Degeneracy-projected polarization formulas for Hall-type conductivities

Noga Bashan and Assa Auerbach
Physics Department, Technion, 32000 Haifa, Israel
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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. \( \sigma_{xy}, \alpha_{xy}, \) and \( \kappa_{xy} \), 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][2]. 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 [11][3] 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 \( \sigma_{xy}, \alpha_{xy} \) and \( \kappa_{xy} \) 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 transport coefficients is defined by,

\[
S_{\alpha \beta \gamma}^{xy-de} \equiv \lim_{V^2 \to \infty} S_{\alpha \beta \gamma}^{xy}(\varepsilon, V), \quad \alpha, \beta, \gamma \in \{c, t\},
\]

where the charge (C) and thermal (T) Hall-type conductivities are \( \sigma_{xy} \equiv S_{xy}^{xy}/T \), \( \alpha_{xy} \equiv S_{xy}^{xy}/T \), and \( \kappa_{xy} \equiv S_{xy}^{xy}/T \).

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 \( \{\varepsilon_n, |n\rangle\} \). The Hall-type Kubo formulas in the Lehmann representation are,

\[
S_{\alpha \beta \gamma}^{xy} = \frac{\hbar}{V} \text{Im} \sum_{n,m} \langle \rho_n - \rho_m \rangle \langle m| j_{\alpha |n} \rangle \langle n| j_{\beta |m} \rangle \frac{\langle m| j_{\gamma |n} \rangle \langle n| j_{\gamma |m} \rangle}{(\varepsilon_n - \varepsilon_m) + i\varepsilon}, \quad (\varepsilon, V)
\]

where \( \rho_n(T) \) are Boltzmann weights at temperature \( T \). The magnetization terms \( \propto \langle M_{\alpha \beta \gamma} \rangle \) eliminate circulating magnetization currents from the first term [10].

The currents \( j_{\alpha |n} \) and magnetizations \( M_{\alpha \beta \gamma} \) are defined as follows. The Hamiltonian is spatially decomposed on the lattice \( H = \sum_i h_i \) [20]. The charge and thermal polarizations are,

\[
P_C^\alpha \equiv \frac{\hbar}{V} \sum_i n_i x_i^\alpha, \quad P_T^\alpha \equiv \sum_i h_i x_i^\alpha, \quad \alpha = x, y, (3)
\]

\[
j_C^\alpha = \frac{i}{\hbar} [H, P_C^\alpha], \quad \alpha = c, t. (4)
\]

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,

\[
M_{CT} = -i \frac{1}{\hbar} [P_C^\alpha, P_T^\alpha], \quad M_{TT} = -i \frac{1}{\hbar} [P_T^x, P_T^y]. (5)
\]

Note that \( M_{CC} = 0 \), since the two charge polarizations commute. For anomalous bosonic Hamiltonians \( \langle M_{TT} \rangle/T \) may diverge as \( \lim_{V \to 0} \). 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,

\[
\text{Re}(\langle n|j^x_\rho|n\rangle \langle n|j^y_\rho|m\rangle) = 0.
\]

(6)

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

\[
\text{Re} \frac{1}{\Delta_{nm}(\Delta_{nm} - i\varepsilon)} = \frac{1}{\Delta_{nm}^2} - \frac{\varepsilon^2}{\Delta_{nm}^2(\Delta_{nm}^2 + \varepsilon^2)},
\]

(7)

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

\[
\frac{\langle n|O^\dagger_\rho|n\rangle}{\Delta_{nm}} = i \hbar \frac{\langle n|P_\rho^\dagger|m\rangle}{\Delta_{nm} + \varepsilon^2},
\]

(8)

which we insert into Eq. \[2\] to yield,

\[
S_{OO'}^{xy} = \frac{1}{\hbar V} \sum_{mn} (\rho_n - \rho_m) \text{Im} \left( \frac{\langle m|P_{xy}|n\rangle \langle n|P_{xy}^\dagger|m\rangle}{\Delta_{nm}^2 + \varepsilon^2} \right) - \frac{\langle M_{OO'} \rangle}{V}.
\]

(9)

The top row, which is an off-shell sum, can be rewritten as the thermodynamic average of the polarizations’ commutator \([P_{xy}, P_{xy}^\dagger]\)]. Therefore it vanishes for \(\sigma_{xy}\), and precisely cancels with the magnetization corrections \(5\) for \(\alpha_{xy}\) and \(\kappa_{xy}\) (good riddance!).

