Vanishing Hall Constant in the Stripe Phase of Cuprates

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The Hall constant $R_H$ is considered for the stripe structures. In order to explain the vanishing of $R_H$ in La$_{2-y}$Nd$_y$Sr$_2$CuO$_4$ (LNSCO) at $x = 1/8$, we use the relation of $R_H$ to the Drude weight $D$ as well as direct numerical calculation, to obtain results within the $t$-$J$ model, where the stripes are imposed via a charge potential and a staggered magnetic field. The origin of $R_H \sim 0$ is related to a maximum in $D$ and the minimal kinetic energy in stripes with a hole filling $\sim 1/2$. The same argument indicates on a possibility of $R_H \sim 0$ in the whole range of static stripes for $x \leq 1/8$.

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The evidence for the stripe structures in La$_{2-y}$Nd$_y$Sr$_2$CuO$_4$ (LNSCO) emerging from neutron scattering experiments [1] has stimulated in recent years numerous experimental and theoretical investigations, trying to relate this phenomenon to superconductivity and other anomalous properties of cuprates. In the commensurate case $x \sim 1/8$ the stripe structure represents spin and charge ordering, i.e., domain walls within an ordered two-dimensional antiferromagnet (AFM) with the filling of $n_l = N_h/L = 1/2$ hole per unit length (quarter filling in the usual band picture) within each domain wall - stripe. Actually, it was shown in the recent angle-resolved photoemission spectroscopy experiments that the stripes are in the quarter filled state [2]. In contrast to many other systems showing spin-density wave order at low temperatures, the stripe structures in cuprates appear to be metallic [3]. This can be explained with charge carriers - holes being well mobile along the one-dimensional (1D) stripes. Recently, a systematic study of LNSCO ($y = 0.6$) with varying doping $x$ [4] revealed a striking signature of stripes in the behavior of the Hall constant $R_H$. While for $x > 0.15$ $R_H(x,T)$ is very close to that of the reference doped La$_2$Sr$_2$CuO$_4$ (LSCO), $R_H$ appears to be very sensitive to the structural phase transition between the low-temperature tetragonal (LTT) and orthorhombic (LTO) phase for $x < 0.15$. Below the LTT-LTO transition $R_H$ becomes strongly $T$ and $x$ dependent and it eventually vanishes, $R_H \sim 0$, at $T \sim 0$ for $x \sim 0.12$, i.e., in the structure with long range stripe order. At the same time the anomaly is weakly pronounced in the planar resistivity $\rho_{ab}$ [5].

In the present paper, we investigate $R_H$ in stripe structures and in particular a possible explanation for its vanishing. $R_H \sim 0$ in a conducting system is quite unusual and non universal. For instance, it could happen in an ordinary metal due to (accidental) cancellation of band curvatures or due to band crossings. However, cuprates are closer to hole-doped Mott insulators where in the reference LSCO a (semiconductor-like) semi-classical $R_H \propto 1/x$ is followed in a wide range $x < 0.2$ at low $T$. $R_H \sim 0$ in LNSCO at $x \sim 1/8$ is, on the other hand, a very pronounced deviation from the latter. Therefore, one can speculate on more fundamental origin of this most pronounced macroscopic effect of stripes whereby the strong correlations play an essential role. The authors [4] interpreted the experimental finding $R_H \sim 0$ as an evidence for a transport along independent stripes. This requires exclusively 1D transport and therefore can hardly apply. Hall constant can be expressed in terms of planar conductivities $\sigma_{\alpha\beta}$ in a finite magnetic field $B$ as $R_H = \sigma_{xy}[B\sigma_{xx}\sigma_{yy}]$. Assuming a very anisotropic system with stripes, e.g., along the $x$ direction and large $\sigma_{xx}$ it is plausible that $\sigma_{xy}$ scales with the weak hopping between stripes. But $\sigma_{yy}$ is expected usually to scale in the same way leaving the ratio $R_H$ finite. The evidence for the latter behavior can be found in the experiments on very anisotropic quasi-1D metals which reveal nevertheless quite normal metallic values of $R_H$ [6].

Another simple interpretation is that in a stripe structure with hole filling $n_l = 1/2$ we are dealing along the single stripe with an equal concentration of holes and electrons, leading to the cancellation of $\sigma_{xy}$ while both diagonal $\sigma_{xx}$ remain finite. Although it is hard to improve this argument into a more formal theory, to some extent it seems to be closer to our final conclusions further on.

