Hall Number of Strongly Correlated Metals

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(Received 21 February 2018; published 6 August 2018)

An exact formula for the temperature dependent Hall number of metals is derived. It is valid for nonrelativistic fermions or bosons, with an arbitrary potential and interaction. This dc transport coefficient is proven to (remarkably) depend solely on equilibrium susceptibilities, which are more amenable to numerical algorithms than the conductivity. An application to strongly correlated phases is demonstrated by calculating the Hall sign in the vicinity of Mott phases of lattice bosons.

DOI: 10.1103/PhysRevLett.121.066601

The zero field Hall number or “carrier density” of a metal is defined by

\[ n_H \equiv -\left( \frac{d\rho_H}{dB} \right)_{B=0}^{-1}, \]

where \( \rho_H \), \( B \), \( e^* \), and \( c \) are the (magnetic field antisymmetric) Hall resistivity, magnetic field, quasiparticle charge and speed of light, respectively. This definition is rooted in the Drude-Boltzmann [1] theory for weakly interacting conduction electrons (holes) of density \( n \) and charge \( e^* = e (e - e) \). While conductivities \( \sigma_{xx} \), \( \sigma_H \) depend on the quasiparticles’ effective mass and scattering time, for isotropic Fermi liquids, these properties cancel out in \( (d\rho_H/dB) = -\sigma_{xx}^{-1}(d\sigma_H/dB) = -1/(ne^*c) \).

The experimental Hall number, however, has defied a carrier density interpretation in strongly correlated metals. In the normal phase of cuprates [2,3] and in disordered superconducting films [4,5] \( n_H \) exhibits anomalous temperature dependences and sign changes, which have posed a challenge to the theory [6]. When the quasiparticles’ scattering rate is too high, the Boltzmann transport theory has questionable validity.

For gapped phases and finite lattices \( \sigma_{xx} = 0 \), and \( \rho_H = -\sigma_{xx}^{-1} \) can be calculated by Chern numbers on the torus [7–10]; however, computing both \( \sigma_{xx}, \sigma_H \) in the resistive phases \( \sigma_{xx} > 0 \) of strongly correlated systems is notoriously difficult: Diagrammatic expansions of the Kubo formulas require infinite resummations [11]. Exact diagonalization suffers from small lattice sizes [12,13], quantum Monte Carlo simulations [14] from ill-posed analytical continuation [15,16], and continued fraction calculations [8,17,18] require extrapolation schemes. Approximations for \( d\rho_H/dB \) include high frequency [19], retraceable paths [20], Drude weight derivatives [21], and dynamical mean field theory [22]. However an exact (generally valid), computable expression is in dire need.

In this Letter, I derive a summation formula, given by Eq. (26), for the temperature dependent Hall number of nonrelativistic fermions or bosons, in an arbitrary potential and two-body interaction strength. Remarkably, the formula expresses a dc transport coefficient solely in terms of equilibrium susceptibilities. Such a property of the Hall number was previously suggested, but not proven, except in the high frequency limit [19]. Susceptibilities are much more amenable to numerical computation than the conductivity, which miraculously drops out of the Hall number formula given below. Properties of the magnetic Liouvillian in Bogoliubov hyperspace are essential in the derivation. The leading term in the sum recovers Drude-Boltzmann’s result at weak disorder. For strong lattice potentials and interactions, projected Hamiltonians may be used to compute the susceptibilities. As an example, I evaluate the Hall signs for strongly interacting lattice bosons. The results extend previous Chern number calculations [8,9] to finite temperatures. Future applications are discussed.

Hamiltonian and Kubo formulas.—We consider \( N \) interacting particles in volume \( V \) in an arbitrary bounded potential \( \Phi \),

\[ H = \sum_{i=1}^{N} \left( \frac{\mathbf{p}_i - e^* \mathbf{A}(\mathbf{x}_i)}{2m} \right)^2 + \Phi(\mathbf{x}_i) + \frac{1}{2} \sum_{i\neq j} U(|\mathbf{x}_i - \mathbf{x}_j|). \]

(2)

\( \mathbf{A}(\mathbf{x}) = (B/2)(\hat{\mathbf{z}} \times \mathbf{x}) \). The zero wave vector current operators are \( j^\alpha = (e^*/m) \sum_i [p_i^\alpha - (e^*/c)A^\alpha(\mathbf{x}_i)], \alpha = x, y \).

