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**ELECTRONIC PROPERTIES  
OF SOLID**

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## Hall Effect in Doped Mott–Hubbard Insulator

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**Abstract**—We present theoretical analysis of Hall effect in doped Mott–Hubbard insulator, considered as a prototype of cuprate superconductor. We consider the standard Hubbard model within DMFT approximation. As a typical case we consider the partially filled (hole doping) lower Hubbard band. We calculate the doping dependence of both the Hall coefficient and Hall number and determine the value of carrier concentration, where Hall effect changes its sign. We obtain a significant dependence of Hall effect parameters on temperature. Disorder effects are taken into account in a qualitative way. We also perform a comparison of our theoretical results with some known experiments on doping dependence of Hall number in the normal state of YBCO and Nd-LSCO, demonstrating rather satisfactory agreement of theory and experiment. Thus the doping dependence of Hall effect parameters obtained within Hubbard model can be considered as an alternative to a popular model of the quantum critical point.

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### 1. INTRODUCTION

The studies of Hall effect in high - temperature superconductors continues for a long time. The early experiments demonstrated the significant dependence of Hall effect parameters on temperature and doping, which are qualitatively different from the case of ordinary metals [1]. The complete understanding of Hall effects in cuprates at present is absent.

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 realized in very strong external magnetic fields [2–4]. The observed anomalies of Hall effect in these experiments are usually attributed to reconstruction of Fermi surface due to (antiferromagnetic) pseudogap formation and closeness to the corresponding quantum critical point [5].

Since the early days of theoretical studies of cuprates the leading point of view is, that these systems are strongly correlated and metallic (and superconducting) state is realized via doping of the initial Mott insulator phase, which in a simplest case can be described within Hubbard model. However, up to now there are only few papers where systematic studies of Hall effect dependence on doping and temperature were performed within this model [6].

Even the answer to a classical question on the doping level at which the Hall effect changes its sign is not perfectly clear. At small hole doping of an initial insulator, such as  $\text{La}_2\text{CuO}_4$  or YBCO Hall effect is obviously determined by hole concentration  $\delta$ . Then at what doping level Hall effect changes its sign and when the transition from hole – like Fermi surface to electron–like takes place? The answer to this question seems to be important also for the general theory of transport phenomena in strongly correlated systems. This paper is mainly devoted to the solution of this problem.

### 2. HALL CONDUCTIVITY AND HALL COEFFICIENT

One of the most general approaches to the studies of Hubbard model is the dynamical mean field theory (DMFT) [6–8], which gives an exact description of the system in the limit of infinite spatial dimensions (lattice with infinite number of nearest neighbors). General approaches allowing to overcome this rigid limitation are actively developed [9, 10], but as a rule these complicate the analysis very much. In this paper we limit ourselves to the analysis of Hall effect within the standard DMFT approximation. The aim of this work is systematic study of concentration and temperature dependence of Hall effect at different doping

levels of the lower Hubbard band and comparison of theoretical results with experiments on YBCO and Nd-LSCO [3, 4]. Preliminary results were published in [11].

In the standard DMFT [6–8] self-energy of a single-electron Green's function  $G(\mathbf{p}\epsilon)$  is local, i.e. independent of momentum. Due to this locality both the usual and Hall conductivities are completely determined by the spectral density of this Green's function

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

In particular, the usual (diagonal) static conductivity is given by [6]:

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

while Hall (non-diagonal) conductivity is defined as:

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

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

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

is also completely determined by the spectral density  $A(\mathbf{p}\epsilon)$ , which in the following will be calculated within the DMFT [6–8]. Effective Anderson single-impurity model of DMFT in this paper was solved with numerical renormalization group (NRG) [12].

In the following we consider two basic models of the bare electron band. The model with semi-elliptic density of states (DOS) (per elementary cell and single spin projection) is a reasonable approximation for three-dimensional case:

$$N_0(\epsilon) = \frac{2}{\pi D^2} \sqrt{D^2 - \epsilon^2}, \quad (5)$$

where  $D$  is conduction band half-width. We assume that the bare electronic spectrum is isotropic. To find the momentum derivatives of the spectrum in this model, entering Eqs. (2) and (3), we follow the procedure proposed before in [13]. Appropriate technical details are presented in Appendix.

For two-dimensional systems, in anticipation of comparison with experimental data for cuprates, we limit ourselves to the usual tight-binding model of electronic spectrum:

$$\begin{aligned} \epsilon(\mathbf{p}) &= -2t(\cos(p_x a) + \cos(p_y a)) \\ &- 4t' \cos(p_x a) \cos(p_y a). \end{aligned} \quad (6)$$

Within this two-dimensional model we consider a number of cases:

(1) spectrum with only nearest hoppings ( $t' = 0$ ) and full electron-hole symmetry;

(2) spectrum with  $t'/t = -0.25$ , which qualitatively corresponds to electronic dispersion in systems like LSCO;

(3) spectrum with  $t'/t = -0.4$ , which qualitatively corresponds to situation observed in YBCO.

Below we present the results of detailed calculations of Hall coefficient for all these models.

