Noncommutative quantum mechanics and skew scattering in ferromagnetic metals
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Abstract: The anomalous Hall effect is classified into two based on the mechanism. The first one is the intrinsic Hall effect due to the Berry curvature in momentum space. This is a Hall effect that solely arises from the band structure of solids. On the other hand, another contribution to the Hall effect, so-called extrinsic mechanism, comes from impurity scatterings such as skew scattering and side jump. These two mechanisms are often discussed separately; the intrinsic Hall effect is related to the Berry curvature of the band while the skew scattering is studied using the scattering theory approaches. However, we here show that, in an electronic system with finite Berry curvature, the skew scattering by nonmagnetic impurities is described by the noncommutative nature of the real-space coordinates due to the Berry curvature of the Bloch wavefunctions. The anomalous Hall effect due to this skew scattering is estimated and compared with the intrinsic contribution.

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I. INTRODUCTION

Berry phase connection

\[ a(k) = i \langle u_k | \nabla_k | u_k \rangle \]

of the band structures in solids, which describes how the two neighboring Bloch functions overlap in the crystal momentum \( (k) \)-space, plays important roles in a variety of phenomena. \( \langle u_k \rangle \) is the periodic part of the Bloch function with crystal momentum \( k \), and \( \nabla_k \) is the gradient operator with respect to \( k \). This \( a(k) \) plays the role of the vector potential and leads to the Berry curvature \( b(k) = \nabla_k \times a(k) \) analogous to the magnetic field. The Berry connection \( a(k) \) has the physical meaning of the intracell coordinate, i.e., the real-space position of the wavepacket measured from the Wannier coordinate reads

\[ r = i \frac{\partial}{\partial k} + a(k). \] (1)

On the other hand, the Berry curvature \( b(k) \) gives a nonzero commutation relation between the components of the real-space coordinate \( r \). For example,

\[ [x, y] = [i \frac{\partial}{\partial k_x} + a_x(k), i \frac{\partial}{\partial k_y} + a_y(k)] = i \left( \frac{\partial a_y}{\partial k_x} - \frac{\partial a_x}{\partial k_y} \right) = ib_z(k). \] (2)

Therefore, the wavepackets made of the Bloch functions are described by the noncommutative quantum mechanics. This fact leads to the so-called anomalous velocity and also the intrinsic anomalous Hall effect (AHE) in metallic ferromagnets. Namely, the transverse anomalous velocity to the external electric field is induced by the Berry curvature \( b(k) \), which is the dual to the Lorentz force due to the magnetic field in real space. This intrinsic mechanism due to the geometric nature of the Bloch wavefunctions is now confirmed in many materials by the comparison between the first-principles calculations and experiments.

Historically, however, the intrinsic mechanism of the AHE was questioned for a long period, as the impurity scatterings relax the momentum distribution to the steady state under the external electric field. As impurity scatterings are inevitable in solids and they seem to cancel the force acting on the electrons, the anomalous velocity induced by the Berry curvature was expected to vanish; thus, no intrinsic AHE. Therefore, the extrinsic mechanisms due to impurity scattering were established earlier. Historically, Smit was the first to propose the extrinsic mechanism of AHE by the skew scattering, where the transition probability for the scattering \( k \rightarrow k' \) is different from that of \( k' \rightarrow k \), i.e., the detailed balance condition is broken. Later, another extrinsic mechanism called side jump was proposed, where a transverse shift of the electron trajectory occurs at the scatterers. In these mechanisms, the spin-orbit interaction (SOI) plays a key role in the asymmetry of the scattering amplitude.

