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The Hall constant of correlated electrons: Cluster calculation for Hubbard model

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Abstract

We calculate the Hall constant $R_H(\omega, T)$ for the high T_c materials $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{7-x}$ using the 2D Hubbard model, on a cluster of dimension (2×3). Close to half filling, at low temperatures and high frequency, we find that $R_H(\omega)$ is electronlike in the weak correlation regime and in the strong correlation regime it is holelike with roughly $1/T$ + const form. At high frequencies, for $La_{2-x}Sr_xCuO_4$ we obtain a change in the sign of $R_H(\omega)$ at $x \sim 0.3$, which is in good agreement with the experimental data.

The Hall constant in high T_c materials [9] $La_{2-x}Sr_xCuO_4$ (LSCO) and $YBa_2CuO_3O_{7-x}$ (YBCO) and $Nd_{2-x}Ce_xCuO_{4-\delta}$ (NCCO) is of great importance in understanding the charge dynamics in these compounds. The temperature (T) dependence of the Hall constant R_H in both these materials is roughly of the form $1/T$ + const over a wide range of temperature [2, 3]. Further in LSCO as the doping (x) is increased the sign of R_H changes from holelike (positive) to electronlike (negative) at $x \sim 0.3$ [4]. The electron doped High T_c systems, NCCO provide a dramatic example of a system wherein the Fermi surface is holelike and remains so, as one dopes with electrons, as seen in Angle Resolved Photo Emission (ARPES) data [5], whereas the Hall constant changes from being electron like at low doping to holelike at large doping [6]. These striking results have led to the proposal by Shastry et al. (SSS) [7] that in a strongly correlated system, the sign of the Hall constant can be dominated by spectral weight quite far from the Fermi surface, and hence independent of its shape. This work computes a high frequency Hall constant of a t J model using the technique of High temperature expansion. The results of SSS suggests an interesting possibility, namely that the high frequency limit of the Hall resistivity contains information about interactions only, as opposed to the conductivity which contains the effects of scattering in addition. The effect of scattering is "stripped" at these high frequencies and hence it is easier to isolate the effects of interactions. However, the work of SSS does not explore several interesting issues thrown up, namely the behaviour of the Hubbard model for weak and intermediate U wherein one expects a transition from normal Hall constants to anomalous ones as U is increased, in contrast to that of the t–J model, and also the frequency and temperature dependence of the Hall constant. Recent Quantum Monte Carlo (QMC) data [12] lends partial support to these pictures, although it is limited by restrictions of small to moderate $U\beta$.

Motivated by the above, we present in this paper, a series of exact numerical diagonalization studies on a small cluster of Hubbard model, choosing parameters appropriately to fit the physical systems. Accepting *a priori*, the inherent limitation, namely the difficulty in extrapolating to low frequencies, we believe that there is sufficient cause to study in detail the temperature as well as frequency dependence of the Hall constant for small clusters as a function of these as well as other parameters.

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We calculate $R_H(\omega)$ of the Hubbard model on a cluster of dimension (2×3) using exact diagonalisation techniques and an exact evaluation of the Kubo formula [7]. The tight binding parameters for YBCO are chosen such that they reproduce the Fermi surface as observed by ARPES. For LSCO materials since there is no ARPES data available, we model it by simple nearest neighbour hopping.

The Hamiltonian of the two-dimensional Hubbard model with magnetic field along the c-axis, has the form

$$H = -\sum_{\langle i,j\rangle\sigma} t_{ij}(\boldsymbol{A}) c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{\langle\langle i,l\rangle\rangle\sigma} t'_{il}(\boldsymbol{A}) c^{\dagger}_{i\sigma} c_{l\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}$$

where $\langle i,j\rangle$ denotes nearest neighbours and $\langle\langle i,l\rangle\rangle$ denotes next-nearest neighbours. The operator $c^{\dagger}_{i\sigma}(c_{i\sigma})$ creates (annihilates) an electron on site i with the z component of spin σ and the number operator $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$. Due to the presence of a the magnetic field the hopping matrix elements are modified by the Peierls phase factor and have the form

$$t_{ij}(\boldsymbol{A}) = t \exp\left(\frac{2\pi \mathrm{i}}{\Phi_0} \int_i^j \boldsymbol{A}\, d\boldsymbol{l}\right),$$

where $\boldsymbol{A}$ is the vector potential and Φ_0 is the flux quantum (hc/e). In our calculation we have assigned non-zero phase factor Φ for hopping along the horizontal bonds and zero along the vertical and the diagonal bonds in such a way that each closed path encloses the correct flux. The phase factor is related to the applied magnetic field (B) by the relation $2\pi B l^2/\Phi_0 = \Phi$, where l is the lattice constant.

