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The Hall Number of Strongly Correlated Metals

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An exact formula for the temperature dependent Hall number of metals is derived. It is valid for non-relativistic fermions or bosons, with 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.

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

$$n_H \equiv - \left(\frac{d\rho_H}{dB} \Big|_{B=0} e^* c \right)^{-1}. \quad (1)$$

ρ_H, B, e^*, c are the (magnetic field antisymmetric) Hall resistivity, magnetic field, quasiparticle charge and speed of light respectively. This definition is rooted in Drude-Boltzmann[1] theory for weakly interacting conduction electrons (holes) of density n , and charge $e^* = e$ ($-e$). While *conductivities* σ_{xx}, σ_H , depend on the quasiparticles’ effective mass and scattering time, for isotropic Fermi liquids, these properties cancel out in $\frac{d\rho_H}{dB} = -\sigma_{xx}^{-2} \frac{d\sigma_H}{dB} = -1/(ne^*c)$.

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 theory[6]. When quasiparticles’ scattering rate is too high, Boltzmann transport theory has questionable validity.

For gapped phases and finite lattices $\sigma_{xx} = 0$, and $\rho_H = -\sigma_H^{-1}$ can be calculated by Chern numbers on the torus[7–10], however, computing both σ_{xx}, σ_H in the resistive phases ($\sigma_{xx} > 0$) of strongly correlated systems, *is notoriously difficult*: Diagrammatic expansions of the Kubo formulae 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 paper, I derive a summation formula, given by Eq. (26), for the temperature dependent Hall number of non-relativistic fermions or bosons, in an arbitrary po-

tential 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. 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 sign for strongly interacting lattice bosons. The results extend previous Chern number calculations[8, 9] to finite temperatures. Future applications are discussed.

Hamiltonian and Kubo Formulae. — We consider N interacting particles in volume V in an arbitrary bounded potential Φ ,

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

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

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

$$(A|B) = \frac{1}{Z} \sum_{n \neq m} \frac{e^{-\beta E_n} - e^{-\beta E_m}}{E_m - E_n} A_{mn}^* B_{mn} \quad (3)$$

where E_n is the spectrum of H , and Z is the partition function. $(A|B)$ 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 resolvent $\left(\frac{1}{\mathcal{L} - i0^+} \right) \equiv \left(\frac{1}{\mathcal{L}} \right)' + i \left(\frac{1}{\mathcal{L}} \right)''$, separates into the hermitian and antihermitian parts. (The latter’s

eigenvalues are energy conserving delta functions.) The DC conductivities[26] are written in hyperspace notation as (for the derivation see Supplementary Material[27] (SM)),

$$\begin{aligned}\sigma_{xx} &= \frac{\hbar}{V} \text{Re} \left(j^x \left| \left(\frac{1}{\mathcal{L}} \right)'' \right| j^x \right), \\ \sigma_H &= \frac{\hbar}{V} \text{Im} \left(j^x \left| \left(\frac{1}{\mathcal{L}} \right)' \right| j^y \right).\end{aligned}\quad (4)$$

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

$$\sigma_H = -\frac{\hbar}{V} \text{ImTr} \left\{ \rho \left[\left(\frac{1}{\mathcal{L}} \right)' j^x, \left(\frac{1}{\mathcal{L}} \right)' j^y \right] \right\}. \quad (5)$$

Differentiating the density operator yields,

$$\frac{d\rho}{dB} = - \left[\rho, \left(\frac{1}{\mathcal{L}} \right)' M \right] - \beta \langle M \rangle, \quad (6)$$

and differentiating the resolvent yields,

$$\frac{d}{dB} \left(\frac{1}{\mathcal{L}} \right)' = \left(\frac{1}{\mathcal{L}} \right)' \mathcal{M} \left(\frac{1}{\mathcal{L}} \right)' - \left(\frac{1}{\mathcal{L}} \right)'' \mathcal{M} \left(\frac{1}{\mathcal{L}} \right)'', \quad (7)$$

where

$$M \equiv -\frac{dH}{dB}, \quad \mathcal{M} \equiv [M, \bullet], \quad (8)$$

are the magnetization operator, and magnetization hyper-operator, respectively.

The field derivative of the Hall conductivity[29] is given by a sum of five terms:

$$\left. \frac{d\sigma_H}{dB} \right|_{B=0} = \Xi_{\text{osc}} + \Xi_{\text{comm}} + \Xi_j + \Xi'_{\mathcal{M}} + \Xi''_{\mathcal{M}}. \quad (9)$$

I shall now show that the sum over the first 4 terms in (9) vanishes identically.