Usually, the intrinsic and extrinsic mechanisms of AHE are discussed separately; the effect of impurities are often considered to be irrelevant for the intrinsic Hall effect, while the skew scattering is studied as a scattering problem and the effect of the Berry phase is not (explicitly) considered. Indeed, the two contributions are considered to be dominant in different regimes of the longitudinal resistivity \( \rho_{xx} \), the intrinsic one is dominant in the region \( 1 \mu \Omega \text{cm} < \rho_{xx} < 10 \mu \Omega \text{cm} \) while the skew scattering is dominant for \( \rho_{xx} < 1 \mu \Omega \text{cm} \). The side jump mechanism is also effective, but often smaller than these two. Technically, skew scattering appears in the second Born approximation; it appears from the interference of the first order and second order scattering processes.

In this paper, we study the scattering by an impurity potential for the electronic states with finite Berry curvature in terms of the noncommutative quantum mechanics. The key observation is that the nonzero commutators between the components of the real-space coordinates urge to introduce the new canonical coordinates, which satisfies the usual commutation relations. This results in the asymmetric scattering as we see in Eqs. (7) and (13), which leads to the skew scattering. The results imply that the skew scattering is a ubiquitous phenomenon that appears in a system with finite Berry curvature.
The paper is organized as follows. In Sec. II, we introduce the model we consider throughout this paper; a non-interacting electron system with non-magnetic impurities without SOI. A difference from the conventional scattering problem is that the position operators do not commute with each other due to the non-zero Berry curvature. Using this model, in Sec. III, we discuss how the noncommutativity leads to skew scattering using the second Born approximation. In Sec. IV, using the scattering rate obtained in Sec. III, we present the explicit form of the anomalous Hall conductivity using the semiclassical Boltzmann theory. We also discuss the competition between the AHE induced by skew scattering and that by intrinsic mechanism, which both arise from the Berry curvature. Section V is devoted to discussions and summary.

II. MODEL

In this paper, we consider a three-dimensional space denoted by \( \mathbf{x} = (x, y, z) = (x_1, x_2, x_3) \) and its momentums \( \mathbf{p} = (p_x, p_y, p_z) = (p_1, p_2, p_3) \) with the following commutation relations:

\[
\begin{align*}
[x_1, x_2] &= i\hbar, \\
[x_1, x_3] &= 0, \\
[x_1, p_j] &= i\delta_{ij}, \\
[p_i, p_j] &= 0,
\end{align*}
\]

where \( i, j = 1, 2, 3 \). In solids, the noncommutativity of the position operators is a consequence of the Berry curvature; it is briefly explained in Eqs. (1) and (2) of Sec. I. Throughout this paper, we put \( \hbar = 1 \). To study the effect of impurity scattering, we here consider a single particle Hamiltonian of spinless fermion with (non-magnetic) impurities:

\[
\begin{align*}
H &= H_0 + H_V, \\
H_0 &= \frac{\mathbf{p}^2}{2m}, \\
H_V &= V \sum_i \delta(\mathbf{x} - \mathbf{x}_i),
\end{align*}
\]

where \( H_0 \) is the Hamiltonian for the free electrons and \( H_V \) is the impurity Hamiltonian; \( V \) is the strength of potential induced by a scatterer, \( \delta(\mathbf{x}) \) is the three-dimensional delta function, and \( \mathbf{x}_i \) is the position of the impurity. The sum in the second term is over all impurities indexed by \( i \). Note that \( V \) has the dimension of (energy)\( \times \) (length)\( ^3 \); when we consider the case of impurity atoms replacing the host atoms that form a crystal, \( V \) should be replaced by \( v a^3 \), where \( v \) is the potential energy and \( a \) the lattice constant (Hereafter, we take the unit \( a = 1 \)). In the discussion below, we treat \( H_V \) as a perturbation and assume \( V \) is the same for all impurities. However, an extension to a set of impurities with different scattering strength is straightforward.

