i\Gamma(\epsilon),
\]
where
\[
\Gamma(\epsilon) = \frac{\Gamma_W}{2} + \sqrt{\left(\frac{\Gamma_W}{2}\right)^2 + \alpha^2\epsilon^2},
\]
\[
\alpha = \left(1 - \frac{W}{W_c}\right)^{-1},
\]
\[
\Gamma_W = \epsilon_0 \left(\frac{1}{W_c} - \frac{1}{W}\right),
\]
and
\[
W_c = \frac{\pi \epsilon_0}{2 \epsilon_c},
\]
where $\epsilon_c = \hbar v_k l$ is the cut-off energy. The density of states is then written in terms of $\Gamma(\epsilon)$ as
\[
D(\epsilon) = \frac{\epsilon_0}{2\pi^2(\hbar v)^3} \frac{\Gamma(\epsilon)}{W}. 
\]
At ε = 0, in particular, Γ(ε) becomes

\[ Γ(0) = \begin{cases} 0 & (W < W_c) \\ Γ_W & (W > W_c) \end{cases}, \]  

(41)
i.e., the self-energy, and thus the density of states, become zero in the weak disorder regime W < W_c, and abruptly rise in the strong disorder regime W > W_c. The vanishing Γ(0) at a finite W is peculiar to three dimensions, and it is intuitively understood as follows. By assuming a solution of the form Eq. (37), the first equation in Eq. (26) can be written at ε = 0 as

\[ Γ = \frac{ni_0 u_0^2}{2π^2} \int_0^{k_c} k^2dk \frac{Γ}{(hv)^2 + Γ^2}, \]  

(42)
which is to be solved for Γ. For a non-zero Γ, it becomes

\[ 1 = \frac{ni_0 u_0^2}{2π^2} \int_0^{k_c} k^2dk \frac{1}{(hv)^2 + Γ^2}. \]  

(43)
When the right-hand side of Eq. (42) is viewed as a function of Γ, it has an upper bound \( ni_0 u_0^2 k_c / (2π^2 h^2 v^2) \), which is achieved at Γ = 0. When the scattering strength is so small that \( ni_0 u_0^2 k_c / (2π^2 h^2 v^2) \) is smaller than 1, Eq. (43) has no solution, and we are left only with a trivial solution Γ = 0 in Eq. (42). This critical condition exactly corresponds to W < W_c. In contrast, the self-consistent equation in 2D always has a non-zero solution for any scattering strength, because in Eq. (43), \( k^2dk \) is replaced with \( kdk \), and then the right-hand side logarithmically diverges in Γ → 0, giving no upper bound.

In a similar manner, the Bethe-Salpeter equation Eq. (34) is approximately solved as

\[ \begin{pmatrix} J_0 \\ J_1 \\ J_2 \\ J_3 \end{pmatrix} \approx \begin{pmatrix} J \\ 0 \\ 0 \\ 0 \end{pmatrix}, \]  

(44)
where

\[ J = \left[ 1 + \frac{1}{3} \frac{W}{W_c} \right]^{-1}. \]  

(45)
The conductivity is obtained as

\[ σ(ε) = \frac{J}{12π^2} \frac{e^2}{hv} \frac{1}{3Γ(ε)^2 + α^2ε^2} \frac{Γ(ε)^2}{Γ(ε)}. \]  

(46)
When Γ(0) is non-zero, the conductivity at ε = 0 can be simply obtained by replacing Γ(ε) with Γ(0) as

\[ σ(0) = \frac{J}{4π^2} \frac{e^2}{hv} \frac{Γ(0)}{Γ(ε)}. \]  

(47)
In the strong disorder regime W > W_c, this gives

\[ σ(0) = \frac{J}{12π^2} \frac{e^2}{hv} × 3 \left( \frac{1}{W_c} - \frac{1}{W} \right) (W > W_c). \]  

(48)

\[ \text{Density of States (ε = 0)} \]

Fig. 2: (Solid) Density of states at zero energy calculated by the SCBA. (Dotted-dashed) Approximate expression Eq. (40) with Eq. (43), where ε/ε_0 is taken as 0.87. Inset shows the density of states near W_c ≈ 1.806 in a smaller scale.

