



CHORUS

This is the accepted manuscript made available via CHORUS. The article has been published as:

Intrinsic Anomalous Hall Conductivity in a Nonuniform Electric Field

Vladyslav Kozii, Alexander Avdoshkin, Shudan Zhong, and Joel E. Moore

Phys. Rev. Lett. **126**, 156602 — Published 12 April 2021

DOI: [10.1103/PhysRevLett.126.156602](https://doi.org/10.1103/PhysRevLett.126.156602)

Intrinsic anomalous Hall conductivity in non-uniform electric field

Vladyslav Kozii,^{1,2,*} Alexander Avdoshkin,^{1,*} Shudan Zhong,^{1,*} and Joel E. Moore^{1,2}

¹*Department of Physics, University of California, Berkeley, CA 94720, USA*

²*Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*

(Dated: February 1, 2021)

We study how the intrinsic anomalous Hall conductivity is modified in two-dimensional crystals with broken time-reversal symmetry due to weak inhomogeneity of the applied electric field. Focusing on a clean non-interacting two-band system without band crossings, we derive the general expression for the Hall conductivity at small finite wavevector q to order q^2 , which governs the Hall response to the second gradient of the electric field. Using the Kubo formula, we show that the answer can be expressed through the Berry curvature, Fubini-Study quantum metric, and the rank-3 symmetric tensor which is related to the quantum geometric connection and physically corresponds to the gauge-invariant part of the third cumulant of the position operator. We further compare our results with the predictions made within the semiclassical approach. By deriving the semiclassical equations of motion, we reproduce the result obtained from the Kubo formula in some limits. We also find, however, that the conventional semiclassical description in terms of the definite position and momentum of the electron is not fully consistent because of singular terms originating from the Heisenberg uncertainty principle. **We thus present a clear example of a case when the semiclassical approach inherently suffers from the uncertainty principle, implying that it should be applied to systems in non-uniform fields with extra care.**

Introduction. — One of the most spectacular manifestations of quantum mechanics in solids is the effect of band geometry and topology on transport coefficients. Examples include the anomalous Hall effect [1], Chern insulators [2], topological insulators [3, 4], and topological semimetals [5]. Remarkably, some intriguing transport properties of these materials can be solely explained by the peculiarities of the band structure [6]. For instance, the intrinsic anomalous Hall effect in magnetic materials can be elegantly described in terms of the Berry curvature on the Brillouin zone [1, 6–9]. Another interesting example is the explanation of natural optical activity at low frequencies, also known as gyrotropic magnetic effect, via the intrinsic magnetic moment of the Bloch electrons on the Fermi surface [10, 11].

Recently, attention has been drawn to the conducting properties of metals and insulators in an inhomogeneous electric field. One set of studies focused on the momentum-dependent part of the Hall conductivity in magnetic field and its profound connection to the Hall viscosity in Galilean invariant and lattice systems [12–17]. Moreover, it was shown that the Hall viscosity determines the size-dependent part of the Hall resistance and can be used as an indication of the hydrodynamic flow of the electron fluid [14, 15], which was recently probed experimentally [18]. Other works studied the modifications of the semiclassical equations of motion in inhomogeneous field due to the non-zero Fubini-Study quantum metric and the manifestation of these modifications in transport and optical measurements [19, 20].

In this work, we study the intrinsic contribution to the anomalous Hall current in a non-uniform electric field. Instead of an external magnetic field, we assume that time-reversal symmetry in a crystal is broken by, e.g., magnetic order, leading to nonzero Berry curvature. The

correction due to the electric field inhomogeneity is captured by the momentum dependence of the Hall conductivity, which at small momenta q can be expanded as (choosing vector \mathbf{q} to be along the x -axis)

$$\sigma_{AH}(q) = \sigma_{AH}^{(0)} + q^2 \sigma_{AH}^{(2)} + \dots \quad (1)$$

Here we explicitly defined the antisymmetric part of the conductivity tensor as $\sigma_{AH}(\mathbf{q}) \equiv [\sigma_{xy}(\mathbf{q}) - \sigma_{yx}(\mathbf{q})]/2$, and the subscript “AH” stands for “anomalous Hall” [21]. We calculate $\sigma_{AH}^{(2)}$ for a generic clean two-dimensional two-band system (without any external magnetic field) and show that it is expressed through three gauge-invariant objects defined on the Brillouin zone: Berry curvature, quantum metric, and the fully symmetric rank-3 tensor defined through the symplectic connection [22]. The latter object determines the gauge-invariant part of the third cumulant of the position operator (analogous to how quantum metric determines the second cumulant of the position operator) and was recently shown to enter the answer for the shift photocurrent in Weyl semimetals [23, 24]. We assume that the two bands are separated by a finite energy gap everywhere in the Brillouin zone. We use the Kubo formula to obtain the most general microscopic answer.

