Non-adiabatic Hall effect at Berry curvature hot spot

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Abstract

Hot spot of Berry curvature is usually found at Bloch band anti-crossings, where the Hall effect due to the Berry phase can be most pronounced. With small gaps there, the adiabatic limit for the existing formulations of Hall current can be exceeded in a moderate electric field. Here we present a theory of non-adiabatic Hall effect, capturing non-perturbatively the across gap electron-hole excitations by the electric field. We find a general connection between the field induced electron-hole coherence and intrinsic Hall velocity. In coherent evolution, the electron-hole coherence can manifest as a sizeable ac Hall velocity. When environmental noise is taken into account, its joint action with the electric field favors a form of electron-hole coherence that is function of wavevector and field only, leading to a dc non-linear Hall effect. The Hall current has all odd order terms in field, and still retains the intrinsic role of the Berry curvature. The quantitative demonstration uses the example of gapped Dirac cones, and our theory can be used to describe the bulk pseudospin Hall current in insulators with gapped edge such as graphene and 2D MnBi\textsubscript{2}Te\textsubscript{4}.

1. Introduction

Intrinsic Hall current arising from Berry phase effect ofBloch electrons is of long standing interest [1, 2]. The Hall conductivity is determined by the Berry curvature, which, being inversely proportional to the square of the band separation, is most pronounced at band anti-crossings with small gap. A seminar example is the gapped Dirac cones found in graphene with inversion symmetry breaking[3–10], surface bands of ultrathin films of topological insulators [11–13] and magnetic topological insulators such as MnBi\textsubscript{2}Te\textsubscript{4} [14–21], which are all drawing great interest. Berry curvature distribution features hot spot at the Dirac point, where a small momentum space area can enclose a sizeable flux, underlying a strong Hall response.

Existing formulations of Hall effects are limited to the adiabatic regime, i.e. assuming a sufficiently large gap preventing electric field to create interband excitations [2]. The first order adiabatic approximation gives the linear response, with an intrinsic Hall conductivity equal to the Berry curvature flux enclosed by the equilibrium Fermi sea [22]. Generalization of the Hall effect to second order in electric field has also been progressed along two lines, both in the adiabatic limit [23–29], by either including a field correction to the Berry curvature, [23] or the extrinsic mechanism of disorder scatterings and non-equilibrium carrier distribution [24–29]. Experimental observations of second order Hall effect have been reported in 2D WTe\textsubscript{2} [30–32], where the Fermi energy also lies near a Berry curvature hot spot from a band anti-crossing [30, 31]. These findings have stimulated remarkable interests on non-linear Hall responses.

A Berry curvature hot spot, however, is always accompanied by a small gap. In the aforementioned materials, the gap is within a few tens of meV [4–6, 14, 15, 30, 31, 33], which is not sufficient to guarantee adiabaticity in experimental conditions, especially when a large current is desired. In addressing the strong Hall effect at such Berry curvature hot spots, going beyond the adiabatic regime is therefore highly relevant, which can in principle lead to non-perturbative response to the electric field.

It is also known that, when Fermi energy lies in the gap, the Dirac cone has a half-quantized Hall conductivity in the linear response, \(\frac{1}{2}\text{sgn}(\Delta)\frac{e^2}{\hbar}\), where \(\Delta\) is the Dirac mass (gap) [34, 35]. In reality, Dirac cones come in pairs. For example, graphene has a pair of cones with opposite (same) \(\Delta\) forming the \(K\)
and \(-K\) valleys at Brillouin zone corners [3], when the gap is opened by inversion (time reversal) symmetry breaking [3, 36]. And the recently discovered even-layer MnBi\(_2\)Te\(_4\) ultrathin films feature two cones with opposite (same) \(\Delta\) on the top and bottom surfaces respectively, when the magnetic order is layer anti-ferromagnetic (ferromagnetic) [15]. Two cones of same \(\Delta\) makes a quantum anomalous Hall insulator, where the bulk-edge correspondence dictates a chiral edge channel inside the bulk gap. Opposite \(\Delta\) for the pair of cones, labeled by the valley or layer pseudospin, means a half-quantized pseudospin Hall conductance in the gap. In such case, however, the edge can also remain gapped as in the case of graphene and MnBi\(_2\)Te\(_4\) [16, 35], and the absence of conduction channels at Fermi energy raises the intriguing issue of how the valley or pseudospin current is sustained [6–8].