We use the Kubo formula to calculate the conductivity tensor $\sigma_{\alpha,\beta}$ [7, 10], which is given by the relation,

$$\sigma_{\alpha,\beta}(\omega) = \frac{\mathrm{i}e^2 l^2}{\Omega \omega Z \hbar^2}\left[\sum_{\mu} \exp(-\beta\varepsilon_\mu)\langle\mu|\tau_{\alpha,\beta}|\mu\rangle + \sum_{\mu,\nu} \frac{\exp(-\beta\varepsilon_\mu) - \exp(-\beta\varepsilon_\nu)}{\omega + \varepsilon_\mu - \varepsilon_\nu + \mathrm{i}\eta} \times \langle\mu|J_\alpha|\nu\rangle\langle\nu|J_\beta|\mu\rangle\right]. \tag{2}$$

In the above equation $\tau_{\alpha,\beta}$ is the stress tensor defined as $\tau_{\alpha,\beta} = (1/e^2)\,\delta^2 T/\delta A_\alpha \delta A_\beta$ which for $\alpha = \beta = x$ has the form $\tau_{xx} = \sum_{i\sigma}\{t_{ii+x}(\boldsymbol{A}) c^{\dagger}_{i\sigma} c_{i-x\sigma} + \text{H.c.}\}$, and the current operator J_α is given by $J_\alpha = -i\sum_{i\sigma}\{t_{ii-\alpha}(\boldsymbol{A}) c^{\dagger}_{i\sigma} c_{i+\alpha\sigma} - \text{H.c.}\}$.

The relevant part of the Hall conductivity $\sigma_{xy}(\omega)$ is antisymmetric in x, y, and hence we may write $\sigma_{[x,y]}(\omega) = \frac{1}{2}(\sigma_{xy}(\omega) - \sigma_{yx}(\omega))$ which has the form,

$$\sigma_{[x,y]}(\omega) = \frac{\mathrm{i}e^2 l^2}{\Omega Z \hbar^2} \sum_{\mu,\nu} \frac{\exp(-\beta\varepsilon_\mu) - \exp(-\beta\varepsilon_\nu)}{(\omega + \mathrm{i}\eta)^2 - (\varepsilon_\nu - \varepsilon_\mu)^2} \times \langle\mu|J_x|\nu\rangle\langle\nu|J_y|\mu\rangle. \tag{3}$$

The Hall resistivity at frequency ω, $R_H(\omega)$, is obtained from the relation,

$$R_H(\omega) = \frac{1}{B}\frac{\sigma_{[x,y]}(\omega)}{\sigma_{xx}(\omega)^2}.$$

In all the above equations Z is the partition function, β is the inverse temperature and Ω is the crystal volume [11].

Since we are working on a finite cluster, the energy level broadening factor η is taken to be a finite number, roughly as the mean energy level separation on a lattice of the same size. All the data on $R_H(\omega)$ that we present in this paper is checked to be η invariant, i.e. when η is varied in the range from say 0.1 eV to 0.001 eV the change in $R_H(\omega)$ is less than one percent. As further checks we have also verified that for the noninteracting case (U = 0) at low temperatures, large frequencies $(\omega \gg (\varepsilon_\mu - \varepsilon_\nu))$, and small electronic fillings (n) σ_{xx} behaves as $i2t/\omega \sum_k \cos(k_x) n_k$ and $\sigma_{[x,y]}$ as $4t^2\Phi/\omega^2 \sum_k \cos(k_x)\cos(k_y) n_k$, these combine to give the correct high frequency Hall constant R^*_H [7]. In the special case when $t' = 0$ the lattice is bipartite and our data exhibits particle–hole symmetry as required. We also checked the linear response of the Hall data with respect to the applied magnetic field over a wide region in B ranging from 20 to 0.2 T.

It is experimentally found that in $La_{2-x}Sr_xCuO_4$ as the doping (x) is increased the sign of the Hall constant changes from holelike at half filling $(x = 0)$ to electronlike at $x \sim 0.3$ [4]. In Fig. 1 we present our high frequency R_H versus x data for two different values of U in absolute

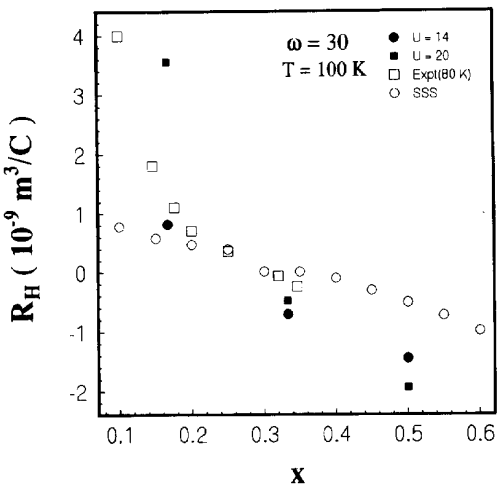

Fig. 1. $R_H(\omega)$ versus x of $La_{2-x}Sr_xCuO_4$ at $\omega = 30$ and $T = 100$ K. The open squares is experimental data [4] at $T = 80$ K and the open circle is data from SSS [7] with $t/J = 3$ and $T = 2$.

