Reactive Hall Response

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The zero temperature Hall constant R_H, described by reactive (nondissipative) conductivities, is analyzed within linear response theory. It is found that in a certain limit R_H is directly related to the density dependence of the Drude weight, implying a simple picture for the change of sign of charge carriers in the vicinity of a Mott-Hubbard transition. This novel formulation is applied to the calculation of R_H in quasi-one-dimensional and ladder prototype interacting electron systems.

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It is now well known that in strongly correlated systems, zero temperature ($T = 0$), the reactive part of the conductivity can be used as a criterion of a metallic or insulating ground state [1]. In particular, following the work of Kohn, the imaginary part of the conductivity, $\sigma''(\omega \to 0) = 2D/\omega$, characterized by D (now called the "Drude weight" or charge stiffness), can be related to the ground state energy density ϵ^0 dependence on an applied fictitious flux ϕ as $D = (1/2)\partial^2\epsilon^0/\partial\phi^2|_{\phi\to 0}$.

A similar question is posed by the doping of an insulating state, where it would be interesting to have a simple description of the charge carriers sign as probed in a Hall experiment. For instance, we would like to describe the doping of a Mott-Hubbard insulator; within a semiclassical approach it is expected that the Hall constant $R_H \simeq +1/e\delta$, holelike (positive) near half filling ($\delta = 1 - n$, $n =$ density), changing to $R_H \simeq -1/en$, electronlike at low densities, the turning point depending on the interaction.

Over the recent years, ingenious ways have been proposed [2,3] for characterizing this sign change and strongly correlated electron systems, such as the t-J model, have been studied. In particular, following the suggestion to focus on the $T = 0$ Hall constant within linear response theory [4], the R_H of a hole in the t-J model was analyzed and a numerical method was proposed for calculating the Hall response in ladder systems [5]. This activity is partly motivated by the physics of high temperature superconductors viewed as doped Mott-Hubbard insulators and related Hall measurements showing a change of the sign of carriers with doping [6].

In this Letter, we show that within a certain frequency ω, wave vector q limiting procedure, the $T = 0$, $\omega \to 0$, thus "reactive" Hall constant, is simply related to the density dependence of the Drude weight. Following this point of view, we recover in a straightforward way: (i) the semiclassical expressions for R_H at low density and near an insulating state, (ii) a physical picture of the sign change of carriers in the vicinity of a Mott-Hubbard transition and its dependence on interaction strength, (iii) a common expression used to describe the Hall constant in quasi-one-dimensional conductors described by a band picture [7], (iv) good accord with R_H for ladder systems calculated using the numerical method proposed in [5].

The Hamiltonian.—In the following we will consider a generic Hamiltonian for fermions on a lattice, where for simplicity we describe the kinetic energy term by a one-band tight binding model; it is straightforward to extend this formulation to a many-band or continuum system. The sites are labeled $l(m)$ along the $x(y)$ direction with periodic boundary conditions in both directions:

$$
\begin{aligned}
H = &(-t)\sum_{l,m} e^{i\phi^x(t)} e^{iA_m} c^\dagger_{l+1,m} c_{l,m} + \text{H.c.} \\
&+ (-t')\sum_{l,m} e^{i\phi^y_{m+1/2}(t)} c^\dagger_{l,m+1} c_{l,m} + \text{H.c.} \\
&+ \hat{U}, \qquad l = 1,\ldots,L_x;\ m = 1,\ldots,L_y\,. \quad (1)
\end{aligned}
$$

$c_{l,m}$ ($c^\dagger_{l,m}$) is an annihilation (creation) operator at site (l,m) and the spin is neglected as it enters in a trivial way in the formulation. The $\hat{U}$ term can represent a many-particle interaction or a one-particle potential. We take the lattice constant so as to consider a unit volume, electric charge $e = 1$ and $\hbar = 1$. We add a magnetic field along the z direction, modulated by a one component wave vector q along the y direction, generated by the vector potential A_m; this allows one to take the zero magnetic field limit smoothly [8]:

$$
\begin{aligned}
A_m &= e^{iqm}\frac{iB}{2\sin(q/2)} \simeq e^{iqm}\frac{iB}{q}, \\
B_{m+1/2} &= -(A_{m+1} - A_m) = Be^{iq(m+1/2)}
\end{aligned} \quad (2)
$$

[for convenience, we present the long wavelength limit, substituting $2\sin(q/2) \to q$]. Electric fields along the x,y directions are generated by time dependent