### 3. HALL COEFFICIENT IN TWO-DIMENSIONAL MODEL OF TIGHT-BINDING SPECTRUM OF ELECTRONS

Let us start with simplest qualitative analysis. It is easy to understand that deep in Mott insulator state with well defined upper and lower Hubbard bands the Hall coefficient under hole doping is in fact determined by filling the lower Hubbard band (the upper band is significantly higher in energy and is practically unfilled). In this situation in the model with electron-hole symmetry (in two dimensions this corresponds to spectrum with  $t' = 0$ ), an estimate of band filling corresponding to the sign change of the Hall coefficient can be obtained using very simple arguments. Let us consider the paramagnetic phase with  $n_\uparrow = n_\downarrow = n$ , so that in the following  $n$  denotes electron density per one spin projection, so the complete density of electrons is given by  $2n$ . Qualitatively the situation is illustrated in Fig. 1. In lower Hubbard band (in the vicinity of the Fermi level  $E = 0$ )  $2n$  electrons occupy states below the Fermi energy  $E_F$ . An additional electron can go to the upper Hubbard band in the vicinity of  $E \sim U$ , where we also have  $2n$  states. It also can go to the lower Hubbard band, where there still remain  $2(1 - 2n)$  empty states in the region of  $E > E_F$ . Summing we obtain  $2n + 2(1 - 2n) + 2n = 2$  as it should be. The sign of the Hall coefficient will change at the half filling of the lower band, when  $2n = 2(1 - 2n)$ . Now it is clear that the value of the critical concentration is  $n_c = 1/3$ .

The same result is easily obtained in Hubbard I approximation, where the Green's function spin-up electron takes the form [14]:

$$G_\uparrow^R(\mathbf{p}\epsilon) = \frac{1 - n_\downarrow}{\epsilon - \epsilon_-(\mathbf{p}) + i\delta} + \frac{n_\downarrow}{\epsilon - \epsilon_+(\mathbf{p}) + i\delta}, \quad (7)$$

where  $\epsilon_\pm(\mathbf{p})$  is quasiparticle spectrum in upper and lower Hubbard bands. We see that in this approximation the number of states with upper spin projection in the lower Hubbard band (first term in Eq. (7)) is in fact  $1 - n_\downarrow$ . During hole doping of Mott insulator

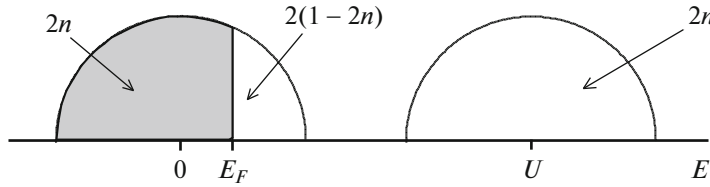


Fig. 1. Schematic picture of doping in Hubbard bands for the case of complete electron-hole symmetry.

practically all filling takes place in the lower Hubbard band, so that:

$$n = n_{\uparrow} \approx (1 - n_{\downarrow}) \int_{-\infty}^{\infty} d\epsilon f(\epsilon) \times \left( -\frac{1}{\pi} \text{Im} \sum_{\mathbf{p}} \frac{1}{\epsilon - \epsilon_{-}(\mathbf{p}) + i\delta} \right) \equiv (1 - n) n_0. \tag{8}$$

Then at half-filling of the lower Hubbard band we have  $n_0 = 1/2$  and the Hall coefficient (effective mass of the quasiparticles) changes its sign at  $n = n_c = 1/3$ , corresponding to our previous estimate.

In general case situation is obviously more complicated. In strongly correlated systems Hall coefficient (and other electronic properties) become significantly dependent on temperature. At low temperature in these systems DMFT approximation leads, besides the formation of lower and upper Hubbard bands, to the appearance of a narrow quasiparticle band, or quasiparticle peak in the density of states [6–8]. In hole doped Mott insulator (in the following we consider only hole doping) such a peak appears close to the upper edge of the lower Hubbard band (cf. Fig. 2). Thus at low temperatures the Hall coefficient is mainly determined by filling of this quasiparticle band. At high enough temperature (of the order or higher than quasiparticle peak width) quasiparticle peak is damped and the Hall coefficient is mainly determined by filling of the lower Hubbard band. Thus, in general case it is necessary to consider two different temperature regimes for Hall coefficient.

In low temperature regime both the width and the amplitude of quasiparticle peak depend on filling and temperature. Increasing temperature leads to widening of quasiparticle peak and some shift of the Fermi level below the maximum of this peak (cf. Fig. 2). This may lead to a significant drop of the Hall coefficient, though further increase of the temperature leading to the damping of the quasiparticle peak leads to the growth of this coefficient. Thus the relevant dependence of the quasiparticle peak on band filling in the low temperature regime leads to the regions of non-monotonous filling dependence of the Hall coefficient (cf. Fig. 3a).

From Fig. 3a it is easy to see that high-temperature behavior of the Hall coefficient in doped Mott insulator ( $U/2D = 4; 10$ ) in a model with full electron-hole

symmetry ( $t' = 0$ ), completely confirms the qualitative estimate given above. However, this estimate becomes invalid in the case of noticeable breaking of electron-hole symmetry (cf. Fig. 3b).

It should be noted that damping and disappearance of quasiparticle peak can be not only due increasing temperature, but also due to disordering [9, 13] (cf. Fig. 4) or due to pseudogap fluctuations, which are entirely neglected within local DMFT [9, 15]. Thus, in reality the region of applicability of simplest estimates given above may be much wider.

In general case taking into account disorder scattering (more so pseudogap fluctuations) in calculations of the Hall effect is rather complicated problem. As a simple estimate we present below results of calculations using Eqs. (2)–(4), where we have used the values of the spectral density  $A(\mathbf{p}\epsilon)$  for disordered Hubbard model obtained within DMFT+ $\Sigma$  approach [9, 15]. Disorder parameter  $\Delta$  denotes the effective scattering rate of electrons by random field (in self-consistent Born approximation). It is clear that this approach based only on the account of disorder in spectral density is oversimplified, but it seems reasonable for qualitative analysis.