We further compare our result with the answer obtained within the semiclassical approach. To do that, we derive the semiclassical equations of motion in a non-uniform electric field up to the second order in the field gradients. We find that semiclassics reproduces the terms dominating $\sigma_{AH}^{(2)}$ in the insulating regime in the limit when the two bands are well separated. However, we also show that the Heisenberg uncertainty principle does not allow for a reliable semiclassical description in terms

of the wave packet dynamics when dealing with the second gradients of the electric field. In particular, we find that the equations of motion for the electron wave packet contain some terms which formally become divergent in the case when the wave packet is narrow in momentum space (i.e., corresponds to the state with a well-defined momentum). The origin of these terms is clear: the semiclassical Boltzmann approach relies on the assumption that the particles are described by the well-defined momentum and coordinate, which is inherently incompatible with the basics of quantum mechanics. **This contradiction does not cause serious problems when dealing with the uniform part of the electric field or with its first gradient, and we also show that the semiclassics well agrees with the Kubo formula in some limits once these wavepacket-dependent terms are discarded. However, our work presents a clear example of how the uncertainty principle dramatically reveals itself in the conventional semiclassical description of the systems in inhomogeneous fields, imposing the natural limits of its applicability.**

Kubo formula result. — The most straightforward way to calculate the intrinsic Hall conductivity from the microscopic band structure is to use the Kubo formula. For simplicity, we consider generic two-band Hamiltonian $\hat{H}_0(\mathbf{k})$ defined in the two-dimensional quasimo-

mentum space, which is diagonal in the basis of Bloch wavefunctions $|u_{V,C}(\mathbf{k})\rangle$ with the spectrum $\varepsilon_{V,C}(\mathbf{k})$, $\hat{H}_0(\mathbf{k})|u_{V,C}(\mathbf{k})\rangle = \varepsilon_{V,C}(\mathbf{k})|u_{V,C}(\mathbf{k})\rangle$. Indices “V” and “C” stand for the “valence” and “conduction” band, respectively.

The Hall conductivity is given by the antisymmetric part of the conductivity tensor $\sigma_{\alpha\beta}(i\omega_n, \mathbf{q})$ which is related to the current-current correlation function, $K_{\alpha\beta}(i\omega_n, \mathbf{q}) = \langle \hat{j}^\alpha(i\omega_n, \mathbf{q}) \hat{j}^\beta(-i\omega_n, -\mathbf{q}) \rangle$, as $\sigma_{\alpha\beta}(i\omega_n, \mathbf{q}) = -K_{\alpha\beta}(i\omega_n, \mathbf{q})/\omega_n$ [25]. Strictly speaking, the correlator $K_{\alpha\beta}$ only describes the paramagnetic contribution to conductivity and, in principle, the diamagnetic term should also be included. The latter, however, does not contribute to the (antisymmetric) Hall component of conductivity and will be omitted hereafter.

We find that the simplest and most physically intuitive result is obtained in the case when the chemical potential lies within the band gap, i.e., when the system is in the insulating state. The uniform part of the anomalous Hall conductivity is then quantized and given by $\sigma_{AH}^{(0)} = -\frac{e^2}{\hbar} \frac{1}{S} \sum_{\mathbf{k}} \Omega_{xy}(\mathbf{k}) = \frac{e^2}{\hbar} C$, where S is the total area of the system, integer C is the Chern number, and $\Omega_{ij}(\mathbf{k}) = -2 \text{Im} \langle \partial_{k_i} u_V | \partial_{k_j} u_V \rangle$ is the Berry curvature of the valence band [1]. As for the q^2 component of the Hall conductivity, we find that in the static limit $\omega \rightarrow 0$ it equals to

$$\sigma_{AH}^{(2)} = \frac{e^2}{2\hbar} \frac{1}{S} \sum_{\mathbf{k}} g_{xx} \Omega_{xy} - \frac{\hbar}{\varepsilon_C - \varepsilon_V} \left[\frac{v_{Cx} - v_{Vx}}{3} \frac{\partial \Omega_{xy}}{\partial k_x} + \frac{v_{Cx} - v_{Vx}}{2} T_{xxy} - \frac{v_{Cy} - v_{Vy}}{2} T_{xx} \right] - \frac{2\hbar^2 v_{Cx} v_{Vx}}{(\varepsilon_C - \varepsilon_V)^2} \Omega_{xy}, \quad (2)$$