**Surprisingly, it is the seemingly negligible \(\varepsilon^2\)-term which fully determines \(S_{OO'}^{xy}\) !** The Kubo formulas reduce to a purely on-shell expression,

\[
S_{OO'}^{xy} = - \lim_{V \to \infty} \frac{1}{\hbar V} \sum \rho_n \langle n|H_{xy}^\text{sp}|n\rangle \text{Im} \langle [\hat{P}_O, \hat{P}^\dagger_O]|n\rangle, \tag{10}
\]

where \(\hat{P}_O\) is the DPP in the \(O\) direction,

\[
\langle n|\hat{P}_O|n\rangle = \langle n|P_\rho^\dagger|n\rangle |E_n - E_m|, \tag{11}
\]

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

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

\[
H_{xy}^\text{sp} = \sum_{ij} h_{ij}(B) a_i^\dagger a_j = \sum_{\alpha} \epsilon_{\alpha}(B) a_\alpha^\dagger a_\alpha. \tag{12}
\]

**Eq. \(10\)** reduces to

\[
S_{OO'}^{xy} = - \lim_{V \to \infty} \frac{1}{\hbar V} \sum |n_\alpha| \langle [\hat{P}_O, \hat{P}^\dagger_O]|_{\alpha\alpha}, \tag{13}
\]

where \(n_\alpha\) is the Fermi-Dirac or Bose-Einstein occupation of SP state \(a_\alpha^\dagger|0\rangle\). The DPPs are \([23]\).

\[
\hat{P}_O^\gamma = \sum_{\alpha\beta} \langle \alpha|P_\rho^\gamma|\beta\rangle a_\alpha^\dagger a_\beta, \quad \langle \alpha|\langle \gamma(\delta - \epsilon_\beta)\rangle|\beta\rangle.
\]

(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

\[
P_{xy}^\text{cc} = eR^x + eB(\pi \times \hat{z})\gamma, \tag{15}
\]

where \(l_B = \sqrt{\hbar / eB}\). \(\pi\) connects adjacent Landau levels. \(R\) are guiding center coordinates which satisfy \([R^x, R^y] = -i\hbar B, \quad [R^x, \pi^z] = 0\).

On OBC, \(H_{xy}^\text{sp}\) includes a confining potential \(V(x)\) on its edges. A smooth potential \([23]\) with \(\nabla \log V \ll l_B\) can be approximated by an intra-Landau level operator \(V_{xy}^\text{eff}(R)\). \(V_{xy}^\text{eff}(R)\) (which commutes \(\pi\)) acts only within a single Landau level labelled by \(\nu\). One can choose the eigenstate basis of say \(R^\nu|\nu, k\rangle = k|\nu, k\rangle\), in which \(\langle \nu, k|V_{xy}^\text{eff}|\nu', k'\rangle\) is generally not diagonal. \(U_{\nu,k}(V_{xy}^\text{eff})\) is the unitary matrix which diagonalizes \(V_{xy}^\text{eff}(R)\), and defines the energy eigenbasis \(|\nu, \alpha\rangle\). Since \([R^x, R^y] = -i\hbar B, \quad [U^\dagger R^\nu U, U^\dagger R^{\nu'} U] = -i\hbar B, \quad [U^\dagger R^\nu U, U^\dagger R^{\nu'} U] = -i\hbar B\), the expectation value of the second commutator is used in Eq. \(15\) to obtain \(\langle \nu, \epsilon_{xy}\rangle = \frac{e\epsilon_{xy}}{m\omega_c}\) 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 \(\omega_c T \ll 1\), where \(T\) is the transport scattering time and \(\omega_c = eB/mc\) is the cyclotron frequency. The DB Hall conductivity yields,

\[
\sigma_{xy} = \frac{n e^2 \omega_c \tau^2}{m}. \tag{16}
\]

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. \(\hat{P}_O^\gamma \simeq e(\omega_c T)^\gamma R^\gamma\), in Eq. \(13\).

**Numerical calculations** – Eq. \(10\) are significantly less costly than the off-shell formulas Eq. \(2\). Having eliminated \(-\frac{M_{\alpha\beta}}{\ell_B^2}, -\frac{h_{ij}}{\ell_B^2}\) in \(\sigma_{xy}\) and \(\kappa_{xy}\) 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 \([27]\).
Contrary to the initial off-shell formulation of Eq. (2), \( H \) in (10) may be replaced by its low energy effective Hamiltonian in the thermodynamic limit, of Eq. (1). If \( S_{\text{OO}}^x(\varepsilon, L_x) \) is computed for a sequence of linear dimensions \( \{L_x\} \), “optimal” values of \( \varepsilon(L_x) \) can be extracted by the extrema conditions,

\[
\partial_{\varepsilon} S_{\text{OO}}^x(\varepsilon, L_x^i) = 0 \Rightarrow \varepsilon(L_x^i).
\]

The DC limit is obtained by extrapolating the extrema, \( \varepsilon(\varepsilon, L_x^i) \) for the square lattice Hamiltonian, shown in Fig. 1. Inset: The Hall conductivities at different disorder strengths extrapolate linearly in the inset of Figure 1, the Hall conductivities at different disorder strengths extrapolate linearly in the inset of Figure 1, the Hall conductivities at different disorder strengths extrapolate linearly in the inset of Figure 1, the Hall conductivities at different disorder strengths extrapolate linearly. The DC limit is obtained by extrapolating the extrema, as defined in Fig. 1 for the square lattice Hamiltonian, \( \varepsilon(L_x^i) \) may be replaced by its low energy effective field theories for magnets and superconductors.