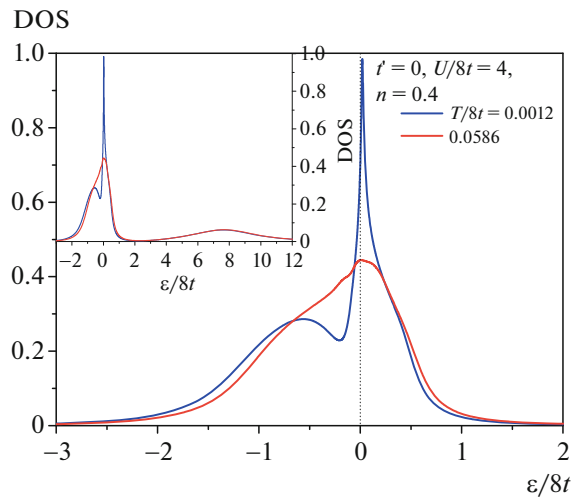
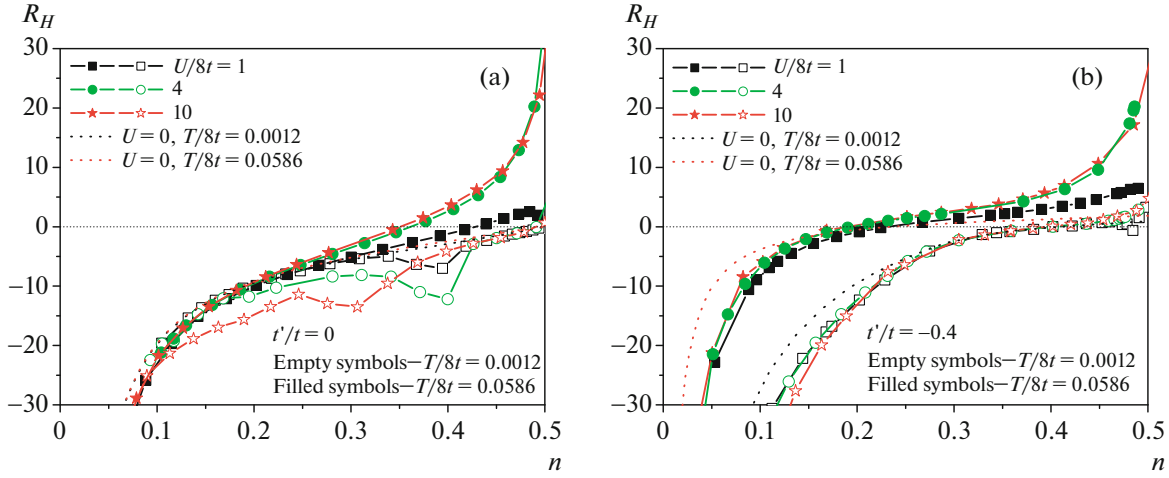
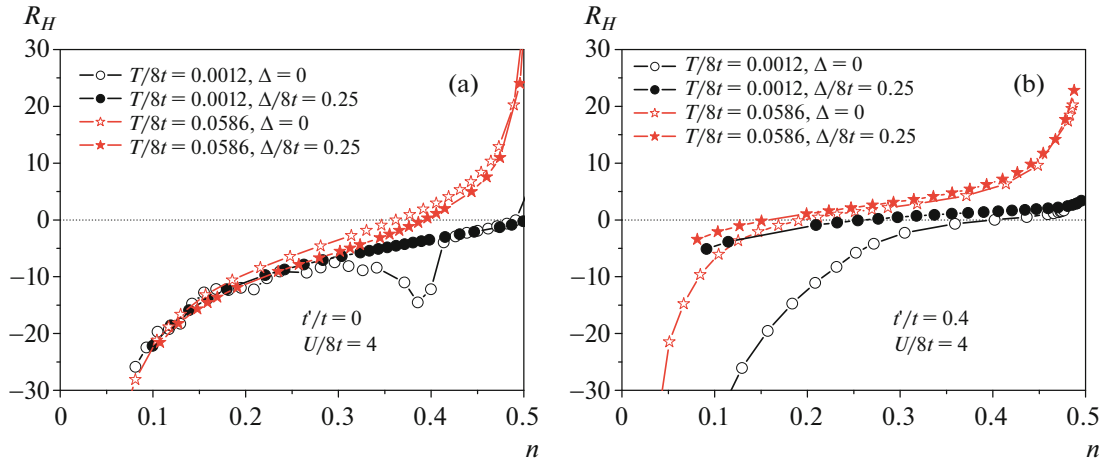


Fig. 2. Density of states (DOS) in doped Mott insulator at different temperatures. Parameters of the Hubbard model are shown in figure,  $8t$  is the initial band-width. At the insert—the density of states in a wide energy interval including the upper Hubbard band.



**Fig. 3.** Dependence of Hall coefficient on correlation strength  $U$  on band filling for  $t'/t = 0$  (a) and  $t'/t = -0.4$  (b) in low temperature regime (empty symbols) and in high temperature regime (filled symbols).