The Bogoliubov hyperspace of operators is defined by inner products [23–25]. For any two operators (hyperstates) \( A, B \),

\[ \langle A|B \rangle = \frac{1}{Z} \sum_{n\neq m} \frac{e^{-\beta E_n} - e^{-\beta E_m}}{E_m - E_n} A_{mn}^* B_{mn} \]

(3)

where \( E_n \) is the spectrum of \( H \) and \( Z \) is the partition function. \( \langle A|B \rangle \) is a thermodynamic susceptibility. In this hyperspace, the Liouvillian \( \mathcal{L} \equiv [H, \bullet] \) is a Hermitian hyperoperator and \( \bullet \) is any operator. The Liouvillian

0031-9007/18/121(6)/066601(6) 066601-1 © 2018 American Physical Society
resolvent $[(1/L - i0^+)] = [(1/L)]^* + i[(1/L)]''$ separates into the Hermitian and anti-Hermitian parts. (The latter's eigenvalues are energy conserving delta functions.) The dc conductivities [26] are written in hyperspace notation as (for the derivation, see the Supplemental Material [27])

$$
\sigma_{xx} = \frac{\hbar}{V} \text{Re} \left[ j^x \left( \frac{1}{L} \right)^n |j^x| \right],
$$

$$
\sigma_H = \frac{\hbar}{V} \text{Im} \left[ j^x \left( \frac{1}{L} \right)^n |j^y| \right].
$$

(4)

Defining $\rho = e^{-\beta H}/Z$ the operators can be reorganized as [28]

$$
\sigma_H = -\frac{\hbar}{V} \text{Im} \text{Tr} \left\{ \rho \left( \frac{1}{L} \right)^{M'} \left( \frac{1}{L} \right)^{M''} \right\}.
$$

(5)

Differentiating the density operator yields

$$
\frac{d\rho}{dB} = -\left[ \rho \left( \frac{1}{L} \right)^{M'} - \beta \langle M \rangle \right],
$$

(6)

and differentiating the resolvent yields

$$
\frac{d}{dB} \left( \frac{1}{L} \right)^{M'} = \left( \frac{1}{L} \right)^{M'} \left( \frac{1}{L} \right)^{M''} - \left( \frac{1}{L} \right)^{M''} \left( \frac{1}{L} \right)^{M'},
$$

(7)

where

$$
M \equiv -\frac{dH}{dB}, \quad M \equiv [M, \ast],
$$

(8)

are the magnetization operator and the magnetization hyperoperator, respectively.

The field derivative of the Hall conductivity at $B = 0$ [29] is given by a sum of five terms:

$$
\frac{d\sigma_H}{dB} \bigg|_{B=0} = \Xi_{\text{osc}} + \Xi_{\text{comm}} + \Xi_j + \Xi_{M'} + \Xi_{M''}.
$$

(9)

I shall now show that the sum over the first four terms in Eq. (9) vanishes identically.

The first term, using Eq. (6), is

$$
\Xi_{\text{osc}} = \frac{\hbar \beta}{V} \text{Im} \text{Tr} \left\{ \rho M^{\text{diag}} \left( \frac{1}{L} \right)^{M'} \left( \frac{1}{L} \right)^{M''} \right\} + \beta \langle [M^{\text{diag}}] \rangle \sigma_H = 0,
$$

(10)

where $M^{\text{diag}}$ is the energy-diagonal part of $M$, which vanishes at the zero field.

