Linear and nonlinear Hall conductivity in presence of interaction and disorder

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(Dated: 13–May–21)

The theory of the nonlinear Hall effect has been established by I. Sodemann and L. Fu [Phys. Rev. Lett. 115, 216806 (2015)] in a semiclassical framework: therein, the effect appears as a geometrical property of Bloch electrons, originating from their anomalous velocity. Here I present a more general theory, addressing correlated and/or noncrystalline systems as well, where the expressions of both linear and nonlinear Hall conductivities originate from the many-electron anomalous velocity. The independent-electron results are retrieved as special cases.

It is known since long time that transverse dc conductivity is allowed—to linear order in the field—only in materials which spontaneously break time-reversal (T) symmetry: it goes then under the name of anomalous Hall conductivity (AHC) [1]. More recently it has been pointed out that second-order transverse dc conductivity can be nonzero even in T-symmetric materials, provided that inversion (I) symmetry is absent: the quadratic dc response is then called nonlinear Hall conductivity (NHC); the theory so far is based on geometrical concepts at the independent-electron level for crystalline systems, and the relevant expressions are obtained semiclassically [2–4]. In this Letter I show how to formulate the theory at a much more general level, encompassing correlated and/or disordered systems as well. Even in the present case the theory is based on geometrical concepts, although in a many-body framework: in particular on the many-body Berry curvature, whose root is in a seminal paper by Niu and Thouless [5]. The known independent-electron NHC formula [2, 3] will be retrieved as a special case; a few other known results will be also presented en passant, obtained here via somewhat unconventional proofs.

The independent-electron geometrical theory for a pristine crystal only provides the intrinsic AHC term; extrinsic terms are necessarily present in the case of metals [1]. The present formulation allows in principle for the inclusion of disorder and accounts therefore for a part of the extrinsic effects as well, thus generalizing a previous work at the independent-electron level [6].

An outstanding qualitative difference exists between AHC and NHC. In the former case the geometrical intrinsic term is nondissipative: it yields a dc current without any mechanism accounting for dissipation (e.g. relaxation times); in the latter case, instead, the geometrical expressions yield a transverse free acceleration; one gets a dc current only after some dissipation mechanism is accounted for. NHC can therefore be assimilated to a skewed nonlinear Drude-like conductivity.

The starting point of the present theory is a milestone paper published by Kohn in 1964 [7]. Following him, we consider a system of \(N\) interacting \(d\)-dimensional electrons in a cubic box of volume \(L^d\), and the family of many-body Hamiltonians parametrized by \(\kappa\), called “flux” or “twist”:

\[
\hat{H}_\kappa = \frac{1}{2m} \sum_{i=1}^{N} \left[ \mathbf{p}_i + \frac{e}{c} \mathbf{A}^{(\text{micro})}(\mathbf{r}_i) + \hbar \kappa \right]^2 + \hat{V},
\]

where \(\hat{V}\) includes the one-body potential (possibly disordered) and electron-electron interaction, while the microscopic vector potential \(\mathbf{A}^{(\text{micro})}(\mathbf{r})\) summarizes all the intrinsic T-breaking terms, as e.g. those due to spin-orbit coupling to a background of local moments. We assume the system to be macroscopically homogeneus; the eigenstates \(|\Psi_{n\kappa}\rangle\) are normalized to one in the hypercube of volume \(L^N\). The thermodynamic limit \(N \to \infty\), \(L \to \infty\), \(N/L^d = n\) constant, is understood throughout this Letter. In order to simplify notations we will set \(\hat{H}_0 \equiv \hat{H}, |\Psi_{n0}\rangle \equiv |\Psi_n\rangle, E_{n0} \equiv E_n\).

We assume Born-von-Kármán periodic boundary conditions (PBCs): the many-body wavefunctions are periodic with period \(L\) over each electron coordinate \(\mathbf{r}_i\) independently; the potential \(\hat{V}\) and the intrinsic vector potential \(\mathbf{A}^{(\text{micro})}(\mathbf{r})\) enjoy the same periodicity. The flux \(\kappa\)—cast into inverse-length dimensions for convenience—corresponds to perturbing the Hamiltonian with a vector potential \(\mathbf{A} = \hbar \kappa / e\), constant in space. Kohn only considered a time-independent \(\kappa\), which amounts to a pure gauge transformation; the latter has nontrivial effects, given that PBCs violate gauge-invariance in the conventional sense [7]. Here we additionally consider even a time-dependent flux, which amounts to perturbing the Hamiltonian with the macroscopic field \(\mathbf{E}(t) = -\mathbf{A}(t)/c = -\hbar \kappa(t)/e\).

