Faraday Rotation and the Hall Constant in Strongly Correlated Fermi Systems

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We observe that the semiclassical Hall constant for a strongly correlated Fermi system is most directly related to the high frequency Hall conductivity. For the square lattice, the sign of the latter is found to be holelike (while the Fermi surface is electronlike) for fillings close to half, and electronlike for almost empty bands. For the t-J model on the square lattice in two dimensions the change of sign occurs at roughly 1/3 hole filling in good agreement with measurements on $La_{2-x}Sr_xCuO_4$ compounds, and is weakly temperature dependent. We suggest that the high frequency Hall constant can be directly measured in a Faraday rotation experiment.

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The measurements of the Hall constant in high-T_c materials [1] raise two major questions. The first one is how to reconcile the positive (holelike) sign of the Hall constant observed in $La_2Sr_xCu_{2-x}O_4$, as well as $YBa_2Cu_3O_{7-\delta}$ families of compounds [1, 2], with the "electronlike" shape of the Fermi surface. The latter follows from the band structure calculations [3], and is consistent with the photoemission data in these and related Bi compounds [4]. One could introduce terms in a tight binding model that give holelike curvature to parts of the Fermi surface, but such modifications cannot, even in principle, give a Hall constant that has an unbounded increase as half filling is approached. The second question is the unusual temperature dependence: it shows considerable universality in the high-T_c compounds, especially upon taking the Hall angle as the central variable, as suggested by Anderson [5]. In this work we shall only consider the first question which concerns the dependence of the sign of the Hall constant on doping for the Mott-Hubbard system. Of course, it is expected that R_H is electronlike at very low filling (since in this Galitskii limit, the lattice is presumably irrelevant) and holelike very near half filling, as seems reasonable from the point of view of an antiferromagnet with a few holes, or the Nagaoka limit, although these extreme pictures involve magnetic order and lead to non-Luttinger Fermi surfaces.

It is well known that the interpretation of the Hall resistivity is notoriously nontrivial even in relatively simple metals [6]. The reason is that while the familiar semiclassical expression $R_H = 1/n^*ec$, with n^* the effective carrier density, does not contain the relaxation time τ, the Hall resistivity is in fact a transport measurement and the effects of scattering drop out only in the single relaxation time approximation. In practice (as is already the case for the metals with complex Fermi surfaces) the relaxation time at low T is anisotropic and depends on the wave number resulting in a nontrivial dependence of R_H on $\tau(k)$ on the Fermi surface [6]. Thus, the magnitude and sign of Hall resistivity R_H do not provide a direct measurement of the number and the sign of the carriers. One is then led to ask if there is a direct experimental access to the "semiclassical" quantity $R_H^* = 1/n^*ec$ with the familiar interpretation. The "answer" that we propose here is the Faraday rotation experiment which measures Hall resistivity at finite frequency, $R_H(\omega)$. For sufficiently high ω, $R_H(\omega) \to R_H^*$. In the case of Mott-Hubbard systems such as the CuO based materials, we will be interested in ω high compared to the bandwidth, but still below the Mott-Hubbard "gap" or optical edge. In this way R_H^* will be free of the low energy scattering effects but will include the correlation effects. The motivation to consider a high frequency measurement is the observation that the semiclassical formula for the Hall effect is essentially the Lorentz force acting on moving carriers normalized to the charge current. As such, it is an instantaneous measurement and is not sensitive to the details of the irreversible processes involved in setting up the current in contrast to the $\omega = 0$ transverse resistivity measurement. On the other hand, the consequence of R_H^* being defined at finite ω is that it is not, in general, related to the shape of the Fermi surface. This helps one to understand the "paradox" of the holelike Hall effect coexisting with the electronlike Fermi surface. We have studied the minimal models for high-T_c systems, the Hubbard and the t-J models on a square lattice using the moments scheme to calculate R_H^*. We shall find below that for the Hubbard model with strong on-site repulsion, R_H^* changes sign at a filling $n \sim \frac{2}{3}$, in good agreement with the transport measurements [1, 2].

