Unconventional Spin Hall Effect and Axial Current Generation in a Dirac Semimetal

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We investigate electrical transport in a three-dimensional massless Dirac fermion model that describes a Dirac semimetal state realized in topological materials. We derive a set of interdependent diffusion equations with 8 local degrees of freedom, including the electric charge density and the spin density, that respond to an external electric field. By solving the diffusion equations for a system with a boundary, we demonstrate that a spin Hall effect with spin accumulation occurs even though the conventional spin current operator is zero. The Noether current associated with chiral symmetry, known as the axial current, is also discussed. We demonstrate that the axial current flows near the boundary and that it is perpendicular to the electric current.

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Introduction.—Massless Dirac fermions (MDFs) have been widely studied not only in particle physics but also in condensed matter physics. In the latter context, MDF models describe materials whose conduction and valence bands touch with linear dispersion at isolated (Dirac) points in momentum space. Such a band structure has been found in two-dimensional systems such as graphene [1] and topological insulator surface states [2, 3]. In recent years, three-dimensional analogues of these materials called Dirac semimetals (DSMs) have been theoretically predicted [4–7], Na$_3$Bi [8, 9] and Cd$_3$As$_2$ [10, 11] are thought to be experimentally realized DSMS with symmetry protected Dirac points. The DSM state is also believed to be realized in topological materials such as TlBi(S$_{1+x}$Se$_2$)$_2$ [12–14] and (Bi$_{1−x}$In$_x$)$_2$Se$_3$ [15, 16].

One of the important differences between two- and three-dimensional MDF systems is the number of local degrees of freedom (DOFs) such as the electric charge density and the spin density. For a Dirac fermion field $\psi$, the low energy effective Hamiltonian in $d$ spatial dimensions is given by

$$H = \int \frac{d^dp}{(2\pi)^d} \psi^\dagger \hat{H} p \psi_p = \int \frac{d^dp}{(2\pi)^d} \psi^\dagger \left[ \sum_{i=1}^{d} v_i p_i \hat{\alpha}_i \right] \psi_p,$$

(1)

where $\hat{H}$ is a $2^d$-1 $\times$ $2^d$-1 Hermitian matrix, $\psi$ is a $2^d$-1-component spinor, $v_i = (v_1, \ldots, v_d)$ is the Fermi velocity, $p_i = (p_1, \ldots, p_d)$ is the crystal momentum measured from the Dirac point, $\hat{\alpha}_i$ are the alpha matrices obeying the Clifford algebra $\{\hat{\alpha}_\mu, \hat{\alpha}_\nu\} = 2\delta_{\mu\nu}$, and we use $\hbar = 1$ henceforth. Thus, in two dimensions, the largest number of linearly independent local operators is 4, which is the number of the independent components of a $2 \times 2$ Hermitian matrix, is 4, e.g., the particle density $N = \psi^\dagger \psi$ and the spin density $S = \psi^\dagger (S_x, S_y, S_z) \psi$ in a topological insulator surface state [18]. In three dimensions, on the other hand, that number is 16. It follows that the potential for interesting new effects is greater in three dimensions.

In this paper, we derive a set of interdependent diffusion equations in the presence of an electric field, involving 8 local DOFs for a DSM state in topological materials. We show that an unconventional spin Hall effect occurs in the bulk of the system, while the axial current, which is unique to massless Dirac fermion systems, flows near the boundary (See Fig. 1).

Spin transport in a Dirac Semimetal.—We start with a $d = 3$ MDF Hamiltonian Eq. (1) with $v_i = v$. We assume an explicit representation of the alpha matrices: $\hat{\alpha}_i = \hat{\sigma}_i \otimes \hat{\tau}_i$, with $\hat{\sigma}_i$ and $\hat{\tau}_i$ being the Pauli matrices in spin and orbital space, respectively. Although the Hamiltonian includes spin-orbit interaction terms, the conventional spin Hall coefficient $\sigma_{x y}^{S \psi}$ is zero because the conventional spin current operator is given by

$$\hat{j}_y^{S \psi} = \left\{ \hat{S}_x, \frac{\partial\hat{p}_y}{\partial\hat{p}_x} \right\} = 0,$$