It is evident that the Hall effect in cuprates [7], as well as in systems with strongly correlated electrons in general, still lacks proper theoretical understanding. This applies for most investigated reference cuprate LSCO and $R_H$ dependence on $T$ and hole doping $n_l$. While the theoretical formulation of the Hall linear response $R_H(\omega,T)$ is well established [8], there are very few theoretical results and numerical studies for models with strong correlation in particular in the relevant low $T$ and low doping regime [9]. Recently an approach and a numerical procedure have been designed [10] which yield for a static d.c. $R_H$ at $T = 0$ (although for a ladder system) the desired
result, namely a semi-classical behavior $R_H^* = 1/e_0n_h$ in a magnetic insulator at low hole doping $n_h = N_h/N$ ($e_0$ being the electric charge), as found experimentally in cuprates [12]. Moreover, for a reactive (non-dissipative) $R_H(T = 0)$ it was possible to find an useful relation to the variation of the Drude weight (charge stiffness) $D$ with the electron density $n$,

$$R_H = -\frac{1}{e_0 D} \frac{\partial D}{\partial n}.$$ (1)

The latter relation is derived using the non-standard $D$-system where $\omega \rightarrow \omega_0$ first, then $q \rightarrow 0$. Nevertheless, it has very attractive properties for the analysis of strongly correlated electrons: a) $D$ at $T = 0$ is the central quantity distinguishing the Mott-Hubbard insulator from a conductor, b) close to the Mott insulator $D \propto n_h = 1 - n$ directly implies a plausible semi-classical result $R_H^* = 1/e_0n_h$, which is hard to be established by other methods. While so far the relation has not been justified for the general case in the proper transport limit ($q \rightarrow 0$ first, then $\omega \rightarrow 0$) it appears to be valid for a strongly anisotropic system where $D = D_{\alpha\alpha}$ should be taken along the most conducting direction $\alpha$ [13].

There is also a qualitative similarity of the relation [1] with the proposal in Ref. [14] where the authors correlate Hall ($B > 0$) conductivity $\sigma_{xy}$ with the doping dependence of the kinetic energy, i.e., $\partial \langle K \rangle/\partial n$. Note that in a (tight binding) strongly correlated system $K$ and $D$ are related through the sum rule

$$ND_{\alpha\alpha} = \frac{1}{2}(-K_{\alpha\alpha}) - \frac{1}{e_0} \int_0^\infty \sigma_{\alpha\alpha}^{reg}(\omega)d\omega,$$ (2)

where $\sigma^{reg}$ is the regular part of the optical conductivity and $K_{\alpha\alpha}$ involves only the hopping in the $\alpha$ direction.

Theoretical modeling of stripes in cuprates has proven to be quite delicate just due to their $n_l = 1/2$ filling and metallic character. Stripe solutions of relevant (Hubbard and analogous) models within simplest mean-field approximations generally show a tendency towards $n_l = 1/2$ filling and an insulating behavior. More recently extensive numerical analyses within the relevant $t$-$J$ model [15] confirm the relative stability of metallic stripes at commensurate doping $n_h = 1/8$. These results and other approaches [15,16] all indicate a crucial interplay of the hole kinetic energy and the spin Heisenberg interaction in metallic stripes, both being crucially related to strong electron correlation.

Equation (1) suggests an explanation of $R_H \sim 0$ in $x = 1/8$ stripes, namely that $D(n)$ is a local maximum for $n_l = 1/2$, this being closely related to the minimum kinetic energy ($K$) in this configuration. In order to support this conjecture we perform a numerically exact-diagonalization study of $D$ and $R_H$ within the prototype $t$-$J$ model,

$$H = -t \sum_{\langle ij \rangle} (\hat{c}_{i \sigma}^\dagger \hat{c}_{j \sigma} + \text{H.c.}) + J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j),$$ (3)

where no double occupancy of sites is allowed. In numerical studies we use $J/t = 0.4$ to be in the strong-correlation regime relevant to cuprates.