The first term, using (6), is

$$\begin{aligned}\Xi_{\text{osc}} &= \frac{\hbar\beta}{V} \text{ImTr} \left\{ \rho M^{\text{diag}} \left[\left(\frac{1}{\mathcal{L}} \right)' j^x, \left(\frac{1}{\mathcal{L}} \right)' j^y \right] \right\} \\ &\quad - \beta \langle M^{\text{diag}} \rangle \sigma_H = 0, \quad (10)\end{aligned}$$

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

The other terms, using (6,7), are,

$$\Xi_{\text{comm}} = \frac{\hbar}{V} \text{Im} \left(M \left| \left[\left(\frac{1}{\mathcal{L}} \right)' j^x, \left(\frac{1}{\mathcal{L}} \right)' j^y \right] \right| \right), \quad (11)$$

$$\Xi_j = \frac{\hbar}{V} \text{Im} \left(\left(\frac{dj^x}{dB} \left| \left(\frac{1}{\mathcal{L}} \right)' \right| j^y \right) + \left(j^x \left| \left(\frac{1}{\mathcal{L}} \right)' \right| \frac{dj^y}{dB} \right) \right), \quad (12)$$

$$\Xi'_{\mathcal{M}} = \frac{\hbar}{V} \text{Im} \left(j^x \left| \left(\frac{1}{\mathcal{L}} \right)' \mathcal{M} \left(\frac{1}{\mathcal{L}} \right)' \right| j^y \right) - (j^x \leftrightarrow j^y), \quad (13)$$

$$\Xi''_{\mathcal{M}} = -\frac{\hbar}{V} \text{Im} \left(j^x \left| \left(\frac{1}{\mathcal{L}} \right)'' \mathcal{M} \left(\frac{1}{\mathcal{L}} \right)'' \right| j^y \right) + (j^x \leftrightarrow j^y). \quad (14)$$

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

$$\begin{aligned}\left(\frac{1}{\mathcal{L}} \right)' \mathbf{j} &= \frac{ie^*}{\hbar} \mathbf{d}, \\ [M, \mathbf{d}] &= -i \frac{\hbar e^*}{2mc} \hat{\mathbf{z}} \times \mathbf{d} \\ \frac{d\mathbf{j}}{dB} &= -\frac{(e^*)^2}{2mc} \hat{\mathbf{z}} \times \mathbf{d},\end{aligned}\quad (15)$$

where $\mathbf{d} = \sum_i \mathbf{x}_i$ is the total polarization operator.

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

$$\left[\left(\frac{1}{\mathcal{L}} \right)' j^x, \left(\frac{1}{\mathcal{L}} \right)' j^y \right] = -\left(\frac{e^*}{\hbar} \right)^2 [\mathbf{d}^x, \mathbf{d}^y] = 0. \quad (16)$$

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

$$\begin{aligned}\Xi_j &= \frac{(e^*)^3}{2mcV} \text{Re} \left((d^x | d^x) + (d^y | d^y) \right) \\ \Xi'_{\mathcal{M}} &= \frac{(e^*)^2}{\hbar V} \text{Im} (d^x | [M, d^y]) - (x \leftrightarrow y) = -\Xi_j.\end{aligned}\quad (17)$$

Thus we are left with just $\Xi''_{\mathcal{M}}$,

$$\left. \frac{d\sigma_H}{dB} \right|_{B=0} = -\frac{\hbar}{V} \text{Im} \left(j^x \left| \left(\frac{1}{\mathcal{L}} \right)'' \mathcal{M} \left(\frac{1}{\mathcal{L}} \right)'' \right| j^y \right) + (j^x \leftrightarrow j^y). \quad (18)$$

Krylov states and recurrences — We set $B=0$. H is assumed to have $x \leftrightarrow y$ symmetry, for simplicity. Two or-

thonormal Krylov bases $|n, \alpha\rangle$, $\alpha = x, y$ are constructed,

$$\begin{aligned} |0, \alpha\rangle &\equiv \frac{|j^\alpha\rangle}{(j^\alpha|j^\alpha)^{\frac{1}{2}}}, \\ |n, \alpha\rangle &\equiv (1 - \mathcal{P}_{n-2, \alpha})\mathcal{L}(1 - \mathcal{P}_{n-3, \alpha}) \cdots \mathcal{L}|0, \alpha\rangle \\ |n, \alpha\rangle &= \frac{1}{N_n}|n, \alpha\rangle, \end{aligned} \quad (19)$$

where $|\bullet\rangle$ ($|\bullet\rangle$) denote unnormalized (normalized) hyperstates, where 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,

$$L_{n', n} = \delta_{n', n+1}\Delta_n + \delta_{n', n-1}\Delta_{n-1}. \quad (20)$$

