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Degeneracy-projected polarization formulas for Hall-type conductivities

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Kubo formulas for Hall, transverse thermoelectric and thermal Hall conductivities are simplified into on-shell commutators of degeneracy projected polarizations. The new expressions are computationally economical, and apply to general Hamiltonians without a gap restriction. We show that Hall currents in open boundaries are carried by gapless chiral excitations. Extrapolation of finite lattice calculations to the DC-thermodynamic limit is demonstrated for a disordered metal.

Electric, thermoelectric, and thermal Hall conductivities, a.k.a. σ_{xy} , α_{xy} , and κ_{xy} , respectively, characterize charge and thermal carriers of condensed matter phases, and identify their topology [1–3]. Anomalous Hall and thermal Hall behavior have been reported in strongly interacting systems e.g. cuprates [4, 5] and correlated insulators [6, 7]. In principle, they might be explained by computing Kubo formulas [8–10].

Unfortunately, DC Hall-type Kubo formulas are computationally costly. Their *off-shell* (energy non-conserving) matrix elements of the currents, require full diagonalization of the Hamiltonian on large systems. In addition, divergent magnetization subtractions [10] for thermal Hall coefficients require careful cancellation [11, 12].

Berry curvature (Chern) integrals [1, 13] and Streda (equilibrium) formulas [14, 15], approximate the Kubo formula by *reversing* the DC order of limits (i.e. setting frequency to zero before taking the large volume limit [16]). Thus, they only apply to bulk-gapped phases with vanishing longitudinal conductivities, e.g. Quantum Hall (QH) and topological insulators (TI).

This paper simplifies the Kubo formulas in the proper DC order of limits. The new formulas are compact and valid for general Hamiltonians, including gapless phases with disorder and interactions. Physical insight is gained by expressing σ_{xy} , α_{xy} and κ_{xy} as commutators of degeneracy-projected polarizations (DPPs). The DPPs generalize the role of Landau guiding centers to gapless phases. The formulas imply that Hall and thermal Hall currents are carried by extended chiral excitations which may be supported on the sample edges (for e.g. QH and TI) or may percolate through the bulk.

The conductivities are expressed by a smaller sum over *on shell* matrix elements, which is computationally economical. Problematic magnetization subtractions in the thermal conductivities are eliminated. At low temperatures, the relevant eigenstates are confined to low energies, which allows one to replace the microscopic model by a simpler low energy effective Hamiltonian.

Finite lattice calculations require extrapolation to the DC-thermodynamic limit. A finite size scaling scheme is demonstrated for the metallic phase of disordered electrons at weak magnetic fields. The numerical results recover Drude-Boltzmann (DB) theory, and Wiedemann-Franz law for that model.

Kubo formulas – The DC-thermodynamic limit of trans-

port coefficients is defined by,

$$S_{OO'}^{xy-\text{dc}} \equiv \lim_{\substack{\varepsilon \rightarrow 0 \\ V \rightarrow \infty}} S_{OO'}^{xy}(\varepsilon, V), \quad O, O' = C, T, \quad (1)$$

where the charge (C) and thermal (T) Hall-type conductivities are $\sigma_{xy} \equiv S_{CC}^{xy}$, $\alpha_{xy} \equiv S_{CT}^{xy}/T$, and $\kappa_{xy} \equiv S_{TT}^{xy}/T$. ε, V are finite imaginary frequency and volume respectively. The DC order of limits is taken from bottom to top [17].

Here we consider a general many-body lattice Hamiltonian H on open boundary conditions (OBC) [18], C4 symmetry in the xy plane [19], and a magnetic field B in the z direction. Its spectrum and eigenstates are $\{E_n, |n\rangle\}$. The Hall-type Kubo formulas in the Lehmann representation are,

$$S_{OO'}^{xy} = \frac{\hbar}{V} \text{Im} \sum_{n,m} \frac{(\rho_m - \rho_n) \langle m | j_O^x | n \rangle \langle n | j_{O'}^y | m \rangle}{(E_n - E_m)(E_n - E_m - i\varepsilon)} - \frac{\langle M_{OO'} \rangle}{V}. \quad (2)$$

$\rho_n(T)$ are Boltzmann weights at temperature T . The magnetization terms $\propto \langle M_{OO'} \rangle$ eliminate circulating magnetization currents from the first term [10].