III. ASYMMETRIC SCATTERING RATE

We first investigate the scattering problem with one impurity at the center, i.e., \( \mathbf{x}_0 = 0 \). We discuss that an asymmetric scattering term arises from the noncommutativity of position operators, which has the same form as the skew scattering. For simplicity, we set \( \mathbf{b} = (0, 0, b) \) to be constant. The eigenstates of single particle Hamiltonians with the commutation relation in Eq. (3) can be obtained by introducing an alternative set of commutative “position” operators, \( X_1 \) and \( X_2 \), that gives two sets of canonical coordinates and momenta, \( (X_1, p_1) \) and \( (X_2, p_2) \):

\[
\begin{align*}
X_1 &= x_1 + \frac{b}{2} p_2, \\
X_2 &= x_2 - \frac{b}{2} p_1, \\
X_3 &= x_3.
\end{align*}
\]

Using \( X_i \) instead of \( x_i \) in Eq. (3), we obtain three sets of canonical coordinates and momenta:

\[
\begin{align*}
[X_1, X_j] &= 0, \\
[X_1, p_j] &= i\delta_{ij}, \\
[p_i, p_j] &= 0.
\end{align*}
\]

We, here, use this new coordinate to calculate the scattering amplitude of the Hamiltonian in Eq. (4a). Using \( X_1 \), the impurity Hamiltonian reads

\[
\begin{align*}
\langle k'|V \delta(\mathbf{x})|k\rangle &= \langle k'| \left( \frac{V}{2\pi i} \int dq \ e^{iq \cdot \mathbf{x}} \right) |k\rangle, \\
&= \langle k'| \left( \frac{V}{2\pi} \int dq \ e^{iq \cdot \mathbf{x}} e^{i\frac{b}{2} (p \times q)} \right) |k\rangle, \\
&= e^{i\frac{b}{2} (k \times k')_3},
\end{align*}
\]

where \( (\cdots)_3 \) is the \( i = 3 \) component of the vector in the round bracket. Here, we used Baker-Campbell-Hausdorff formula to factorize the exponential function.

To calculate the scattering rate \( W_{k \to k'} \), we here use the Born approximation\(^{29,35} \). Within the second Born approximation, \( W_{k \to k'} \) reads

\[
W_{k \to k'} = 2\pi |F^{(1)}(k', k) + F^{(2)}(k', k)|^2 \delta(\varepsilon_k - \varepsilon_{k'}),
\]

where

\[
F^{(1)}(k', k) = \langle k'| V \delta(\mathbf{x}) |k\rangle, \quad F^{(2)}(k', k) = \langle k'| V \delta(\mathbf{x}) G(0, \varepsilon_k) V \delta(\mathbf{x}) |k\rangle,
\]

and

\[
F^{(1)}(k', k) = \langle k'| V \delta(\mathbf{x}) |k\rangle, \quad F^{(2)}(k', k) = \langle k'| V \delta(\mathbf{x}) G(0, \varepsilon_k) V \delta(\mathbf{x}) |k\rangle,
\]

are the first and second Born terms, respectively. Here, \( |k\rangle \) is the eigenstate for \( p, p|k\rangle = k|k\rangle, \varepsilon_k = k^2 / 2m \) is the
been shown to be a useful approach for studying AHE that can take into account the intrinsic and other impurity-induced mechanisms. For simplicity, however, we here focus on the skew scattering term and calculate the explicit formula for the anomalous Hall conductivity that arise from the impurity scattering studied in Sec. III. In the leading order, the contribution from other terms are given as a simple sum of the different contributions such as side-jump. Therefore, it should be straightforward to evaluate the Hall conductivity in presence of all different contributions.

\[ G(x, \omega) = \int \frac{dK'}{(2\pi)^3} \mathcal{G}(K', \omega)e^{ik' \cdot r}, \]

(11)

where \( \mathcal{G}(K', \omega) \) is the Fourier transform of \( G(x, \omega) \).

\[ G(K', \omega) = \frac{1}{\omega - \frac{e^2}{2m} + i \epsilon} \frac{\Lambda^2}{\hbar^2 + \Lambda^2}. \]

(12)

In Eq. (12), \( \Lambda \) is the cutoff introduced to avoid the divergence that appears in the integral for \( k' \) in Eq. (11); we take the \( \Lambda \to \infty \) limit at the end of the calculation of \( F^{(2)} = (k', k) \). The result in Eq. (10) is after taking the \( \Lambda \to \infty \) limit; it turns out \( F^{(2)}(k', k) \) converges to a finite value in the limit.

