Study of spin transport in Dirac systems

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Abstract. We investigate spin Hall effect in a three-dimensional Dirac electron system. We derive diffusion equations in the Keldysh formalism and define a spin current from a spin diffusion equation. We solve the obtained diffusion equations in a steady state in the bulk and find that the bulk spin Hall conductivity is non-zero, though that for the conventional spin current is zero.

1. Introduction
Spintorronics is one of the most important fields in recent condensed matter physics. In particular, studies of spin currents in materials with spin-orbit coupling (SOC) led to discoveries such as intrinsic [1, 2] (and extrinsic [3]) spin Hall effect (SHE) and topological insulators [4, 5, 6].

In such materials, however, spin currents are often not conserved currents because SOC breaks spin rotational symmetry. Conventionally, a spin current is defined as a Hermitian operator

$$\hat{j}S_i = \frac{\{\hat{S}_i, \hat{j}\}}{2},$$

where $\hat{S}_i$ ($i = 1, 2, 3$) is the spin operator and $\hat{j}$ is the electric current divided by $|e|$. The spin current defined in eq.(1) is a conserved Noether current in the systems with spin rotational symmetry. In the systems with SOC, however, this conventional spin current does not satisfy the continuity equation and sometimes leads crucial problems [7]. Hence it is not clear whether or not we can use the definition to each system.

Instead of using the conventional definition, we define a spin current from a spin diffusion equation [8] in this paper. We derive the spin diffusion equation from a quantum kinetic equation [9]. In this formalism, we do not need any assumption for the spin current operator. In order to investigate intrinsic SHE in a spin-non-conserved system, we choose a three-dimensional semi-metallic Dirac electron system with spin-mixing terms. We find that the spin Hall conductivity (SHC) can be non-zero even when the conventional SHC is zero.

This paper is organized as follows. In section 2 we introduce a three-dimensional Dirac Hamiltonian and derive its quantum kinetic equation. Then we outline the derivation to obtain diffusion equations. In section 3 we define 16 charges which describe the transport of the system and choose a specific form of alpha matrices. In section 4 we define a spin current and calculate the SHC. In section 5 we briefly summarize this paper.
2. Model and Formalism

In this section, we introduce a three-dimensional Dirac Hamiltonian. Then we derive its quantum kinetic equation and diffusion equations in the same formalism as previous works [10]. We consider only the effect of nonmagnetic impurities and ignore electron-electron interactions.

We investigate a 4×4 three-dimensional massless Dirac Hamiltonian with impurities

\[ H = H_0 + H_{imp}, \]

\[ H_0 = \int dx \psi^\dagger(x) v (-i \partial_i - eA_i) \hat{\alpha}_i \psi(x), \]

\[ H_{imp} = \int dx \psi^\dagger(x) V(x) \psi(x) = \int dx \psi^\dagger(x) \left[ u_0 \sum_i \delta(x - x_i) \right] \psi(x), \]

where \( v \) is the Fermi velocity, \( A_i \) is a vector potential, \( V(x) \) is a nonmagnetic impurity potential, \( \psi \) is a four-component spinor field, and alpha matrices \( \hat{\alpha}_i \) obey the anticommutation relations

\[ \{ \hat{\alpha}_i, \hat{\alpha}_j \} = 2 \delta_{ij} \hat{1}, \quad (i, j = 1, 2, 3). \]

In order to investigate a non-equilibrium state of this system, we work on the Keldysh formalism. We start from the following equations:

\[ \hat{G}^{\text{R}(A)} = \left[ \hat{G}^{(0)} \right]^{-1} - \hat{\Sigma}^{R(A)} \]

\[ \left[ \hat{G}^R \right]^{-1} \hat{G}^K - \hat{G}^K \left[ \hat{G}^A \right]^{-1} = \hat{\Sigma}^K \hat{G}^A - \hat{G}^R \hat{\Sigma}^K, \]

where \( \hat{G}^{R(A)} \) is the retarded (advanced) Green’s function, \( \hat{G}^K \) is the Keldysh Green’s function, and \( \hat{\Sigma}'s \) are their self-energies.