where the summation is over the states in the completely filled valence band and we fix our coordinate system such that \mathbf{q} is along the x -axis. We also suppressed the indices \mathbf{k} in the above expression for brevity. Band velocities $v_{V(C)}$ and the quantum metric tensor of the valence band g_{ij} are defined as $v_{V(C)i}(\mathbf{k}) = \partial_{k_i} \varepsilon_{V(C)}(\mathbf{k})/\hbar$ and $g_{ij}(\mathbf{k}) = \text{Re} [\langle \partial_{k_i} u_V | \partial_{k_j} u_V \rangle - \langle \partial_{k_i} u_V | u_V \rangle \langle u_V | \partial_{k_j} u_V \rangle]$, respectively. The answer for $\sigma_{AH}^{(2)}$ in Eq. (2) also contains the components of a fully symmetric tensor

$$T_{ijl} = \frac{1}{3} \text{Im}(c_{ijl} + c_{jli} + c_{lij}), \quad (3)$$

where

$$c_{ijl} = \langle u_V | (\partial_{k_i} \partial_{k_j} P_C) (\partial_{k_l} P_C) | u_V \rangle \quad (4)$$

is the quantum geometric connection of the valence band [24] and $P_C = |u_C\rangle\langle u_C| = 1 - |u_V\rangle\langle u_V|$ is the projector onto the conduction band. **The real part of the tensor c_{ijl} is just the Christoffel symbols of the quantum metric, while the imaginary part was identified as the**

symplectic Christoffel symbols in Ref. [24]. All the geometric quantities that determine the answer in Eq. (2), Ω_{ij} , g_{ij} , and T_{ijl} , are invariant under the gauge transformation $|u(\mathbf{k})\rangle \rightarrow e^{i\phi_{\mathbf{k}}} |u(\mathbf{k})\rangle$.

Equation (2) is one of the main results of the present work. We see that in case when the bandwidth is much smaller than the band gap, i.e., when bands are nearly flat, $\sigma_{AH}^{(2)}$ is mainly determined by the first term, involving product of the Berry phase Ω_{xy} and quantum metric g_{xx} . That this term indeed dominates σ_{AH} in this limit has been verified numerically for a Haldane model with flattened bands [26]. This result can be qualitatively understood as follows. The size of the maximally localized Wannier orbital is known to be given by the quantum metric tensor g_{ij} [27, 28]. The effective electric field averaged over the size of the wave packet that the particle experiences in a slowly varying electric field can be estimated as $\mathbf{E}(0) + [\partial^2 \mathbf{E}(0)/\partial x^2] g_{xx}$. The correction to the anomalous velocity then equals $\delta v_j \sim \delta E_i \Omega_{ij} \sim (\partial^2 E_i / \partial x^2) g_{xx} \Omega_{ij}$, which in Fourier space gives exactly $\sigma_{AH}^{(2)} \propto q^2 g_{xx} \Omega_{xy}$.

Since the tensor T_{ijl} is not well known in the con-

densed matter context, we briefly comment on its significance. Defined as the fully symmetric part of the symplectic Christoffel symbols, T_{ijl} encapsulates certain geometric information about the band structure similar to the Berry curvature and quantum metric [29]. Physically, it determines the gauge-invariant part of the third cumulant (skewness) of the position operator averaged over the electron configuration. This observation reconciles the results of Refs. [23] and [24] which computed the circular shift photocurrent in topological semimetals and expressed the answers in terms of the third cumulant and the symplectic Christoffel symbols, correspondingly. We also note that the real part of the quantum geometric connection, the Christoffel symbols, was shown to determine the linear shift photocurrent [24].

As an example, we consider the case of a massive Dirac fermion described by the Hamiltonian $\hat{H}_0(\mathbf{k}) = \hbar v_F(k_x \sigma_x + k_y \sigma_y) + \Delta \sigma_z$, where σ_i are the Pauli matrices. We find that its Hall conductivity is given by

$$\sigma_{AH}^{\text{Dirac}}(q) \approx -\frac{e^2}{2h} \left(1 - \frac{\hbar^2 v_F^2 q^2}{12 \Delta^2} \right). \quad (5)$$

An extra prefactor 1/2 appears due to the fact that the realistic band structure (e.g., a Haldane model) always contains an even number of Dirac points. We further emphasize that this result as well as Eq. (2) are obtained for a system with the chemical potential inside the band gap (an insulator). In principle, one can generalize the answer for a metallic system with the chemical potential residing in a partially filled band. In this case, the final result also contains the contributions from the vicinity of the Fermi surface which are rather complicated and require extra care. In particular, these contributions are very sensitive to the order in which frequency ω and wavevector q are taken to zero and demonstrate singular dependence on the electron's density in the clean limit. These and related questions are discussed in more detail in the Supplemental Materials [29].

It is known that, for the Galilean invariant quantum Hall states, $\sigma_{AH}^{(2)}$ is determined by the Hall viscosity at large magnetic fields [12–14]. However, the direct comparison of our result for the anomalous Hall conductivity, Eq. (2), and Hall viscosity for the lattice systems found in Ref. [30] does not reveal any obvious connection between these two quantities. This is not surprising since a generic crystal does not possess Galilean invariance.