We shall proceed by using Kubo formulas and the moment expansion to define R_H^* and its relation to R_H. The resulting explicit expression for the R_H^* in terms of the equal time many-body correlation functions will then be evaluated for (i) small Hubbard U/t, by perturbation theory and for (ii) large U/t by a high-temperature expansion for the t-J model using the projected fermions. Finally, in the conclusion, we will quote an estimate of the expected Faraday rotation angle via the high-

temperature series.

We recall the Peierls phase factor, governing the coupling between the electromagnetic field and the lattice fermions; the kinetic energy is written as $T = -t\sum_{\delta=\mathbf{x},\mathbf{y}}\{\exp[ie\mathbf{A}(\mathbf{r})\cdot\delta]c^\dagger(\mathbf{r}+\delta)c(\mathbf{r}) + \text{H.c.}\}$, where $\mathbf{A}$ is the vector potential. The (matter) current operator $J_\alpha = -\frac{1}{e}\delta T/\delta A_\alpha$ and the stress tensor $\tau_{\alpha,\beta} = \frac{1}{e^2}\delta^2 T/\delta A_\alpha \delta A_\beta = \sum_k[\delta^2\epsilon(k)/\delta k_\alpha \delta k_\beta]c^\dagger(k)c(k)$ are defined as usual, in terms of which the conductivity tensor is [7, 8]

$$\sigma_{\alpha,\beta}(\omega) = \frac{ie^2}{\omega\Omega}\left[\langle\tau_{\alpha,\beta}\rangle - \frac{1}{\mathcal{Z}}\sum\frac{\exp-(\beta\epsilon_\nu)-\exp-(\beta\epsilon_\mu)}{\epsilon_\mu-\epsilon_\nu-\omega-i\eta}\langle\nu|J_\alpha|\mu\rangle\langle\mu|J_\beta|\nu\rangle\right]. \tag{1}$$

The Hall resistivity, at a frequency ω, may be obtained from

$$R_H(\omega) = a_0^3\frac{\partial}{\partial B}\left(\frac{\sigma_{x,y}(\omega)}{\sigma_{x,x}(\omega)\sigma_{y,y}(\omega)-\sigma_{x,y}(\omega)\sigma_{y,x}(\omega)}\right)_{B=0} \tag{2}$$

in the weak field regime. The relevant part of $\sigma_{x,y}$ is antisymmetric in x, y, and hence we may write

$$\sigma_{[x,y]}(\omega) = -\frac{ie^2}{\mathcal{Z}\Omega}\sum\frac{\exp-(\beta\epsilon_\nu)-\exp-(\beta\epsilon_\mu)}{(\epsilon_\mu-\epsilon_\nu)^2-\omega^2}\langle\nu|J_x|\mu\rangle\langle\mu|J_y|\nu\rangle. \tag{3}$$

For large ω ($>> \epsilon_\mu - \epsilon_\nu$), we have

$$\sigma_{[x,y]}(\omega) = \frac{ie^2}{\Omega\omega^2}\left[\langle[J_x,J_y]\rangle + \frac{1}{\omega^2}\langle[[[J_x,H],H],J_y]\rangle + O(1/\omega^4)\right], \tag{4}$$

while

$$\sigma_{x,x}(\omega) = \frac{ie^2}{\Omega\omega}\left[\langle\tau_{x,x}\rangle + \frac{1}{\omega^2}\langle[[J_x,H],J_x]\rangle + O(1/\omega^4)\right]. \tag{5}$$

We will assume cubic symmetry and substituting these expansions into Eq. (2) generates a moment expansion, and we may use a standard Stieltjes trick to resum it in the form of a high frequency "residue" R_H^*, and a "self-energy" $\Sigma_H(\omega)$ as

$$R_H(\omega) = \frac{R_H^*}{1-\Sigma_H(\omega)}, \tag{6}$$

with

$$R_H^* = \lim_{B\to 0}\left(-\frac{ia_0^3 N}{Be^2}\frac{\langle[J_x,J_y]\rangle}{\langle\tau_{x,x}\rangle^2}\right). \tag{7}$$

where the self-energy $\Sigma \to 1/\omega^2$ for large ω. In the case of purely elastic scattering by impurities, as in the Drude model, the self-energy Σ_H *vanishes identically*, and the frequency dependence of $R_H(\omega)$ drops out completely, in contradistinction to that of the Hall conductivity $\sigma_{[x,y]}(\omega)$. The functional form of Eq. (6) expresses a decomposition of R_H with the self-energy carrying all the information about inelastic scattering, and the numerator, namely, R_H^*, the information about the kinematics of the problem, and also, as we shall show, the interaction between particles in a strongly correlated Fermi system.