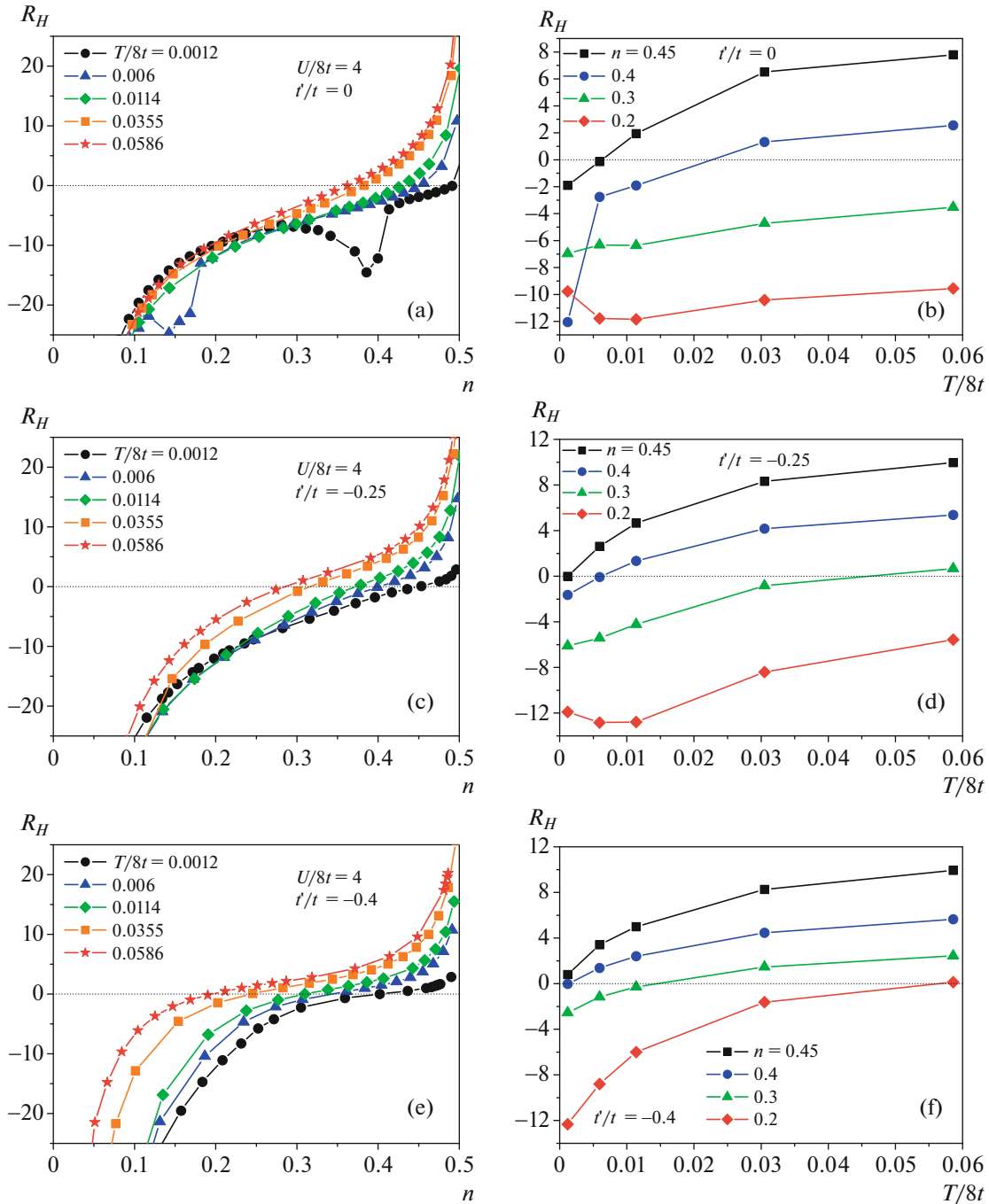
**Fig. 4.** Dependence of Hall coefficient on band filling in presence of impurity scattering ( $\Delta/8t = 0.25$ , filled symbols) and in its absence ( $\Delta = 0$ , empty symbols) for two models of two-dimensional electronic spectrum: (a) full electron-hole symmetry ( $t'/t = 0$ ); (b)  $t'/t = -0.4$ .

In Fig. 4 we compare the dependencies of Hall coefficient on band filling in the absence of disorder and for the case of impurity scattering with  $\Delta/8t = 0.25$  for Mott insulator with  $U/8t = 4$ . It is seen that for different values of  $t'$  in high temperature limit disorder only slightly affects the Hall coefficient by rather insignificant shift of the value of filling, where  $R_H$  changes its sign. In low temperature regime impurity scattering, damping the quasiparticle peak, lead to disappearance of the anomalies of  $R_H$ , connected with its existence (cf. Fig. 4a) and weakening differences between low temperature and high temperature regimes.

In Fig. 5 we show dependencies of Hall coefficient on band filling and temperature for the case of Mott insulator with  $U/8t = 4$  for different models of elec-

tronic spectrum, both for the case of full electron-hole symmetry with  $t' = 0$  and for  $t'/t = -0.25$  and  $t'/t = -0.4$ , characteristic for cuprate systems LSCO and YBCO respectively. On the dependence of  $R_H$  on band filling with the growth of temperature we observe smooth evolution from low to high temperature regime with smooth weakening of the anomalies of Hall coefficient related to quasiparticle peak, which are most clearly seen in Figs. 3a and 5a. For all cases of electronic spectrum under consideration ( $t'/t = 0; -0.25; -0.4$ ) increasing temperature leads to a shift of the value of filling corresponding to  $R_H = 0$  into the region of larger hole dopings.

