Hall Coefficient in the doped Mott Insulator

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We compute the (zero frequency) Hall coefficient $R_H$, and the high frequency Hall constant $R_H^*$ for the strong coupling Hubbard model away from half-filling, in the $d = \infty$ local approximation, using the new iterated perturbation scheme proposed by Kajntner and Kotliar. We find quantitative agreement of our $R_H^*$ with the QMC results obtained in two dimensions by Assaad and Imada [Phys. Rev. Lett. 74, 3868 (1995)]. However while the sign of $R_H$ is quite accurately reproduced by $R_H^*$ the doping dependence of its magnitude at large $U$ is not. We report results for the complete temperature ($T$), doping ($x$) and $U$ dependence of $R_H$ and $R_H^*$ and discuss their possible relevance to doped cuprates.

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Hall measurements are normally regarded as a standard probe for the density and sign of charge carriers in electronic systems. Within a Boltzmann, continuum ($\epsilon \sim k^2$) picture, the Hall coefficient, $R_H$, is given by $1/ne$, where $n$ is the density and $e$ the charge of the carriers. In the presence of a lattice, and for weak scattering, $R_H$ depends on the curvature ($\partial^2 \epsilon / \partial k^2$, etc) of the Fermi surface (FS) and need not have the same sign as $e$; an “electron-like” (positive curvature) FS implies $R_H < 0$ and a “hole-like” (negative curvature) FS implies $R_H > 0$.

An obvious question of great interest is whether this correspondence would survive for strong correlations. Experiments on some of the high $T_c$ systems reveal a hole-like FS while $R_H$ changes from electron-like to hole-like with electron doping. In addition, both the doping and temperature dependence of $R_H$ are “anomalous”: $R_H$ shows unbounded growth as the “half-filled” state is approached, while the temperature dependence is roughly $1/T$, with a saturation as $T \to T_c$, the superconducting transition temperature, from above.

The physics of the cuprates is believed to be governed by strong electron-electron repulsion (large $U$, in the Hubbard context) and low dimensionality ($d = 2$). This has motivated the search for controlled approximations that help to isolate the generic correlation effects in transport in strongly correlated models. For the Hubbard model in $d = 2$ the only controlled calculations that exist are for the high frequency Hall constant, $R_H^*$, defined by

$$R_H^* = \lim_{B \to 0} \lim_{\omega \to \infty} \sigma_{x,y}(\omega)/[B \sigma_{x,x}(\omega)]$$

Unlike the usually measured (zero frequency) Hall coefficient, $R_H$, which involves low energy scattering processes, $R_H^*$ defined above involves only the reactive response. Nevertheless, as demonstrated first by Shastry et al., $R_H^*$ encodes information about correlation effects in the system and (unlike $R_H$) is accessible within controlled calculations. For the Hubbard model it has been computed through Quantum Monte Carlo and finite cluster calculations, and for the $t-J$ model through high temperature series expansion and cluster calculations. Finite size effects and analytic continuation problems which hinder low frequency transport calculations in these contexts do not significantly affect the results on $R_H^*$.

One significant result of these studies is the finite temperature crossover from electron-like to hole-like $R_H^*$ as the hole doping concentration, $x$, away from half-filling is reduced below $\sim 30\%$. This is consistent with some of the high $T_c$ data on $R_H$ and raises the intriguing possibility that $R_H^*$ may mimic all the features of $R_H$. Hence it would be interesting to calculate both $R_H$ and $R_H^*$ for a strongly correlated model within a single scheme and clarify the connection between them. The recently developed $d = \infty$ or local approximation does provide us with a controlled scheme for studying this connection in a strongly interacting system. We report and discuss the results of such a study of the $R_H$ and $R_H^*$ for the doped Mott insulator phase of the Hubbard model in this paper. Our primary results can be summarised as follows. (i) The results for $R_H^*$ computed in the local approximation are quantitatively consistent with QMC results obtained for $d=2$. (ii) There is a complete correspondence of the sign of $R_H$ and $R_H^*$ computed within this approximation at intermediate $T$ over a wide range of $x$ and $U$. (iii) However, $R_H$ and $R_H^*$, differ in sign as $T \to 0$, and their magnitudes have qualitatively different dependences on $x$, for intermediate $T$ and large $U$, close to half-filling.