Using the \( F^{(1)}(k', k) \) and \( F^{(2)}(k', k) \), we calculate the leading part of the scattering rate \( W^{(\text{sym})}_{k \to k'} \). We find that the leading order of the asymmetric part is \( V^3 \); it arises from the products \( F^{(1)}(k', k)F^{(2)}(k', k) \) and \( F^{(2)}(k', k) \). The leading order of \( W^{(\text{ asym})}_{k \to k'} \) reads

\[ W^{(\text{asym})}_{k \to k'} = \frac{1}{2} \left( W_{k \to k'} - W_{k' \to k} \right), \]

\[ = - \frac{(2\pi)^3}{\Omega} \frac{n_i V^3}{(2\pi)^2} \frac{m}{|b(k_3 - k'_3)|} \delta(\varepsilon_k - \varepsilon_{k'}), \]

\[ \sim - \frac{(2\pi)^3}{\Omega} \frac{n_i V^3}{(2\pi)^2} \frac{m}{b(k \times k')} \delta(\varepsilon_k - \varepsilon_{k'}). \]

(13)

Here,

\[ w_{k', k}(b) = \sin \left[(b/2)(k \times k')_3\right] \sin \left[(k/2)|b(k_3 - k'_3)|\right], \]

(14)

\( n_i = N_i/\Omega \) is the density of impurities, \( \Omega \) is the volume, and \( N_i \) is the number of impurities. In Eq. (13), we expanded \( w_{k', k}(b) \) by assuming \( k_3^2 b \ll 1 \); it has the same \( k \) dependence as that of skew scattering induced by an impurity with spin-orbit interaction.

**IV. ANOMALOUS HALL CONDUCTIVITY**

In this section, we evaluate the Hall conductivity using the Boltzmann transport theory. Recently, this method has been shown to be a useful approach for studying AHE that can take into account of the intrinsic and other impurity-induced mechanisms. For simplicity, however, we here focus on the skew scattering term and calculate the explicit formula for the anomalous Hall conductivity that arise from the impurity scattering studied in Sec. III. In the leading order, the contribution from other terms are given as a simple sum of the different contributions such as side-jump. Therefore, it should be straightforward to evaluate the Hall conductivity in presence of all different contributions.

The semiclassical Boltzmann equation reads:

\[ q v_k \cdot E f_0' (\varepsilon_k) = -\frac{g_k}{\tau} + \frac{1}{(2\pi)^3} \int dq' k' \rightarrow k q' g_{k'}, \]

\[ = -\frac{g_k}{\tau} + \frac{1}{4\pi} \int d\theta' d\phi' \rho(\varepsilon_F) \tilde{V}(k) \cdot \frac{k \times k'}{k'^2} g_{k'}. \]

(15)

where \( q \) is the charge of the particle, \( E \) is the external d.c. electric field, \( v_k = \nabla \varepsilon_k \) is the velocity of the electron in \( k \) state, \( f_0' (\varepsilon) = d f_0(\varepsilon)/d\varepsilon \) with \( f_0(\varepsilon) \) is the Fermi-Dirac distribution function, and \( \rho(\varepsilon_k) = n_k/2\pi^2 \) is the density of states for \( H_0 \) at energy \( \varepsilon_k \). Here we assumed the occupation of electrons \( f_k \) is close to \( f_0(\varepsilon_k) \), i.e.,

\[ f_k = f_0(\varepsilon_k) + g_k, \]

that is, the scattering term that involves \( W^{(\text{sym})}_{k \to k'} \) is replaced by \( -g_k/\tau \). where \( \tau \) is the relaxation time.