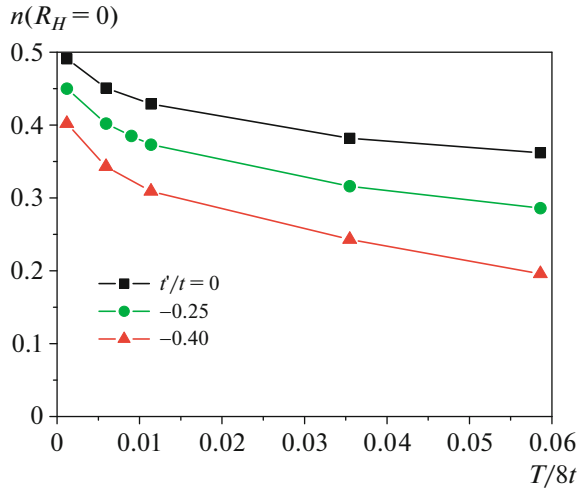
Also in the r.h.s. part of Figs. 5b, 5d, 5f we show the temperature dependencies of Hall coefficient for different band fillings. In all case we observe the signifi-



**Fig. 5.** Dependence of Hall coefficient on band filling for different values of temperature—left column (a, c, e) and temperature dependence of  $R_H$  for different band fillings—right column (b, d, f).

cant dependence of  $R_H$  on temperature and for small hole dopings ( $n = 0.45-0.3$ )  $R_H$  grows with increasing temperature and we obtain the sign change of  $R_H$  at larger hole dopings ( $n = 0.3-0.2$ ). For small enough values of  $t'$  ( $t'/t = 0; -0.25$ ) we can observe non monotonous dependence of Hall coefficient on temperature, when  $R_H$  decreases with increasing temperature, while it grows at high  $T$ .

The sign change of Hall coefficient is usually connected to a change of the type of charge carriers. Hall coefficient approaching zero corresponds to divergence of Hall number  $n_H \sim 1/R_H$ . At Fig. 6 we show temperature dependence of the band filling corresponding to the sign change of the Hall coefficient for all three values of  $t'/t$  considered here. We see that in all models the band filling at which  $R_H$  changes its sign



**Fig. 6.** Temperature dependence of band filling corresponding to a sign change of Hall coefficient in doped Mott insulator for three different values of  $t'/t$ .

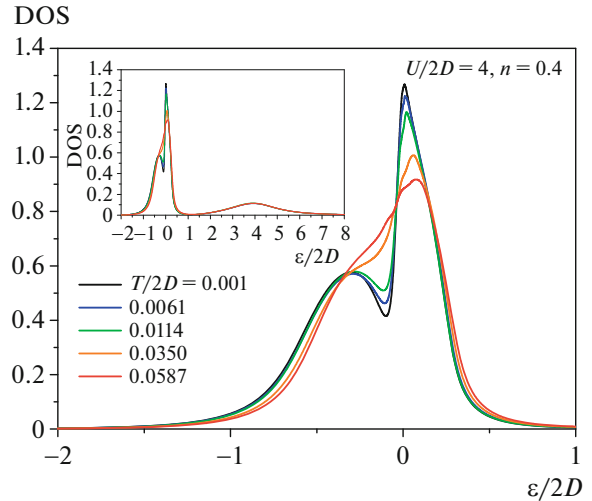
decreases with temperature. In case of the full electron-hole symmetry  $t' = 0$  we see, that in high temperature regime hole doping  $\delta = 1 - 2n$  corresponding to the sign change of  $R_H$  really tends to  $1/3$ . However, with increasing  $|t'/t|$  we observe the significant decrease of the value of hole doping where  $R_H$  changes its sign.

#### 4. HALL COEFFICIENT IN THE MODEL WITH SEMI-ELLIPTIC DENSITY OF STATES

Let us briefly discuss results obtained in the model of electronic band with semi-elliptic density of states, which has the full electron-hole symmetry. The main results are qualitatively similar to the case two-dimensional tight-binding electronic spectrum with  $t' = 0$  also having the complete electron-hole symmetry. Similarly to two-dimensional case the Hall coefficient in three-dimensional strongly correlated system is significantly dependent on temperature and it is necessary to consider separately the low and high temperature regimes for  $R_H$ , as in the low temperature regime the Hall coefficient is mainly determined on filling the quasiparticle band (quasiparticle peak).

Increasing temperature leads to damping of quasiparticle peak (cf. Fig. 7) and in high temperature regime Hall coefficient is mainly determined by filling of the lower (for the case of hole doping considered here) Hubbard band.

In Fig. 8a we show the Hall coefficient dependence on electronic band filling if low temperature (unfilled symbols) and in high temperature (filled symbols) regimes, both for the case of strongly correlated metal ( $U/2D = 1$ ) and for doped Mott insulator ( $U/2D = 4$ ; 10). We can see that in the low temperature regime, as in two dimensional model with  $t' = 0$  ( $R_H$  is negative



**Fig. 7.** Density of states (DOS) in doped Mott insulator with semi-elliptic band (three-dimensional case) for different temperatures.

practically at all band fillings) at small hole dopings there is a significant non monotonous dependence of  $R_H$  on doping.

In high temperature regime the Hall coefficient at small hole dopings is positive (hole-like), decreasing with increasing hole doping, while at larger dopings  $R_H$  becomes negative, changing its sign (in Mott insulator) at hole doping  $\delta = 1 - 2n \approx 1/3$ , which again confirms qualitative estimates given above. A smooth evolution of Hall coefficient dependence of filling as temperature increases from low temperature to high temperature regime in Mott insulator ( $U/2D = 4$ ) is shown in Fig. 8b.