Our calculations are based on the (by now well known) mapping of Hubbard model in the $d \to \infty$ limit to a self-consistently embedded impurity problem. At half-filling this model shows a transition from a Fermi-liquid to a Mott insulating phase at $U = U_c \sim 2.5$ (in units of $D$, the half-bandwidth, which we set to 1) at $T = 0$, as long as there is sufficient frustration in the lattice to suppress magnetic order. Away from half-filling...
the system is metallic, and there is no evidence of magnetic order [12]. Most of this has been learnt [13] using a combination of Quantum Monte Carlo, exact diagonalisation, the NCA [14], and iterated perturbation theory (IPT) [10,15,16] schemes for solving the impurity problem. Of these, the IPT scheme, because of its simplicity, has been particularly useful in clarifying the physics at half-filling. It reproduces Fermi-liquid behaviour for \( U < U_c \) and is exact in both the atomic \((t = 0)\) and the band \((U = 0)\) limits. Although it does not reproduce the exact critical behaviour as \( U \rightarrow U_c \) at \( T = 0 \), it gives excellent results at intermediate temperatures and allows one to directly calculate the continuous real-frequency spectra of the system. The absence of a similar approximation away from half-filling, where the proximity to a correlation driven insulating state is expected to profoundly affect the ‘metallic’ behaviour, had until recently been a bottleneck. A recent paper by Kajueter and Kotliar [17] achieves a significant advance by devising an interpolation scheme which is exact in the atomic and band limits at any filling and obtains the correct low energy physics by imposing the Friedel sum rule. Our calculations are based on this new scheme, which as originally proposed was for \( T = 0 \), but has been adapted by us to \( T \neq 0 \) in a straightforward way.

We refer the reader to the original paper [17] for the detailed formulation of this scheme and comparison with exact results. For our purposes it is enough to note that in this scheme the self-energy at \( T = 0 \) is approximated as \( \Sigma_{\text{int}}(\omega) = A \Sigma_2(\omega)/[1 - B \Sigma_2(\omega)] \) where \( \Sigma_2 \) is the analytically continued second order self-energy

\[
\Sigma_2(\omega) = \left[ \frac{U^2}{\beta^2} \sum_{n_1,n_2} G_{n-n_1} G_{n_2} G_{n_1+n_2} \right]_\omega \quad (2)
\]

with \( G_n \equiv G(\omega_n) \) etc. Here \( A \equiv \frac{n(1-n)}{n(1+n)\beta^2} \) and \( B \equiv \frac{(1-n)U/\mu + \tilde{\mu}_0}{n(1+n)\beta^2} \) have been chosen so as to reproduce the atomic limit and the high frequency behaviour of the self-energy at any filling; \( n \equiv \int_{-\infty}^{0} \rho_G(\omega)\text{d}\omega \) and \( n_0 \equiv \int_{-\infty}^{0} \rho_G(\omega)\text{d}\omega \), where \( \rho_G(\omega) \text{ and } \rho_G(\omega) \) are the spectral functions of the full local propagator \( G(\omega) \) and the 'bare' local propagator \( G(\omega_n) \) respectively; \( G^{-1}(\omega) = \omega + \tilde{\mu}_0 - \Delta(\omega) \), where \( \Delta(\omega) \) is the hybridisation of the self-consistently embedded impurity problem and \( \tilde{\mu}_0 \) is a free parameter fixed by imposing the Friedel sum rule. At \( T = 0 \) and for a given \( U \), the chemical potential \( \mu \), "quasi chemical -potential" \( \tilde{\mu}_0 \) and occupation number \( n \) are related uniquely through the interpolation and sum rule constraints.

The ground state averages \( n \) and \( n_0 \) which enter the interpolating self-energy \( \Sigma_{\text{int}}(\omega) \) trivially generalise to \( T \neq 0 \) as thermal averages \((n = \langle \hat{n} \rangle) = \int_{-\infty}^{0} \rho_C(\omega)f(\omega)\text{d}\omega, \quad f \equiv [\exp(\omega/T) + 1]^{-1}, \text{ etc } \) and still yield a sensible interpolation. For \( T \neq 0 \) and a desired \( n \) we fix \( \tilde{\mu}_0(n, T) \) as \( \tilde{\mu}_0(n, T = 0) \) and solve for \( \mu(n, T) \) self-consistently. Thus once the connection between \( \mu, n \) and \( \tilde{\mu}_0 \) is established at \( T = 0 \) for a given \( U \), the \( T \neq 0 \) calculations only involve the \( d = \infty \) consistency loop and are computationally quite affordable. We compute the self-energy, \( \Sigma(\omega) \) of the lattice problem as the self-consistent self-energy \( \Sigma_{\text{int}}(\omega) \) of the impurity problem directly for real frequencies, and use it to study \( R_H \) and \( R_H^* \) for large \( U \), \((U/D \sim 4 - 6)\) as a function of \( T \) and \( x \). \( R_H \) is computed from the conductivity tensor \( \sigma_{\alpha\beta}(\omega = 0) \). In the \( d \rightarrow \infty/\text{local approximation the transport coefficients do not involve vertex corrections} [19] \) and the dc conductivity is given by