In the weak disorder regime W < W_c, Eq. (17) is no longer valid since Γ(0) = 0, and then we need to take a limit ε → 0 to consider σ(0). We expand Γ(ε) in Eq. (45) as

\[ Γ(ε) ≈ \frac{α^2ε^2}{|Γ_W|} (W < W_c), \]  

(49)
and obtain

\[ \lim_{ε→0} σ(ε) = \frac{J}{12π^2} \frac{e^2}{hv} × \left( \frac{1}{W} - \frac{1}{W_c} \right) (W < W_c). \]  

(50)
From Eqs. (48) and (50), we see that the Weyl-point conductivity \( σ(0) \) vanishes at W = W_c, and it increases as W goes away from W_c in either direction.

In the vicinity of the critical point W = W_c, α becomes large and Γ(ε) and σ(ε) approximate linear functions,

\[ Γ(ε) ≈ |αε|, \]  

(51)
\[ σ(ε) ≈ \frac{1}{4π^2} \frac{e^2 |αε|}{hv} (W ≈ W_c), \]  

of which gradient diverges at W = W_c.

IV. NUMERICAL RESULTS

We solve the SCBA equations Eq. (26) and (34) by numerical iteration and calculate the density of states and the conductivity. Fig. 3 shows the density of states at ε = 0 as a function of W. The behavior is qualitatively
FIG. 3: Density of states (a,c) and the conductivity (b,d) calculated by the SCBA, as a function of the Fermi energy. The panels (c) and (d) show the detailed plots near $\varepsilon = 0$ of (a) and (b), respectively. The dotted-dashed line in Fig. (c) and (d) represent the approximate SCBA solution, Eq. (40) and Eq. (46), respectively.

similar to the approximate analysis in the previous section. There is a critical disorder strength $W_c \approx 1.806$, and the density of states rapidly increases once $W$ enters the strong disorder regime $W > W_c$. The dotted-dashed line in Fig. 2 shows the approximate SCBA solution of Eq. (40) at $\varepsilon = 0$, where $\varepsilon_c/\varepsilon_0$ is taken as $\approx 0.87$ to fit $W_c$ to the numerically obtained value. It nicely reproduces the increase in $W > W_c$, though the approximation fails in larger $W$ because the assumption $\Gamma \ll \varepsilon_c$ in deriving Eq. (38) becomes no longer valid as $\Gamma$ increases. Actually, the density of states in the weak disorder regime $W < W_c$ does not completely vanish in the numerics unlike the analytic approximation, but an exponentially small value remains as shown in the inset in Fig. 2. The rapid increase in $W < W_c$ is roughly expressed by $\propto 1/(W_c - W)$. As we will argue later, this small residue leads to a significant difference in the zero-energy conductivity between the numerical calculation and the analytic approximation.

Figs. 3(a) and (b) show the density of states and the
 conductivity as a function of the Fermi energy, respectively, which are numerically calculated by the SCBA. Figs. 3(c) and (d) are the detailed plots around zero energy for Figs. 3(a) and (b), respectively. We see that the density of states is enhanced in all the energy region with the increase of the scattering strength $W$. In the weak disorder regime $W < W_c$, it approximates a quadratic curve in the vicinity of $\varepsilon = 0$, and it nearly sticks to zero at the origin. At the critical point $W_c$, the curve exhibits a wedge-like shape, and in the strong disorder regime $W > W_c$, the bottom of the curve departs from zero as already argued. The dotted-dashed line in Fig. 3(c) represents the approximate SCBA solution near zero energy, Eq. (40). It reproduces the qualitative behavior of the numerical curve. At $W = 1.8$, slightly away from the critical point $W_c \approx 1.806$, the density of states is approximated by a linear function in accordance with Eq. (51).

