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CONDENSED MATTER

Hall Effect in a Doped Mott Insulator: DMFT Approximation

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In the framework of dynamical mean-field theory, we analyze the Hall effect in a doped Mott insulator as a parent cuprate superconductor. We consider the partial filling (hole doping) of the lower Hubbard band and calculate the dependence of the Hall coefficient and Hall number on hole doping, determining the critical concentration for sign change of the Hall coefficient. Significant temperature dependence of the Hall effect is noted. Good agreement is demonstrated with the concentration dependence of the Hall number obtained in experiments in the normal state of YBCO.

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1. INTRODUCTION

In recent years much interest was attracted to experimental studies of Hall effect at low temperatures in the normal state of high-temperature superconductors (cuprates), which is achieved in very strong external magnetic fields [1–3]. The observed anomalies of Hall effect in these experiments are usually attributed to Fermi surface reconstruction due to formation of (antiferromagnetic) pseudogap and corresponding quantum critical point [4].

At the same time, rather commonly accepted view is that cuprates are strongly correlated systems and their metallic (superconducting) state is realized as a result of doping of a parent Mott insulator, which can be described most simply within the Hubbard model. However, there are almost no works devoted to systematic studies of doping dependence of Hall effect in this model. A common question here is what is determining the sign of the Hall coefficient? At small hole doping of a parent insulator like La_2CuO_4 or oxygen-depleted YBCO, it is obviously determined by hole concentration δ. Then at what doping level shall we observe the sign change of Hall coefficient, when is there a transition from a small Fermi surface to a large electron one? Solution of this problem is quite important also for the general transport theory in strongly correlated systems.

Rather general approach to study the Hubbard model is the dynamical mean-field theory (DMFT) [5–7]. The aim of the present paper is a systematic study of concentration and temperature dependence of Hall effect for different doping levels in the lower Hubbard band within DMFT approach, as well as comparison of theoretical results with experiments on YBCO [2]. We shall see that surprisingly good agreement with experiment at quantitative level can be achieved even for this elementary model.

2. BASIC RELATIONS

In DMFT [5–7] the electron self-energy in single-particle Green's function $G(\mathbf{p}\varepsilon)$ is local and independent of momentum. Due to this locality both the usual and Hall conductivities are completely determined by the spectral density:

$$A(\mathbf{p}\varepsilon) = -\frac{1}{\pi}\operatorname{Im}G^R(\mathbf{p}\varepsilon). \quad (1)$$

In particular the static conductivity is given by the expression

$$\sigma_{xx} = \frac{\pi e^2}{2\hbar a}\int_{-\infty}^{\infty} d\varepsilon\left(-\frac{df(\varepsilon)}{d\varepsilon}\right)\sum_{\mathbf{p}\sigma}\left(\frac{\partial\varepsilon(\mathbf{p})}{\partial p_x}\right)^2 A^2(\mathbf{p}\varepsilon), \quad (2)$$

while Hall conductivity has the form [5]

$$\sigma_{xy}^H = \frac{2\pi^2 e^3 aH}{3\hbar^2}\int_{-\infty}^{\infty} d\varepsilon\left(\frac{df(\varepsilon)}{d\varepsilon}\right)\sum_{p\sigma}\left(\frac{\partial\varepsilon(\mathbf{p})}{\partial p_x}\right)^2 \times \frac{\partial^2\varepsilon(\mathbf{p})}{\partial p_y^2}A^3(\mathbf{p}\varepsilon). \quad (3)$$