Semiclassical description. — To get more intuition about the answer obtained within the Kubo formula, we now apply the semiclassical approach to the same problem. While we show that this approach is useful for obtaining certain insight into the origin of the most relevant terms in some limits, it still has a number of limitations which do not allow for an accurate quantitative description. The most restrictive limitation is imposed by the uncertainty principle. This principle forbids a quantum

particle to have a definite position and momentum simultaneously, which, in turn, is the key assumption of the semiclassical Boltzmann formalism.

We consider an electron moving in a periodic potential of a lattice with the Hamiltonian \hat{H}_0 in an inhomogeneous static electric field $\mathbf{E}(\mathbf{r}) = -\nabla\phi(\mathbf{r})$, such that the full Hamiltonian is given by

$$\hat{H} = \hat{H}_0 - e\varphi(\hat{\mathbf{r}}). \quad (6)$$

Hamiltonian $\hat{H}_0(\mathbf{k})$ used in the Kubo-formula derivation is the second-quantized version of \hat{H}_0 , written in momentum space. In our further derivation, we closely follow the approach of Ref. [19]. In particular, we assume that the periodic part of the Hamiltonian (without the electrostatic potential), \hat{H}_0 , is diagonal in the basis of the Bloch wavefunctions $|\psi_{\mathbf{k}}\rangle = e^{i\mathbf{k}\cdot\hat{\mathbf{r}}}|u(\mathbf{k})\rangle$, $\hat{H}_0|\psi_{\mathbf{k}}\rangle = \varepsilon_{\mathbf{k}}|\psi_{\mathbf{k}}\rangle$, where $\hbar\mathbf{k}$ is quasimomentum and the function $u_{\mathbf{k}}(\mathbf{r}) \equiv \langle \mathbf{r}|u(\mathbf{k})\rangle$ has the periodicity of the crystal in real space, with the normalization condition $\langle \psi_{\mathbf{k}'}|\psi_{\mathbf{k}}\rangle = \delta(\mathbf{k} - \mathbf{k}')$.

The goal now is to derive the corrections to the semiclassical equations of motion due to the finite gradients of the electric field. More specifically, we are interested in the second gradient, which is equivalent to the q^2 term in the Hall conductivity calculated above. To obtain the correction, we consider the dynamics of the wave packet constructed of the states within the same band and defined as $|\Psi(t)\rangle = \int d\mathbf{k} a(\mathbf{k}, t)|\psi_{\mathbf{k}}\rangle$. Within this single-band approximation, the Schrödinger equation $i\hbar(\partial/\partial t)|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$ determines the dynamics of $a(\mathbf{k}, t)$ as

$$i\hbar \frac{\partial a(\mathbf{k}, t)}{\partial t} = \varepsilon_{\mathbf{k}} a(\mathbf{k}, t) - e \int d\mathbf{k}' a(\mathbf{k}', t) \langle \psi_{\mathbf{k}}|\varphi(\hat{\mathbf{r}})|\psi_{\mathbf{k}'}\rangle, \quad (7)$$

with the normalization condition $\int d\mathbf{k} |a(\mathbf{k}, t)|^2 = 1$ [19].

To take into account weak inhomogeneity of the electric field, we expand the electrostatic potential near $\mathbf{r} = 0$ as $\varphi(\mathbf{r}) = -E^\mu r_\mu - \frac{1}{2} E^{\mu\nu} r_\mu r_\nu - \frac{1}{6} E^{\mu\nu\xi} r_\mu r_\nu r_\xi - \dots$, where $E^{\mu\nu\xi}$, $E^{\mu\nu}$, and E^μ are fully symmetric tensors that do not depend on \mathbf{r} , and the summation over the repeated indices is implied. The electric field near $\mathbf{r} = 0$ is then given by $E^\mu(\mathbf{r}) \approx E^\mu + E^{\mu\nu} r_\nu + \frac{1}{2} E^{\mu\nu\xi} r_\nu r_\xi$. The correction to the electron's velocity proportional to $E^{\mu\nu\xi}$ determines the q^2 term in the Hall conductivity, $\sigma_{AH}^{(2)}$.