The kinetic-energy term in Eq. (1) defines the extensive many-electron velocity as

\[
\mathbf{v}_\kappa = \frac{1}{m} \sum_{i=1}^{N} \left[ \mathbf{p}_i + \frac{e}{c} \mathbf{A}^{(\text{micro})}(\mathbf{r}_i) + \hbar \kappa \right] = \frac{1}{\hbar} \partial_\kappa \hat{H}_\kappa. \tag{2}
\]

When \(\kappa\) is adiabatically varied in time the instantaneous current density is the sum of two terms: the expectation value of the current operator, and the Niu-Thouless
adiabatic current \([5, 8]\). Their expression is cast as:

\[
j_\alpha = -\frac{\hbar e}{L^d} \langle \Psi_{\alpha\mathbf{k}} | \partial_{\kappa_\alpha} \hat{H}_{\mathbf{k}} | \Psi_{\alpha\mathbf{k}} \rangle \\
+ \frac{ie}{L^d} \left( \langle \partial_{\kappa_\alpha} \Psi_{\alpha\mathbf{k}} | \Psi_{\alpha\mathbf{k}} \rangle - \langle \Psi_{\alpha\mathbf{k}} | \partial_{\kappa_\alpha} \Psi_{\alpha\mathbf{k}} \rangle \right) \\
= -\frac{e}{L^d} \left( \frac{1}{\pi} \partial_{\kappa_\alpha} E_{\alpha\mathbf{k}} - \Omega_{\alpha\beta}(\mathbf{k}) \kappa_\beta \right),
\]

(3)

where the sum over repeated Cartesian indices is understood, and \(\Omega_{\alpha\beta}(\mathbf{k})\) is the many-body Berry curvature

\[
\Omega_{\alpha\beta}(\mathbf{k}) = -2\text{Im} \langle \partial_{\kappa_\alpha} \Psi_{\alpha\mathbf{k}} | \partial_{\kappa_\beta} \Psi_{\alpha\mathbf{k}} \rangle.
\]

(4)

The extensive quantity \(\Omega_{\alpha\beta}(\mathbf{k})\kappa_\beta\) is the many-electron anomalous velocity. In the static case (\(\dot{\kappa} = 0\)) no dc current may flow through an insulating sample, ergo the ground-state energy \(E_{\alpha\mathbf{k}} = E_0\) is \(\mathbf{k}\)-independent; in metals, instead, \(E_{\alpha\mathbf{k}}\) does depend on \(\mathbf{k}\) \([7]\).

The linear conductivity is by definition

\[
\sigma_{\alpha\beta}(\omega) = \frac{\partial j_\alpha(\omega)}{\partial \mathcal{E}_\beta(\omega)} = \frac{\partial j_\alpha(\omega)}{\partial A_\beta(\omega)} \frac{dA(\omega)}{d\mathcal{E}(\omega)};
\]

(5)

since \(\mathcal{E}(\omega) = i\omega A(\omega)/c\), causal inversion yields the last factor as \([9]\)

\[
\frac{dA(\omega)}{d\mathcal{E}(\omega)} = -\frac{ie}{\omega + i\eta} = -c \left[ \pi\delta(\omega) + \frac{i}{\omega} \right].
\]

(6)

At finite \(\omega\), the linear response \(\partial j_\alpha(\omega)/\partial A_\beta(\omega)\) is provided by time-dependent perturbation theory \(\text{i.e. Kubo formulæ}\) \([10]\); here instead we only address the response to a dc macroscopic field. The physical perturbation is therefore static; it enters the Hamiltonian as a dynamical one in the adiabatic limit, owing to the vector-potential gauge, mandatory within PBCs \([11]\). Hence we set

\[
\frac{\partial j_\alpha(\omega)}{\partial A_\beta(\omega)} \equiv \frac{\partial j_\alpha(0)}{\partial A_\beta(0)},
\]

(7)

where the symbol “\(\equiv\)” means “equal in the dc limit”.