Here we present a theory of non-adiabatic Hall effect, capturing the across gap excitation by the electric field in the non-perturbation regime. In the coherent evolution in constant electric field, a massive Dirac electron is shown to develop a sizeable ac Hall velocity, lying in the field induced interband coherence dependent on evolution history. When environmental noise is taken into account, the joint action of electric field and decoherence favors certain form of interband coherence that is function of wavevector and field only, with memory effect erased. The corresponding Hall velocity is given by the Berry curvature times a normalization factor non-perturbative in field. This leads to a dc non-linear Hall current, where the intrinsic contribution contains all odd order terms in field. A general connection between field induced interband (electron-hole) coherence and intrinsic Hall effect is thus established in both the coherent and incoherent dynamics, with the known linear response result properly reproduced. For insulator with gapped edge like the graphene and MnBi\(_2\)Te\(_4\) examples, the pseudospin Hall current can be sustained in the bulk as the interference of the field induced electron-hole pair excitations with the Fermi sea background. Our result is applicable to a general band anti-crossing with a narrow gap.

2. Results

In a homogeneous electric field \(E\), the time evolution of an electron is described by

\[
\mathcal{H}(k)|u_k\rangle = i\hbar \dot{|u_k}\rangle,
\]

where \(\hbar \dot{u_k} = -eE\). The instantaneous eigenstates of \(\mathcal{H}(k)\) are the Bloch functions: \(\mathcal{H}(k)|u_{n,k}\rangle = \varepsilon_{n,k}|u_{n,k}\rangle\), \(\varepsilon_{n,k}\) giving the band dispersion. For electron initially in a band \(n\), the zeroth order adiabatic evolution is given by \(|u_k\rangle \approx \hat{\phi}_{\text{ad}}(t)|\varepsilon_{n,k}\rangle |u_{n,k}\rangle\), \(\hat{\phi}_{\text{ad}}\) is the dynamical phase, and \(\gamma_{n}(k) = \frac{\hbar}{k_{\text{F}}} d k'\). \([\mathcal{R}_{k}]_{n,m}\) is the Berry phase, where \(\mathcal{R}_{k} = \langle u_{m,k} | i \frac{\partial}{\partial k} | u_{n,k}\rangle\) is the Berry connection between bands \(n\) and \(m\).

A finite electric field causes non-adiabaticity, where the wavefunction in general is a superposition of multiple bands: \(|u_k\rangle = \sum_{n} \eta_{n}(t) e^{i\gamma_{n}(k)} |u_{n,k}\rangle\). The electron velocity then has two parts \(\dot{x} \equiv \langle u_k | \frac{\partial \mathcal{H}(k)}{\partial k} | u_k\rangle = v_h + v_\eta\),

\[
v_h = \sum_{n} |\eta_{n}\rangle \frac{\partial \varepsilon_{n,k}}{\hbar \partial \varepsilon_{n,k}}, \tag{2}
\]

\[
v_\eta = \sum_{m \neq n} \eta_{m}^{*} \eta_{n} e^{i(\varepsilon_{n,k} - \varepsilon_{m,k})} \left\langle u_{m} | \frac{\partial \mathcal{H}}{\hbar \partial \varepsilon_{n,k}} | u_{n}\rangle \right\rangle + \text{c.c.} \tag{3}
\]

\(v_h\) is the normal part from band dispersions. \(v_\eta\) is the anomalous velocity from interband coherences, which is our focus here. The band amplitudes \(\eta_{n}\) are subject to the equation of motion,

\[
\hat{\mathcal{H}} \eta = i\hbar \dot{\eta}, \tag{4}
\]

where \(\eta\) is a column vector whose entries are \(\eta_{n}\). For example of massive Dirac fermion with only two bands \((n = \xi, \nu)\),

\[
\hat{\mathcal{H}} = \begin{pmatrix}
\varepsilon_{\nu,k} & \left[\mathcal{R}_{k}\right]_{\nu\nu} e^{i\gamma(k)} \\
\left[\mathcal{R}_{k}\right]_{\nu\nu}^{*} e^{-i\gamma(k)} & \varepsilon_{\nu,k}
\end{pmatrix}, \tag{5}
\]

where \(
\left[\mathcal{R}_{k}\right]_{\nu\nu} = e^{-i\gamma(k)} \left[\mathcal{R}_{k}\right]_{\nu\nu} e^{i\gamma(k)}\)