(2)

![FIG. 1. Schematic illustration of electrical transport in the DSM state realized in TlBi(S$_{1+x}$Se$_2$)$_2$. The electric field $E$ induces the $i$-component spin current $\hat{j}_i^{S \psi}$ in the $\hat{e}_i \times E$ direction in the bulk, and the $i$-component spin density $\hat{S}_i$ accumulates near the boundary with the normal vector $\hat{e}_i$. The axial current $\hat{j}_i^{ax}$ flows near the boundary in the $-\hat{e}_i$ direction. See text for a detailed discussion.](cond-mat-mes-hall/1602.01179v2)
which apparently indicates the absence of non-trivial spin transport. When spin is not conserved, however, the conventional spin current operator has no theoretical foundation and often leads to unphysical results. For instance, Rashba \[23\] constructed an example in which the conventional spin current is non-zero even in equilibrium. The definition of the spin current operator is still controversial, and there are other proposals for the definition \[20, 21\].

Instead of spin current operators, we herein use the spin density, which is always a well-defined observable. We introduce a momentum- and energy-dependent density matrix \(\hat{g}(\mathbf{p}, \epsilon, \mathbf{x}, t)\). In the Born approximation for non-magnetic impurity scattering, we start with a quantum kinetic equation \[(1)\] for the spin density, which is always a well-defined observable \[20, 21\]. The definition of the spin current operator is still controversial. For instance, the conventional spin current operator has no theoretical foundation, and often leads to unphysical results. For instance, the conventional spin current is non-zero even in equilibrium. The definition of the spin current operator is still controversial, and there are other proposals for the definition \[20, 21\].

To obtain the diffusion equations, we solve Eq. \[(3)\] with respect to \(\hat{\rho}(\epsilon, \mathbf{x}, t)\), where \(\hat{\rho} = \hat{\rho}(\epsilon, \mathbf{x}, t)\) is the energy-dependent density matrix. Here, \(\nu = \mu^2/(2\pi^2 v^3)\) is the density of states per band at the Fermi energy.

To obtain the diffusion equations, we solve Eq. \[(3)\] approximately. For convenience, we introduce the time Fourier transforms \(\hat{g}_\omega(\mathbf{p}, \epsilon, \mathbf{x})\) and \(\hat{\rho}_\omega(\epsilon, \mathbf{x})\). The Fourier transform of Eq. \[(3)\] can be formally solved as

\[
\partial_t \hat{g}_\omega + \frac{1}{2} \left\{ \partial_\omega \hat{g}_\omega, \frac{\partial \hat{H}}{\partial \mathbf{p}_i} \right\} = i \epsilon \hat{g}_\omega + i \epsilon (4 E_p^2 - \Omega^2) \hat{F} + 2 E_p^2 \alpha_{\theta \phi} F \alpha_{\theta \phi} - \Omega \epsilon E_p \left[ \alpha_{\theta \phi} \hat{F} \right]
\]

\[
\equiv \hat{g}_\omega(0) + \hat{G}_{\text{grad}}[\hat{g}_\omega],
\]

\[(5)\]

where \(\hat{F} = \hat{F}_0 + \hat{F}_{\text{grad}}, \hat{F}_0 = i/\tau (\hat{G}_R \hat{\rho} - \hat{\rho} \hat{G}_A), \hat{F}_{\text{grad}} = -\left\{ \partial_\omega \hat{g}_\omega, \frac{\partial \hat{H}}{\partial \mathbf{p}_i} \right\}/2, \alpha_{\theta \phi} = \sin \theta \cos \phi \alpha_1 + \sin \theta \sin \phi \alpha_2 + \cos \theta \alpha_3, \Omega = \omega + i/\tau, \) and \(E_p = |\mathbf{p}|\). \(\hat{g}_\omega(0)\) and \(\hat{G}_{\text{grad}}[\hat{g}_\omega]\) are \(\hat{F}_0\) and \(\hat{F}_{\text{grad}}\) dependent parts of the first line, respectively. \(\theta\) and \(\phi\) are the polar and azimuthal angles of the momentum \(\mathbf{p}\). Assuming \(\partial_\omega \ll p_F \equiv \mu/v\), we regard \(\hat{G}_{\text{grad}}\) as a perturbation and perform a gradient expansion \[23\]. Solving Eq. \[(3)\] with respect to \(\hat{g}_\omega\) by a second order iteration, integrating over both \(\epsilon\) and \(\mathbf{p}\), and performing an inverse Fourier transform with respect to \(\omega\) \[23\], we obtain the diffusion equation for the density matrix \(\hat{D}(\mathbf{x}, t) = \nu \int d \epsilon \hat{\rho}(\epsilon, \mathbf{x}, t)\) \[23\].