We chose the perturbing vector potential in the form \(A(t) = A(\omega) e^{-i\omega t}\), ergo we set

\[
\kappa(t) = \frac{e}{hc} A(\omega) e^{-i\omega t}, \quad \dot{\kappa}(t) = -\frac{ie\omega}{hc} A(\omega) e^{-i\omega t},
\]

(8)

whence (to lowest nonvanishing order in \(\omega\)):

\[
\kappa \equiv \frac{e}{hc} A(0), \quad \dot{\kappa} = -\frac{ie\omega}{hc} A(0).
\]

(9)

From Eqs. (3) and (9) it follows that

\[
\frac{\partial j_\alpha(\omega)}{\partial A_\beta(\omega)} \equiv \frac{\partial j_\alpha(0)}{\partial A_\beta(0)} = -\frac{e^2}{hcL^d} \left( \frac{1}{\hbar} \frac{\partial^2 E_0}{\partial \kappa_\alpha \partial \kappa_\beta} - i\omega \Omega_{\alpha\beta}(0) \right).
\]

(10)

The product of Eq. (10) times Eq. (6) yields the real parts of symmetric (longitudinal) and antisymmetric (transverse) dc conductivities as:

\[
\text{Re } \sigma^{(+)}_{\alpha\beta}(\omega) = \frac{\pi e^2}{\hbar^2 L^d} \frac{\partial^2 E_0}{\partial \kappa_\alpha \partial \kappa_\beta} \delta(\omega) = D_{\alpha\beta}(\omega);
\]

(11)

\[
\text{Re } \sigma^{(-)}_{\alpha\beta}(\omega) = \text{Re } \sigma^{(-)}_{\alpha\beta}(0) = -\frac{e^2}{\hbar^2 L^d} \Omega_{\alpha\beta}(0).
\]

(12)

Both these equations are not new, and can be alternatively obtained by the standard sum-over-states Kubo formulae \([10]\) in the \(\omega \to 0\) limit.

The present unconventional derivation has the virtue of being easily generalizable to nonlinear dc conductivity, which is the major focus of the present work. Eq. (11) is Kohn’s milestone expression for the Drude term in longitudinal conductivity \([7]\); the derivation given here is inspired by Ref. \([9]\). As for Eq. (12), it holds for either insulators or metals, for either \(d = 2\) or \(d = 3\), and yields the geometric (or intrinsic) term in the AHC; extrinsic effects are discussed in the final part of the present Letter.

AHC is nonzero only if the Hamiltonian of Eq. (1) breaks T-symmetry at \(\mathbf{k} = 0\) (see also the discussion below about symmetry).

The case of a two-dimensional insulator deserves a separate discussion. Transverse conductivity is quantized:

\[
\sigma^{(-)}_{xy}(0) = -\frac{e^2}{\hbar} C_1,
\]

(13)

where \(C_1 \in \mathbb{Z}\) is a Chern number. This famous relationship was first established at the independent-electron level, where \(C_1\) is also known as TKNN invariant \([12]\); it was later generalized by Niu, Thouless, and Wu, who provided the many-body expression for \(C_1\) \([13]\). Following Ref. \([8]\) (Sec. III.C) the same invariant is conveniently recast as

\[
C_1 = \frac{1}{2\pi} \int_0^{2\pi} d\kappa_x \int_0^{2\pi} d\kappa_y \Omega_{xy}(\kappa);
\]

(14)

Eq. (14) is quantized because it is equivalent to the integral over a torus. In order to show this, we remind that in insulators the ground-state energy \(E_{0\mathbf{k}}\) is \(\mathbf{k}\)-independent, and we observe that whenever the components of \(\mathbf{k} - \mathbf{k}'\) are integer multiples of \(2\pi/L\), then the state \(e^{i(\mathbf{k} - \mathbf{k}') \cdot \hat{r}} | \Psi_{\mathbf{0}\mathbf{k}} \rangle\) is eigenstate of \(H_{\mathbf{k}'}\) with the same eigenvalue as \(| \Psi_{\mathbf{0}\mathbf{k}} \rangle\). The eigenstates which define \(\Omega_{xy}(\kappa)\) have therefore the required toroidal periodicity:

\[
| \Psi_{\mathbf{0}\mathbf{k}'} \rangle = e^{i(\mathbf{k} - \mathbf{k}') \cdot \hat{r}} | \Psi_{\mathbf{0}\mathbf{k}} \rangle.
\]