\(\mathcal{H}\) is effectively a Hamiltonian in the moving frame of the carrier, whose \(k\)-space motion by the electric field gives rise to the coherent hybridization between the Bloch bands, manifested as the off-diagonal term of equation (5). The solution of \(\eta\), formally expressed by

\[
\eta(t) = \hat{T} \exp \left\{-i \int_{0}^{t} \text{d} \tau \hat{\mathcal{H}}(k(\tau), E(\tau)) \right\} \eta(0), \tag{6}
\]

with \(\hat{T}\) the time ordering operator, necessarily contains non-perturbative effects of electric field to all orders. Keeping the electric field effect to the leading order only, the above solution for an electron initially in band \(\nu\) reduces to [37]

\[
|u_{\nu}(t)\rangle = \hat{\phi}_{\text{ad}}(t) \left( e^{i\gamma(\nu,k)} |u_{\nu,k}\rangle + r(k,E) e^{i\gamma(k)} |u_{\nu,k}\rangle \right),
\]

where,

\[
r(k,E) = \frac{-\left[\mathcal{R}_{k}\right]_{\nu\nu}^{*} (eE)}{\varepsilon_{\nu,k} - \varepsilon_{\nu,k}}, \tag{7}
\]

a dimensionless quantity measuring the ratio between the field strength to the gap size. The anomalous velocity from the interband coherence then becomes,

\[
v_\eta = r(k,E) e^{i(\gamma_{\nu}(k) - \gamma_{\nu}(k))} \left\langle u_{\nu} | \frac{\partial \mathcal{H}(k)}{\hbar \partial \varepsilon_{n,k}} | u_{\nu}\rangle \right\rangle + \text{c.c.}
\]
Here by retaining the leading order band hybridization of the moving electron driven by electric field (equation (5)), the intrinsic Hall effect from the band Berry curvature \( \Omega_e = \nabla \times [R |_{k}] \) is recovered. Importantly, concerning the Hall current for an ensemble of electrons, \( J^I = -e \int dk f(k) v_h \),\(^{(9)}\) in this first order adiabatic approximation, \( v_h \) is purely a function of \( k \) without other time dependence, so the Hall conductance is completely determined by the instantaneous Fermi distribution \( f(k) \). A steady state dc Hall current is obtained when \( f(k) \) is stabilized by momentum relaxation. In contrast, in the general non-adiabatic dynamics at large \( r \), when the electric field is retained to all orders in equation (6), \( v_h \) is not a pure function of \( k \), but has additional time dependence determined by the evolution history. Figure 1 shows examples of numerically calculated exact evolutions for a massive Dirac cone with the mass \( \Delta = 0.01 \text{ eV} \) in an electric field of \( 1 \text{ V/\mu m} \), which corresponds to \( r \approx 6 \) at the Dirac point. \( v_h(t) \) are oscillating functions of time, with amplitudes and phases dependent on the initial \( k_0 \). Interestingly, when \( k \) evolves far away from the Dirac point, the component parallel to the electric field \( v^\parallel_h \) damps out, while the perpendicular component \( v^\perp_h \) reaches a constant amplitude, corresponding to an ac Hall velocity. This is evident by applying equation (3) to the Dirac Hamiltonian, which leads to

\[
\begin{align*}
 v^\perp_h &= \frac{2v_D}{k} \left( k_{||} \text{Im}Z - \frac{k_{||} \Delta}{\nu_{\perp} - \nu_{\perp}} \text{Re}Z \right), \\
 v^\parallel_h &= \frac{2v_D}{k} \left( -k_{||} \text{Im}Z - \frac{k_{||} \Delta}{\nu_{\parallel} - \nu_{\parallel}} \text{Re}Z \right),
\end{align*}
\]

where \( Z = e^{i\gamma_z(k_{||} - \gamma_z(k_{||}))\eta_i \eta_j} \), \( v_D \) is the Dirac velocity and \( k_{||} (k_{\perp}) \) denotes the component of \( k \) parallel (perpendicular) to \( E \). On the other hand, this oscillation, and the history dependence, apparently raise the issue of how steady state dc current can be reached in the non-adiabatic regime.