The conductivity exhibits significantly different behaviors between the weak and strong disorder regimes. In Fig. 4, we compare the SCBA conductivity and the Boltzmann conductivity Eq. (12) at several $W$’s in (a) wide and (b) narrow energy regions. We see that the SCBA
agrees well with the Boltzmann conductivity in small \( W \), while the discrepancy becomes significant as \( W \) increases. The Boltzmann theory works well when the condition that the self-energy is much smaller than the Fermi energy, so that the theory naturally stands in the weak disorder regime. In the strong disorder regime \( W > W_c \), the Boltzmann approximation fails and the SCBA conductivity is enhanced in increasing \( W \) as observed in Figs. 4 (b) and (d), contrary to the usual metallic behavior. When \( W \) is too strong to violate the condition Eq. (50), the SCBA is no longer valid and the correction from the quantum interference effect would be important.

In the weak disorder regime \( W < W_c \), we notice that the conductivity \( \sigma(\varepsilon) \) exhibits a sharp dip at the zero energy, as shown in Fig. 5 (d) in a greater scale. The dotted-dashed line in Fig. 5 (d) indicates the approximate SCBA solution near zero energy, Eq. (51), with \( \varepsilon_c/\varepsilon_0 = 0.87 \) (the same value used in the DOS plot). We see that the analytic approximation fails to describe the zero-energy dip observed in the numerics, while, in the flat region outside the dip, the approximation qualitatively reproduces the \( W \)-dependence of the numerical conductivity.

The conductivity dip actually originates from an exponentially small self-energy remaining at \( \varepsilon = 0 \), which is missing in the analytic approximation. Indeed, the entire curve including the dip is qualitatively reproduced by Eq. (46), when \( \Gamma(\varepsilon) \) of Eq. (39) is modified by

\[
\Gamma(\varepsilon) \approx \Gamma_{\text{num}} + \frac{\alpha^2\varepsilon^2}{|W|} (W < W_c),
\]

where \( \Gamma_{\text{num}} \) is the small residue of the selfenergy at \( \varepsilon = 0 \) in the numerical calculation. The conductivity \( \sigma(0) \) is then given by Eq. (47), and thus is exponentially small. In increasing the Fermi energy \( \varepsilon \), \( \Gamma_{\text{num}} \) becomes less important in Eq. (52), and the conductivity gradually approaches the original analytic expression Eq. (50). The energy width of the dip is roughly estimated by the condition \( \alpha^2\varepsilon^2/|\Gamma W| \sim \Gamma_{\text{num}} \).

In Fig. 5 (a), the SCBA conductivity (solid) and the Boltzmann conductivity (dashed) at fixed Fermi energies are plotted as a function of \( 1/W \) (not \( W \)). In the weak disorder regime \( W < W_c \), the SCBA conductivity is proportional to \( 1/W \), and it coincides nicely with the Boltzmann conductivity Eq. (12) except for a constant shift. In increasing the disorder (i.e., decreasing \( 1/W \)), on the other hand, the SCBA conductivity reaches a minimum at a certain point, and it turns to increase nearly in proportional to \( W \). The scattering strength for the turning point is of the order of \( W_c \), and moves toward larger \( W \) (i.e., smaller \( 1/W \)) for larger Fermi energy.

Fig. 5 (b) presents a similar plot at zero energy, where the approximate SCBA solution, Eqs. (48) and (50), is plotted as a dotted-dashed line. We also show the numerical SCBA conductivity at \( \varepsilon = 0.001\varepsilon_0 \), slightly away from the Weyl point. In the weak disorder regime \( W < W_c \), the SCBA conductivity is very sensitive to \( \varepsilon \) as expected from the sharp dip structure in Fig. 5 (d). The energies \( \varepsilon = 0 \) and \( \varepsilon = 0.001\varepsilon_0 \) correspond to the bottom of the dip and the flat region outside the dip, respectively. The conductivity in \( W < W_c \) is exponentially small at \( \varepsilon = 0 \) as already argued, while at \( \varepsilon = 0.001\varepsilon_0 \) it linearly rises approximately in accordance with the analytical expression Eq. (51).