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vector potentials:

$$\phi^{x,y}(t) = \frac{E^{x,y}(t)}{iz}, \qquad \phi^{y}_{m+1/2}(t) = e^{iq(m+1/2)}\phi^{y}(t);$$
$$E^{x}(t) = E^{x}e^{-izt}, \qquad E^{y}(t) = iE^{y}e^{-izt}; \tag{3}$$
$$z = \omega + i\eta .$$

Currents are defined through derivatives of the Hamiltonian expanded to second order in $\phi^{x,y}$:

$$J^{x} = -\frac{\partial H}{\partial \phi^{x}}, \qquad J^{y}_{q} = -\frac{\partial H}{\partial \phi^{y}}, \tag{4}$$

with the paramagnetic parts:

$$j^{x} = t\sum_{l,m}(ie^{iA_m}c^{\dagger}_{l+1,m}c_{l,m} + \text{H.c.}),$$
$$j^{y}_{q} = t'\sum_{l,m}e^{iq(m+1/2)}(ic^{\dagger}_{l,m+1}c_{l,m} + \text{H.c.}). \tag{5}$$

The reactive Hall response.—From standard linear response theory we obtain

$$\langle J^{x}\rangle = \sigma_{j^x j^x}E^{x}(t) + \sigma_{j^x j^y_q}E^{y}(t),$$
$$\langle J^{y}_{q}\rangle = \sigma_{j^y_q j^x}E^{x}(t) + \sigma_{j^y_q j^y_q}E^{y}(t). \tag{6}$$

$\langle\ldots\rangle$ are ground state expectation values in the presence of the magnetic field, with the conductivities

$$\sigma_{j^\alpha j^\beta} = \frac{i}{z}\left(\left\langle\frac{\partial^2 H}{\partial\phi^\alpha\partial\phi^\beta}\right\rangle - \chi_{j^\alpha j^\beta}\right),$$
$$\chi_{AB} = i\int_0^\infty dt\, e^{izt}\langle[A(t),B]\rangle. \tag{7}$$

Now, in contrast to the usual derivation of the Hall constant expression, we will keep the q dependence explicit by converting the current-current to current-density correlations using the continuity equation:

$$\langle J^{x}\rangle = \sigma_{j^x j^x}E^{x}(t) + \frac{1}{q}\chi_{j^x n_q}E^{y}(t),$$
$$\langle J^{y}_{q}\rangle = -\frac{1}{q}\chi_{n_q j^x}E^{x}(t) + \left(\frac{z}{q}\right)^2\chi_{n_q n_q}\frac{i}{z}E^{y}(t), \tag{8}$$

with $n_q = \sum_{l,m}(-ie^{iqm})c^{\dagger}_{l,m}c_{l,m}$.

At $T = 0$, the response is nondissipative so we will study the reactive (out-of-phase) induced currents. Furthermore, at this point we will consider the "screening" (or slow) response in the y direction, by taking the (q,ω) limits in the order $\omega \to 0$ first and $q \to 0$ last; in the usual "transport" (or fast) response the limits are in the opposite order [9]. As we discuss below, this approach leads to a simple physical picture for the Hall constant and it might be argued that at least for certain cases, for example, for a system of finite size in the y direction, it is indeed the right one. The expressions (8) for the currents become

$$\langle J^{x}\rangle_0 = \sigma''_{j^x j^x}(\omega\to 0)[iE^{x}(t)] + \frac{1}{q}\chi'_{j^x n_q}(\omega = 0)E^{y}(t),$$
$$\langle J^{y}_{q}\rangle_0 = -\frac{1}{q}\chi'_{n_q j^x}(\omega = 0)E^{x}(t) + \left(\frac{\omega}{q}\right)^2\frac{1}{\omega}\chi'_{n_q n_q}(\omega = 0)[iE^{y}(t)], \tag{9}$$

where the subscript zero denotes the leading order in ω response,

$$\chi'_{AB}(\omega = 0) = \sum_{n>0}\frac{\langle 0|A|n\rangle\langle n|B|0\rangle + \text{H.c.}}{E_n - E_0}, \tag{10}$$

and $|n\rangle\,(E_n)$ are eigenstates (eigenvalues) of the Hamiltonian in the presence of the magnetic field.