The other terms, using Eqs. (6) and (7), are

$$
\Xi_{\text{comm}} = \frac{\hbar}{V} \text{Im} \text{Tr} \left\{ M \left( \frac{1}{L} \right)^{M'} \left( \frac{1}{L} \right)^{M''} \right\},
$$

(11)

The following identities hold for $H(B = 0)$:

$$
\left( \frac{1}{L} \right)^{M'} \left( \frac{1}{L} \right)^{M''} \left( \frac{1}{L} \right)^{M''} = \left( \frac{1}{L} \right)^{M'} \left( \frac{1}{L} \right)^{M''} - \left( \frac{1}{L} \right)^{M''} \left( \frac{1}{L} \right)^{M'},
$$

(12)

$$
\Xi_j = \frac{\hbar}{V} \text{Im} \left\{ \left( \frac{1}{L} \right)^{M'} \left( \frac{1}{L} \right)^{M''} \right\}.
$$

(13)

$$
\Xi_{M'} = \frac{\hbar}{V} \text{Im} \left\{ \left( \frac{1}{L} \right)^{M'} \left( \frac{1}{L} \right)^{M''} \right\}.
$$

(14)

The following identities hold for $H(B = 0)$:

$$
\left( \frac{1}{L} \right)^{M'} \left( \frac{1}{L} \right)^{M''} = \left( \frac{1}{L} \right)^{M'} \left( \frac{1}{L} \right)^{M''} - \left( \frac{1}{L} \right)^{M''} \left( \frac{1}{L} \right)^{M'},
$$

(15)

where $d = \sum_i x_i$ is the total polarization operator.

$$
\Xi_{\text{comm}} = 0 \text{ since the two polarizations commute [30],}
$$

$$
\Xi_j = \left( \frac{e^x}{\hbar} \right)^2 \left( d^x, d^y \right) = 0.
$$

(16)

It also follows from Eq. (15), that the next two terms cancel each other:

$$
\Xi_j = \frac{(e^x)^3}{2mcV} \text{Re} \left\{ (d^x |d^y) + (d^y |d^x) \right\}
$$

(17)

$$
\Xi_{M'} = \frac{(e^x)^2}{\hbar V} \text{Im} \left\{ (d^x |M, d^y) - (x \leftrightarrow y) \right\} = \Xi_j.
$$

Thus in Eq. (9), we are left with just $\Xi_{M''}$ i.e.,

$$
\frac{d\sigma_H}{dB} \bigg|_{B=0} = \Xi_j + \Xi_{M'} + \Xi_{M''}.
$$

(18)

Krylov states and recurrences.—We set $B = 0$. $H$ is assumed to have $x \leftrightarrow y$ symmetry, for simplicity. Two orthonormal Krylov bases $|n, \alpha \rangle$, $\alpha = x, y$ are constructed

$$
|0, \alpha \rangle = \left| j^\alpha \right| (j^y |j^\alpha)^2, \quad |1, \alpha \rangle = \frac{L |j^\alpha \rangle}{(j^y |j^\alpha)^2}.
$$

(19)

$$
|n, \alpha \rangle = (1 - \mathcal{P}_{n-2, \alpha}) L (1 - \mathcal{P}_{n-3, \alpha}) \cdots L |0, \alpha \rangle \quad n \geq 2,
$$

$$
|n, \alpha \rangle = \frac{1}{N_n} |n, \alpha \rangle,
$$

(19)

where $\ast$ ($\ast$) denote unnormalized (normalized) hyperstates, and $N_n$ are the normalizations of $|n, \alpha \rangle$. $\mathcal{P}_{n\alpha} = |n, \alpha \rangle \langle n, \alpha |$ are projectors.
In Krylov space, the Liouvillian acts as a hopping Hamiltonian on two semi-infinite chains, as shown in Fig. 1.

\[
\langle n, \alpha | L | n', \alpha \rangle = L_{n,n'} = \delta_{n',n+1} \Delta_n + \delta_{n,n-1} \Delta_{n-1} \quad (20)
\]

\[\Delta_n = \langle n + 1, \alpha | L | n, \alpha \rangle\] are the recurrences [17]. The conductivity moments \(\mu_{2k} = \hbar^{-2k} V^{-1} (L^k j^i | L^k j^i)\) are computable as thermodynamic susceptibilities. \(\Delta_n\) is obtained directly from \(\mu_{2k}\) by the recursive relations [27] \(\mu_{2k} = \hbar^{-2k} \tau_{xx} (L^{2k}[\Delta])/0,0\), which depend only on \(\Delta_n, n = 1, 2, \ldots, k\).