For the integral in Eq. (15), we assumed the form

\[ W^{(\text{sym})}_{k \to k'} = \tilde{V}(k) \cdot \frac{k \times k'}{k'^2}, \]

(16)

with \( \tilde{V}(k) = [\tilde{V}_1(k), \tilde{V}_2(k), \tilde{V}_3(k)] \) being the function of \( k \); this is a generalization of the antisymmetric scattering term in Eq. (13). The integral is written using the polar coordinate \( k' = (k' \cos \theta' \cos \phi', k' \cos \theta' \sin \phi', k' \sin \theta') \); the radius is fixed to \( k' = k \) due to the energy conservation, i.e., the delta function in Eq. (13).

Equation (15), is solved using a self-consistent approach. For this, we introduce a new parameter

\[ P(k) = \int d\theta' d\phi' \sin \theta' k' g_{k'}. \]

(17)

Using Eqs. (15) and (17), \( g_k \) become

\[ g_k = -\frac{\tau q v_k \cdot E f_0' (\varepsilon_k)}{4\pi} \delta \rho(\varepsilon_F) \tilde{V}(k) \times P(k), \]

(18)

Substituting Eq. (18) into \( g_k \) in the integrand of Eq. (17), the solution for \( P(k) \) reads

\[ P(k) = -\frac{\tau q}{m} 2\pi k^2 f_0' (\varepsilon_k) E + \frac{\tau q}{2} \rho(\varepsilon_F) K \times \tilde{V}(k), \]

\[ \sim -\frac{\tau q}{m} 2\pi k^2 f_0' (\varepsilon_k) E. \]

(19)

Here, we assumed \( \tilde{V} \perp E \). In the second line, we expanded the result to the leading order in \( \tau \). Therefore, to the leading order in \( E \) and \( \tau \), Eq. (18) reads

\[ g_k = -\frac{\tau q f_0' (\varepsilon_k) v_k}{2} \left( E + \frac{\tau q}{2} \rho(\varepsilon_F) \tilde{V}(k) \times E \right). \]

(20)
Hence, the contribution from impurity scattering to the transverse conductivity reads
\[ \sigma_{xy} = -\frac{nq^2\tau^2}{2m} \rho(\varepsilon_F)\tilde{V}(k_F), \]  
where \( k_F \) is the Fermi velocity and \( \varepsilon_F \) is the Fermi energy. For the \( W_{k'\rightarrow k}^{\text{any}} \) in Eq. (13), \( \tilde{V}(k) \) reads
\[ \tilde{V}(k) = -2\pi n_i V^3 mk^3 \hat{a}_3, \]
where \( \hat{a}_3 = (0, 0, 1) \) is the unit vector along the \( x_3 \) axis. Therefore, the transverse conductivity becomes
\[ \sigma_{xy} = \frac{nq^2\tau^2 n_i}{2\pi} V^3 mk^3 b. \]

In the last, we discuss the scaling relation of the skew scattering induced Hall effect. When the major source of scattering is the elastic scattering by the impurities, \( \tau \) in Eq. (21) is estimated to be \( 1/\tau \sim n_i V^2 \rho(\varepsilon_F) \). On the other hand, from Eq. (13), we see that the leading order of \( \tilde{V}(k) \) reads
\[ \tilde{V}(k) \sim n_i V^3 \rho(\varepsilon_F)b k_F^3. \]  Therefore, similar to the skew scattering by an impurity with SOI, the Hall conductivity is \( \sigma_{xy} \sim \rho(\varepsilon_F) V^2 k_F^3 b \sigma_{xx} \) with \( \sigma_{xx} = nq^2\tau/m \) being the longitudinal conductivity. Hence, the Hall angle for the AHE due to skew scattering is estimated as \( \sigma_{xy}/\sigma_{xx} \sim V^2 \rho(\varepsilon_F) k_F^3 b \). This result indicates a relation between the longitudinal (\( \rho_{xx} \)) and transverse (\( \rho_{yx} \)) resistivities as \( \rho_{yx} \propto \rho_{xx} \) with the fixed strength of the impurity potential \( V \).