To derive the semiclassical expression for the wave packet velocity, we define its position $R_\alpha(t)$ and momentum $K_\alpha(t)$ as

$$\begin{aligned} R_\alpha(t) &\equiv \langle \Psi(t)|\hat{r}_\alpha|\Psi(t)\rangle, \\ K_\alpha(t) &\equiv \langle \Psi(t)|\hat{k}_\alpha|\Psi(t)\rangle, \end{aligned} \quad (8)$$

where $\hbar\hat{k}_\alpha$ is the quasimomentum operator satisfying $\hat{k}_\alpha|\psi_{\mathbf{k}}\rangle = k_\alpha|\psi_{\mathbf{k}}\rangle$. Parameterizing function $a(\mathbf{k}, t)$ as $a(\mathbf{k}, t) = |a(\mathbf{k}, t)|e^{-i\gamma(\mathbf{k}, t)}$, one easily finds that

$$\begin{aligned} R_\alpha(t) &= \int d\mathbf{k} \tilde{R}_\alpha(\mathbf{k}, t) |a(\mathbf{k}, t)|^2, \\ K_\alpha(t) &= \int d\mathbf{k} k_\alpha |a(\mathbf{k}, t)|^2, \end{aligned} \quad (9)$$

with

$$\tilde{R}_\alpha(\mathbf{k}, t) \equiv \frac{\partial\gamma(\mathbf{k}, t)}{\partial k_\alpha} + A_\alpha(\mathbf{k}), \quad (10)$$

and $A_\alpha(\mathbf{k}) = i\langle u(\mathbf{k})|\partial_{k_\alpha}u(\mathbf{k})\rangle$ is the Berry connection. If the wave packet is strongly peaked at momentum \mathbf{K} , $|a(\mathbf{k}, t)|^2 \approx \delta(\mathbf{k}-\mathbf{K})$, semiclassical coordinate of the wave packet becomes simply $R_\alpha \approx \tilde{R}_\alpha(\mathbf{K})$.

Thus far, our semiclassical analysis was similar to that of Ref. [19]. In what follows, however, we are mostly interested in the second-order gradient correction to the semiclassical equations of motion which, to the best of our knowledge, has never been studied before. Assuming that the wavepacket is narrowly peaked in the momentum space, we find up to the order $\partial^2\mathbf{E}(\mathbf{R})/\partial R_\mu\partial R_\nu$ (equivalently, up to the order $E^{\mu\nu\xi}$):

$$\begin{aligned} \dot{K}^\alpha(t) &= -\frac{e}{\hbar}E^\alpha(\mathbf{R}) - \frac{e}{2\hbar}E^{\alpha\mu\nu} [g_{\mu\nu}(\mathbf{K}) + f_{\mu\nu}\{|a(\mathbf{k}, t)|\}], \\ \dot{R}_\alpha(t) &= \frac{1}{\hbar}\frac{\partial\varepsilon_{\mathbf{k}}}{\partial k_\alpha} - \frac{e}{\hbar}E^\mu(\mathbf{R})\Omega_{\mu\alpha} + \frac{e}{2\hbar}\frac{\partial E^\mu(\mathbf{R})}{\partial R_\nu}\frac{\partial g_{\mu\nu}}{\partial K_\alpha} \\ &\quad - \frac{e}{6\hbar}E^{\mu\nu\xi}\left(3g_{\mu\nu}\Omega_{\xi\alpha} - \frac{\partial T_{\mu\nu\xi}}{\partial K_\alpha} - \frac{\partial^2\Omega_{\xi\alpha}}{\partial K_\mu\partial K_\nu}\right) - \\ &\quad - \frac{e}{2\hbar}E^{\mu\nu\xi}\tilde{f}_{\mu\nu\xi\alpha}\{|a(\mathbf{k}, t)|\}, \end{aligned} \quad (11)$$

with functionals $f_{\mu\nu}$ and $\tilde{f}_{\mu\nu\xi\alpha}$ given by

$$\begin{aligned} f_{\mu\nu}\{|a(\mathbf{k}, t)|\} &\equiv \int d\mathbf{k} \frac{\partial|a(\mathbf{k}, t)|}{\partial k_\mu} \frac{\partial|a(\mathbf{k}, t)|}{\partial k_\nu}, \\ \tilde{f}_{\mu\nu\xi\alpha}\{|a(\mathbf{k}, t)|\} &\equiv \int d\mathbf{k} \frac{\partial|a(\mathbf{k}, t)|}{\partial k_\mu} \frac{\partial|a(\mathbf{k}, t)|}{\partial k_\nu} \Omega_{\xi\alpha}(\mathbf{k}). \end{aligned} \quad (12)$$

Equations (11) represent the second main result of the present work. The derivation is straightforward but tedious, so we delegate it to the Supplemental Materials [29]. The first gradient correction, $E^{\mu\nu}\partial g_{\mu\nu}/\partial K_\alpha$, has been obtained and discussed in Refs. [19, 20], and our answer agrees with it. The second-order gradient term containing $E^{\mu\nu\xi}$ is a new result that deserves further discussion.

Within the kinetic equation approach, current density equals $j_\alpha = -(e/S)\sum_{\mathbf{K}}\dot{R}_\alpha f_{\mathbf{K}}$, where $f_{\mathbf{K}}$ is the distribution function. To the leading order, $f_{\mathbf{K}}$ is given by

the Fermi-Dirac distribution, and the current is given by $-e\dot{R}_\alpha$ summed over the filled states, thus allowing for a simple interpretation of all the terms in Eq. (11).