First, we consider the system without an electromagnetic field. Ignoring the weak-localization effects, we perform the disorder average in the Born approximation and obtain the following relations [10]:

\[ \hat{G}^{R,A}(p, \epsilon) = \frac{1}{(\epsilon - \mu) - v p_i \hat{\alpha}_i \pm \frac{i}{2} \tau}, \]

\[ \hat{\Sigma}^K(x, x') = \frac{1}{\pi \nu \tau} \delta(x - x') \hat{G}^K(x, x), \]

\[ \tau = \frac{1}{\pi \nu u_0^2 n_i}, \]

where \( \mu \) is the chemical potential, \( \nu \) is the density of states of one band at the Fermi energy, and \( n_i \) is the density of impurities. In this approximation, eq.(5) becomes

\[ \left[ \hat{\epsilon}, \hat{G}^K \right] + \left[ \hat{G}^K, \hat{H} \right] + \frac{i}{\tau} \hat{G}^K = \hat{\Sigma}^K \hat{G}^A - \hat{G}^R \hat{\Sigma}^K. \]

All we have to do is determine the Keldysh Green’s function and its self-energy in eq.(9).

In order to obtain the quantum kinetic equation, we consider the Wigner transformation of eq.(9). The Wigner transformation of a function \( A(x + \frac{\delta x}{2}, x - \frac{\delta x}{2}) \) is defined as

\[ A_{\delta x}(x, t) = \int d(\delta x)d(\delta t)e^{-i p \delta x + i e \delta t} A \left( x + \frac{\delta x}{2}, x - \frac{\delta x}{2} \right), \]
where \( x = (x, t) \). Applying the semi-classical approximation (See Appendix A), the Wigner transformation of eq.(9), or the quantum kinetic equation, can be written as

\[
\frac{\partial}{\partial t} \hat{g}_{pc}(x, t) - i [\hat{g}_{pc}(x, t), v \alpha \cdot p] + \frac{i}{2} \{ \nabla \hat{g}_{pc}(x, t), v \alpha \} + \frac{1}{\tau} \hat{g}_{pc}(x, t) = \frac{i}{\tau} \left( G_{pc}^R \hat{\rho}_e(x, t) - \hat{\rho}_e(x, t) G_{pc}^A \right).
\]

(11)

Here we define the non-equilibrium distribution function \( \hat{g}_{pc}(x, t) \) and the density matrix \( \hat{\rho}_e(x, t) \) as

\[
\hat{g}_{pc}(x, t) = \frac{1}{2i} \hat{G}^K(xt, pc),
\]

\[
\hat{\rho}_e(x, t) = \frac{1}{\pi \nu} \int \frac{dp}{(2\pi)^3} \hat{g}_{pc}(x, t).
\]

(12)

The details of the derivation is included in Appendix A.

The effect of a uniform static electric field can be taken by a replacement

\[
\nabla \rightarrow \tilde{\nabla} = \nabla + eE\partial_e
\]

and a modification of the Wigner transformation as

\[
A_{pc}(x, t) = \int d(\delta x)d(\delta t) e^{-i(p+eA(t))\delta x + ic\delta A} \left( x + \frac{\delta x}{2}, x - \frac{\delta x}{2} \right)
\]

(14)

in eq.(11).

In the following, we outline the derivation to solve eq.(11) by iterations. We consider the Fourier transformation of eq.(11) with respect to time. Using the following notations:

\[
\Omega \equiv \omega + \frac{i}{\tau}, \quad E_p \equiv vp, \quad \hat{\alpha}_{\theta \phi} \equiv \sin \theta \cos \phi \hat{\alpha}_1 + \sin \theta \sin \phi \hat{\alpha}_2 + \cos \theta \hat{\alpha}_3,
\]

\[
\tilde{F}_0 \equiv \frac{i}{\tau} \left( G_{pc}^R \hat{\rho}_e - \hat{\rho}_e G_{pc}^A \right), \quad \tilde{F}_{grad} \equiv -\frac{1}{2} \{ \nabla \hat{g}_{pc}, v \alpha \},
\]

(15)

we can rewrite eq.(11) as

\[
\Omega \hat{g}_{pc}(x, \omega) = \tilde{F}_0 + \tilde{F}_{grad} - E_p [\hat{g}_{pc}(x, \omega), \hat{\alpha}_{\theta \phi}].
\]

(16)

Equation (16) can be formally solved as

\[
\hat{g}_{pc} = A_{pc,0} \tilde{F}_0 + B_{pc,0} \hat{\alpha}_{\theta \phi} \tilde{F}_0 \hat{\alpha}_{\theta \phi} + C_{pc,0} \left[ \hat{\alpha}_{\theta \phi}, \tilde{F}_0 \right] + A_{pc} \tilde{F}_{grad} + B_{pc} \hat{\alpha}_{\theta \phi} \tilde{F}_{grad} \hat{\alpha}_{\theta \phi} + C_{pc} \left[ \hat{\alpha}_{\theta \phi}, \tilde{F}_{grad} \right]
\]

\[
\equiv \hat{g}_{pc}^{(0)} + \tilde{G}_{grad} [\hat{g}_{pc}],
\]