The spectral matrix \(G_{0,0}'' = \text{Im}(i 0^+ - L)/0,0\) yields the continued fraction representation of \(\sigma_{xx}\) [8]

\[\sigma_{xx} = -\hbar \tau_{xx} G_{0,0}'' = -\hbar \tau_{xx} \text{Im} \frac{1}{i 0^+ - (\Delta^2)/0^+ - (\Delta)/0} \quad (21)\]

where

\[\tau_{xx} = \frac{1}{V} \left( \langle j^i | j^i \rangle \right) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \sigma_{xx}(\omega) \quad (22)\]

is the “f-sum rule.” While computation of low order recurrences is commonly feasible, determination of \(\sigma_{xx}\) requires extrapolation [17,18] of \(\Delta_n\) to \(n \to \infty\), a procedure which can suffer from some ambiguity. I will now show that, fortunately, \(\sigma_{xx}\) drops out of the Hall number.

**Summation formula for \(n_H\).**—Inserting (partial) resolutions of identity \(1 = \sum_n P_{n,0}\) between the hyperoperators in \(\Xi M''\) of Eq. (14) leads to the following sums:

\[
\frac{d\sigma_H}{dB} \bigg|_{B=0} = -\frac{\hbar \tau_{xx}}{V} \sum_{n,m} G_{0,n}'' G_{m,0}'' M''_{n,m},
\]

\[M''_{n,m} = \text{Im}(\langle n,x | M|m,y \rangle - \langle n,y | M|m,x \rangle) \quad (23)\]

All the odd terms \(G_{0,2j+1}\) are purely real [27] and do not contribute to \(\Xi M''\), while the even terms are given by

\[G''_{0,2j} = G_{0,0}'' R_j = -\frac{\sigma_{xx}}{\hbar \tau_{xx}} R_j, \quad R_0 = 1, \quad R_{j>0} = \prod_{i=1}^{j} \left( \frac{-\Delta_{2i-1}}{\Delta_{2i}} \right) \quad (24)\]

Assuming a metal with time reversal symmetry, \(\sigma_{xx} > 0\), and \(d\sigma_{xx}/dB|_{B=0} = 0\), one can write

\[
\frac{d\rho_H}{dB} \bigg|_{B=0} = -\sigma_{xx}^2 \frac{d\sigma_H}{dB} \bigg|_{B=0} \quad (25)
\]

Hence, by Eqs. (1), (23), and (24), the prefactor of \(\sigma_{xx}^2\) is eliminated and we arrive at

\[
\frac{1}{n_H} = \frac{1}{n_H[0]} + \frac{e^c}{\hbar \tau_{xx}} \sum_{j,k=1}^{\infty} R_j R_k M''_{2j,2k}, \quad \frac{1}{n_H[0]} = \frac{e^c}{\hbar \tau_{xx}} \text{Im}(\langle j^i | M | j^i \rangle - \langle j^i | M | j^i \rangle). \quad (26)
\]

**Discussion.**—Equation (26) is the key result of this paper. Since for a noncritical metal \(|d\rho_{xx}/dB| < \infty\), this is a conditionally convergent sum. When truncated, a finite subset of recurrences \(\Delta_n\) and magnetization matrix elements \(M''_{n,m}\) need to be computed. The truncation error may be estimated by various perturbative methods, depending on the Hamiltonian, or numerically. Remarkably, all coefficients depend solely on static thermodynamic susceptibilities as defined by Eq. (3). Hence they are amenable to well controlled algorithms. A partial list is as follows.

(i) Quantum Monte Carlo simulations [14,31] (for sign free models), which compute imaginary time correlators \(\langle A | B \rangle = \int_0^\beta d\tau \langle \Lambda(\tau) | B \rangle\), (ii) High temperature series expansion [32]. (iii) Variational methods, including the density matrix renormalization group [33], which can compute \(\langle A | B \rangle = -\langle \partial^2 F/\partial \Lambda | \partial \Lambda \rangle\), where \(F\) is a variational free energy which includes the source terms \(-\hbar A^1 - h_B B\). (iv) Equation (3) may be computed by exact diagonalization on finite clusters, whose linear length exceeds the correlation length.

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Formula (26) will now be demonstrated for weak and strong interaction models.