One can easily show that the term with $g_{\mu\nu}\Omega_{\xi\alpha}$ exactly reproduces the first term in Eq. (2). The remaining terms in Eq. (2) contain first or second powers of the bandgap $(\varepsilon_C - \varepsilon_V)$ in the denominator and could in principle be perturbatively captured by the semiclassical approach [20, 31]; we, however, do not present such analysis in this work. Other two terms in Eq. (11) contain full derivatives $\partial T_{\mu\nu\xi}/\partial K_\alpha$ and $\partial^2\Omega_{\xi\alpha}/\partial K_\mu\partial K_\nu$, consequently, their contribution to the current vanishes in the case of a completely filled band, so they do not appear in Eq. (2) [32].

Finally, there are terms $f_{\mu\nu}$ and $\tilde{f}_{\mu\nu\xi\alpha}$ in Eq. (11) which pose the main problem for the semiclassical description of the wave packet dynamics to the second order in the electric field gradients. These terms are given by Eq. (12) and are very non-universal in a sense that they strongly depend on the shape of the wave packet, i.e., function $a(\mathbf{k}, t)$. To estimate the magnitude of these terms, we may assume that $a(\mathbf{k}, t)$ has form of the Gaussian distribution with the width Δk . It is clear then that $f_{\mu\nu} \propto 1/(\Delta k)^2$ and $\tilde{f}_{\mu\nu\xi\alpha} \propto \Omega_{\xi\alpha}/(\Delta k)^2$, thus diverging as $\Delta k \rightarrow 0$, which corresponds to the limit of well-defined quasiparticles in momentum space. These terms originate from the correlators $\langle\Psi(t)|\hat{r}_\mu\hat{r}_\nu|\Psi(t)\rangle$ (and higher moments) and clearly represent the Heisenberg uncertainty principle, which implies that the wavefunctions strongly localized in momentum space experience large variation with the position. While this fundamental principle is not an obstacle for the quasiclassical description at the zeroth and first order in field gradients, it clearly manifests itself at the second order. We see, however, that once the terms $f_{\mu\nu}$ and $\tilde{f}_{\mu\nu\xi\alpha}$ are neglected, our semiclassical answer well agrees with the Kubo formula calculation for an insulating case in the limit when the band separation is much larger than the bandwidth.

It is also instructive to demonstrate an alternative derivation of Eq. (11), which is less rigorous but more physically intuitive. The first equation is simply the Newton's law stating that the rate of the momentum change equals the external force: $\hbar\dot{\mathbf{K}} = -e\langle\Psi(t)|\mathbf{E}(\hat{\mathbf{r}})|\Psi(t)\rangle$. To derive the second equation, we introduce the effective quasiparticle energy $\varepsilon_{eff}(\mathbf{R}, \mathbf{K}) = \langle\Psi(t)|\hat{H}_0 - e\varphi(\hat{\mathbf{r}})|\Psi(t)\rangle$, where $\hbar\mathbf{K}$ is the momentum of the wave packet. The equation for the effective velocity then reads as $\hbar\dot{R}_\alpha \approx (\partial\varepsilon_{eff}/\partial K_\alpha) - \hbar\Omega_{\alpha\mu}\dot{K}_\mu$, while the Newton's law can be rewritten as $\hbar\dot{\mathbf{K}} \approx -\partial\varepsilon_{eff}/\partial\mathbf{R}$ [19]. It is straightforward to check that the resulting equations are equivalent to Eq. (11). The only subtle difference originates from the singular terms analogous to Eq. (12), which we discuss in more detail in the Supplemental Materials [29].

This approach has the further advantage of elucidating the physical meaning and origin of different terms.

For example, the singular terms $f_{\mu\nu}$ and $\tilde{f}_{\mu\nu\xi\alpha}$ originate from the correlator $\langle\Psi|\hat{r}_\mu\hat{r}_\nu|\Psi\rangle$, which determines the real-space width of the state and appears in the expression for $\hbar\dot{\mathbf{K}}$. While these terms are singular for the wave packets narrowly peaked in momentum space, they vanish in case of maximally localized Wannier functions, $|a(\mathbf{k})| = \text{const}$. In the latter case, the correlator can be roughly estimated by the averaged quantum metric $g_{\mu\nu}$ [27, 28]. In fact, there is a well-established procedure for how to define the width in such a way that the corresponding cumulant averaged over the filled band does not suffer from any divergencies and is given exactly by the quantum metric averaged over the same filled band [33, 34]. If for some reason further development of the semiclassical approach is necessary, it seems likely that this approach would allow for a formulation which is free of any singularities and completely agrees with the Kubo formula results found in this work. Finally, when calculating ε_{eff} , we notice that the tensor $T_{\mu\nu\xi}$ determines the gauge-invariant part of the third cumulant of the position operator $\hat{\mathbf{r}}$, $T_{\mu\nu\xi} \approx \langle\Psi|\delta\hat{r}_\mu\delta\hat{r}_\nu\delta\hat{r}_\xi|\Psi\rangle_{\text{g.-i.}}$, where $\delta\hat{r}_\mu \equiv \hat{r}_\mu - \langle\hat{r}_\mu\rangle$ [29].