Here, a is the lattice parameter, $\varepsilon(\mathbf{p})$ is the electronic dispersion, $f(\varepsilon)$ is the Fermi distribution, and H is the magnetic field along the z axis. Thus, the Hall coefficient

$$R_H = \frac{\sigma_{xy}^H}{H\sigma_{xx}^2} \quad (4)$$

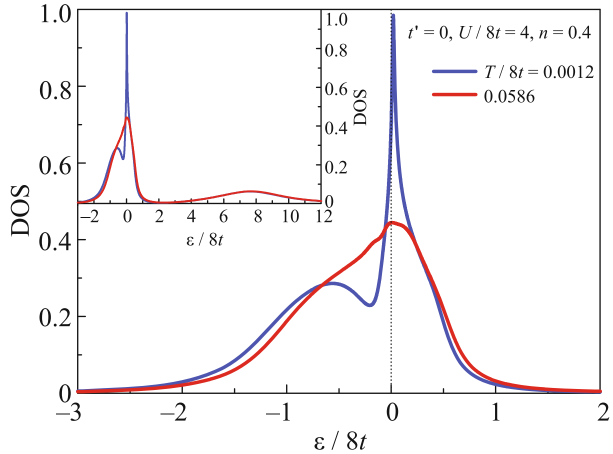

Fig. 1. (Color online) Density of states in the doped Mott insulator for different temperatures obtained with the Hubbard model parameters shown in the figure, $8t$ is the initial bandwidth from Eq. (5). The inset shows the density of states in a wider energy interval including the upper Hubbard band.

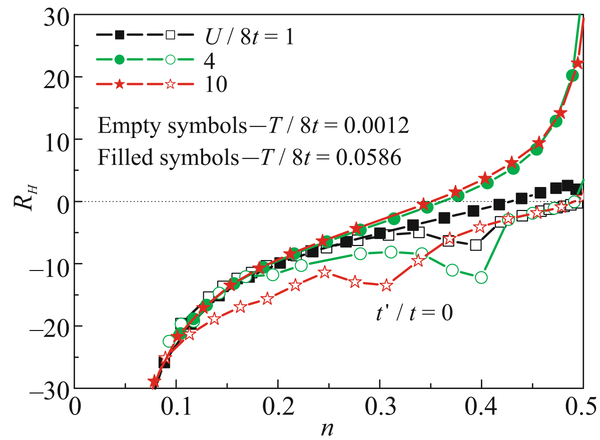

Fig. 2. (Color online) Hall coefficient versus band filling at (empty symbols) low and (filled symbols) high temperatures for the model of the two-dimensional electron spectrum (5) with transfers only between nearest neighbors ($t' = 0$).

is also completely determined by the spectral density $A(\mathbf{p}\varepsilon)$, which will be calculated within DMFT [5–7]. To solve an effective single-impurity Anderson model in DMFT, we used numerical renormalization group [8].

We performed rather extensive calculations of Hall effect for different models of electronic spectrum. Below, keeping in mind comparison with the experimental data on YBCO, we limit ourselves to the results obtained for two-dimensional tight-binding model of electronic spectrum:

$$\varepsilon(\mathbf{p}) = -2t(\cos(p_x a) + \cos(p_y a)) - 4t'\cos(p_x a)\cos(p_y a). \quad (5)$$

In this model we shall consider here two cases:

(i) the model with electron transfers only between nearest neighbors ($t' = 0$) and with complete electron–hole symmetry;

(ii) the case of $t'/t = -0.4$, which qualitatively corresponds to YBCO.

For other cuprates we should use different values of t'/t ratio.

Further on, for two-dimensional models used, the static and Hall conductivities will be measured in the units of universal two-dimensional conductivity $\sigma_0 = e^2/\hbar$ and $e^3a^2H/\hbar^2$, respectively. Correspondingly, the Hall coefficient (4) is measured in units of a^2/e.

3. RESULTS OF CALCULATIONS AND COMPARISON WITH EXPERIMENT

For strongly correlated systems Hall coefficient is essentially dependent on temperature. At low temperatures in these systems, when treated in DMFT approximation, besides the upper and lower Hubbard bands also a narrow band appears close to a narrow band forms close to Fermi level forming the so-called quasiparticle peak in the density of states. In the hole doped Mott insulator (in the following we consider only the hole doping) this peak lies close to the upper edge of the lower Hubbard band (cf. Fig. 1). Thus, at low temperatures the Hall coefficient is mainly dependent on the filling of this quasiparticle band. At higher temperatures (of the order or higher than the width of quasiparticle peak) the quasiparticle peak broadens and the Hall coefficient is determined by the filling of the lower Hubbard band. Thus, it is necessary to consider two rather different temperature regimes for Hall effect.