Now, following Kohn's observation [1], we can identify the different terms as derivatives of the ground state energy density ϵ^0 of a fictitious Hamiltonian depending on static ϕ^x, μ_q fields:

$$H = (-t)\sum_{l,m}(e^{i\phi^x}e^{iA_m}c^{\dagger}_{l+1,m}c_{l,m} + \text{H.c.}) + (-t')\sum_{l,m}(c^{\dagger}_{l,m+1}c_{l,m} + \text{H.c.}) + \mu_q n_q + \hat{U}. \tag{11}$$

For $H(\lambda,\mu)$, using the following identity,

$$\epsilon^0_{\mu\lambda} = \frac{\partial^2\epsilon^0}{\partial\mu\partial\lambda} = \langle 0|\frac{\partial^2 H}{\partial\mu\partial\lambda}|0\rangle - \sum_{n>0}\frac{\langle 0|\frac{\partial H}{\partial\mu}|n\rangle\langle n|\frac{\partial H}{\partial\lambda}|0\rangle + \text{H.c.}}{E_n - E_0}, \tag{12}$$

we can rewrite the currents as

$$\langle J^{x}\rangle_0 = \frac{\epsilon^0_{\phi^x\phi^x}}{\omega}[iE^{x}(t)] + \left(\frac{-1}{q}\right)\epsilon^0_{\phi^x\mu_q}E^{y}(t),$$
$$\langle J^{y}_{q}\rangle_0 = \frac{1}{q}\epsilon^0_{\mu_q\phi^x}E^{x}(t) - \frac{\omega}{q^2}\epsilon^0_{\mu_q\mu_q}[iE^{y}(t)]. \tag{13}$$

Finally, setting $\langle J^{y}_{q}\rangle_0 = 0$ we determine the reactive Hall constant:

$$R_H \equiv -\frac{1}{B}\frac{E^y}{\langle J^x\rangle_0} = \frac{q}{B}\frac{\epsilon^0_{\mu_q\phi^x}}{\epsilon^0_{\phi^x\phi^x}\epsilon^0_{\mu_q\mu_q} + \epsilon^0_{\mu_q\phi^x}\epsilon^0_{\phi^x\mu_q}}. \tag{14}$$

Neglecting the $O(B^2)$ cross term $\epsilon^0_{\mu_q\phi^x}\epsilon^0_{\phi^x\mu_q}$ and Taylor expanding the numerator in B, we can rewrite R_H as

$$R_H = q\frac{\frac{\partial^3\epsilon^0}{\partial B\partial\mu_q\partial\phi^x}}{\epsilon^0_{\phi^x\phi^x}\epsilon^0_{\mu_q\mu_q}} = q\frac{\frac{\partial}{\partial\mu_q}\left(\frac{\partial^2\epsilon^0}{\partial B\partial\phi^x}\right)}{\epsilon^0_{\phi^x\phi^x}\epsilon^0_{\mu_q\mu_q}}. \tag{15}$$

Using (12) we find the final expression

$$R_H = -\frac{\frac{\partial D_q}{\partial\mu_q}}{D\kappa_q}, \tag{16}$$

where

$$D_q = \frac{1}{2}\Bigg[\langle 0| - T_q^x|0\rangle - \sum_n \frac{\langle 0|j^x|n\rangle\langle n|j_q^x|0\rangle + \text{H.c.}}{E_n - E_0}\Bigg],$$

$$j_q^x = (-t)\sum_{l,m}(-ie^{iqm})\,(ic_{l+1,m}^\dagger c_{l,m} + \text{H.c.}),$$

$$T_q^x = (-t)\sum_{l,m}(-ie^{iqm})\,(c_{l+1,m}^\dagger c_{l,m} + \text{H.c.}). \tag{17}$$

$D = \frac{1}{2}\epsilon^0_{\phi^x\phi^x}$, the Drude weight, is identical to D_q by the replacement of j_q^x (T_q^x) by j^x (T^x). $\kappa_q = \epsilon^0_{\mu_q\mu_q} = \partial n_q/\partial\mu_q$ is the compressibility corresponding to the density modulation n_q. Notice that the spatial dependence of j_q^x and n_q is the same as that of A_m.

Taking the $q \to 0$ limit, we obtain a particularly simple expression for R_H:

$$R_H = -\frac{1}{D}\frac{\partial D}{\partial n}. \tag{18}$$

A handwaving argument leading to expression (18) for $t' \to 0$ is as follows: A_m corresponds to a twist of boundary conditions on chain m, inducing an extra current on each chain proportional to D (besides the uniform one induced by the flux ϕ^x); minimization of the energy at fixed x current gives rise to an m-dependent charge density. The "Hall potential" μ_q is then determined by requiring the cancellation of this induced charge density, leading to the above expression by the definition of the Hall constant (14). Note that a similar idea, analyzing the Hall constant in terms of independent channels (edge states), exists in the literature of the quantum Hall effect [10].