(15)

Since \(\Omega_{xy}(\kappa)\) is gauge-invariant, an arbitrary \(\mathbf{k}\)-dependent phase factor may relate the two members of Eq. (15). It is worth stressing that in the topological case a globally smooth periodic gauge does not exist; in other words we can enforce Eq. (15) as it stands (with no extra phase factor) only locally, not globally; we also
notice that Eq. (15) may be regarded as the many-body analogue of the periodic gauge in band-structure theory [14].

Eq. (14) is independent of the L value, and its integrand is extensive: therefore in the large-L limit the integration domain contracts to a point:

\[ C_1 = \frac{1}{2\pi} \left( \frac{2\pi}{L} \right)^2 \Omega_{xy}(0). \]  

(16)

By comparing this to Eq. (12) for \( d = 2 \), Eq. (13) is immediately retrieved.

Next we move on to deal with nonlinear conductivity; for the symmetric longitudinal term we adopt the same definitions as in Refs. [10, 15]. The same logic as adopted above yields

\[ \sigma^{(\alpha\beta)}(\omega_1, \omega_2) \equiv \frac{e^3}{\hbar^3 L^4} \partial^3 E_0 \frac{i}{\omega_1 + i\eta} \omega_2 + i\eta : \]

(17)

not surprisingly, this is indeed identical to the recent finding of Ref. [15].

In order to address the antisymmetric second-order term, we expand the many-electron anomalous velocity as

\[ \Omega_{\alpha\beta}(\mathbf{k})(\kappa_\beta \sim \Omega_{\alpha\beta}(0)\kappa_\beta + \partial_{\kappa_\alpha} \Omega_{\alpha\beta}(0) \kappa_\beta \kappa_\gamma. \]

(18)

The first term yields the AHC, Eq. (12); we focus on the second term in the following, and we evaluate it in the adiabatic limit. Eq. (3) yields, to second order,

\[ j_\alpha^{(2)}(\omega) \equiv \frac{e}{L^2} \partial_{\kappa_\alpha} \Omega_{\alpha\beta}(0) \kappa_\beta \kappa_\gamma \]

\[ = -\frac{e^2}{\hbar L^4} \partial_{\kappa_\alpha} \Omega_{\alpha\beta}(0) E_\beta \kappa_\gamma, \]

(19)

where the second equality owes to \( \mathbf{E}(t) = -\hbar \kappa(t)/e \) in the dc limit; the \( \kappa_\gamma \) factor is dealt with in the same way as in Eqs. (6) and (8), i.e.

\[ \kappa_\gamma(t) = \frac{e}{\hbar c} A_t/(\omega)e^{-i\omega t} = -\frac{i}{\omega + i\eta} \mathbf{E}_\gamma(\omega)e^{-i\omega t}. \]

(20)

Therefore, to leading order in \( \omega \),

\[ j_\alpha^{(2)}(\omega) \equiv \frac{e^3}{\hbar^2 L^2} \partial_{\kappa_\alpha} \Omega_{\alpha\beta}(0) \left( \frac{i}{\omega + i\eta} \mathbf{E}_\beta \mathbf{E}_\gamma \right) \]

\[ = \frac{i}{\omega + i\eta} \chi_{\alpha\beta\gamma} \mathbf{E}_\beta \mathbf{E}_\gamma, \quad \chi_{\alpha\beta\gamma} = \frac{e^3}{\hbar^2 L^2} \partial_{\kappa_\alpha} \Omega_{\alpha\beta}(0). \]

(21)

This is the major result of the present work: the sought for general NHC formula, which also applies to cases with interaction and/or disorder. For a crystalline system of independent electrons, Eq. (21) converges—in the large-sample limit—to the original Sodemann-Fu formula: see Eq. (25) below.