In 3D Weyl electron, the Weyl-point conductivity is highly \( W \)-dependent since Eq. (17) is proportional to \( \Gamma(0) \), and it abruptly rises when \( W \) exceeds \( W_c \) just in the same way as the density of states. This is in a sharp contrast to the 2D case, where the Weyl-point conductivity becomes nearly universal value of the order of \( e^2/h \). The 3D Weyl system does not have such a universal conductivity, because the conductivity in 3D has a dimension of \( e^2/h \) times the inverse of the length scale, and this is given by \( \Gamma(0)/(h\nu) \) in the present system.

V. CONCLUSION

We have studied the electronic transport in disordered three-dimensional Weyl electron system using the self-consistent Born approximation. The scattering strength is characterized by the dimensionless parameter \( W \) determined by the scattering amplitude, and the conductivity significantly changes its behavior at the certain scattering strength \( W \sim 1.806 \). In the weak disorder regime \( W < W_c \), the SCBA conductivity off the Weyl point mostly agrees with the Boltzmann conductivity which is proportional to \( 1/W \), while in the strong disorder regime \( W > W_c \), the conductivity becomes larger in increasing the disorder contrary to the usual metallic behavior. The conductivity at Weyl point is not universal unlike in 2D, but highly \( W \)-dependent just in the same way as the density of states. It is exponentially small in the weak disorder regime, and abruptly rises when \( W \) exceeds \( W_c \).

Throughout the paper, we assumed a single-node 3D Weyl Hamiltonian with Gaussian impurity scatterers. We expect that the theory applies to the Weyl semimetals as long as different Weyl nodes are well separated in \( k \)-space, and the disorder potential is sufficiently smooth not to mix up the different nodes. The valley mixing effect should be important when two or more Weyl nodes are degenerate in \( k \)-space. In the 2D Weyl electron system, it was reported that the valley mixing effect does not change the qualitative behavior of the SCBA conductivity, while the same problem in 3D requires a further investigation.

The dependence of the transport property on the specific form of impurity potential \( u(q) \) is also an important problem. In Gaussian impurities, the existence of the critical disorder strength \( W_c \) is attributed to the fact that the self-consistent equation Eq. (12) only allows the trivial solution \( \Gamma = 0 \) in \( W < W_c \), and this restriction is imposed by the upper limit of the integral in Eq. (13). The existence of \( W_c \) for other long range impurities should be
examined by a detailed SCBA calculation, while it is roughly estimated by a similar argument. For Coulomb impurities \( u(q) \propto 1/q^2 \), for example, the squared matrix element \( u(q)^2 \) gives an extra \( 1/k^4 \) term in \( k \)-integral in Eq. (43). Then there is no upper limit in the integral, so that we always have non-zero solution for \( \Gamma \), giving no \( W_c \). We expect that \( W_c \) exists in the type of impurity such that \( u(q) \) remains finite at \( q = 0 \).

A 3D Weyl electron system in condensed matter always has the end of the linear dispersion in high energy, and this may affect the transport property. In this work, we showed that the SCBA conductivity in Gaussian impurities is well described by an analytic approximation, where \( u(q) \) is approximated by a constant and a \( k \)-space cut-off \( k_c \). On the contrary, if we regard the end of the linear band in a real system as a cut-off, it would be effectively described by the present theory with an appropriate \( k_c \).

**Note added.** We recently became aware of recent works\textsuperscript{28,30} which predict the rise density of states at the critical disorder strength in the 3D Weyl electron system.

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