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

The spectral matrix $G''_{0,0} = \text{Im}(i0^+ - L)_{0,0}^{-1}$ yields the

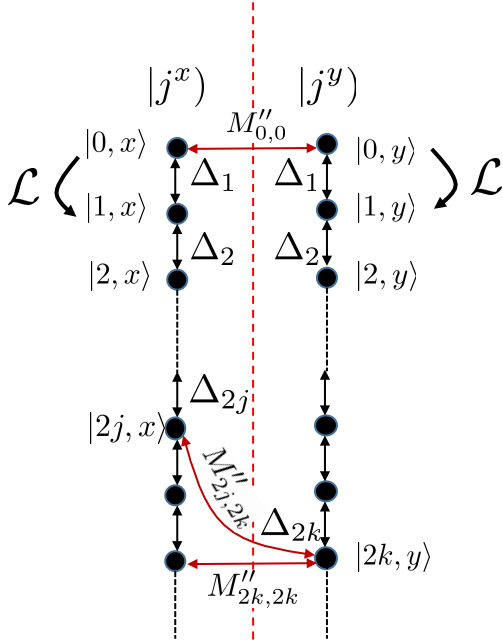


FIG. 1. The orthonormal Krylov bases, Eq. (19), constructed (for $B = 0$) from j^x and j^y by repeated application of the Liouvillian \mathcal{L} . Δ_n are the recurrents of σ_{xx} . $M''_{n,m}$ are the magnetization matrix elements defined in Eq. (23).

continued fraction representation [8],

$$\begin{aligned} \sigma_{xx} &= -\hbar\tau_{xx}G''_{0,0} \\ &= -\hbar\tau_{xx}\text{Im}\frac{1}{i0^+ - \frac{|\Delta_1|^2}{i0^+ - \frac{|\Delta_2|^2}{i0^+ - \frac{|\Delta_3|^2}{\dots}}}}, \end{aligned} \quad (21)$$

where,

$$\tau_{xx} = \frac{1}{V}(j^x|j^x) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \sigma_{xx}(\omega), \quad (22)$$

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

Summation formula for n_H – Inserting (partial) resolutions of identity $1 = \sum_n \mathcal{P}_{n,\alpha}$ between the hyperoperators in $\Xi''_{\mathcal{M}}$ of (14) leads to the following sums,

$$\begin{aligned} \frac{d\sigma_H}{dB}\Big|_{B=0} &= -\frac{\hbar\tau_{xx}}{V} \sum_{n,m} G''_{0,n} G''_{m,0} M''_{n,m}, \\ M''_{n,m} &\equiv \text{Im}(\langle n, x|\mathcal{M}|m, y\rangle - \langle n, y|\mathcal{M}|m, x\rangle). \end{aligned} \quad (23)$$

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

$$\begin{aligned} G''_{0,2j} &= G''_{0,0} R_j = -\frac{\sigma_{xx}}{\hbar\tau_{xx}} R_j, \\ R_j &\equiv \prod_{i=1}^j \left(-\frac{\Delta_{2i-1}}{\Delta_{2i}} \right). \end{aligned} \quad (24)$$

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

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

Hence, by (1), (23) and (24), the prefactor of σ_{xx}^{-2} is eliminated, and we arrive at,

$$\begin{aligned} \frac{1}{n_H} &= \frac{1}{n_H^{(0)}} + \frac{e^*c}{\hbar\tau_{xx}} \sum_{j,k=1}^{\infty} R_j R_k M''_{2j,2k}, \\ \frac{1}{n_H^{(0)}} &= \frac{e^*c}{V\hbar\tau_{xx}^2} \text{Im}\left((j^x|\mathcal{M}|j^y) - (j^y|\mathcal{M}|j^x)\right). \end{aligned} \quad (26)$$

Discussion. — Eq. (26) is the key result of this paper. Since for a non critical metal, $|d\rho_{xy}/dB| < \infty$, this is

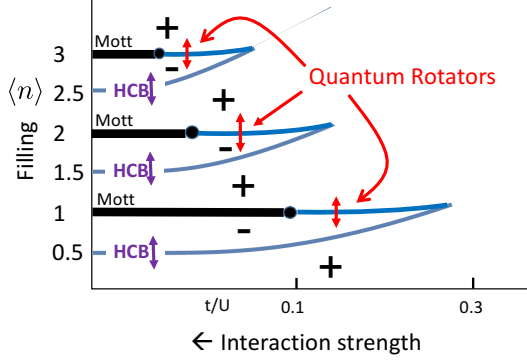


FIG. 2. Hall signs in strong interactions regime of the Bose Hubbard model Eq. (28). Mott insulators are thick black lines, ending at critical points (black circles). Solid blue lines mark Hall sign changes at zero temperature, computed by Huber and Lindner[9]. At high temperatures, we find the same sign changes using Quantum Rotators, and Hard Core Bosons (HCB) in Eqs. (32,36).