The real part of the \( \omega \)-dependent factor in Eq. (21) equals \( \pi \delta(\omega) \): the many-electron system undergoes a transverse free acceleration. One gets a dc current upon replacement of the infinitesimal \( \eta \) with an inverse relaxation time \( 1/\tau \). This is in stark contrast with AHC, Eq. (12), accounting for a \( \tau \)-independent dc current (some extrinsic AHC contributions are \( \tau \)-dependent; see below).

As for the symmetry properties of Eq. (21), we remind that in presence of T-symmetry \( \Omega_{\alpha\beta}(\mathbf{k}) = -\Omega_{\alpha\beta}(-\mathbf{k}) \), while in presence of I-symmetry \( \Omega_{\alpha\beta}(\mathbf{k}) = \Omega_{\alpha\beta}(-\mathbf{k}) \) [8]: therefore in a T-symmetric system \( \Omega_{\alpha\beta}(0) = 0 \) and the AHC vanishes. In the case of NHC the parity is swapped: the gradient of \( \Omega_{\alpha\beta}(\mathbf{k}) \) is even in T-symmetric systems, and odd in I-symmetric systems. Therefore the NHC requires breaking of I-symmetry; in the special case of a T-symmetric and I-breaking system, nonzero transverse conductivity appears at second order only.

Since the responses to \( \mathbf{E}_\beta \mathbf{E}_\gamma \) and to \( \mathbf{E}_\beta \mathbf{E}_\gamma \) coincide, \( \chi_{\alpha\beta\gamma} \) is symmetrical in the \( \beta, \gamma \) indices, while instead it is antisymmetrical in the \( \alpha, \beta \) and \( \alpha, \gamma \) indices. Therefore the current is always orthogonal to the field: if—for an arbitrary \( \mathbf{E} \) orientation—we set the \( x \)-axis along \( \mathbf{E} \), then \( j_x \propto \chi_{xxy} = 0 \), while \( j_y \propto \chi_{xyx} \) and \( j_z \propto \chi_{zzz} \) are not constrained to be zero by (this) symmetry.

At the independent-electron level (either Hartree-Fock or Kohn-Sham) the many-electron wavefunction is a Slater determinant of Bloch orbitals \( \langle \psi_{jk}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}|u_{jk}\rangle \); we normalize them to one over the crystal cell. The Berry curvature of band \( j \) is [14]

\[ \Omega_{j,\alpha\beta}(\mathbf{k}) = -2 \text{Im} \langle \partial_{\kappa_\alpha} u_{jk} | \partial_{\kappa_\beta} u_{jk} \rangle, \]

(22)

and the many-body curvature per unit volume is [10]

\[ \frac{1}{L^2} \Omega_{\alpha\beta}(0) = \sum_j \int_{BZ} (2\pi)^d \frac{dk}{L^4} f_j(\mathbf{k}) \bar{\Omega}_{j,\alpha\beta}(\mathbf{k}), \]

(23)

where BZ is the Brillouin zone, and \( f_j(\mathbf{k}) \) is the Fermi factor at \( T = 0 \).

The equality holds in the \( L \to \infty \) limit. The convergence of Eq. (23) with \( 1/L \) has been indeed investigated by means of tight-binding simulations in the simple case of a Chern insulator, where the r.h.s. is quantized: Fig. 2 in Ref. [16].

It is then easy to prove [10] that

\[ \frac{1}{L^2} \partial_{\kappa_\alpha} \Omega_{\alpha\beta}(0) = \sum_j \int_{BZ} (2\pi)^d f_j(\mathbf{k}) \partial_{\kappa_\beta} \bar{\Omega}_{j,\alpha\beta}(\mathbf{k}), \]

(24)

whence

\[ \chi_{\alpha\beta\gamma} = \frac{e^3}{\hbar^2} \sum_j \int_{BZ} (2\pi)^d f_j(\mathbf{k}) \partial_{\kappa_\alpha} \bar{\Omega}_{j,\alpha\beta}(\mathbf{k}). \]

(25)

This is equivalent—in the single-band case—to the semiclassical expression which first appeared in the founding NHC paper by Sodemann and Fu [2]. The current induced by a monochromatic field of frequency \( \omega \) has a
dc (i.e. rectifying) component and a second-harmonic component. The adiabatic limit of the two terms is considered separately in Ref. [2], hence a factor 1/2 in each of them [17].