\[
\sigma_{xx}(0) = c_{xx} \int \text{d}\rho(\epsilon) \int \text{d}\omega A^2(\epsilon, \omega)(-\partial f/\partial \omega) \quad (3)
\]

where \( c_{xx} = e^2 \pi/(d\hbar a_0) \) is the lattice spacing, \( \rho(\epsilon) = (2/\pi D)\sqrt{1 - (\epsilon/D)^2} \) is the bare density of states (DOS), and \( A(\epsilon, \omega) = -\frac{1}{2} \text{Im}\{(\mu + \epsilon - \Sigma(\omega))^{-1} \} \) is the spectral function. The transverse conductivity is given by [18,20]

\[
\sigma_{xy}(0) = B c_{xy}(\epsilon) \int \text{d}\omega A^4(\epsilon, \omega)(-\partial f/\partial \omega) \quad (4)
\]

where \( c_{xy} = |e|^3 \pi^2 a_0/(3d^2 \hbar^2) \) and \( \sigma_{xy}(0)/[\text{Ba}_x^*(\omega)] \). For \( R_H^* \) we use the expression for a hypercubic lattice [18]

\[
R_H^*(0) = (a_0^3/|e|^2) \sum_{k,\sigma} \text{cos}k_x \text{cos}k_y \langle n_{k,\sigma} \rangle / \left[ \sum_{k,\sigma} \text{cos}k_x \langle n_{k,\sigma} \rangle \right]^2 \quad (5)
\]

In the spirit of the local approximation we compute \( \langle n_{k,\sigma} \rangle \), the momentum distribution function, from our self-energy and do the \( \vec{k} \) sums over a 2d Brillouin zone.

We first discuss \( R_H(x, T) \) since 2d QMC [3] and cluster calculations [3] provide us with results to compare with. For large \( U \), \((U/t \sim 16) \) QMC results are available only above \( T/t \sim 0.25 \), \((T \sim 0.06 \text{ in our units, } D \sim 4t)\) and there is a clear peak structure in \( R_H^*(T) \) with the location of the maxima \( T^{QMC}_{\text{max}} \) gradually shifting to lower \( T \) as \( U \) increases at a fixed doping \((x = 0.05)\). This is consistent with our results; but as \( T \rightarrow 0 \) we find an "anomalous" region \((R_H^* > 0) \) in the \( U - x \) plane which could not be accessed within QMC but is clearly seen in cluster calculations [3]. The detailed comparison is shown in Fig.1.

Exploring the detailed \( x, T \) dependence of \( R_H^* \) and \( R_H \) for \( U/D = 4 \) (roughly \( U = 16t \) in 2d), we find that \( R_H^* \) remains hole-like down to \( T = 0 \) for \( x \lesssim 0.12 \) (Fig.2a) while for \( x \gtrsim 0.20 \), \( R_H^* \) is electronlike for all \( T \). \( R_H \) however is electron-like for all \( x \) at \( T = 0 \) (Fig.2b). This, as we discuss below, is a consequence of the Friedel sum rule which forces \( R_H \) to preserve its non-interacting, band structure determined, value at \( T = 0 \). For small \( x \) however there is a rapid crossover to a hole-like \( R_H^* \) with increasing
Fig. 3 shows the crossover temperature $T_{cr}$ as located from the numerically evaluated $R_H$. $T_{cr} \propto x^2$ for small, $x$ (Fig. 3), and rises more steeply as $x \to x_c \sim 0.25$, beyond which there is no crossover. For $x < x_c \sim 0.25$ there is a high temperature branch of $T_{cr}(x)$ across which there is a "re-entrant" change of sign in $R_H$. For $x \gtrsim 0.25$ $R_H$, like $R_H^*\rho$, is electron-like for all $T$. While the $T$ dependence illustrates the similarity in the sign of $R_H$ and $R_H^*$ at intermediate $T$ ($T \gtrsim 0.15 \sim O(J)$ in 2d) the $T \to 0$ result illustrates their essential difference. This difference arises from the fact, that for $T \to 0$, $R_H$ is a Fermi surface object, completely dominated by the coherent part of the spectra (which leads to the divergent $\sigma_{\alpha\beta}$), while $R_H^*$ being a "high-frequency" object gets contribution from all over the Brillouin zone.