In addition to the skew scattering we discussed here, an electronic band with a finite net Berry curvature shows intrinsic AHE\(^4,17,18\); the intrinsic Hall conductivity is proportional to the number of carriers and Berry curvature, \( \sigma_{xy}^{\text{int}} \sim nq^2 b \).

A key difference is that \( \sigma_{xy}^{\text{int}} \) is insensitive to the longitudinal conductivity while the anomalous Hall conductance by skew scattering is \( \sigma_{xy}^{(sk)} \propto \sigma_{xx} \). Therefore, it is expected that the skew scattering becomes the major cause of Hall effect when the system is clean while the intrinsic Hall effect dominates when \( \sigma_{xx} \) is small\(^27,31\). The crossover occurs when \( \sigma_{xy}^{(sk)}/\sigma_{xy}^{(int)} \sim \varepsilon_F/(n_i V) \sim 1 \): this indicates that the crossover of AHE from intrinsic to skew scattering occurs at \( \sigma_{xx} \sim q^2/(mV) \). Therefore, the skew scattering is dominant when \( V \lesssim \varepsilon_F \) while the intrinsic AHE is dominant if \( V \gtrsim \varepsilon_F \).

In addition to the intrinsic contribution, side-jump mechanism also contributes to the AHE in magnetic metals\(^30\). While the side-jump contribution is generally considered to be smaller than the other two\(^27\), it has been discussed that the contribution can be large for the constant Berry curvature case considered in this manuscript\(^37\). However, even for this case, the magnitude of side-jump effect is the same as that of the intrinsic one. Therefore, the above argument should hold even when there exists an observable contribution from the side-jump mechanism.

V. DISCUSSION AND SUMMARY

To summarize, in this work, we studied the anomalous Hall effect from the viewpoint of noncommutative quantum mechanics. In presence of the Berry curvature \( b(k) \), we find that a non-magnetic impurity generally contributes to the skew scattering regardless of the spin-orbit interaction. Using a Boltzmann theory, we present the explicit form of the anomalous Hall conductivity induced by this mechanism. Analogous to the case of the skew scattering by an impurity with spin-orbit interaction, the skew scattering in the current mechanism also results in a Hall conductivity that is linearly proportional to the longitudinal conductivity.

We note that a similar idea on the skew scattering proportional to Berry curvature was pointed out in Ref.\(^5\). This preceding paper, however, introduces the asymmetric scattering as a phenomenological scattering term; in general, the derivation of the asymmetric scattering term becomes a complicated task due to the noncommutativity of the position operators. In contrast, in this paper, we used a method of noncommutative quantum mechanics and derived the scattering term microscopically within the second Born approximation.

The results indicate that the Berry curvature of the electronic bands is the sufficient condition for skew scattering to occur. This shows that the skew scattering is a ubiquitous phenomenon that appears in the materials with nonzero Berry curvature. For instance, magnets with non-coplanar magnetic orders show nontrivial electronic states with nonzero Berry curvature\(^40-42\); such states are expected to appear in frustrated magnets\(^43-45\). Our results indicate that, the anomalous Hall effect due to skew scattering by nonmagnetic impurities also appears in these magnets as long as the Berry curvature is there, although the spin-orbit interaction does not appear in the electronic Hamiltonian.

Regarding the relation to anomalous Hall effect in collinear ferromagnets, in these systems, the Berry curvature often arises as a consequence of the spin-orbit interaction. Therefore, our theory provides a different view on the skew scattering induced by the host spin-orbit interaction. Remarkably, Smit already discussed that the spin-orbit interaction at the impurity potential is not required for the skew scattering\(^29\). Further studies on such possibilities were explored in various systems considering multiple bands and the scattering between them\(^32,46-51\). Our study, in contrast, considered a single band model with Berry curvature, i.e., the multiple band effects are taken into account as the Berry curvature.

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