In the final part of this Letter I revert to AHC in order to comment on the extrinsic effects. First of all I stress the quite different role of the impurities between the AHC in metals and the quantized AHC in 2d insulators: in the former case there must necessarily be extrinsic effects, while in the latter case extrinsic effects are ruled out. In fact—as a basic tenet of topology—any impurity has no effect on linear Hall conductivity insofar as the system remains insulating.

In principle the dc longitudinal conductivity is infinite: the Drude term is proportional to $\delta(\omega)$. Extrinsic mechanisms are necessary to warrant Ohm’s law, and are accounted for by relaxation time(s) $\tau$; in absence of T-symmetry, extrinsic effects contribute to AHC as well. Two distinct mechanisms have been identified: they go under the name of “side jump” and “skew scattering” [1]. The side-jump term is nondissipative (independent of $\tau$). Since a crystal with impurities actually is a (very) dilute alloy, it was previously argued [6] that the sum of the intrinsic and side-jump terms can be regarded as the intrinsic (geometrical) term of the dirty sample, whose AHC is given by Eq. (12) as it stands, provided that the potential $\tilde{V}$ includes the effect of the impurities. At the independent-electron level, the same effect can in principle be retrieved from the supplementary real-space formulation of AHC [18]. The other extrinsic term (skew scattering) is dissipative, proportional to $\tau$ in the single-relaxation-time approximation, and presumably cannot be explained by means of geometrical concepts. Remarkably, NHC is also proportional to $\tau$, yet it is a geometrical effect.

In this Letter I have started addressing linear dc conductivity (longitudinal and transverse), showing that their many-body expressions can be retrieved in an alternative way, making no use of the standard sum-over-states Kubo formulæ; in this formulation AHC owes to the many-electron generalization of the anomalous velocity. Then I have adopted the same logic to second order in the field. In the longitudinal case the present approach retrieves the same result as in Ref. [15]; in the transverse case the quadratic expansion of the anomalous velocity yields a compact generalization of the semiclassical NHC formula of Ref. [2]. Even in presence of electron-electron interaction and/or disorder, NHC is dominated by the quantum geometry of the electronic system. Finally, it is worth observing that—as it often happens when dealing with transport phenomena [8, 19]—the semiclassical NHC coincides with the exact one at the independent-electron level.

I thank Gabriele Bellomia and Ivo Souza for illuminating discussions, and for bringing some relevant papers to my attention. Work supported by the Office of Naval Research (USA) Grant No. N00014-17-1-2803.

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Linear and nonlinear Hall conductivity in presence of interaction and disorder: Supplemental material

(Dated: 13–May–21)

Many-body Kubo formulæ

We define the matrix elements of the many-body velocity operator at \( \mathbf{k} = 0 \):

\[
\mathcal{R}_{n,\alpha\beta} = \text{Re} \langle \Psi_0 | \hat{v}_{n,\alpha} | \Psi_n \rangle \langle \Psi_n | \hat{v}_{\beta} | \Psi_0 \rangle,
\]
\[
\mathcal{I}_{n,\alpha\beta} = \text{Im} \langle \Psi_0 | \hat{v}_{n,\alpha} | \Psi_n \rangle \langle \Psi_n | \hat{v}_{\beta} | \Psi_0 \rangle,
\]

where \( \mathcal{R}_{n,\alpha\beta} \) is symmetric and \( \mathcal{I}_{n,\alpha\beta} \) antisymmetric; we further set \( \omega_0 = (E_n - E_0)/\hbar \). The longitudinal (symmetric) conductivity is:

\[
\sigma^{(+)}_{\alpha\beta}(\omega) = D_{\alpha\beta} \left[ \delta(\omega) + \frac{i}{\pi \omega} \right] + \sigma^{(\text{regular})}_{\alpha\beta}(\omega),
\]

\[
D_{\alpha\beta} = \frac{\pi e^2}{L^d} \left( \frac{N}{m} \delta_{\alpha\beta} - \frac{2}{\hbar^2} \sum_{n \neq 0} \mathcal{R}_{n,\alpha\beta} \frac{\omega_0}{\omega_0} \right),
\]

\[
\text{Re} \sigma^{(\text{regular})}_{\alpha\beta}(\omega) = \frac{\pi e^2}{\hbar L^d} \sum_{n \neq 0} \mathcal{R}_{n,\alpha\beta} \delta(\omega - \omega_0), \omega > 0,
\]

\[
\text{Im} \sigma^{(\text{regular})}_{\alpha\beta}(\omega) = \frac{2\pi e^2}{\hbar L^d} \sum_{n \neq 0} \mathcal{R}_{n,\alpha\beta} \frac{\omega}{\omega_0^2 - \omega^2},
\]

the Drude weight \( D_{\alpha\beta} \) vanishes in insulators.