In the low temperature regime both the amplitude and width of quasiparticle peak depend on band filling and temperature. Temperature growth leads to the broadening of the quasiparticle peak and to some displacement of the Fermi level below the maximum of this peak (cf. Fig. 1). This may lead to a noticeable drop of Hall coefficient, though further increase in the temperature broadens the quasiparticle peak and leads to the growth of this coefficient. Significant dependence of quasiparticle peak on band filling in low temperature regime leads to the regions of nonmonotonic doping dependence of the Hall coefficient (cf. Fig. 2).

In high temperature regime the quasiparticle peak is strongly broadened and is practically absent due to temperature. In this case, deeply in the hole doped Mott insulator the Hall coefficient is in fact deter-

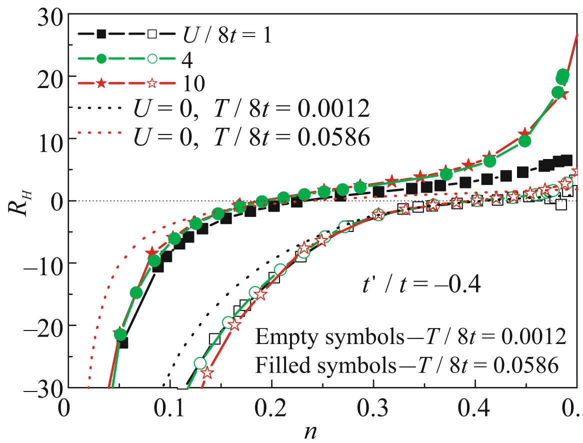

Fig. 3. (Color online) Hall coefficient versus band filling at (empty symbols) low and (filled symbols) high temperatures for the model of the two-dimensional electron spectrum (5) with transfers between nearest and next-nearest neighbors ($t'/t = -0.4$).

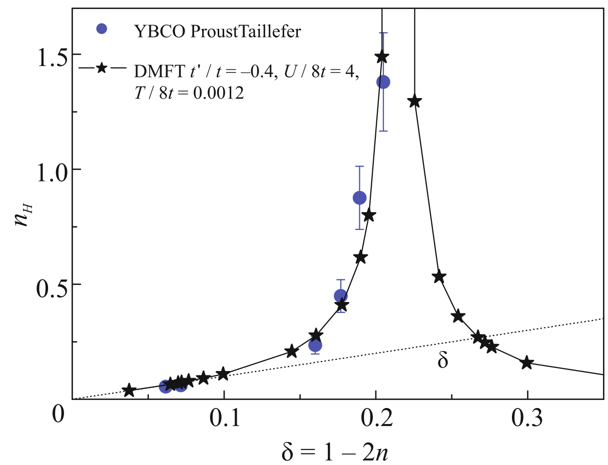

Fig. 4. (Color online) (Stars) Hall number n_H calculated in this work versus doping in comparison with (blue circles) experiment [2] on YBCO, $\delta = 1 - 2n$ is the hole concentration.

mined by filling of the lower Hubbard band (the upper Hubbard band is significantly higher in energy and is practically empty). In this situation, in the model with electron–hole symmetry ($t' = 0$) we can qualitatively estimate the band filling corresponding to sign change of Hall coefficient as follows. Consider paramagnetic phase with $n_\uparrow = n_\downarrow = n$, so that in the following n denotes electron density per single spin projection, while the total electron density is $2n$. It is natural to assume that the sign change of the Hall coefficient takes place close to half-filling of the lower Hubbard band $n_0 \approx 1/2$. Consider the states with "upper" spin projection, then the total number of states in the lower Hubbard band is $1 - n_\downarrow = 1 - n$. Then the band filling is obtained as $n = n_\uparrow = n_0(1 - n) \approx 1/2(1 - n)$. Thus, for the band filling corresponding to a sign change of the Hall coefficient we get $n_c \approx 1/3$.