The fact that at $T = 0$ all correlation effects cancel out of $R_H$ is easily seen by using the $\omega \to 0, T \to 0$ Fermi liquid parametrisation of the spectral function: $A(\epsilon, \omega) \sim \Gamma/[(\epsilon^2 + m^2\omega - \epsilon)^2 + \pi^2\Gamma^2]$ for $\Gamma \equiv -(1/\pi)\text{Im} \Sigma(\omega = 0) + m^* \equiv 1 - (\partial \Sigma_R/\partial \omega)|_{\omega=0}$ and $\bar{\mu} \equiv \mu(x, T) - \Sigma_R(x, T, \omega = 0)$. Since $-\partial \tilde{\rho}/\partial \omega \to \delta(\omega)$ as $T \to 0$, $\sigma_{xx} \sim \rho_0(\bar{\mu})/\Gamma$, $\sigma_{xy} \sim B\rho_0(\bar{\mu})/\Gamma^2$ and $R_H \sim \bar{\mu}$ so long as $\Gamma \ll D$. Since the sum rule requires $\tilde{\mu}(x, T = 0) = \bar{\mu}(x, T = 0, U = 0) = \rho_0(x)$, $R_H$ is pinned to its band value at $T = 0$. The small $x$ behaviour of the lower $T_{cr}$ (Fig. 3) can also be understood within this phenomenon. For $x \to 0$ (accessible within our numerics so far up to $x \sim 0.06$) $\tilde{\rho}(x, T)$ increases rapidly with $T$. We find $\tilde{\mu}(x, T) \sim \rho_0(x) + (\alpha T^2/x^3)$, where $\alpha > 0$ depends on $U$. Since the free band chemical potential $\mu_0(x) \sim -x$ for $x \to 0$, the crossover scale $T_{cr} \sim x^2$. The rapid rise of $\tilde{\mu}$ with increasing $T$ is primarily due to the reduction of $\Sigma_R(x, T, \omega = 0)$ This in turn is due to the redistribution of spectral weight in $\text{Im} \Sigma(\omega)$ which rises rapidly at low frequencies as $T$ increases, causing the disappearance of the resonant feature in $\rho_G(\omega)$ at the Fermi level.

The difference between $R_H$ and $R_H^*$ is further highlighted in their doping dependence as $x \to 0$ at intermediate $T$. $R_H \sim g(T)/x$ with $g(T)$ increasing with $T$. This behaviour is seen down to the lowest accessible $x$ ($\sim O(0.04)$ at these $T$), despite particle-hole symmetry which should force $R_H(T = 0) = 0$ at $x = 0$. This indicates that due to the large finite $T$ resistivity in the "metal" for $x \to 0$ (and the absence of any coherence/sum rules unlike at $T = 0$), $R_H$ "diverges", as if the doped holes could be treated as effective carriers within a "Boltzmann like" scenario. $R_H^*$ on the other hand shows a peak as $x$ reduces and then a clear turnaround, with $R_H^* \sim x$ for $x \to 0$. Thus as the "Mott" phase is approached for $T \neq 0$, $R_H^*$ is "divergent" (with possibly an exponentially small turnaround scale because $\sigma_{\alpha\beta}$ is finite) while $R_H^*$ is benign. This feature of $R_H^*$ has been seen within QMC and confirms that for a one band model with particle-hole symmetry $R_H^*$ is regular as $x \to 0$. The "divergence" in $R_H$ as $x \to 0$ had been seen earlier within

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[1] e.g. see J. M. Ziman, *Electrons and Phonons* (Clarendon, Oxford, 1960)
[2] N. P. Ong, Y. F. Fan and J. M. Harris, CCAST Symposium, Beijing 1994 (to be published by Gordon and Breach)
[3] B. Batlogg et al, Jl of Low Temperature Physics, 95, 23 (1994)
[4] D. M. King et al, Phys. Rev. Lett. 70, 3159 (1993)
FIG. 1 $R_H^*$ in units of $a_0^3/|e|$, for different $U/D$. Triangle $U/D = 4$; inverted triangle $U/D = 3$; cross $U/D = 2$. Inset: QMC data [7], same legend for $U/4t$.

FIG. 2 $R_H^*$ (a) and $R_H$ (b) in units of $a_0^3/|e|$, for $U = 4$.

FIG. 3 Crossover temperature $T_{cr}(x)$ for $U = 4$. The line is a quadratic fit for $x \rightarrow 0$. “normal” and “anomalous” refer to $R_H < 0$ and $R_H > 0$ respectively.

FIG. 4 $R_H$ (a) and $R_H^*(b)$ in units of $a_0^3/|e|$ for $U = 4$. 
$U = 4$

"anomalous"

"normal"