The real part of longitudinal conductivity obeys the \( f \)-sum rule

\[
\int_0^\infty d\omega \text{Re} \sigma_{\alpha\beta}(\omega) = \frac{D_{\alpha\beta}}{2} + \int_0^\infty d\omega \text{Re} \sigma^{(\text{regular})}_{\alpha\beta}(\omega)
\]

\[
= \frac{\omega_0^2}{8} \delta_{\alpha\beta} = \frac{\pi e^2 n}{2m} \delta_{\alpha\beta},
\]

where \( n = N/L^d \) is the electron density and \( \omega_p \) is the plasma frequency.

Using then the relationship

\[
|\partial_{\kappa_n} \Psi_0 \rangle = - \sum_{n \neq 0} |\Psi_n \rangle \frac{\delta_{\alpha\beta} |\Psi_0 \rangle}{\omega_0},
\]

the Drude weight can be recast as a geometrical property of the electronic ground state:

\[
D_{\alpha\beta} = \frac{\pi e^2 N}{m L^d} \delta_{\alpha\beta} - \frac{2\pi e^2}{\hbar^2 L^d} \text{Re} \langle \partial_{\kappa_n} \Psi_0 | (\hat{H} - E_0) | \partial_{\kappa_n} \Psi_0 \rangle.
\]

If we then start from the identity \( \langle \Psi_0 \kappa | (\hat{H}_{\kappa} - E_{0\kappa}) | \Psi_0 \kappa \rangle \equiv 0 \), we take two derivatives, and we set \( \kappa = 0 \), we arrive at Kohn’s famous expression for the Drude weight:

\[
D_{\alpha\beta} = \frac{\pi e^2}{\hbar^2 L^d} \frac{\partial^2 E_0}{\partial \kappa_{\alpha} \partial \kappa_{\beta}},
\]

proved in the main text in an alternative way.

Transverse conductivity is nonzero only when T-symmetry is absent. The Kubo formulæ for the transverse (antisymmetric) conductivity are:

\[
\text{Re} \sigma^{(-)}_{\alpha\beta}(\omega) = \frac{2e^2}{\hbar L^d} \sum_{n \neq 0} \mathcal{I}_{n,\alpha\beta} \frac{\omega_0}{\omega_0^2 - \omega^2},
\]

\[
\text{Im} \sigma^{(-)}_{\alpha\beta}(\omega) = \frac{\pi e^2}{\hbar L^d} \sum_{n \neq 0} \mathcal{I}_{n,\alpha\beta} \delta(\omega - \omega_0), \omega > 0.
\]

Using again Eq. (8) the dc transverse conductivity is easily recast in terms of the many-body Berry curvature at \( \mathbf{k} = 0 \):

\[
\text{Re} \sigma^{(-)}_{\alpha\beta}(0) = -\frac{e^2}{\hbar L^d} \Omega_{\alpha\beta}(0);
\]

the expression holds for metals and insulators, in either 2d or 3d. Even this expression in the main text is obtained in an alternative way, by means of the anomalous velocity in its many-body formulation.

Second-order conductivity

In the time domain, the second-order conductivity is by definition

\[
\sigma_{\alpha\beta\gamma} = \frac{\delta j_{\alpha}(t)}{\delta \mathcal{E}_{\beta}(t')} \frac{\delta \mathcal{E}_{\gamma}(t'')}{\delta \mathcal{E}_{\beta}(t')}.
\]

or equivalently (for a time-independent system)

\[
\bar{j}_{\alpha}(t) = \frac{1}{2} \int_0^\infty dt' \int_0^\infty dt'' \sigma_{\alpha\beta\gamma}(t-t', t-t'') \mathcal{E}_{\beta}(t') \mathcal{E}_{\gamma}(t'');
\]

therein all quantities are real and \( \sigma \) is causal.