a conditionally convergent sum. When truncated, a finite subset of recurrences Δ_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 (3).* Hence they are amenable to well controlled algorithms. A partial list is: (i) Quantum Monte Carlo simulations[14, 30] (for sign free models) which compute imaginary time correlators, $\langle A|B \rangle = \int_0^\beta d\tau \langle A^\dagger(\tau)B \rangle$. (ii) High temperature series expansion[31]. (iii) Variational methods, including Density Matrix Renormalization Group[32], which can compute $\langle A|B \rangle = -\frac{\partial^2 F}{\partial h_A \partial h_B}$, where F is a variational free energy which includes the source terms $-h_A A^\dagger - h_B B$. (iv) Eq. (3) may be computed by exact diagonalization on finite clusters, whose linear length exceeds the correlation length. We note that exact diagonalizations are problematic when approaching e.g. superconducting, magnetic or charge density wave instabilities.

Formula (26) will now be demonstrated for weak and

strong interaction models.

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

$$\left(\frac{\Delta_1}{\Delta_2}\right)^2 \propto \frac{\sum_{\mathbf{q}} q_x^2 |\Phi_{\mathbf{q}}|^2 \kappa_{\mathbf{q}}}{\epsilon_F} \ll 1, \quad (27)$$

where $\kappa_{\mathbf{q}}$ is the wavevector dependent isothermal compressibility, and ϵ_F is the Fermi energy. Thus the sum in Eq. (26) produces systematic corrections to 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 \mathbf{j} , in Eq. (18), and thus in Eq. (26), by renormalized effective Hamiltonian and its derivatives [33]. The Krylov states, recurrences and magnetization matrix elements are modified accordingly. Formula (26) can then be computed for the effective Hamiltonians, such as the Hubbard, t-J [34] and Kondo lattice models[35]. 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 [36].

Here we study the Bose Hubbard model (BHM),

$$H^{\text{BHM}} = -t \sum_{\langle ij \rangle} e^{-ie^* A_{ij}} a_i^\dagger a_j + \text{h.c.} + \frac{U}{2} \sum_i n_i^2 - \mu n_i, \quad (28)$$

where a_i^\dagger creates a lattice boson on site i , with occupations $n_i = 0, 1, \dots$. 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^{BHM} by Quantum Rotators (QR),

$$H^{\text{QR}} = \int d^d x \frac{1}{2\chi_c} (\rho(\mathbf{x}) - n_0 a^{-d})^2 + \frac{1}{2} \rho_s \left(\nabla \varphi(\mathbf{x}) + \frac{e^*}{c} \mathbf{A} \right)^2 (1 + \gamma \rho(\mathbf{x})^2) + \Phi(\mathbf{x}) \rho(\mathbf{x}). \quad (29)$$

a is the lattice constant, χ_c is the local compressibility,

and ρ_s is the local superfluid stiffness. $\gamma > 0$ since

the superfluid order parameter increases away from the Mott phases. The canonical density-phase commutations are [37],

$$[\rho(\mathbf{x}), \varphi(\mathbf{x}')] = -i\delta(\mathbf{x} - \mathbf{x}'). \quad (30)$$

The QR currents and magnetization densities are,

$$\begin{aligned} \mathbf{j}(\mathbf{x}) &= -e^* \rho_s \nabla \varphi (1 + \gamma \rho^2), \\ m(\mathbf{x}) &= -\frac{e^*}{2c} (x j^y(\mathbf{x}) - y j^x(\mathbf{x})). \end{aligned} \quad (31)$$

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

$$\frac{1}{n_H^{(0)}} \propto \frac{\gamma}{e^* \rho_s c} \langle (\rho a^d - n_0) \rangle + \mathcal{O}(\langle (\rho a^d - n_0)^2 \rangle). \quad (32)$$

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 (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],

$$H^{\text{HCB}} = -t \sum_{\langle ij \rangle} e^{-ie^* A_{ij}} S_i^+ S_j^- + \text{h.c.} \quad (33)$$

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

The HCB currents and magnetization are,

$$\begin{aligned} j^\alpha &= -ie^* t \sum_i \left(e^{-ie^* A_{ii+\alpha}} S_i^+ S_{i+\alpha}^- - \text{h.c.} \right), \\ M &= \frac{e^*}{2} \sum_i x_i j_{i+y}^y - y_i j_{i+x}^x. \end{aligned} \quad (34)$$

Expanding (3) at high temperature yields,

$$(A|B) = \beta \text{Tr} \rho_\infty A^\dagger B - \frac{\beta^2}{2} \text{Tr} \rho_\infty \{H, A^\dagger\} B + \mathcal{O}(\beta^3). \quad (35)$$

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

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

High order terms include $M_{2j,2k}''$, 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 lattice effect resembles the behavior at infinite frequency [38].

Summary - Eq. (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, non relativistic 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 formulae for conductivities. We look forward to its application in experimentally relevant models of strongly correlated electron systems.

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