Conclusions. — We have calculated the q^2 contribution to the intrinsic anomalous Hall conductivity in the inhomogeneous electric field in clean crystals without time-reversal symmetry. To do that, we have applied the Kubo formula to a generic two-band model and then compared the results with the predictions obtained from the semiclassical approach. We showed that the two approaches agree with each other in some limits once the uncertainty principle limitations of the semiclassics are neglected. We expect that this new contribution can be directly probed by the high-precision optical measurement, thus providing valuable information about the geometry of the band structure. As a next step, it would be interesting to relate the newly found q^2 correction to the Hall current to possible experiments revealing the hydrodynamics of electrons in solids [35]. In particular, it is interesting to study whether $\sigma_{AH}^{(2)}$ determines the finite size correction to the Hall resistivity in the crystals with broken time-reversal symmetry, analogous to how the Hall viscosity η_{xy} does it in the narrow channel or Corbino geometry experiments in the Galilean-invariant systems in strong external magnetic field [14, 15]. We leave the study of these questions for future work.

Acknowledgements. — We thank Vir Bulchandani, Daniel Parker, Fedor Popov, and Jonathan Ruhman for stimulating discussions. This work was supported by the Quantum Materials program at LBNL, funded by the US Department of Energy under Contract No. DE-AC02-05CH11231 (V. K. and J. E. M.), the National Science Foundation under Grant No. DMR-1918065 (A. A.), a Kavli ENSI fellowship at UC Berkeley (A. A.), and a Simons Investigatorship (J. E. M.).

* These authors contributed equally.

- [1] Naoto Nagaosa, Jairo Sinova, Shigeki Onoda, A. H. MacDonald, and N. P. Ong, “Anomalous Hall effect,” *Rev. Mod. Phys.* **82**, 1539–1592 (2010).
- [2] F. D. M. Haldane, “Model for a quantum Hall effect without Landau levels: Condensed-matter realization of the “parity anomaly,”” *Phys. Rev. Lett.* **61**, 2015–2018 (1988).
- [3] M. Z. Hasan and C. L. Kane, “Colloquium: Topological insulators,” *Rev. Mod. Phys.* **82**, 3045–3067 (2010).
- [4] Xiao-Liang Qi and Shou-Cheng Zhang, “Topological insulators and superconductors,” *Rev. Mod. Phys.* **83**, 1057–1110 (2011).
- [5] N. P. Armitage, E. J. Mele, and Ashvin Vishwanath, “Weyl and Dirac semimetals in three-dimensional solids,” *Rev. Mod. Phys.* **90**, 015001 (2018).
- [6] Di Xiao, Ming-Che Chang, and Qian Niu, “Berry phase effects on electronic properties,” *Rev. Mod. Phys.* **82**, 1959–2007 (2010).
- [7] Ming-Che Chang and Qian Niu, “Berry phase, hyperorbital, and the Hofstadter spectrum: Semiclassical dynamics in magnetic Bloch bands,” *Phys. Rev. B* **53**, 7010–7023 (1996).
- [8] Ganesh Sundaram and Qian Niu, “Wave-packet dynamics in slowly perturbed crystals: Gradient corrections and Berry-phase effects,” *Phys. Rev. B* **59**, 14915–14925 (1999).
- [9] F. D. M. Haldane, “Berry curvature on the Fermi surface: Anomalous Hall effect as a topological Fermi-liquid property,” *Phys. Rev. Lett.* **93**, 206602 (2004).
- [10] Shudan Zhong, Joel E. Moore, and Ivo Souza, “Gyrotropic magnetic effect and the magnetic moment on the Fermi surface,” *Phys. Rev. Lett.* **116**, 077201 (2016).
- [11] Jing Ma and D. A. Pesin, “Chiral magnetic effect and natural optical activity in metals with or without Weyl points,” *Phys. Rev. B* **92**, 235205 (2015).
- [12] Carlos Hoyos and Dam Thanh Son, “Hall viscosity and electromagnetic response,” *Phys. Rev. Lett.* **108**, 066805 (2012).
- [13] Barry Bradlyn, Moshe Goldstein, and N. Read, “Kubo formulas for viscosity: Hall viscosity, Ward identities, and the relation with conductivity,” *Phys. Rev. B* **86**, 245309 (2012).
- [14] Thomas Scaffidi, Nabhanila Nandi, Burkhard Schmidt, Andrew P. Mackenzie, and Joel E. Moore, “Hydrodynamic electron flow and Hall viscosity,” *Phys. Rev. Lett.* **118**, 226601 (2017).
- [15] Tobias Holder, Raquel Queiroz, and Ady Stern, “Unified description of the classical Hall viscosity,” *Phys. Rev. Lett.* **123**, 106801 (2019).
- [16] Fenner Harper, David Bauer, T. S. Jackson, and Rahul Roy, “Finite-wave-vector electromagnetic response in lattice quantum Hall systems,” *Phys. Rev. B* **98**, 245303 (2018).
- [17] YingKang Chen, Guodong Jiang, and Rudro R. Biswas, “Geometric response of quantum Hall states to electric fields,” [arXiv:1812.04000](https://arxiv.org/abs/1812.04000) (2018).
- [18] A. I. Berdyugin, S. G. Xu, F. M. D. Pellegrino, R. Krishna Kumar, A. Principi, I. Torre, M. Ben Shalom, T. Taniguchi, K. Watanabe, I. V. Grigorieva, M. Polini, A. K. Geim, and D. A. Bandurin,