(17)

where

\[
A_{pc,0} = i \frac{2E_p^2 - \Omega^2}{\Omega(4E_p^2 - \Omega^2)}, \quad B_{pc,0} = i \frac{2E_p^2}{\Omega(4E_p^2 - \Omega^2)}, \quad C_{pc,0} = i \frac{\tilde{E}_p}{4E_p^2 - \Omega^2}.
\]

(18)

Solving eq.(17) with respect to \( \hat{g}_{pc} \) by the second order iteration and performing momentum integration, we obtain the diffusion equation of \( \hat{\rho}_e \), which is the momentum-integral of \( \hat{g}_{pc} \) (eq.(12)). The inverse Fourier transformation with respect to \( \omega \) can be performed when we assume \( \Omega \approx i/\tau \) in eq.(18).
3. Definition of charges
The density matrix $\hat{\rho}_e$ is a 4×4 Hermitian matrix. Every 4×4 Hermitian matrix can be decomposed into the following 16 matrices:

$$\begin{align*}
1, \\
\hat{\alpha}_0, \\
\hat{\alpha}_i (i = 1, 2, 3), \\
\hat{\alpha}_5 \equiv \hat{\alpha}_0 \hat{\alpha}_1 \hat{\alpha}_2 \hat{\alpha}_3, \\
\hat{\alpha}_{\mu\nu} \equiv i\hat{\alpha}_\mu \hat{\alpha}_\nu (\mu < \nu \text{ and } \mu, \nu = 0, 1, 2, 3, 5).
\end{align*}$$

Therefore the density matrix $\hat{\rho}_e$ can be written as

$$\hat{\rho}_e = \frac{1}{4} \left[n_e \mathbf{1} + \rho^a_\mu \hat{\alpha}_\mu + \rho^a_{\mu\nu} \hat{\alpha}_{\mu\nu}\right].$$

Here we define 16 "charges" as coefficients corresponding to 16 matrices. Using these charges, we can derive 16 diffusion equations (to be published). For example, diffusion equations for $n_e$, $\rho^1_e$, and $\rho^{12}_e$ can be written as

$$\begin{align*}
\frac{\partial n_e}{\partial t} &= \frac{v^2}{3} \nabla^2 n_e - \frac{v}{3} \partial_x \rho^1_e - \frac{v}{3} \partial_y \rho^2_e - \frac{v}{3} \partial_z \rho^3_e, \\
\frac{\partial \rho^1_e}{\partial t} &= \frac{v^2}{5} \partial_x^2 \rho^1_e + \frac{v^2}{15} \partial_y^2 \rho^1_e + \frac{v^2}{15} \partial_z^2 \rho^1_e + \frac{2v^2}{15} \partial_x \partial_y \rho^1_e + \frac{2v^2}{15} \partial_x \partial_z \rho^1_e \\
&\quad - \frac{v}{3} \partial_x n_e - \frac{v}{6\mu_T} \partial_y \rho^2_e - \frac{v}{6\mu_T} \partial_z \rho^3_e - \frac{\rho^1_e}{(3/2)}, \\
\frac{\partial \rho^{12}_e}{\partial t} &= \frac{v^2}{15} \partial_x^2 \rho^{12}_e + \frac{v^2}{15} \partial_y^2 \rho^{12}_e + \frac{v^2}{5} \partial_z^2 \rho^{12}_e - \frac{2v^2}{15} \partial_x \partial_y \rho^{12}_e + \frac{2v^2}{15} \partial_x \partial_z \rho^{12}_e \\
&\quad - \frac{v}{6\mu_T} \partial_x \rho^2_e + \frac{v}{6\mu_T} \partial_y \rho^1_e - \frac{v}{3} \partial_z \rho^{05}_e - \frac{\rho^{12}_e}{(3/2)}.
\end{align*}$$

We use these equations in the next section, which describe z-component SHE.