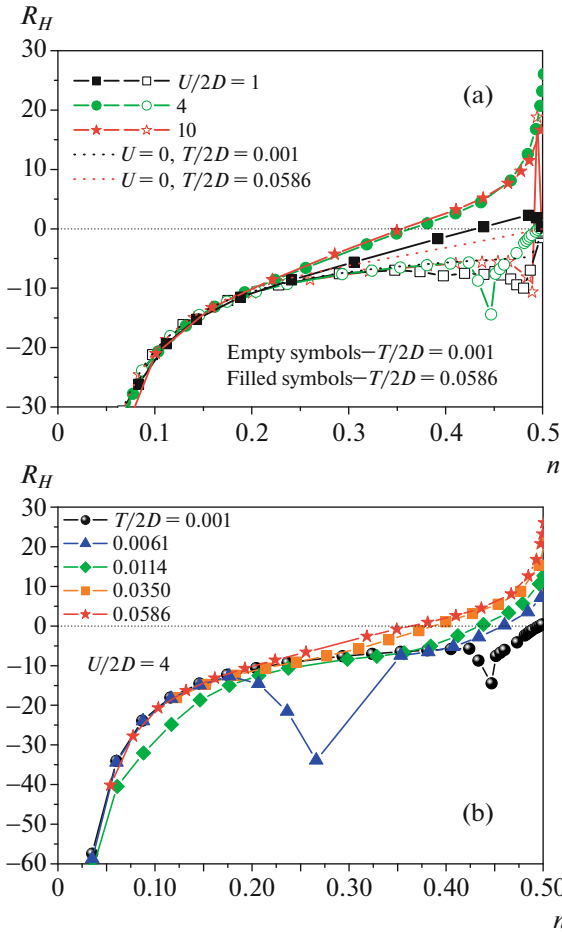
In Fig. 9 we demonstrate disorder influence on Hall coefficient in Mott insulator. In high temperature limit impurity scattering practically does not influence  $R_H$  at all, while in low temperature limit damping the quasiparticle peak by disorder removes the anomalous non monotonous behavior of  $R_H$  dependence on  $n$ .

#### 5. COMPARISON WITH EXPERIMENTS

As we mentioned before in recent years the unique experimental studies were performed measuring Hall effect at low temperatures in the normal state of high-temperature superconductors (cuprates), which was achieved in very strong external magnetic fields [2–4]. These experiments revealed the dependence of Hall

number  $n_H = \frac{a^2}{|eR_H|}$  on doping with a smooth transition from linear dependence on hole concentration  $\sim \delta$  at small dopings to the values  $\sim (1 + \delta)$  for high enough concentrations of the order of critical hole concentration of vanishing (closing) pseudogap. These data are usually interpreted within the picture of Fermi surface





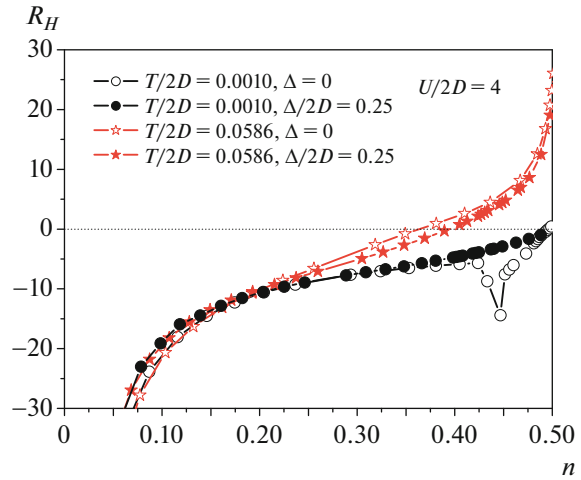
**Fig. 8.** Dependence of Hall coefficient on band filling for semi-elliptic density of states: (a) for different values of  $U$  in low temperature (empty symbols) and high temperature (filled symbols) regimes; (b) for different temperatures at fixed  $U/2D = 4$ .

reconstruction in the vicinity of the expected quantum critical point in the framework of rather specific model of cuprates with inhomogeneous localization of carriers [5, 16]. It should be noted, that in none of papers known to us were in fact presented experimental points reliably demonstrating the dependence  $\sim(1 + \delta)$ , and clearly established experimental fact is only the observed growth of the Hall number.

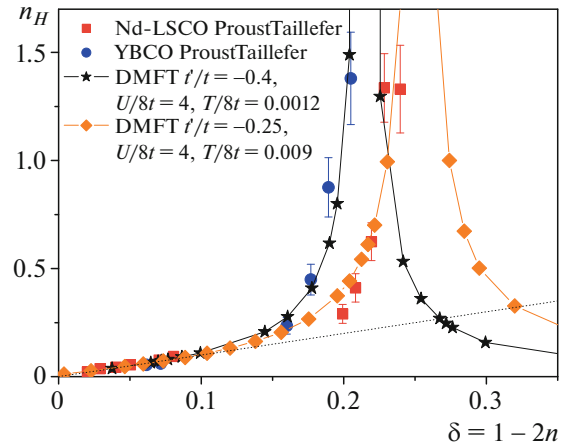
Below we propose an alternative interpretation of the growth of Hall number in these experiments as reflecting the approach of the system to critical concentration of carriers at which Hall effect just changes its sign (Hall coefficient  $R_H$  becomes zero) [11].

In Fig. 10 we show the comparison of the results of our calculations for Hall number (Hall concentration)

$n_H = \frac{a^2}{|eR_H|}$  for typical parameters of the model with experimental data for YBCO and Nd-LSCO from [3, 4]. We can see that even for this, rather arbitrary,



**Fig. 9.** Dependence of Hall coefficient on band filling in low temperature regime (black curves) and high temperature regime (red curves) in the absence of disorder  $\Delta = 0$  (empty symbols) and for  $\Delta/2D = 0.25$  (filled symbols).