The currents j_O^α and magnetizations $M_{OO'}$ are defined as follows. The Hamiltonian is spatially decomposed on the lattice $H = \sum_i h_i$ [20]. The charge and thermal polarizations are,

$$P_C^\alpha \equiv e \sum_i n_i x_i^\alpha, \quad P_T^\alpha = \sum_i h_i x_i^\alpha, \quad \alpha = x, y, \quad (3)$$

where en_i is the local charge density, and x_i is the position of lattice site i . The electric and thermal currents are,

$$j_O^\alpha = \frac{i}{\hbar} [H, P_O^\alpha], \quad O = C, T. \quad (4)$$

In the literature one often finds first quantized expressions for the magnetizations [21]. Here we use more general definitions which apply to any form of the hamiltonian,

$$M_{CT} = -\frac{i}{\hbar} [P_C^x, P_T^y], \quad M_{TT} = -\frac{i}{\hbar} [P_T^x, P_T^y]. \quad (5)$$

Note that $M_{CC} = 0$, since the two charge polarizations commute. For anomalous bosonic Hamiltonians $\langle M_{TT} \rangle / T$ may diverge as $\lim_{T \rightarrow 0}$. Such divergence must be precisely cancelled by the current correlators, as shown

for non-interacting QH systems [11, 22]. Such cancellations could be problematic if one applies separate approximations to the two terms in Eqs. (2).

DPP formulas – Eqs. (2) are simplified as follows. The real part of the summands' numerator vanishes by C4 symmetry,

$$\text{Re}\langle m|j_O^x|n\rangle\langle n|j_{O'}^y|m\rangle = 0. \quad (6)$$

The real part of the denominator is written as two terms,

$$\text{Re}\frac{1}{\Delta_{nm}(\Delta_{nm} - i\varepsilon)} = \frac{1}{\Delta_{nm}^2} - \frac{\varepsilon^2}{\Delta_{nm}^2(\Delta_{nm}^2 + \varepsilon^2)}, \quad (7)$$

where $\Delta_{nm} \equiv E_n - E_m$. The matrix elements of Eq. (4) in the eigenstates basis are,

$$\frac{\langle n|j_O^\alpha|m\rangle}{\Delta_{nm}} = \frac{i}{\hbar}\langle n|P_O^\alpha|m\rangle, \quad (8)$$

which we insert into Eq. (2) to yield,

$$S_{OO'}^{xy} = \frac{1}{\hbar V} \sum_{nm} (\rho_n - \rho_m) \text{Im} \left(\langle m|P_O^x|n\rangle\langle n|P_{O'}^y|m\rangle - \frac{\varepsilon^2 \langle m|P_O^x|n\rangle\langle n|P_{O'}^y|m\rangle}{(\Delta_{nm}^2 + \varepsilon^2)} \right) - \frac{\langle M_{OO'} \rangle}{V}. \quad (9)$$

The top row, which is an off-shell sum, can be rewritten as the thermodynamic average of the polarizations' commutator $\langle [P_O^\alpha, P_{O'}^\beta] \rangle$. Therefore it vanishes for σ_{xy} , and precisely cancels with the magnetization corrections (5) for α_{xy} and κ_{xy} (good riddance!).

Surprisingly, it is the seemingly negligible ε^2 -term which fully determines $S^{xy-\text{dc}}$! The Kubo formulas reduce to a purely on-shell expression,

$$S_{OO'}^{xy-\text{dc}} = - \lim_{\varepsilon \rightarrow 0} \frac{1}{\hbar V} \text{Im} \sum_n \rho_n \langle n | [\tilde{P}_O^x, \tilde{P}_{O'}^y] | n \rangle, \quad (10)$$

where \tilde{P}_O^α is the DPP in the α direction,

$$\langle n | \tilde{P}_O^\alpha | m \rangle = \langle n | P_O^\alpha | m \rangle \Theta_\varepsilon(|E_n - E_m|), \quad (11)$$

and the Lorentzian $\Theta_\varepsilon(x) = \frac{\varepsilon^2}{x^2 + \varepsilon^2}$ can be replaced by a projector Heaviside function $\Theta_\varepsilon(x) \rightarrow \Theta(\pi\varepsilon/2 - |x|)$ in the limit $\varepsilon \rightarrow 0$.

Reduction to single particle (SP) Hamiltonians – For non-interacting fermions or bosons,

$$H^{\text{SP}} = \sum_{ij} h_{ij}(B) a_i^\dagger a_j = \sum_\alpha \epsilon_\alpha(B) a_\alpha^\dagger a_\alpha, \quad (12)$$

Eq. (10) reduces to

$$S_{OO'}^{xy-\text{sp}} = - \lim_{\varepsilon \rightarrow 0} \frac{1}{\hbar V} \text{Im} \sum_\alpha n_\alpha [\tilde{P}_O^x, \tilde{P}_{O'}^y]_{\alpha\alpha}, \quad (13)$$

where n_α is the Fermi-Dirac or Bose-Einstein occupation

of SP state $a_\alpha^\dagger |0\rangle$. The DPPs are [23],

$$\begin{aligned} \tilde{P}_O^\gamma &= \sum_{\alpha\beta} \left(\tilde{P}_O^\gamma \right)_{\alpha\beta} a_\alpha^\dagger a_\beta, \\ \left(\tilde{P}_O^\gamma \right)_{\alpha\beta} &= \langle \alpha | P_O^\gamma | \beta \rangle \Theta_\varepsilon(|\epsilon_\alpha - \epsilon_\beta|). \end{aligned} \quad (14)$$

A version of Eq. (13) was derived by Bradlyn and Read [22] for integer QH states without disorder.