In the following, we assume that alpha matrices can be written as

$$\hat{\alpha}_i = \hat{\sigma}_i \times \hat{\tau}_1, \ (i = 1, 2, 3),$$

where $\hat{\sigma}_i$ and $\hat{\tau}_1$ are Pauli matrices in spin and orbital space, respectively. In this system, the particle density $N$, the spin density $S_i$, and other charge density $\rho^a$ can be calculated as

$$\begin{align*}
N(x, t) &= \nu \int dx \ n_e(x, t), \\
S_1(x, t) &= \nu \int dx \ \frac{1}{2} \left[-\rho^{23}_e(x, t)\right], \\
S_2(x, t) &= \nu \int dx \ \frac{1}{2} \left[\rho^{13}_e(x, t)\right], \\
S_3(x, t) &= \nu \int dx \ \frac{1}{2} \left[-\rho^{12}_e(x, t)\right], \\
\rho^a(x, t) &= \nu \int dx \ \rho^a_e(x, t).
\end{align*}$$
4. Spin Hall effect
In this paper, we focus on z-component SHE when the electric field $E = (E_x, 0, 0)$ is applied. We assume that the system size is infinite in x and z directions and finite in y direction. Under this condition, we can drop x and z derivatives. Rewriting diffusion equations (21) with eqs.(13), (14) and (23), we obtain the following equations:

$$\frac{\partial N}{\partial t} = \frac{v^2 \tau}{3} \frac{\partial^2 N}{\partial y^2} - \frac{v}{3} \frac{\partial y^2}{\partial t},$$

$$\frac{\partial \rho^1}{\partial t} = \frac{v^2 \tau}{15} \frac{\partial^2 \rho^1}{\partial y^2} + \frac{ve(2\nu)}{3} E_x + \frac{v}{3\mu \tau} \frac{\partial y S_3}{\partial t} - \frac{\rho^1}{(3\tau)},$$

$$\frac{\partial S_3}{\partial t} = \frac{v^2 \tau}{15} \frac{\partial^2 S_3}{\partial y^2} - \frac{v}{12\mu \tau} \frac{\partial y \rho^1}{\partial t} - \frac{S_3}{(3\tau)}.$$  (24)

Here we have kept only the first order with respect to the electric field and neglected

$$eE_x \partial_y \rho^\alpha, (\alpha = \mu, \mu \nu),$$  (25)

which are the second order contributions.

When $j^{S_3}$ is the z-component spin current and $\tau_s$ is the spin relaxation time,

$$\frac{\partial S_3}{\partial t} = -\nabla \cdot j^{S_3} - \frac{S_3}{\tau_s}.$$  (26)

Comparing eqs.(24) and (26), we obtain

$$j_y^{S_3} = -\frac{v^2 \tau}{15} \frac{\partial y S_3}{\partial t} + \frac{v}{12\mu \tau} \rho^1,$$  (27)

$$\tau_s = \frac{3}{2 \tau}.$$  (28)

This is our definition of the spin current which is naturally defined from the obtained spin diffusion equation.

In the steady state in the bulk, we can drop time and space derivatives in eq.(24). In this case, we have

$$\rho^1 = \tau v e \nu E_x.$$  (29)

Combining eqs.(27) and (29), we obtain non-zero bulk spin current:

$$j_y^{S_3} = \frac{e\mu}{24\pi^2 \nu} E_x \equiv \sigma_{xy}^{S_3} E_x.$$  (30)

Here we have used $\nu = \mu^2 / 2\pi^2 v^3$ and defined the z-component SHC $\sigma_{xy}^{S_3}$. In the system with $\hat{\alpha}_i = \hat{\sigma}_i \times \hat{\tau}_1$, the conventional spin current operator can be defined as

$$j_y^{S_3} = \frac{\{\hat{S}_3, j_y\}}{2} = 0.$$  (31)

Therefore the SHC of this system is 0 for the conventional definition. In our definition, however, we obtain non-zero SHC

It is important to note that we do not assume the form of the spin current operator, while the conventional spin current has no justification.
5. Summary
In this paper, we have derived diffusion equations of a three-dimensional massless Dirac electron system from the quantum kinetic equation. Assuming the specific form of alpha matrices \( \hat{\sigma}_i = \hat{\sigma}_i \times \tau_1 \), we have investigated diffusion equations of the Dirac electron system in terms of spin transport. We have defined the spin current from diffusion equations and found that the system has a finite SHC, though the conventional SHC is zero.

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Appendix A. Semi-classical approximation
In this appendix, we derive the quantum kinetic equation in the semi-classical approximation.