The quantity R_H^* is the effective high frequency Hall "constant" of the system, which controls the sign of $R_H(\omega)$. The fundamental nature of R_H^* is apparent from Eq. (7) which expresses it as a ratio of two equal time correlation functions: The current commutator in the numerator vanishes in the absence of magnetic field and is similar to the magnetic translation commutator, while the expectation value in the denominator is the same one that appears in the f-sum rule and counts the total oscillator strength. The nice thing is that R_H^* is directly measurable provided the probe frequency ω exceeds a typical electronic level separation inside a band, i.e., say, ~ 1 eV. In a typical Mott-Hubbard situation, we have the relevant bands with mobile holes sandwiched in energy, between filled and empty "inert bands," and it presumably suffices to have ω avoid resonant energy level spacings (as evinced say in the peaks in the dielectric function). We distinguish between two cases, a weakly interacting Fermi system where the effective $U \sim t$, and a strongly interacting Fermi system where $U \gg t$. In the first case, it suffices to have $\omega > \max\{U,t\}$, while in the second we require $t < \omega \ll U$.

In the weak coupling case, we have $\omega > \max\{t,U\}$, and the expression for R_H^* simplifies considerably and we find

$$R_H^* = r_0\frac{\sum_{k,\sigma}\cos k_x \cos k_y\langle c_\sigma^\dagger(k)c_\sigma(k)\rangle}{[\sum_{k,\sigma}\cos k_x\langle c_\sigma^\dagger(k)c_\sigma(k)\rangle]^2}, \tag{8}$$

where r_0 is the dimensionful constant [7], and the sums are normalized to unity. It must be first remarked that the expression Eq. (8) reduces to the familiar expression $1/ne$, for any interaction strength, provided the filling of the electrons is very low; i.e., as $n \to 0$, by simple kinematics, the cosine functions can be expanded in powers of k and to leading order we may set them equal to unity, the sums reduce to densities and hence the result. The second point is that the final sign of the R_H^* is not necessarily that of e, but rather depends on that of the weighted integral of $\langle c^\dagger(k)c(k)\rangle$. For an interact-

ing system, the entire Brillouin zone tends to get populated. The dynamics determines the favored regions of occupations and Eq. (8) suggests that, for the sign of R_H^* to reverse, we must have a preferential occupation of regions where $\cos(k_x)\cos(k_y) < 0$. In fact, we can calculate the change of $n_k \equiv \langle c^\dagger(k)c(k)\rangle$ out to second order in U using perturbation theory at $T = 0$ to evaluate the numerator of Eq. (8); one finds that close to half filling, $\delta = 1 - n \sim 0$ the perturbative result $\langle c_1^\dagger c_3\rangle = -0.3\delta\{1 - 0.8(U/4t)^2\} + O(\delta^2)$. This implies that R_H^* changes sign at small δ for $U/4t > 1.1$, which is strictly speaking outside the perturbative regime. This change of sign has, of course, nothing to do with the shape of the Fermi surface, which remains electronlike. Exact diagonalization of small Hubbard clusters should give reliable results for the short distance correlations involved in Eqs. (8), demarcating regions in the $\{\delta, U\}$ space where R_H^* is holelike. However, if the interactions are turned off, then the numerator of Eq. (8) can be rewritten by Stokes theorem as an integral over the Fermi surface yielding a standard relation [6] between the Hall constant and the curvature of the Fermi surface.