This expression is appealing as it gives a direct, intuitive understanding for the change of sign of charge carriers in the vicinity of a metal-insulator transition. First, at low densities, $D \propto n$ giving $R_H \simeq -1/n$; close to a Mott insulator $D \propto \delta = 1 - n$, implying $R_H \simeq +1/\delta$. Furthermore, we obtain a change of sign in the vicinity of a Mott transition at a density which depends on the interaction strength and is given by the position of the maximum of D. Second, for independent electrons, where D is proportional to the kinetic energy, by taking the limit $t' \to 0$ and calculating D as a sum of D's for individual x chains, we obtain from (18)

$$D = \frac{2t}{\pi}\sin\!\left(\frac{\pi n}{2}\right), \qquad R_H = -\frac{\pi}{2}\frac{1}{\tan(\frac{\pi n}{2})}, \tag{19}$$

an expression used for the Hall constant of quasi-one-dimensional compounds [7]. Considering that the $t' \to 0$ limit might by subtle, it is of particular theoretical and experimental interest whether the Hall constant of quasi-one-dimensional correlated systems [11] is indeed given by the expression and thus related to the Drude weight of the individual chains. The same applies for the transverse Hall effect of weakly coupled planes.

Examples.—In this section we present a generic picture for the behavior of the Hall constant for models of strongly correlated fermions showing a Mott-Hubbard metal-insulator transition. This picture emerges, on the one hand, by an exact calculation of R_H for ladder systems using the numerical method of Ref. [5] and on the other hand, from the expression (18) assuming nearly decoupled chains ($t' \to 0$) and calculating $D(n)$ for each chain analytically using the Bethe ansatz method [12,13]. It is clear that this analytical approach refers to either ladder (with $t' \to 0$) or quasi-one-dimensional models.

Three prototype models will be discussed: the Hubbard model, as the most experimentally relevant, the spinless fermions model ("t-V") showing both a metallic and an insulating phase depending on interaction strength, and the supersymmetric t-J model.

(i) The *Hubbard model* is given by the Hamiltonian

$$H = (-t)\sum_{l,m}(c_{l+1,m,\sigma}^\dagger c_{l,m,\sigma} + \text{H.c.}) + (-t')\sum_{l,m}(c_{l,m+1,\sigma}^\dagger c_{l,m,\sigma} + \text{H.c.}) + U\sum_{l,m} n_{l,m,\uparrow}n_{l,m,\downarrow}. \tag{20}$$

$c_{l,m,\sigma}$ ($c_{l,m,\sigma}^\dagger$) is an annihilation (creation) operator at site (l,m) of a fermion with spin $\sigma = \uparrow,\downarrow$. R_H extracted from a Bethe ansatz calculation of $D(n)$ for the one-dimensional Hubbard model [13] is shown in Fig. 1.

This behavior is characteristic of correlated systems undergoing a metal-insulator transition at half filling: at low densities $R_H \simeq -1/n$, while near half filling $R_H \simeq +1/\delta$, the position of change of sign of the carriers depending on the details of the interaction.

(ii) The t-V model on a ladder is given by

$$H = (-t)\sum_{l,m}(c_{l+1,m}^\dagger c_{l,m} + \text{H.c.}) + (-t')\sum_{l}(c_{l,1}^\dagger c_{l,2} + \text{H.c.}) + V\sum_{l,m} n_{l,m}n_{l+1,m}. \tag{21}$$

Here and in the following $l = 1,\ldots,L_x, m = 1,2$. For a

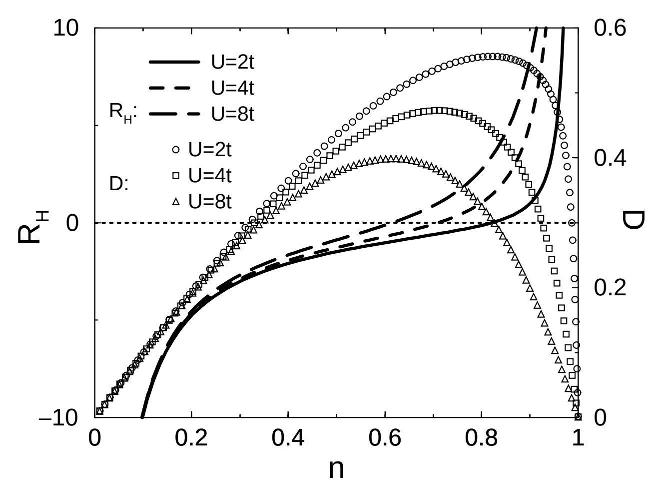

FIG. 1. R_H for the Hubbard model from expression (18) for $t' \to 0$.