For convenience, we decompose the density matrix \(\hat{D}\) into 16 linearly independent components:

\[
\hat{D} = \frac{1}{4} \left( N1 + \sum_{a=0,1,2,3,5} \rho^a \alpha_a + \sum_{a,b=0,1,2,3,5} \rho^{ab} (i \alpha_a \alpha_b) \right)
\]

\[(6)\]

Here, \(\alpha_5 = \alpha_0 \alpha_1 \alpha_2 \alpha_3\), and we define 16 local DOFs: \(N, \rho^a, \) and \(\rho^{ab}\). In the DSM state with \(\hat{\alpha}_i = \hat{\sigma}_i \otimes \hat{n}\), the spin operator is \(\hat{S} = (\hat{\sigma} \otimes \mathbf{1})/2 = (-i \hat{\sigma}_2 \hat{\alpha}_3, i \hat{\alpha}_1 \hat{\alpha}_3, -i \hat{\alpha}_1 \hat{\alpha}_2)/2\), and the spin density is \(\hat{S}(\mathbf{x}, t) = (-\rho^{23}(\mathbf{x}, t), \rho^{13}(\mathbf{x}, t), -\rho^{12}(\mathbf{x}, t))/2\). By using these local DOFs, we obtain a set of interdependent diffusion equations with 16 local DOFs. In practice, however, we can limit the discussion to the following closed equations for 8 local DOFs including the particle density \(N(\mathbf{x}, t)\) and the spin density \(\hat{S}(\mathbf{x}, t)\):

\[
\frac{\partial N}{\partial t} = -\nabla \cdot \left[ -D \nabla N + D e(2\nu) \mathbf{E} \right] - \frac{v}{3} \nabla \cdot \mathbf{p},
\]

\[(7a)\]

\[
\frac{\partial p^a}{\partial t} = D \frac{\partial^2}{\partial \mathbf{p}^2} p^a + 2 p^b \frac{\partial E_p}{\partial \mathbf{p}^a} \nabla \cdot \mathbf{p} - \frac{2v}{3} \nabla N + \frac{v e(2\nu)}{3} \mathbf{E} \nabla \cdot \mathbf{p},
\]

\[(7b)\]

\[
\frac{\partial S}{\partial t} = D \frac{\partial^2}{\partial \mathbf{p}^2} S + 2 D \frac{\partial E_p}{\partial \mathbf{p}^a} \nabla \cdot \mathbf{p} + \frac{v}{6} \nabla \rho^{05} \nabla \times \mathbf{S} - \frac{v}{12 \mu \tau} \nabla \times \mathbf{S} - \frac{S}{\tau},
\]

\[(7c)\]

where \(D = v^2 \tau/3\) is the diffusion constant, and \(\mathbf{p} = (\rho^1, \rho^2, \rho^3)\). Here, we have derived Eqs. \[(7)\] in the quasi particle approximation \(\tau \ll \mu\) and have used only the zeroth and first order terms of the electric field. As a result, the electric field only appears in the form \(\nabla \mathbf{N} - \mathbf{e}(2\nu) \mathbf{E}\). Note that \(\rho_0, \rho_5, \rho_0, \) and \(\rho_5\) do not respond to the first-order electric field. Thus, we ignore these local DOFs henceforth.