**Fig. 10.** Dependence of Hall number  $n_H$  on doping—comparison with experiments [3, 4] on YBCO and Nd-LSCO,  $\delta = 1 - 2n$ —hole concentration. Stars and diamonds—results of our calculations, blue circles and red squares—experiment.

choice of parameters we can obtain almost quantitative agreement with experiment, with no assumptions about the connection of Hall effect with reconstruction of Fermi surface by pseudogap and closeness to corresponding quantum critical point, which were used in [3–5, 16]. Thus it seems reasonable to interpret Hall effect in cuprates within picture of lower Hubbard model doping in Mott insulator, as an alternative to the scenario based upon closeness to a quantum critical point.

In this respect it seems to be quite important to try to perform more detailed studies of the Hall effect in the vicinity of a critical concentration corresponding to sign change of the Hall effect (divergence of the

Hall number). It requires the studies of systems (cuprates) where such sign change can be achieved under doping.

## 6. CONCLUSIONS

We have studied Hall effect in metallic state appearing while doping Mott insulator. Main attention was to the case of hole doping, characteristic for a major part of cuprates. We considered a number of two-dimensional tight-binding models of electronic spectrum appropriate for description of electronic structure of cuprates, as well as three-dimensional model with semi-elliptic bare density of states. In all models the Hall coefficient  $R_H$  in doped Mott insulator is significantly dependent on temperature. In low temperature limit  $R_H$  is mainly determined by the filling of quasiparticle peak, which may lead to non monotonous dependence of Hall coefficient on doping. In high temperature limit, when quasiparticle peak is essentially damped,  $R_H$  is mainly determined by filling of the lower (for hole doping) Hubbard band. In this limit the sign change of the Hall coefficient and corresponding divergence of the Hall number takes place, in the simplest (symmetric) case close to the band filling  $n = 1/3$  per single spin projection or  $2/3$  for total density of electrons, which corresponds to hole doping  $\delta = 1 - 2n = 1/3$ , though in general case this filling may strongly depend on the choice of parameters of the model. This concentration follows from simple qualitative estimates and not related with more complicated factors like changing the topology of Fermi surface or the presence of quantum critical points.

Rather satisfactory agreement of obtained concentration dependencies of Hall number with experiments on YBCO and Nd-LS CO [3, 4] shows, that our model may serve as a reasonable alternative to a picture of Hall effect in the vicinity of quantum critical point related to closing the pseudogap [5, 16].

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## APPENDIX

### “BARE” ELECTRONIC DISPERSION AND ITS DERIVATIVES FOR BAND WITH SEMIELLIPIC DENSITY OF STATES

Let us assume that electronic spectrum corresponding to density of states (5) is isotropic  $\varepsilon(\mathbf{p}) = \varepsilon(p) \equiv \varepsilon(p)$ . To calculate derivatives in (2) and (3) it is

necessary to perform “angle” averaging of these derivatives by momentum components

$$\left\langle \left( \frac{\partial \varepsilon(\mathbf{p})}{\partial p_x} \right)^2 \right\rangle_{\Omega} = \varepsilon'^2(p) \left\langle \frac{p_x^2}{p^2} \right\rangle_{\Omega} = \frac{1}{d} \varepsilon'^2(p) = \frac{1}{3} \varepsilon'^2(p), \quad (9)$$

where  $\langle \dots \rangle_{\Omega} = \int \frac{d\Omega}{4\pi} \dots$  is solid angle averaging in three-dimensional system ( $d = 3$ ) and  $\varepsilon'(p) = \frac{d\varepsilon(p)}{dp}$  is derivative over the absolute value of momentum.

$$\begin{aligned} & \left( \frac{\partial \varepsilon(\mathbf{p})}{\partial p_x} \right)^2 \frac{\partial^2 \varepsilon(\mathbf{p})}{\partial p_y^2} \\ &= \varepsilon'^2(p) \left[ \varepsilon''(p) \frac{p_x^2 p_y^2}{p^4} + \frac{\varepsilon'(p)}{p} \frac{p_x^2 p^2 - p_x^2 p_y^2}{p^4} \right], \end{aligned} \quad (10)$$

where  $\varepsilon''(p) = \frac{d^2 \varepsilon(p)}{dp^2}$ . Thus we have a problem of finding the angle average

$\left\langle \frac{p_x^2 p_y^2}{p^4} \right\rangle_{\Omega}$ . Let us introduce notations:  $\left\langle \frac{p_x^4}{p^4} \right\rangle_{\Omega} \equiv a$  and  $\left\langle \frac{p_x^2 p_y^2}{p^4} \right\rangle_{\Omega} \equiv b$ . First of all we have:

$$\begin{aligned} & \left\langle \frac{(p_x^2 + p_y^2 + p_z^2)^2}{p^4} \right\rangle_{\Omega} \\ &= \left\langle \frac{(p_x^4 + p_y^4 + p_z^4) + 2p_x^2 p_y^2 + 2p_x^2 p_z^2 + 2p_y^2 p_z^2}{p^4} \right\rangle_{\Omega} \\ &= d \left\langle \frac{p_x^4}{p^4} \right\rangle_{\Omega} + d(d-1) \left\langle \frac{p_x^2 p_y^2}{p^4} \right\rangle_{\Omega} = 3a + 6b = 1. \end{aligned} \quad (11)$$

Similarly:

$$\begin{aligned} & \left\langle \frac{(p_x^2 + p_y^2)^2}{p^4} \right\rangle_{\Omega} \\ &= \left\langle \frac{p_x^4 + p_y^4 + 2p_x^2 p_y^2}{p^4} \right\rangle_{\Omega} = 2a + 2b = \frac{8}{15}. \end{aligned} \quad (12)$$