Let us now evaluate R_H^* for the large U case. The point here is that even though R_H^* is defined by the high ω limit, we are interested in the order of limits where both $\omega/t, U/t \to \infty$, with $\omega \ll U$. Before proceeding further, we note that the Hall resistivity in this limit has been considered by Brinkman and Rice [9], who also used the moment expansion but concentrated on $R_H(\omega = 0)$. The $U \to \infty$ limit can be taken simply by replacing the fermion operators $c_\sigma(r)$ by the projected fermions $\hat{c}_\sigma(r)$. We can compute R_H^* in a high-temperature limit in a very instructive calculation. The numerator of Eq. (7) is

$$\langle [J_x, J_y]\rangle = \frac{\beta^2}{2}\mathrm{Tr}H^2[J_x, J_y] + O(\beta^4). \tag{9}$$

The trace can be evaluated directly, giving

$$\lim_{B\to 0}\frac{1}{iB}\langle [J_x, J_y]\rangle = -t^4\beta^2 N\delta(1-\delta)\left[\delta^2 - \frac{1}{4}(1-\delta)^2\right] + O(\beta^4), \tag{10}$$

where $\delta = 1 - n$ is the number of holes per site. The two terms in this expression correspond to a single electron hopping around the square (occupied by three holes), and a single hole hopping around the square (occupied by three electrons). In the second case, the trace over the electron spin gives an extra factor of $\frac{1}{4}$. The denominator of Eq. (7) to the leading order in T^{-1} is $\langle \tau_{xx}\rangle = -\beta N\,\mathrm{Tr}H\tau_{xx} + O(\beta^3) = -2\beta t^2\delta(1-\delta)$ so that finally

$$R_H^* = r_0\left[\frac{1}{4\delta} - \frac{1}{1-\delta} + \frac{3}{4}\right]. \tag{11}$$

The second term in this expression diverges at low particle fillings $\delta \to 1$ with the coefficient expected from the Galitskii limit, and is electronlike. The first term, on the other hand, is lattice dependent and holelike [10]. The usual attempt at extracting the carrier density from a holelike Hall constant, naively yields four holes as an effective carrier for the square lattice. This number is renormalized as a function of J, T, as will become clear later [see, e.g., Eq. (12)]. Also, note that the gauge theory calculations [11–14] of the Hall constant have very similar functional dependence as our Eq. (11), but with coefficients that are also functions of δ.

The consequence of Eq. (10) is that R_H^* computed to leading order in β, changes sign at $\delta = \frac{1}{3}$. We evaluate further terms out to order $(\beta)^7$ using the high-temperature series developed in [15]. This technique was tested by evaluating the exact result for Eq. (7) of noninteracting electrons on the square lattice, where we found that the seventh order terms in β are sufficient to reproduce the answer to within a few percent for $T > t/2$. The results are presented in detail below and in the figures, but it is remarkable that the leading order term contains essentially most of the final answer (approximately 60% numerically for the range considered). The two leading terms in the expansion are

$$R_H^* = \frac{r_0}{4}\left[\frac{1 - \frac{3\beta J}{2}}{\delta} - \frac{4}{1-\delta} + 3 + \frac{3\beta J}{2}\right] + O(\beta^2). \tag{12}$$

We can work out an order of magnitude estimate of the Faraday rotation angle in transmission through $YBa_2Cu_3O_7$ films of thickness z_0, say, 1000 Å, in a field of a Tesla, using known optical constants [16], $n_{x,x} = 3.5$ at a wavelength of 0.5 μm. Taking $R_H^* = 0.3 \times 10^{-3}$ cm^3/C, we find the angle $\theta = 2\pi\frac{z_0}{\lambda} i\epsilon_{x,y}/\sqrt{\epsilon_{x,x}}$ of rotation of the plane of polarization, to be ~ 0.1 mrad. This value appears to be well within the limits of resolution achieved so far [16], and it should be interesting to measure it. Figures 1 and 2 display typical results obtained from the series analysis for the t-J model.

In summary, we have focused attention on the Hall

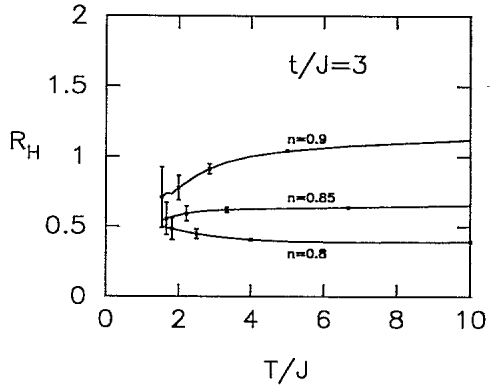

FIG. 1. R_H^* (in units of 0.3×10^{-3} cm^3/C) vs T/J at $n = 0.9, 0.85, 0.8$ for $t/J = 3$.