The same result is easily obtained also in the Hubbard I approximation, where the Green's function for spin up electrons is written as [9]

$$G^R_\uparrow(\varepsilon\mathbf{p}) = \frac{1 - n_\downarrow}{\varepsilon - \varepsilon_-(\mathbf{p}) + i\delta} + \frac{n_\downarrow}{\varepsilon - \varepsilon_+(\mathbf{p}) + i\delta}, \qquad (6)$$

where $\varepsilon_\pm(\mathbf{p})$ is the quasiparticle spectrum in upper and lower Hubbard bands. We can see that in this approximation the number of states with spin-up projection in the lower Hubbard band (first term in (6)) is really $1 - n_\downarrow$. During hole doping of Mott insulator, the main band filling goes into the lower Hubbard band, so that

$$n = n_\uparrow \approx (1 - n_\downarrow) \times \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon)\left(-\frac{1}{\pi}\mathrm{Im}\sum_{\mathbf{p}}\frac{1}{\varepsilon - \varepsilon_-(\mathbf{p}) + i\delta}\right) = (1 - n)n_0. \qquad (7)$$

Then for half-filled lower Hubbard band $n_0 = 1/2$ and the sign of Hall effect (effective mass of quasiparticles) changes, so that we get $n = n_c = 1/3$ again.

From Fig. 2 it is easily seen that the high-temperature behavior of Hall coefficient in doped Mott insulator ($U/2D = 4;10$) in case of the complete electron–hole symmetry ($t' = 0$) fully supports this estimate. In case of noticeable breaking of this symmetry the simple estimate does not work, as even in the absence of correlations the sign change of Hall coefficient is observed not at half-filling (cf. Fig. 3).

It should be noted that the quasiparticle peak in the density of states is widened and suppressed not only by temperature but also by disorder [10, 12], as well as by pseudogap fluctuations, which are completely ignored in local DMFT approach [11, 12]. Thus, the range of applicability of the simple estimates made above for electron–hole symmetric case in reality may be significantly wider.

In Fig. 4 we show the comparison of our calculations for the Hall number (Hall concentration) $n_H = \frac{a^2}{|eR_H|}$ for typical model parameters with experimental data for YBCO from [2]. We can see that even for this, rather arbitrary, choice of parameters we obtain almost quantitative agreement with experiment, with no assumptions on Hall effect connection with the Fermi surface reconstruction by pseudogap and closeness to corresponding quantum critical point, which were used in [2–4]. It is more or less obvious that similar data of [3] for NLSCO can be interpreted within our model with appropriate change of parameters t/t' and U. Thus, it is quite possible that our interpretation of Hall effect in cuprates based on the doping of lower Hubbard band of Mott insulator can be a viable alternative to the picture of quantum critical point.

It may be of great interest to make the detailed studies of the Hall effect in the vicinity of critical concentration corresponding to the sign change of Hall coefficient (divergence of Hall number). This can be done in the systems (cuprates), where such sign change takes place under doping.

4. CONCLUSIONS

We have studied the behavior of the Hall coefficient in metallic phase appearing due to hole doping of the lower Hubbard band of Mott insulator. The change of sign of Hall effect in simplest (symmetric) case takes place close to doping $n_c = 1/3$ per single spin projection or total electron density 2/3 in the lower Hubbard band, corresponding to hole doping $\delta = 1 - 2n = 1/3$, though in general case it depends rather strongly on the choice of model parameters. This concentration follows from simple qualitative estimates and is not related to more sophisticated factors, such as change of topology of Fermi surface or quantum critical points.

More than satisfactory agreement of theoretical concentrations dependencies obtained in the experiments on YBCO [2] shows, that our model may be a reasonable alternative to the picture of Hall effect in the vicinity of quantum critical point, related to closing pseudogap [4].

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CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

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