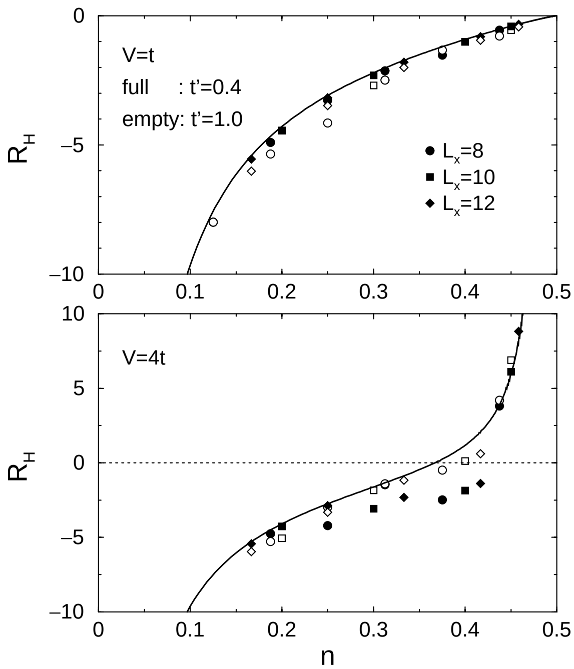

FIG. 2. R_H for the t-V ladder from expression (18) for $t' \to 0$ (continuous line) and from a numerical evaluation (symbols). $V = t(4t)$; metallic (insulating) phase at $n = 0.5$.

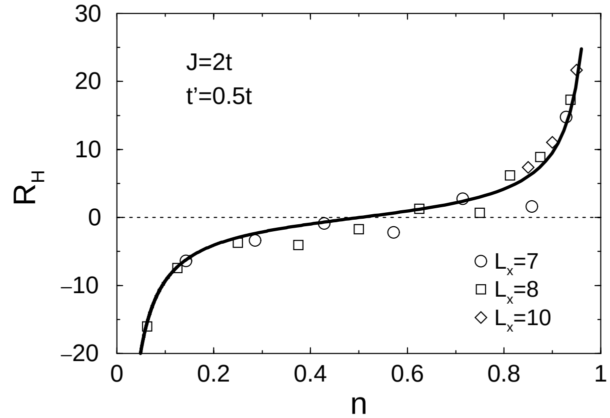

FIG. 3. R_H for the t-J ladder from expression (18) for $t' \to 0$ (continuous line) and from a numerical evaluation (symbols).

single chain, this model describes a metallic phase at all densities for $V < 2t$, while for $V > 2t$ it is an insulator at half filling. In Fig. 2 we show R_H calculated numerically on finite systems for two values of t' and analytically from (18) in the $t' \to 0$ limit. The numerical evaluation being especially sensitive to finite size effects for $t' \to 0$, we study relatively large values of t'.

Results for R_H clearly show the difference between the metallic regime $V = t$, where at half filling ($n = 0.5$) we get $R_H = 0$, while in the insulating regime $V = 4t$, we are dealing with $R_H(n \to 0.5) \to \infty$.

(iii) The t-J model on a ladder is given by the Hamiltonian

$$H = (-t)\sum_{l,m}(c^{\dagger}_{l+1,m,\sigma}c_{l,m,\sigma} + \text{H.c.}) + (-t')\sum_{l}(c^{\dagger}_{l,1,\sigma}c_{l,2,\sigma} + \text{H.c.}) + J\sum_{l,m}\left(\vec{S}_{l,m}\vec{S}_{l+1,m} - \frac{1}{4}\,n_{l,m}n_{l+1,m}\right). \quad (22)$$

$\vec{S}_{lm}$ is the spin operator at site (l, m) and the double occupancy on a site is forbidden.

In Fig. 3 we show again R_H calculated analytically for the "supersymmetric" model, $J = 2t$, and by numerical evaluation for $t' = 0.5t$ and different size systems.

The above three examples show a remarkable agreement between the numerical evaluation of R_H on finite size systems using the method of Ref. [5] (at finite t') and the analytical calculation using (18) for $t' \to 0$, indicating a relative insensitivity on the transverse coupling t' for ladders. These results confirm the intuitive picture for the behavior of the Hall constant in the vicinity of a metal-insulator transition and present an intriguing link between the Hall constant and the Drude weight. It is possible that R_H is dominated at low temperatures by correlations and not the relaxation mechanism so this formulation could have more general validity.

In conclusion, the emerging simple physical picture raises the question of the relation of this novel formulation to the traditional semiclassical approach to the Hall constant, its range of validity, and the role of relaxation in the description of the Hall effect and of the perspectives for an extension at finite temperatures.

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