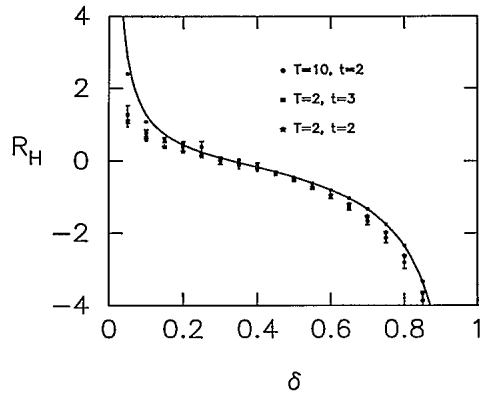

FIG. 2. Solid curve is R_H^* (in units of 0.3×10^{-3} cm^3/C) vs δ at $T = \infty$, Eq. (11), and the three sets of points are from the Padé approximants at three sets of values of T and t in units of J.

constant at high frequencies, and shown that it contains valuable information on the role of interaction on the Hall effect. The sign of the Hall constant is shown to be hole-like close to half filling and electronlike close to empty bands, within a t-J model on the square lattice, with a change occurring at a filling $\delta \sim 0.33$. The sign is shown to be unrelated to the topology and curvature of the fermi surface, when the interaction effects dominate. The result for the change of sign of R_H^* agrees well with the experiments of Takagi *et al.* [2], which report $R_H(\omega = 0)$ changing sign at $\delta \sim 0.3$. On the other hand, the absolute magnitude of the observed $R_H(\omega = 0)$ is about an order of magnitude higher at, say, $\delta = 0.1$ than the calculated R_H^*. It is also strongly temperature dependent. This indicates that the self-energy in Eq. (6) is important as $\omega \to 0$. The $R_H(\omega = 0)/R_H^*$ enhancement is consistent with Anderson's notion [5] of distinct relaxation rates $\tau_{\rm tr}$ and τ_H for transport and Hall effects. From the Hall angle: $\theta_H \sim \sigma_{[x,y]}/\sigma_{xx} \sim \omega_c \tau_H \sim T^{-2}$, so that $\tau_H/\tau_{\rm tr} \sim T^{-1}$. The relatively smaller $\tau_{\rm tr}$ at low temperatures then leads to the enhancement of $R_H(\omega = 0) \sim \tau_H/\tau_{\rm tr} \sim T^{-1}$. It then appears that $R_H(\omega = 0)/R_H^* \sim \frac{J}{T}$, which crudely reconciles the calculation with the experiments.

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[7] $\Omega = Na_0^3$ is the crystal volume, N the number of sites, and a_0 the effective unit cell volume. Note that a_0 should be determined suitably in a quasi-two-dimensional system such as the well studied and popular high-T_c compound $La_2Sr_xCu_{2-x}O_4$. Here it is appropriate to choose $a_0^3 = \frac{190}{\nu}$ Å^3, where ν is the number of Cu atoms per unit cell (=2). The dimensional constant $r_0 \equiv \frac{a_0^3}{|e|}$ is extracted from the definition of R_H^* after Eq. (7). We therefore find $r_0 \equiv 0.594 \times 10^{-3}$cm^3/C.

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[10] The lattice structure and the statistics of the particles plays a crucial role in the behavior of R_H^*, and through it on $R_H(\omega)$. This is brought out in a calculation of the leading high-temperature behavior of R_H^* in the triangular lattice t-J model. We find $R_H^* \sim (\beta t)^{-1} \frac{1+\delta}{\delta(1-\delta)}$, which in contrast to the square lattice result, Eq. (11), does not change sign with δ, but rather with t. Furthermore $R_H^* \sim T$ so that, in a sense, the semiclassical limit $1/ne$ does not exist at all. This highly nontrivial behavior is a consequence of a "fermionic frustration" on the triangular lattice, the same calculation for hard core bosons gives $R_H^* \sim -(\beta t)^{-1} \frac{1-3\delta}{\delta(1-\delta)}$, which indeed changes sign at $\delta = \frac{1}{3}$.

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