As

$$\begin{aligned} & \left\langle \frac{(p_x^2 + p_y^2)^2}{p^4} \right\rangle_{\Omega} = \langle \sin^4 \theta \rangle_{\Omega} \\ &= \frac{1}{2} \int_0^{\pi} \sin \theta \sin^4 \theta d\theta = \frac{1}{2} \int_{-1}^1 (1 - \tau^2)^2 d\tau = \frac{8}{15}, \end{aligned} \quad (13)$$



where  $\theta$  is an angle between vector  $\mathbf{p}$  and  $z$ -axis, Then from Eqs. (11), (12) we immediately obtain  $a = \left\langle \frac{p_x^4}{p^4} \right\rangle_{\Omega} = 1/5$  and  $b = \left\langle \frac{p_x^2 p_y^2}{p^4} \right\rangle_{\Omega} = 1/15$ , so that we have:

$$\left\langle \left( \frac{\partial \varepsilon(\mathbf{p})}{\partial p_x} \right)^2 \frac{\partial^2 \varepsilon(\mathbf{p})}{\partial p_y^2} \right\rangle_{\Omega} = \frac{\varepsilon'^2(p)}{15} [\varepsilon''(p) + 4\varepsilon'(p)/p]. \quad (14)$$

To find derivatives  $\varepsilon'(p)$ ,  $\varepsilon''(p)$  for the spectrum determined by semi-elliptic density of states (5) we can use the approach developed in [13]. Equating the number of states in a phase volume element  $d^3p$  and the number of states in an energy interval  $[\varepsilon, \varepsilon + d\varepsilon]$ , we obtain differential equation determining  $\varepsilon(p)$ :

$$\frac{4\pi p^2 dp}{(2\pi)^3} = N_0(\varepsilon) d\varepsilon. \quad (15)$$

Assuming the quadratic dispersion of  $\varepsilon(p)$  close to lower band edge we obtain the initial condition for (15):  $p \rightarrow 0$  for  $\varepsilon \rightarrow -D$ . As a result:

$$p = \left[ 6\pi \left( \pi - \varphi + \frac{1}{2} \sin(2\varphi) \right) \right]^{1/3}, \quad (16)$$

where  $\varphi = \arccos\left(\frac{\varepsilon}{D}\right)$  and momentum is given in units of inverse lattice parameter. This expression implicitly defines the dispersion law  $\varepsilon(p)$  on electronic branch of the spectrum  $\varepsilon \in [-D, 0]$ .

We can determine characteristic momentum  $p_0$  corresponding to  $\varepsilon = 0$ :

$$p_0 = p(\varepsilon = 0) = (3\pi^2)^{1/3}. \quad (17)$$

We are interested in calculating two derivatives of this spectrum over the momentum. From (15) we get:

$$\varepsilon'(p) = \frac{d\varepsilon}{dp} = \frac{p^2}{2\pi^2} \frac{1}{N_0(\varepsilon)}, \quad (18)$$

where  $p$  is defined by (16).

$$\begin{aligned} \varepsilon''(p) &= \frac{d}{dp} \frac{d\varepsilon}{dp} = \frac{1}{2\pi^2} \frac{2pN_0(\varepsilon) - p^2 \frac{dN_0(\varepsilon)}{d\varepsilon}}{N_0^2(\varepsilon)} \frac{d\varepsilon}{dp} \\ &= \frac{1}{N_0(\varepsilon)} \left[ \frac{p}{\pi^2} - \varepsilon'^2 \frac{dN_0(\varepsilon)}{d\varepsilon} \right], \end{aligned} \quad (19)$$

where  $\frac{dN_0(\varepsilon)}{d\varepsilon} = -\frac{2}{\pi D^2} \frac{\varepsilon}{\sqrt{D^2 - \varepsilon^2}}$ ,  $\varepsilon'(p)$  is determined from (18), while  $p$  is defined by (16).

On the hole branch of the spectrum ( $\varepsilon \in [0, D]$ ), to obtain quadratic dispersion law close to the upper edge of the band ( $\varepsilon \rightarrow D$ ) we introduce a hole momentum  $\tilde{p} = 2p_0 - p$  and equate the number of states in a phase volume element  $d^3\tilde{p}$  and in energy interval  $[\varepsilon, \varepsilon + d\varepsilon]$ :

$$\frac{4\pi \tilde{p}^2 d\tilde{p}}{(2\pi)^3} = -N_0(\varepsilon) d\varepsilon. \quad (20)$$

Demanding  $\tilde{p} \rightarrow 0$  at the upper band edge  $\varepsilon \rightarrow 0$ , we obtain:

$$\tilde{p} = \left[ 6\pi \left( \varphi - \frac{1}{2} \sin(2\varphi) \right) \right]^{1/3}. \quad (21)$$

For the velocity on the hole branch of the spectrum we get:

$$\varepsilon'(p) = -\frac{d\varepsilon}{d\tilde{p}} = \frac{\tilde{p}^2}{2\pi^2} \frac{1}{N_0(\varepsilon)}. \quad (22)$$

Equations (18), (22) determine the dependence of velocity  $\varepsilon'(p)$  on energy. One is easily convinced that velocity is even in energy and goes to zero at band edges. The second derivative over momentum in this approach is explicitly defined on electronic branch of the spectrum ( $\varepsilon \in [-D, 0]$ ), but on the hole branch it is more difficult to do. However, we can require full electron-hole symmetry of the model, which reduces to demanding the square of velocity, entering Eq. (2), being even in  $\varepsilon(p)$ , while Eq. (14) entering Eq. (3) for Hall conductivity being odd (sign change under change of the type of charge carriers). With the account of such symmetry the results obtained in this Appendix allow to replace summation over momenta in Eqs. (2), (3) by integration over energy.

## CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

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