**Weak disorder and interactions.**—The $f$-sum rule (gauge invariance) yields $\tau_s = (n(e^*)^2/m)$. Thus, using Eq. (15) in Eq. (26), Drude’s result is obtained at the zeroth order: $n_H^{(0)} = n$. Higher order terms in Eq. (26) are suppressed by a common factor

$$\left( \frac{\Delta_1}{\Delta_2} \right)^2 \propto \sum q | \Phi_q |^2 \kappa_q \ll 1, \quad (27)$$

where $\kappa_q$ is the wave vector dependent isothermal compressibility and $\epsilon_F$ is the Fermi energy. Thus, the sum in Eq. (26) produces systematic corrections to the Drude theory due to potential fluctuations and interactions.

**Strong interactions.**—In the presence of a large Mott-Hubbard gap, induced by strong interactions, and at low temperatures, one can replace the operators $H$, $M$, and $\bar{J}$ in Eq. (18), and thus in Eq. (26), by the renormalized effective Hamiltonian and its derivatives [34]. The Krylov states, recurrents and magnetization matrix elements are modified accordingly. Formula (26) can then be computed for the effective Hamiltonians, such as the Hubbard, $t$-$J$ [35], and Kondo lattice models [36]. These are relevant to strongly correlated metals, including the normal phase of unconventional superconductors and heavy fermion phases. The Hall number of these modes will be investigated elsewhere [37].

Here we study the Bose Hubbard model (BHM),

$$H_{\text{BHM}} = -t \sum_{\langle ij \rangle} e^{-i e \cdot A_i} a_i^\dagger a_j^\dagger + \text{h.c.} + U \sum_i n_i^2 - \mu n_i, \quad (28)$$

where $a_i^\dagger$ creates a lattice boson on site $i$, with occupations $n_i = 0, 1, \ldots$. The BHM is relevant to superconducting Josephson junction arrays and to cold atoms in optical lattices. At large $U/t$, there are gapped Mott insulator phases at integer fillings $\langle n_i \rangle = \text{integer}$, Huber and Lindner [9] have computed the ground state Chern number on finite tori. Here we obtain the finite temperature Hall number sign for the thermodynamic metal and compare it to the Chern calculations as shown in Fig. 2.

(1) Near the superfluid to Mott insulator critical points at integer fillings $n_0$, we replace $H_{\text{BHM}}$ by quantum rotators (QR). Defining the charge deviation from the Mott insulator density by $\rho(x)$,

$$H_{\text{QR}} = \int d^3 x \left[ \frac{1}{2 \chi c} \rho(x)^2 + \frac{1}{2} \rho_s \left( \nabla \rho(x) + \frac{e^*}{c} A \right)^2 [1 + \gamma \rho(x)^2] + \Phi(x) \rho(x) \right], \quad (29)$$

where $\chi_c$ is the Fermi energy. Thus, the sum in $\langle n \rangle$ results is obtained at the zeroth order: $\langle n_H \rangle = n$. Higher order terms in $\langle n \rangle$ are suppressed by a common factor

$$\frac{1}{\langle n_H \rangle} \propto \frac{\gamma}{e^* \rho_s c} + \mathcal{O}(\rho^2). \quad (30)$$

Thus, we can evaluate the sign of the leading term as

$$\frac{1}{\langle n_H \rangle} \propto \frac{\gamma}{e^* \rho_s c} + \mathcal{O}(\rho^2). \quad (32)$$

Since $\gamma > 0$, the Hall number near the Mott critical point changes sign in the same direction as determined at zero temperature using Chern numbers, as shown in Fig. 2. Higher order terms in Eq. (26) are suppressed in disorder free systems.