The convolution theorem yields

\[
\frac{\partial^2 \bar{j}_{\alpha}(\omega_1 + \omega_2)}{\partial \mathcal{E}_{\beta}(\omega_1) \partial \mathcal{E}_{\gamma}(\omega_2)} = \int_0^\infty dt' \int_0^\infty dt'' e^{i\omega_1 t'} e^{i\omega_2 t''} \sigma_{\alpha\beta\gamma}(t', t''),
\]

where all quantities are complex. The second-order conductivity \( \sigma_{\omega_1, \omega_2} \) is identified with Eq. (16) in Ref. [1], and consistently in our Eq. (17) in the main text.

The current induced to second order by a monochromatic field \( \mathcal{E}(\omega) \) at finite frequency has a dc (i.e. rectifying) component, and a second-harmonic component at frequency \( 2\omega \); in the longitudinal case the dc response goes under the name of “shift photocurrent”. Since the real part of a product is obviously not equal to the
product of the real parts, the second-order conductivity \( \sigma(\omega, \pm \omega) \) can be defined in different ways, related to Eq. (16) by a factor of two [2] or even four [3].

In the main text we deal with the transverse quadratic response, in the \( \omega \rightarrow 0 \) limit only. We avoid mentioning \( \sigma(\omega, \pm \omega) \) altogether, and we explicitly express the current in terms of the field. It is worth reminding that fields can be dealt with directly at the semiclassical level, but the scalar potential \( \phi(r) = -E \cdot r \) is incompatible with PBCs. Therefore we deal here with time-dependent vector potentials in the adiabatic limit.

**Independent-electron results**

The independent-electron AHC of a pristine crystal is

\[
\text{Re} \, \sigma^{(-)}_{\alpha\beta}(0) = -\frac{e^2}{\hbar} \sum_j \int_{\text{BZ}} \left\langle \Omega_j, \alpha\beta \right| \tilde{\Omega}_j, \alpha\beta \left| k \right> \tilde{\Omega}_j, \alpha\beta \left( k \right),
\]

where BZ is the Brillouin zone, \( f_j(k) \) is the Fermi factor at \( T = 0 \), and \( \tilde{\Omega}_j, \alpha\beta \left( k \right) \) is the Berry curvature of band \( j \); comparison to Eq. (13) yields:

\[
\frac{1}{L^d} \Omega_{\alpha\beta}(0) = \sum_j \int_{\text{BZ}} \frac{dk}{(2\pi)^d} f_j(k) \tilde{\Omega}_j, \alpha\beta \left( k \right).
\]  

The \( L \rightarrow \infty \) is implicitly understood in the l.h.s.; it is instead explicit in the r.h.s., given that the Bloch vector therein is a continuous variable.

When \( \kappa \neq 0 \) is set in Kohn’s Hamiltonian \( \hat{H}_K \), the corresponding Kohn-Sham periodic orbitals \( |u_{jk} \rangle \) are eigenstates of the single-particle Hamiltonian

\[
e^{-ikr} e^{ikr} H_K e^{-ikr} = \frac{1}{2m} \left( p + \frac{e}{c} A(r) + \hbar k + \hbar \kappa \right)^2 + V_{KS},
\]

where \( V_{KS} \) is the Kohn-Sham potential, hence

\[
\frac{1}{L^d} \Omega_{\alpha\beta}(\kappa) = \sum_j \int_{\text{BZ}} \frac{dk}{(2\pi)^d} f_j(k) \tilde{\Omega}_j, \alpha\beta \left( k + \kappa \right).
\]

\[
\frac{1}{L^d} \partial_{\kappa} \Omega_{\alpha\beta}(0) = \sum_j \int_{\text{BZ}} \frac{dk}{(2\pi)^d} f_j(k) \partial_{\kappa} \tilde{\Omega}_j, \alpha\beta \left( k \right). \tag{21}
\]

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[2] S. M. Young and A. M. Rappe, Phys. Rev. Lett. 109, 116601 (2012).
[3] J. Ibañez-Azpiroz, S. S. Tsirkin, and I. Souza, Phys. Rev. B 97, 245143 (2018).