units along with the experimental values [4] and data from SSS's work [7]. The zero crossings we obtain is in the proximity of $x \sim 0.3$ which is in good agreement with the experimental data and the result obtained by SSS et al. for the $t-J$ model using high temperature expansions. Further, the slope of the curve at the crossing seems to increase with U.

The temperature dependence of the Hall constant of LSCO has been experimentally measured over a wide range of doping (x) and is found to be strongly temperature dependent [3]. In Fig. 2 we present data from our calculation for $U = 14$, at high frequency and $x = 0.17$ along with experimental values at $x = 0.18$. Interestingly, we find that at low temperatures, order of a few hundreds of Kelvin, and $U < \omega \leq 50$ the Hall constant is holelike and the magnitude increases with decreasing frequency. If we look at the $\omega = 30$ data, the temperature dependence is roughly of the form $1/T$ + const. and has a trend as seen in experiments. However if we look at the data for very large frequency ($\omega \geq 100$), when $R_H(\omega)$ is like R_H^*, the sign is electronlike. For larger values of U, as in Fig. 3 which has data for $U = 20$, $R_H(\omega)$ is holelike at low temperatures for all $\omega > U$. Previous calculations [7, 12] could not go to such low temperatures within the techniques used.

The temperature dependence and the sign of the Hall constant show a clear demarcation between weak and strong correlation regimes. Fig. 4 shows the behaviour of $R_H(\omega)$ at very high frequencies, which is also the behaviour of $R_H^\star$, for doping $x = 0.17$. The data shows that for weak correlation R_H is electronlike at very high temperatures $O(U)$, and also at low temperatures $O(J = 4t^2/U)$, and is holelike in the intermediate temperature range with a maximum at T $O(6t^2/U)$. This result agrees well with the QMC results of Assaad and Imada [12] who could not go to low temperatures at strong correlation, where we find R_H to be holelike. There are thus deviation at low temperatures from the extrapolation of their results.

For broadening-independent mid-frequency data, i.e. $t \ll \omega < U$, we had to go to large values of U (> 20). The trend observed at these frequencies is similar to the high frequency data, i.e. we find an intermediate temperature range where R_H is holelike and also the steep rise at very low temperatures. Exactly at half filling ($x = 0$) we find that $R_H(\omega)$ is relatively zero for all U's at both high and mid-frequencies. This is similar to the QMC result but very much different from the results obtained by SSS, where they find it to diverge.

In $YBa_2Cu_3O_{7-x}$ we concentrate on the $T_c \sim 90$ K system. This phase is observed over a wide range of doping (x) and good ARPES data is available in this doping range [13], especially for $x = 0.1$. The data shows a square holelike Fermi surface centred at the $S(\pi, \pi)$ point. Moreover band structure calculations of the Fermi surface agree quite well with ARPES data [14]. It has been found that within a tight binding model the Fermi surface can be reproduced for parameter values $t'/t \sim 0.5$ [15]. In YBCO the hole count (δ) for the CuO_2 planes is not as straight forward as for LSCO, and there are calculations [16, 17] which give the hole count as a function of doping. For the relevent doping of $x = 0.1$ we take the hole count to be around 0.35 as calculated by Zaanen et al. [16] using band lineup. Alternatively if we calculate

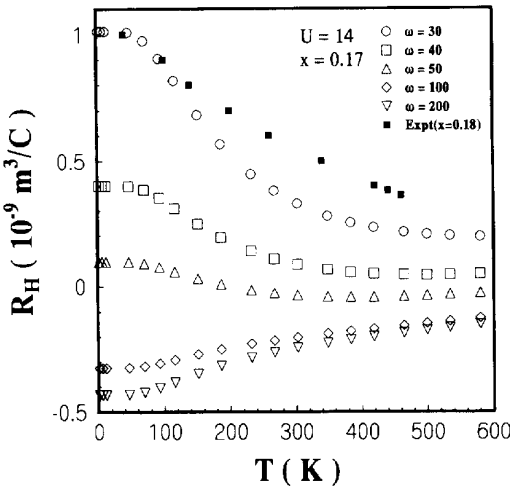

Fig. 2. $R_H(T)$ of $La_{2-x}Sr_xCuO_4$ for $U = 14$ and $x = 0.17$. Filled squares correspond to experimental data [3] for $x = 0.18$.