- “Measuring Hall viscosity of graphene’s electron fluid,” *Science* **364**, 162–165 (2019).
- [19] Matthew F. Lapa and Taylor L. Hughes, “Semiclassical wave packet dynamics in nonuniform electric fields,” *Phys. Rev. B* **99**, 121111 (2019).
- [20] Yang Gao and Di Xiao, “Nonreciprocal directional dichroism induced by the quantum metric dipole,” *Phys. Rev. Lett.* **122**, 227402 (2019).
- [21] The q -linear correction to the conductivity tensor has been studied in detail in Refs. [19, 20]. It is symmetric, so it does not appear in Eq. (1), and requires breaking of both time-reversal and inversion symmetries.
- [22] Boris Fedosov, *Deformation quantization and index theory* (Akademie Verlag, Berlin, 1996).
- [23] Shreyas Patankar, Liang Wu, Baozhu Lu, Manita Rai, Jason D. Tran, T. Morimoto, Daniel E. Parker, Adolfo G. Grushin, N. L. Nair, J. G. Analytis, J. E. Moore, J. Orenstein, and D. H. Torchinsky, “Resonance-enhanced optical nonlinearity in the Weyl semimetal TaAs,” *Phys. Rev. B* **98**, 165113 (2018).
- [24] Junyeong Ahn, Guang-Yu Guo, and Naoto Nagaosa, “Low-frequency divergence and quantum geometry of the bulk photovoltaic effect in topological semimetals,” *Phys. Rev. X* **10**, 041041 (2020).
- [25] Piers Coleman, *Introduction to Many-Body Physics* (Cambridge University Press, Cambridge, 2015).
- [26] Shudan Zhong, *Linear and Nonlinear Electromagnetic Responses in Topological Semimetals*, Ph.D. thesis, University of California, Berkeley (2018).
- [27] Nicola Marzari and David Vanderbilt, “Maximally localized generalized Wannier functions for composite energy bands,” *Phys. Rev. B* **56**, 12847–12865 (1997).
- [28] J. M. Pruneda and Ivo Souza, “Nonadiabatic wavepacket dynamics: k -space formulation,” *Phys. Rev. B* **79**, 045127 (2009).
- [29] See the Supplemental Materials for the details of the Kubo formula and semiclassical calculations.
- [30] Pranav Rao and Barry Bradlyn, “Hall viscosity in quantum systems with discrete symmetry: Point group and lattice anisotropy,” *Phys. Rev. X* **10**, 021005 (2020).
- [31] Yang Gao, Shengyuan A. Yang, and Qian Niu, “Field induced positional shift of Bloch electrons and its dynamical implications,” *Phys. Rev. Lett.* **112**, 166601 (2014).
- [32] These terms, however, do contribute to the Hall conductivity in the metallic regime, though the full answer contains some extra terms which are not captured by the semiclassical approach, see the Supplemental Materials for details [29].
- [33] Ivo Souza, Tim Wilkens, and Richard M. Martin, “Polarization and localization in insulators: Generating function approach,” *Phys. Rev. B* **62**, 1666–1683 (2000).
- [34] Claudia Sgiaravello, Maria Peressi, and Raffaele Resta, “Electron localization in the insulating state: Application to crystalline semiconductors,” *Phys. Rev. B* **64**, 115202 (2001).
- [35] Georgios Varnavides, Adam S. Jermyn, Polina Anikeeva, Claudia Felser, and Prineha Narang, “Generalized electron hydrodynamics, vorticity coupling, and Hall viscosity in crystals,” [arXiv:2002.08976](https://arxiv.org/abs/2002.08976) (2020).