In reality, interband coherence can not be retained in arbitrary form in the presence of decoherence due to the environment. To account for such effect, we introduce a stochastic noise to the evolution. Writing \( \hat{H} \equiv \hat{H}(k) - \sigma \cdot \sigma \) the vector of Pauli matrices, this Hamiltonian-like term in equation (4) is now replaced by \( [H + F(t)\hat{I}] \cdot \sigma \), where \( I \) a unit vector specified by polar angle \( \theta \) and azimuthal angle \( \phi \) with respect to \( h \). The stochastic force has zero mean \( \langle F(t) \rangle_i = 0 \) and noise correlation \( \langle F(t) F(t') \rangle_i = \int \frac{d\omega}{2\pi} \left[ n(\omega)e^{i\omega(t-t')} + e^{-i\omega(t-t')} n(\omega) + 1 \right] J(\omega) \) specified by the spectral density \( J(\omega) \). Instead of the coherent wavefunction \( \eta_i \), we turn to the noise-averaged density matrix \( \rho(t) = \langle \eta_i(t) \eta_j^\dagger(t) \rangle_i \). Under the Born-Markov approximation for the noise spectrum, \([38,40]\)

\[
\dot{\rho} = i \frac{\hbar}{\nu} [\rho, \hat{H}] - \frac{1}{2\nu} [\{n \cdot \sigma, \Gamma_- \rho - \rho \Gamma_+ \}].
\]

\( \Gamma_{\pm} = J(\xi) \sin \theta \left[ e^{i\xi z_+ z_+^\dagger + n(\xi)} + e^{i\xi z_- z_-^\dagger} \right] + J(0) (2n(0) + 1) \cos \theta (z_+ z_+^\dagger - z_- z_-^\dagger) \). \( z_{\pm} \) denote eigenvectors of \( \hat{H} \),

\[
\hat{H}(k, E)z_{\pm} = \pm \left( \xi_+/\xi_- \right) z_{\pm},
\]

which are coherent hybridizations of bands \( c \) and \( v \), and

\[
\xi_\pm = (\epsilon_{c,k} - \epsilon_{v,k}) \sqrt{1 + 4 |\langle k | E \rangle|^2}.
\]

The steady state solution of equation (11) is

\[
\rho = p_+ z_+ z_+^\dagger + p_- z_- z_-^\dagger,
\]

where

\[
p_+ = \frac{n(\xi_+)}{1 + 2n(\xi_+)}, \quad p_- = \frac{1 + n(\xi_-)}{1 + 2n(\xi_-)}.
\]

The joint actions of electric field and the noise thus favor certain forms of coherent interband hybridization, i.e. eigenstates of the effective Hamiltonian \( \hat{H} \). At low temperature \( n(\xi_\pm) \to 0 \), \( p_+ \to 0, p_- \to 1 \), the \( z_- \) state is favored. While the treatment of decoherence here is oversimplified, the above message can be rather general. The decoherence process washes away the coherence between \( z_+ \) and \( z_- \), each of which however has retained the interband coherence induced by the electric field in a non-perturbation manner. Plugging \( \eta_i \) into equations (2) and (3), the velocities that include electric field effects to all orders are obtained

\[
v_h = \frac{\partial \epsilon_{v,k}}{\hbar \partial k} \frac{1}{\sqrt{1 + 4 |\langle k | E \rangle|^2}},
\]

\[
v_h = \frac{\epsilon}{\hbar} E \times \Omega_v(k) \frac{1}{\sqrt{1 + 4 |\langle k | E \rangle|^2}}.
\]

The velocities associated with the \( z_+ \) state has the same form, with the index \( v \) replaced by \( c \). In comparison to equation (8), the non-adiabatic effects of electric field are manifested simply through the prefactor \( 1/\sqrt{1 + 4 |\langle k | E \rangle|^2} \), and the anomalous velocity in the adiabatic limit is reproduced at \( r \ll 1 \). Remarkably, in the non-adiabatic anomalous velocity, its orthogonality to the applied electric field is retained, signifying the intrinsic role of the Berry curvature in generating the anomalous motion. Besides, equa-
Coherent non-adiabatic dynamics. (a) Dirac cone with gap $\Delta = 0.01\text{eV}$. (b) $r$ as function of $k$ at a field of $E = 1\text{V/\mu m}$ (c.f. Equation (7)). (c) Anomalous velocity components perpendicular ($v^\perp_h$, in orange) and parallel ($v^\parallel_h$, in blue) to the field (equation (3)). Solid and dashed trajectories are for the initial $k_0$ labeled as 1 and 2 respectively in (b). (d) The corresponding interband coherence $|\eta^*_c\eta_v|$. (e) and (f) Same plots for the initial $k_0$ labeled as 3 in (b) $v_h$ in unit of $v_D$. The gray-dotted lines in (d) and (f) are steady-state values of $|\eta^*_c\eta_v|$ from incoherent dynamics for comparison.