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tice Hamiltonian, on a lattice of size $L^2$,

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

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

In Drude-Boltzmann theory, the scattering rate is obtained by Fermi golden rule

$$\frac{\hbar}{\tau} = \pi N(\epsilon_F) u^2,$$

where the two clean susceptibilities are,

$$\chi_{\text{CMC}} = 2 \int \frac{d^2 k}{(2\pi)^2} \left( - \frac{\partial f}{\partial \epsilon} \right) \left( \frac{\partial \epsilon_k}{\partial k_x} \right)^2 \left( \frac{\partial^2 \epsilon_k}{\partial k_y^2} \right),$$

$$\chi_{\text{CSR}} = \int \frac{d^2 k}{(2\pi)^2} \left( - \frac{\partial f}{\partial \epsilon} \right) \left( \frac{\partial \epsilon_k}{\partial k_x} \right)^2,$$

where $f$ is the fermi function at temperature $T$ and Fermi energy $\epsilon_F$. $\epsilon_k$ is the square lattice bandstructure,

$$\epsilon_k = -2 \cos(k_x) - 2 \cos(k_y).$$

FIG. 2. DC extrapolated Hall conductivity for weak magnetic field $B = 0.03$ and moderate disorder strength $w$, at Fermi energy $\epsilon_F = -1$. The Hall conductivity scales as $w^{-4}$ as expected by Drude’s theory $\sigma_{xy} \propto \omega_c \tau^2$.

Fig. 2 shows that the disorder averaged Hall conductivity scales as $w^{-4}$. It is also found to be linear in $B$, which agrees with Drude’s theory $\sigma_{xy} \propto \omega_c \tau^2$.

For an additional test, we also compute the zero field Hall coefficient,

$$R_H(w) = \frac{d \sigma_{xy}}{dB} \sigma_{xx}^{-2} \bigg|_{B=0}.$$  

(A3)

The equilibrium Hall coefficient formula [16,29] at low disorder is,

$$R_H = \frac{\chi_{\text{CMC}}}{\chi_{\text{CSR}}} + O(w^2)$$  

(A4)

Eqs. (A4,A5) agree with DB theory in the constant lifetime approximation [29].

In Fig. 3 we plot the disorder averaged Hall coefficient $R_H$ (black circles) of the square lattice model (A1) computed by Eq. (A3), where $\sigma_{xy}^{\text{DC}}$ and $\sigma_{xx}^{\text{DC}}$ are extrapolated to $L_x \to \infty$ and disorder averaged. The leading order equilibrium formula, Eqs. (A4,A5), is shown (dashed line) for comparison.

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On OBC, the wavevector $q$ is continuous and independent on $V$ (in contrast to the finite torus), and $(\lim_{q \to -c}, \lim_{q \to c})$ commute. The complex frequency $\omega + ic \to 0$, can be taken (after $V \to \infty$) along the imaginary axis.

On OBC one can define uniform charge and thermal polarizations, and the charge and thermal magnetizations needed for Eq. (2). Continuous and uniform thermal gradients can only be implemented on OBC. For the mesoscopic regime, boundary conditions matter. Our formulas can be relevant for small mesoscopic samples where the dephasing length scales is of the order of the sample size. Our finite volume formulas can implement the effects of attached leads, by keeping $\varepsilon$ larger than the leads level spacing.

For models with no C4 symmetry, the Hall coefficients, which are antisymmetric in magnetic field $B$, can be defined by antisymmetrizing the Kubo formulas with respect to $j_0 \to j_0'$, in accordance with Onsager’s relations.

For long range interactions, the spatial decomposition may not be unique.

In the literature, one frequently encounters specialized expressions of the magnetization and thermal magnetization $M_{OBC}$ for continuum particle Hamiltonians, $M_{OBC} = -\frac{1}{2} \sum_{j} \sum_{\alpha} \hat{z} \cdot \vec{r}_{j} \times \vec{v}_{j}$, and $M_{OBC} = -\frac{1}{2} \sum_{j} \sum_{\alpha} \hat{z} \cdot \vec{r}_{j}$, where $\alpha = (\vec{p}_{j} - \hat{z} \vec{A}_{j})/m$. Here we consider more general lattice Hamiltonians.

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We describe normal diagonalized hamiltonians. Anomalous bosonic terms e.g. $a \hat{a}^\dagger$ may be present in the energy-diagonalized thermal polarizations. These terms contribute off-shell matrix elements which can be ignored.

The following argument holds also for sharp and well separated edges in the bulk-gapped QH phases.

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