Equations \[(7a)\] and \[(7b)\] have the form of a continuity equation \(\partial_j j^N = -\nabla \cdot \mathbf{j}^N\), where \(j^N\) is the Noether four-current. These relations originate from the fact that MDF systems have \(U(1)\) gauge symmetry, and also chiral symmetry, as will be discussed later. From Eq. \[(7a)\], the electric current \(\mathbf{j}\), which is the Noether current associated with \(U(1)\) gauge symmetry, can be written as

\[
\mathbf{j} = -D \nabla N + D e(2\nu) \mathbf{E} + \mathbf{j}_a,
\]

\[(8)\]

where \(\mathbf{j}_a \equiv \nu \mathbf{p}/3\), and we normalize the electric current by the elementary charge \(e\) henceforth. The first and second terms are the diffusion current and the usual drift current, respectively. The third term is an additional
current that is absent in the electron gas model with quadratic dispersion. We can interpret \( j_z \) as an impurity vertex correction to the longitudinal current in the Kubo formalism. The existence of the vertex correction term is a consequence of the particle conservation law, which holds in our formalism.

To investigate the spin Hall effect, we consider a steady state \( (\partial/\partial t = 0) \) under physical boundary conditions. The solution of the diffusion equations depends on the choice of boundary conditions \([27, 28]\). We here assume that every local DOF is zero on boundaries. Under the boundary conditions, we have the following relations in the steady state:

\[
N = 0, \quad \rho_{05} = 0, \quad \nabla \cdot \rho = 0, \quad \nabla \cdot S = 0, \\
0 = \frac{\partial \rho_i}{\partial t} = \frac{D_i}{5} \nabla^2 \rho_i + \frac{v e (2\mu)}{3} E_i + \frac{v}{3 \mu \tau} \nabla \cdot (S \times \dot{\varepsilon}_i) - \frac{\rho_i}{(\frac{\mu \tau}{2})}, \\
0 = \frac{\partial S_i}{\partial t} = \frac{D_i}{5} \nabla^2 S_i + \frac{v}{12 \mu \tau} \nabla \cdot (\rho \times \dot{\varepsilon}_i) - \frac{S_i}{(\frac{\mu \tau}{2})}, \\
\]

where \( S_i \) and \( \rho_i \) are scalar projections of \( S \) and \( \rho \) on a unit vector \( \varepsilon_i \), respectively. The phenomenological spin diffusion equation for \( S_i \) is given by

\[
\frac{\partial S_i}{\partial t} = D_i \nabla^2 S_i - \nabla \cdot j^{S_i} - \frac{S_i}{\tau_s}, \\
\]

where \( D_i \) is the spin diffusion constant, \( \tau_s \) is the spin relaxation time, and \( j^{S_i} \) is the \( i \)-component spin current. Comparing Eqs. (9) with Eq. (10), we obtain the following expressions:

\[
j^{S_i} = \frac{1}{4 \mu \tau} \varepsilon_i \times j_a, \quad D_s = \frac{D_i}{5}, \quad \tau_s = \frac{3 \tau}{2}. \\
\]

Note that we do not use any definition of the spin current operator to determine the spin current expression. From Eqs. (10), the spin current \( j^{S_i} \) is closely related to the additional current \( j_a \). In the bulk \( (\nabla = 0) \), we obtain non-zero polarization of \( \rho \) from Eqs. (9):

\[
\rho(\text{bulk}) = \tau v e v E, \\
\]

which leads to the non-zero additional current \( j_a = v \rho / 3 \).

Thus, the \( z \)-component spin Hall coefficient \( \sigma_{xy} \) is given by

\[
\sigma_{xy} = \frac{j^{S_z}(\text{bulk})}{E_x} = e \frac{E}{24 \pi \tau P_F}. \\
\]

It is interesting to note that the \( z \)-component spin Hall coefficient is non-zero even though the conventional spin current operator \( j^{S_z} \) is zero. The origin of this spin current is \( [\delta \phi, \hat{F}] \) in Eq. (5), which describes the \( \tau \)-independent correction to the \( \tau \)-dependent transport. Our result is an example of an unconventional spin Hall effect that can not be predicted by the Kubo formula for the conventional spin current operator.