DPP's in clean Landau levels – Eigenstates of electrons of effective mass m in a strong magnetic field are described by degenerate Landau levels. The charge polarizations (whose components commute) can be decomposed as

$$P_C^\gamma = eR^\gamma + el_B(\boldsymbol{\pi} \times \hat{\mathbf{z}})^\gamma, \quad (15)$$

where $l_B = \sqrt{\frac{\hbar c}{eB}}$. $\boldsymbol{\pi}$ connect between adjacent Landau levels. \mathbf{R} are guiding center coordinates which satisfy $[R^x, R^y] = -il_B^2 \mathbb{I}$, and $[R^\alpha, \pi^\beta] = 0$.

On OBC, H^{SP} includes a confining potential $V(\mathbf{x})$ on its edges. A smooth potential [24] with $|\nabla \log V|^{-1} \ll l_B$ can be approximated by an intra-Landau level operator $V^{\text{eff}}(\mathbf{R})$. $V^{\text{eff}}(\mathbf{R})$ (which commutes $\boldsymbol{\pi}$) acts only within a single Landau level labelled by ν . One can choose the eigenstate basis of say $R^y|\nu, k\rangle = kl_B|\nu, k\rangle$, in which $\langle \nu, k | V^{\text{eff}} | \nu, k' \rangle$ is generally not diagonal. $U_{\alpha,k}(V^{\text{eff}})$ is the unitary matrix which diagonalizes $V^{\text{eff}}(\mathbf{R})$, and defines the energy eigenbasis $|\nu, \alpha\rangle$. Since $[R^x, R^y] = -il_B^2 \mathbb{I}$, we know that $[U^\dagger R^x U, U^\dagger R^y U] = -il_B^2 \mathbb{I}$. The expectation value of the second commutator is used in Eq. (13) to obtain $\sigma_{xy} = \frac{ne c}{B}$, where n is the electron density. This result also holds in the presence of translationally invariant many body interactions.

Disordered metals in weak magnetic fields. – This regime can be described by DB theory [25] at small Hall angles $\omega_c \tau \ll 1$, where τ is the transport scattering time and $\omega_c = \frac{eB}{mc}$ is the cyclotron frequency. The DB Hall conductivity yields,

$$\sigma_{xy}^{\text{DB}} = \frac{ne^2 \omega_c \tau^2}{m}. \quad (16)$$

In the weak field regime, disorder strongly mixes the Landau levels and severs the relation between the DPPs and the guiding centers. Eq. (16) can be recovered by a multiplicative renormalization of the DPPs, i.e. $\tilde{P}_C^\gamma \simeq e(\omega_c \tau) R^\gamma$, in Eq. (13).

Numerical calculations – Eq. (10) are significantly less costly than the off-shell formulas Eq. (2). Having eliminated $-\frac{M_{\text{CT}}}{T}$, $-\frac{M_{\text{TT}}}{T}$ in α_{xy} and κ_{xy} respectively, one may apply controlled approximations without worrying about precise cancellations of divergent corrections. While Eq. (2) requires full diagonalization of H and calculations of many current matrix elements, Eq. (10) includes only matrix elements between nearly degenerate eigenstates in the spectrum below temperature T . These states may be numerically accessible by Lanczos algorithms [26] or approximated by variational methods [27].

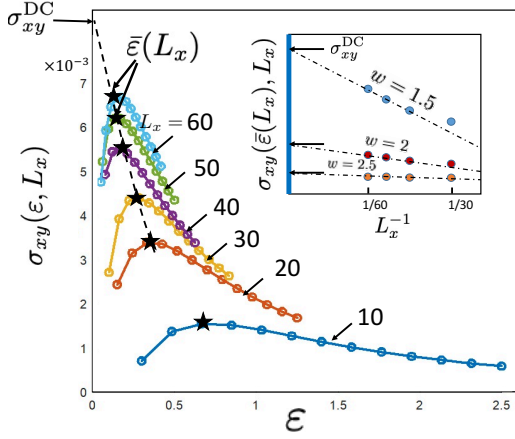


FIG. 1. Extrapolation of numerical Hall conductivities of the square lattice Hamiltonian, Eq. (18). Disorder averaged σ_{xy} are plotted versus ϵ , for a sequence of linear dimensions L_x . Stars mark the values of $\bar{\epsilon}$ as defined in Eq. (17). The disorder strength is fixed at $w = 3$. The temperature, Fermi energy, and magnetic field are $T = 0.3$, $\epsilon_F = -1$ and $B = 0.025$ respectively. **Inset:** The DC limit σ_{xy}^{DC} (marked by black arrows) for three values of disorder strength.