(2) Near half odd integer fillings, between Mott phases, we can use the effective hard core bosons (HCB) model [8],

$$H_{\text{HCB}} = -t \sum_{\langle ij \rangle} e^{-i e \cdot A_i} S_i^+ S_j^- + \text{h.c.}, \quad (33)$$

where $S$ are the effective spin half operators. $S_i^+$ creates a HCB at site $i$, and $S_i^\dagger = n_i - \frac{1}{2}$ measures its occupation relative to half filling.
The HCB currents and magnetization are

\[ j^a = -ie^*T \sum_i (e^{-ie} A_{i;i-a} S_i^a S_{i;i+a} - \text{H.c.}) , \]

\[ M = \frac{e^*}{2} \sum_i \chi_{i;i+y} - \gamma_{i;i+x}. \tag{34} \]

Expanding Eq. (3) at high temperature yields

\[ \langle A|B \rangle = \beta \text{Tr} \rho_\infty A^\dagger B - \frac{\beta^2}{2} \text{Tr} \rho_\infty \{H, A^\dagger\} B + O(\beta^3). \tag{35} \]

The infinite temperature density matrix \( \rho_\infty \) projects onto a fixed particle number \( \sum_i S_i^z = (n - \frac{1}{2}) V \). \( \tau_{xx} = \beta \text{Tr} \rho_\infty \chi_{i;i+x}^2 \). The traces in the magnetization matrix elements \( M_{2j,2k}^m \) vanish unless the operators encircle a magnetic flux. Therefore, for a triangular lattice at high temperatures, \( M_{00,0}^0 \propto -\beta(n - \frac{1}{2}) \), while for a square lattice, \( M_{00,0}^0 \propto -\beta^2(n - \frac{1}{2}) \). Thus, we obtain

\[ \frac{1}{n_H^0} \propto \begin{cases} -T(n - \frac{1}{2}) & \text{triangular} \\ -(n - \frac{1}{2}) & \text{square} \end{cases} \tag{36} \]

High order terms include \( M_{2j,2k}^m \), which decay rapidly with \( j, k \) due to diminishing overlaps between Krylov states. Thus the Hall sign of HCB, in Eq. (36), is depicted in Fig. 2. We note that the lattice effect resembles the behavior at infinite frequency [39].

Summary.—Equation (26) provides an exact computable formula for the Hall number of metals where \( \infty > \sigma_{xx} > 0 \). It should prove useful for numerical studies of disordered and strongly correlated, nonrelativistic fermions and bosons. The formula does not require well defined quasiparticles, as needed for Boltzmann’s equation. It also circumvents numerical difficulties associated with real-time response functions, such as the Kubo formulas for conductivities. We look forward to its application in experimentally relevant models of strongly correlated electron systems.

I thank Yosi Avron, Ilia Khait, Netanel Lindner, and Ari Turner for useful discussions. I acknowledge support from the United States-Israel Binational Science Foundation, Grant No. 2016168, and the Israel Science Foundation, Grant No. 2022061. I thank the Aspen Center for Physics supported by National Science Foundation Grant No. PHY-1607611, and the Kavli Institute for theoretical physics, University of California, Santa Barbara, supported in part by the National Science Foundation under Grant No. NSF PHY-1748958.

[26] The correct order of limits is that the frequency scale of the current, and the $\omega_0$ limit, are taken to zero after the thermodynamic limit $N, V \to \infty$.
[27] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.121.066601, Derivation of the Kubo formula in hyper space notations is provided. The relations between recurrences, moments, and the matrix elements of the Liouvillian resolvent in the Krylov bases at zero magnetic field are explained.
[28] The ambiguity in [(1/$\mathcal{L}(B)$)]$^{\rho}$ (due to the arbitrary addition of operators which commute with $H$) is eliminated by matching the matrix elements at high energies ($E_n, E_m \gg |\Phi|$) as: $f_{nm}^{\rho}/(E_n - E_m) \to (i/\hbar\omega_c)\epsilon_{q\rho} f_{nm}^\rho$. This asymptotic matching respects the semiclassical correspondence principle.
[29] The limit $B \to 0$ is taken after the thermodynamic limit $V \to \infty$.
[30] At zero field, $(1/\hbar) f^\rho$ are defined up to an arbitrary additional operator $f(H)$ will contribute terms to the commutator, Eq. (16), but not to $\Xi_{comm}$, since such terms have different reflection symmetries than $M$.
[34] Using renormalized operators is not advisable for the derivation of Eq. (26), which is based on the microscopic identities of Eq. (15).
[37] I. Khait and A. Auerbach, Hall number of the $t$-$J$ model (to be published).
[38] The minimal coupling $\nabla \varphi(x) + (q/c)A$ is consistent with the sign of the density-phase commutator.