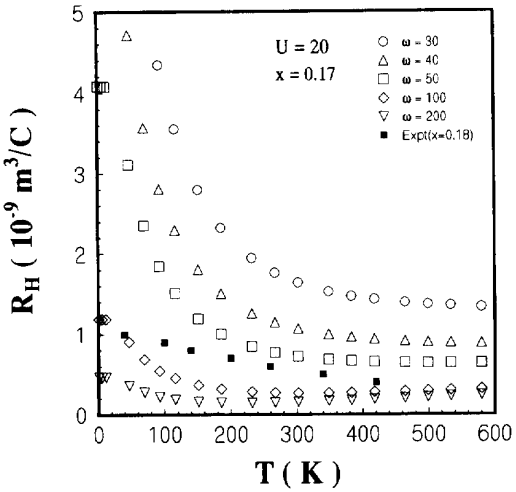

Fig. 3. $R_H(T)$ of $La_{2-x}Sr_xCuO_4$ for $U = 20$ and $x = 0.17$.

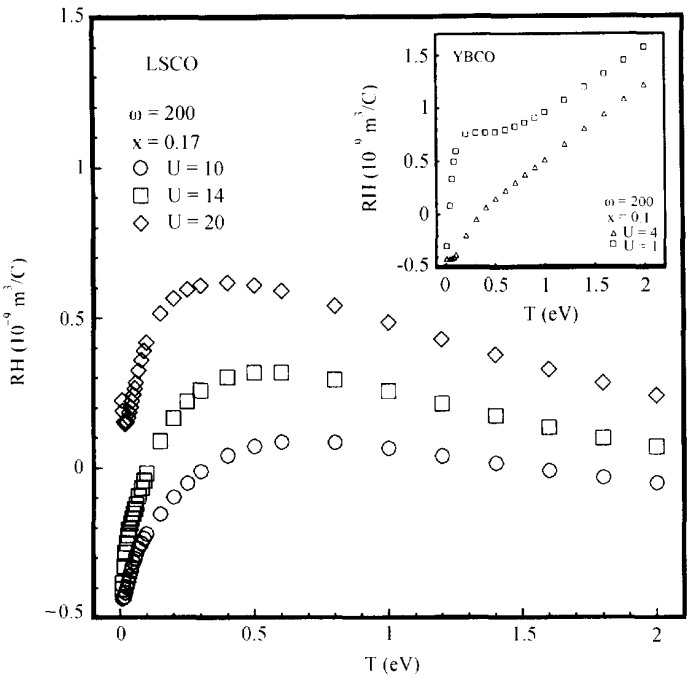

Fig. 4. $R_H(T)$ of $La_{2-x}Sr_xCuO_4$ for $\omega = 200$ and $x = 0.17$. Inset has $R_H(T)$ of $YBa_2Cu_3O_{7-x}$ for $\omega = 200$ and $x = 0.1$ ($\delta = 0.33$).

the area within the FS as measured by ARPES we find the hole count to be around $\delta = 0.15$. We choose parameters $t = 1$ and $t'/t = 0.45$ [18] to model this material and study $R_H(\omega)$ at $\delta = 0.33$.

In the inset of Fig. 4 we look at the temperature dependence of $R_H(\omega)$ for very large frequencies ($\omega \gg U$), which is also the behaviour of R_H^*. Here too we find an intermediate temperature range where R_H is holelike. We could not get any data in the strong correlation regime as the ground state became Ferromagnetic. This we belive is a problem due to the small cluster size.

Lastly we shall comment on $Nd_{2-x}Ce_xCuO_{4-\delta}$ (NCCO) which is an electron doped high T_c material. Like LSCO, the Hall constant of this material changes sign as the doping (x) is increased [19]. It is electronlike at half filling ($x = 0$) and becomes holelike when $x \sim 0.17$. Good ARPES data is available on this compound [5], which clearly shows a holelike Fermi surface centred at the $X(\pi, \pi)$ point, whose area shrinks as the doping is increased. So if we look at the experimental data for $x = 0.15$ there is a clear case of a electronlike Hall constant coexisting with a holelike Fermi surface. To reproduce the Fermi surface within a tight binding model a small but nonzero t' is required. However as a first approximation if we consider $t' = 0$ then we can qualitatively understand the sign change of R_H by using particle–hole symmetry and the results for LSCO. For NCCO this will yield a cross-over at $x \sim 0.3$ rather than the experimentally observed $x \sim 0.17$. This discrepancy might be due to the nonzero t', an issue that we plan to study in a forthcoming work.

In conclusion, we have shown that for LSCO the temperature dependence and the sign change of R_H can be obtained using a strongly correlated Hubbard model.

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