Contrary to the initial off-shell formulation of Eq. (2), H in (10) may be replaced by its low energy effective Hamiltonian in the spectrum range $E_n - E_0 \leq k_B T$. For example, Fermi liquid theory can be used for interacting fermions, or continuum field theories for magnets and superconductors.

Numerical calculations are mostly performed on finite lattices which require extrapolation to the DC-thermodynamic limit, of Eq. (1). If $S_{OO'}(\epsilon, L_x)$ is computed for a sequence of linear dimensions $\{L_x^i\}$, “optimal” values of $\bar{\epsilon}(L_x^i)$ can be extracted by the extrema conditions,

$$\partial_\epsilon S_{OO'}^{xy}(\epsilon, L_x^i) = 0 \Rightarrow \bar{\epsilon}(L_x^i). \quad (17)$$

The DC limit is obtained by extrapolating the extrema, $S^{DC} = \lim_{i \rightarrow \infty} S_{OO'}(\bar{\epsilon}(L_x^i), L_x^i)$. This scheme is demonstrated in Fig. 1 for the square lattice Hamiltonian,

$$H^{SL} = - \sum_{\langle ij \rangle} \left(e^{-iA_{ij}} c_i^\dagger c_j + \text{h.c.} \right) + \sum_i (w_i - \epsilon_F) c_i^\dagger c_i, \quad (18)$$

where $w_i \in [-w/2, w/2]$ is a uniformly distributed random number and $B = \sum_{\square} A_{ij}$ is the magnetic field.

$\bar{\epsilon}$ are marked by black stars which apparently can be fit to a power law $\bar{\epsilon} \simeq 7(L_x)^{-1}$. This scaling is consistent

with level spacings of one dimensional extended states. In the inset of Figure 1, the Hall conductivities at different disorder strengths extrapolate linearly in L_x^{-1} , to their respective DC limits.

In Ref. [28], we show that $\sigma_{xy}^{dc} \sim w^{-4}$, which is consistent with DB result (16), since by Fermi’s golden rule $\frac{1}{\tau} \propto w^2$. The zero field Hall coefficient $R_H = \frac{d}{dB} \sigma_{xy} \sigma_{xx}^{-2}$ varies weakly with w in the moderate disorder regime, as expected by DB theory in the constant life-time approximation. R_H is approximated fairly well by the equilibrium Hall coefficient formula derived in Refs. [16, 29]. In addition, Wiedemann-Franz law $\frac{\kappa_{xy}}{T \sigma_{xy}}$ reaches close proximity to the DB result of $\frac{\pi^2}{3}$ at low temperatures.

Discussion – Since Eq. (10) applies to any Hamiltonian with OBC, we can draw general conclusions concerning Hall effects even in strong disorder and interactions regimes: (i) Quasi-degenerate manifolds of eigenstates are created by the magnetic field. (ii) These manifolds are subjected to *non commutative geometry* by the DPPs, i.e. $\langle [\tilde{P}_O^\alpha, \tilde{P}_{O'}^\beta] \rangle = i\epsilon_{\alpha\beta} c$. In a sense, $c^{-1} \epsilon_{\alpha\beta} \tilde{P}_O^\beta = \Pi_O^\alpha$ generates translations and acts as a conjugate momentum to $\tilde{P}_{O'}^\alpha$. Thus, the DPP’s generalize the algebra of guiding centers to regimes of strong Landau level mixing. (iii) The quasi-degenerate eigenstates are *chiral* as defined by their nonzero vorticity as $\langle \nabla_{\tilde{P}_O} \times \tilde{\Pi}_{O'} \rangle = 2/c \neq 0$.

These gapless chiral wavefunctions may be supported exclusively on the sample edges, as in QH and TI phases, or in the bulk. Bulk chiral states have been derived semiclassically by Chalker and Coddington [30], who described the transition between incompressible plateaux using a percolating network of extended chiral states. Finally, we can also infer that thermal Hall currents in insulators [5–7] are also carried by extended chiral modes.

Summary – Microscopic computations of charge and thermal Hall conductivities are made easier by Eqs. (10, 13), which is especially needed in gapless phases. The new formulas unveil the essential role of non-commuting DPPs and associated quasi-degenerate chiral eigenstates. We expect these formulas to allow better connection between model Hamiltonians and Hall-type measurements in regimes of strong scattering.

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