The Wigner transformation of the convolution \( \hat{A} \hat{B} \) is defined as
\[
[\hat{A} \hat{B}](x,t;\hat{p},\epsilon) = \hat{A}(x,t;\hat{p},\epsilon) \hat{B}(x,t;\hat{p},\epsilon),
\]
where the Moyal product \( * \) is
\[
* = \exp \left[ \frac{i\hbar}{2} \left( \hat{\nabla}_x \cdot \hat{\nabla}_{\hat{p}} - \hat{\nabla}_{\hat{p}} \cdot \hat{\nabla}_x - \hat{\nabla}_t \hat{\nabla}_\epsilon + \hat{\nabla}_\epsilon \hat{\nabla}_t \right) \right].
\]
In the semi-classical approximation, we have kept only zeroth and first order terms with respect to \( \hbar \). Up to this order, eq. (A.1) becomes
\[
A(x,t;\hat{p},\epsilon) * B(x,t;\hat{p},\epsilon) \equiv A(x,t;\hat{p},\epsilon)B(x,t;\hat{p},\epsilon) + \frac{i\hbar}{2} \{ A(x,t;\hat{p},\epsilon), B(x,t;\hat{p},\epsilon) \}_{\text{Poisson}},
\]
where
\[
\{ A(x,t;\hat{p},\epsilon), B(x,t;\hat{p},\epsilon) \}_{\text{Poisson}} = \frac{\partial A}{\partial x} \frac{\partial B}{\partial \hat{p}} - \frac{\partial A}{\partial \hat{p}} \frac{\partial B}{\partial x} - \frac{\partial A}{\partial \epsilon} \frac{\partial B}{\partial t} + \frac{\partial A}{\partial t} \frac{\partial B}{\partial \epsilon}
\]
is the Poisson bracket.

In the following, we consider the Wigner transformation of eq.(9) in the semi-classical approximation. First and second terms of LHS can be written as
\[
\left[ \hat{\epsilon}, \hat{G}^K \right](x,t;\hat{p},\epsilon) \equiv \left[ \epsilon, G^K(x,t;\hat{p},\epsilon) \right] + \frac{i\hbar}{2} \{ \epsilon, G^K \}_{\text{Poisson}} - \frac{i\hbar}{2} \{ G^K, \epsilon \}_{\text{Poisson}}
\]
\[
= \frac{i\hbar}{\partial t},
\]
\[
\left[ \hat{G}^K, \hat{H} \right](x,t;\hat{p},\epsilon) \equiv \left[ G^K(x,t;\hat{p},\epsilon), v\hat{\alpha} \cdot \hat{p} \right] + \frac{i\hbar}{2} \{ G^K, v\hat{\alpha} \cdot \hat{p} \}_{\text{Poisson}} - \frac{i\hbar}{2} \{ v\hat{\alpha} \cdot \hat{p}, G^K \}_{\text{Poisson}}
\]
\[
= \left[ G^K(x,t;\hat{p},\epsilon), v\hat{\alpha} \cdot \hat{p} \right] - \frac{i\hbar}{2} \{ \nabla G^K, v\hat{\alpha} \}. \quad (A.5)
\]
The first term of RHS can be written as
\[
\left[ \hat{\Sigma}^K \hat{G}^A \right] (x_t, p_e) \equiv \sum^K (x_t, p_e) G^A(x_t, p_e)
\]
\[= \int d(\delta x) d(\delta t) e^{-i p \cdot \delta x + i \epsilon \delta t} \Sigma^K \left( x + \frac{\delta x}{2}, x - \frac{\delta x}{2} \right) G^A_{p_e}
\]
\[= \int d(\delta x) d(\delta t) e^{-i p \cdot \delta x + i \epsilon \delta t} \frac{\delta(\delta x)}{\pi \nu \tau} G^K \left( x - \frac{\delta t}{2}; x, t + \frac{\delta t}{2} \right) G^A_{p_e}
\]
\[= \frac{1}{\pi \nu \tau} \int d(\delta t) e^{i \epsilon \delta t} \frac{i}{\pi} \int \frac{d\epsilon' dp'}{(2\pi)^3} g_{p'}(x, t) e^{-i \epsilon' \delta t} G^A_{p_e}
\]
\[= \frac{2i}{\tau} \hat{\rho}_e(x, t) G^A_{p_e}. \]  

(A.6)

Here we have used eq.(7) in the third line. We also obtain
\[
\left[ \hat{G}^R \hat{\Sigma}^K \right] (x_t, p_e) \equiv -\frac{2i}{\tau} G^R_{p_e} \hat{\rho}_e(x, t)
\]

(A.7)

in the same procedure. Finally, we obtain eq.(11).

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