Since this spin Hall effect is a diffusive phenomenon, the spin current causes spin accumulation near the boundary, as shown below. We now solve the diffusion equations \([9]\) in the presence of an electric field \( E = (E_x, 0, 0) \) for \( y \geq 0 \). The physical solution satisfying the boundary conditions \( \rho(y = 0) = S(y = 0) = 0 \) is given by

\[
\rho_x = \tau v e v E_x \left[ 1 - \exp \left( -\frac{y}{l_s} \right) \cos \left( \frac{y}{l_{osc}} \right) \right], \quad \rho_y = \rho_z = 0, \\
S_z = \frac{\tau v e v E_x}{2} \exp \left( -\frac{y}{l_s} \right) \sin \left( \frac{y}{l_{osc}} \right), \quad S_y = S_y = 0, \\
\]

where \( l_s = v \tau / \sqrt{10 - 25/(16 \mu^2 \tau^2)} \) is the spin diffusion length, and \( l_{osc} = 4 \mu \tau v \tau / 5 \) is the oscillation length of local DOFs. The \( z \)-component spin density distribution is plotted for various \( \mu \tau \) in Fig. 2. Although the solution given by Eqs. (13) has oscillations, cancellation of the net spin accumulation is negligibly small for sufficiently large \( \mu \tau \), where the quasi particle approximation \((\mu \tau \gg 1)\) is valid. Note that the accumulated spin is perpendicular to the electric field and parallel to the boundary, while that in the Rashba model, which is a typical model for the spin Hall effect, is not.

For a qualitative estimate, we use the following typical values for the DSM state realized in TlBi(Si_{1-x}Se_x)\(_2\) \([13, 14]\): the scattering time \( \tau \sim 10^{-13} \) s, the Fermi velocity \( v \sim 10^6 \) m/s, and the Fermi wavenumber \( P_F \sim 10^9 \) \( \) m\(^{-1}\). In this material, the quasi particle approximation is justified since \( \mu \tau / h \sim 10^1 > 1 \). By using Eq. (13), we obtain the spin Hall coefficient \( \sigma_{xy} \sim 10^4 (\hbar / e)(\Omega/cm)^{-1} \), which is an order of magnitude larger than the typical value for semiconductors \([20]\). We also obtain the spin diffusion length \( l_s \sim 10^3 \) nm. Thus, our unconventional spin Hall effect is expected to be observed, as in standard
spin Hall materials.

Another interesting feature of DSMs is transport related to chiral symmetry \[30, 31\]. Three-dimensional MDF systems are invariant under a chiral transformation \(\psi \rightarrow e^{i\gamma_5}\psi\), where \(\gamma_5 \equiv i\sigma_0\tilde{\sigma}_5\). From Eq. (7b), the Noether current associated with this symmetry, known as the axial current \(j^{05}\) in quantum field theory, is given by

\[
j^{05} = -\nabla \rho^{05} - \frac{2\mu}{3} \mathbf{S},
\]

where \(\rho^{05}\) is the axial charge density. In the steady state described by Eqs. (9), \(\mathbf{S}\) is a divergenceless vector field, the bulk spin density \(\mathbf{S}(\text{bulk}) = 0\), and \(j^{05}\) is proportional to \(\mathbf{S}\) since \(\rho^{05} = 0\). Thus, we obtain the following expression:

\[
j^{05} = \nabla \times \mathbf{B}^{05},
\]

where \(\mathbf{B}^{05}\) is equivalent to the “magnetic field” for \(\rho^{05}\). Note that the axial current has a similar form to the persistent electric current in the presence of a real magnetic field. The axial current in the bulk is zero, while the axial current flows near the boundary. Because the derivation of the diffusion equations relies only on general properties of three-dimensional massless Dirac fermion models, our discussions can be straightforwardly generalized to other Dirac semimetals such as the recent Dirac semimetal candidate Cd₃As₂.

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