Incoherent non-adiabatic Hall effect in a gapped Dirac cone. (a) The non-perturbative dc Hall conductance as function of electric field, in unit of $e^2/h$. Dashed curve in the inset keeps up to the third order response. (b) Electron-hole pair density as a function of $k$, in the steady state at $E = 2E_0$.

Equation (17) contains only the odd orders of the electric field. This agrees with the intuition that reversing the direction of the electric field reverses the direction of the induced carrier’s motion. The dotted curves in figures 1 (d) and (f) plot the underlying interband coherence $|\eta^*_c\eta_v|$, which is peaked at the Dirac point, i.e. the Berry curvature hot spot. In equation (15), the eigenvalue of $\overline{H}(k)$ is apparently playing the role of renormalized energy in determining the probability distribution of electron at given momentum $k$. This, combined with momentum relaxation, further allows us to discuss a steady state distribution $f(k)$. The Hall current of an electron ensemble then follows from equation (9) and (17). From equation (17), we recover the concerned feature that $v_h$ is a function of $k$ only, and a steady Hall current that is completely determined by $f(k)$ again. Specifically, for a massive Dirac cone at its charge neutrality, the electrons occupy the branch $z_-$ at all $k$, with a thermal excitation gap $\Delta \sqrt{1 + h^2 v_D^2 (eE)^2 / \Delta^4}$. At the low temperature limit, equation (9) becomes,

$$j^I = e^2 / h \int dk \frac{E \times \Omega_e(k)}{\sqrt{1 + 4 |r(k, E)|}}$$

and the Hall conductance up to third order response reads,

$$\sigma_{HI} \approx \frac{\text{sgn}(\Delta)}{2} \frac{e^2}{h} \left[ 1 - \frac{27 h^4 v_D^4 (eE)^2}{35 \Delta^4} \right] .$$

We show in figure 2(a) the field-dependence of the Hall conductance, in comparison with the half-quantized value $\sigma_{HI}(E = 0)$ from the linear response part. Define a critical field $E_0$ by $[\mathcal{R}_{k=0}]_{z_-} = E_0 = \Delta$, i.e. making $r = 1$ at the Dirac point, the deviation $|\sigma_{HI} - \sigma_{HI}(0)| / \sigma_{HI}$ readily grows to 10% when $E/E_0 \approx 0.3$. Keeping up to third order response has limited improve (see the inset of figure 2(a)), showing the non-perturbative nature in this field range marked by $E_0$. For $\Delta = 0.01\text{eV}$, $E_0 = 0.167\text{V/\mu m}$. 
3. Discussion

The above results establish a general connection between interband coherence and intrinsic Hall effect in both the coherent and incoherent dynamics, from the adiabatic to the non-adiabatic regime. This can help to elucidate the current carrying mechanism of the pseudospin Hall effect in an insulator [6–8, 21]. For the Hall current described by equation (9), the underlying steady state can be written as

$$|\Psi\rangle = \prod_{k} (z_{v} + z_{c} a_{v,k}^{\dagger} a_{c,k}) |\text{vac}\rangle,$$

where $|\text{vac}\rangle$ denotes the equilibrium Fermi sea with filled (empty) valence (conduction) band, $z_{v}$ and $z_{c}$ are entries of eigenvector $z_{\pm}$ in equation (12) that depend on both $k$ and $E$. In the non-perturbative regime, the electric field creates electron-hole pairs with sizeable probability on top of the Fermi sea (c.f. Figure 2(b)). This is in contrast to the impression conveyed by the linear response picture where the Fermi sea is considered unperturbed by the infinitesimal field (effect on band filling $\propto E^2$ neglected). Instead of a response purely by the equilibrium Fermi sea, the Hall current, expressed as

$$J^{H} = \sum_{k} z_{v}^{*} z_{c} \left\langle \text{vac} | J_{c,k} a_{c,k}^{\dagger} | \text{vac} \right\rangle + \text{c.c.},$$

where $J$ is the current operator, comes from the interference of the electron-hole pair excitations $a_{c,k}^{\dagger} a_{v,k}$ with the Fermi sea background $|\text{vac}\rangle$. The bulk pseudospin Hall current can thus be sustained without conducting states inside the gap. In the adiabatic limit $r \to 0$, the pair-excitation probability becomes infinitesimally small, and the above picture properly reduces to the linear response one.

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