Since studied systems are too small to inherently reproduce stripes, we impose them through an attractive hole potential $V$ along the stripe [17] and the staggered field $h_i = \pm h$ forming an AFM phase boundary across the stripe [18,19].

$$H_{st} = -V \sum_{i \in st} (1 - n_i) + \sum_{i \in st} h_i S_i^z.$$ (4)

![FIG. 1. Drude weight $D_{xx}/t$ as a function of doping $n_h$ calculated for a $4 \times 4$ system with p.b.c., where the stripes are imposed in the $x$ direction, for various stripe potentials $V$ and staggered fields: (a) $h = 0$ and (b) $h = 0.4$ t.](image)

First we consider numerically a system with $N = 4 \times 4$ sites and periodic boundary conditions (p.b.c.) in both the $x$ and $y$ directions. Two stripes are imposed along the $x$-direction with the inter-stripe distance $d_0 = 2$. $D_{xx} = D$ in such a system can be evaluated by introducing a flux through the torus modifying $t \rightarrow \tilde{t}_{ij} = t \exp[i \theta(x_i - x_j)]$ to find an absolute energy minimum $E^{\min}(\theta)$ at $\theta = \theta_0$ and then by taking the second derivative, i.e., $D = (1/2N)\partial^2 E^{\min}(\theta)/\partial \theta^2 |_{\theta = \theta_0}$. In Figs. 1(a) and (b), we present results for $D$ as a function of hole doping $n_h$ (only even $N_h$ are considered) and various stripe potentials $V$, without the staggered field $h = 0$.
as well as with $h/t = 0.4$. Two limits for $D(n_h)$ are quite easy to understand. For $V = 0$ we are dealing with a homogeneous 2D $t$-$J$ model where $D$ reaches maximum at $n_h \sim 0.5$. On the other hand, for large $V > t$ holes are localized to a 1D motion within each stripe. As in 1D, $D$ then reaches the maximum for stripe filling $n_l = 1/2$, i.e., for $n_h = 1/(2d_0) = 0.25$ (while $D \sim 0$ for $n_l \sim 1$). Using Eq. (4) in the latter case clearly leads to $R_H \sim 0$ for stripes at $n_l = 1/2$. Our results in Fig. 1(a) suggest that the maximum remains pronounced also for far more modest $V \geq t$. The introduction of the staggered field $h$, as shown in Fig. 1(b), enhances but also flattens the maximum which is visible now even at $V/t \sim 0.5$.

For comparison we present in Fig. 2 the related variation of $\langle -K_{xx} \rangle$ with $n_h$. We notice that in analogy to $D$ there is a maximum at $n_l \sim 1/2$, however well pronounced only for larger $V/t$ whereby $\langle K_{xx} \rangle$ is also less sensitive to $h$.

By considering the $t$-$J$ model with open boundary conditions (o.b.c.) in the $y$ direction, i.e., on a ladder system $N = L \times M$, one can study $R_H$ even more directly [1]. If we introduce the Hall electric field in the $y$ direction as $H_{\Delta} = \Delta \sum_i (y_i - \bar{y}) n_i$, as well as the magnetic field $B = \varphi/\epsilon_0$ perpendicular to the planar system entering the hopping $\tilde{t}_{ij} \rightarrow \tilde{t}_{ij} \exp[i\varphi y_i(x_i - x_j)]$, we can express $R_H$ in terms of derivatives of the ground state $E^0(\theta, \Delta, \varphi)$ with respect to external fields [1].

$$R_H = \left. -\frac{N E^0_{\Delta \varphi}}{\epsilon_0 E^0_{\Delta \theta} E^0_{\theta \theta}} \right|_{\Delta=\phi=0, \theta=\theta_0},$$

where derivatives should be taken in general at $\theta = \theta_0$, where $E^0$ is minimum.

For a reasonable approximation of Eq. (5), a system with $L > M$ is required. We therefore restrict our numerical calculations to a $6 \times 3$ system with o.b.c. in the $M$ direction, where a single stripe is introduced via $H_\Delta$, Eq. (5), in the middle leg. The situation with stripe filling $n_l = 1/2$ here corresponds to $N_h = 3$ holes in the system. Odd $N_h$ has some disadvantage leading in general to $\theta_0 \neq 0$ and also to near-degenerate states at $V = 0$.

As a reference for $V = 0$ one should expect at low doping $n_h \ll 1/2$ the semi-classical behavior $R_H^* \sim 1/\epsilon_0 n_h$, which has been in fact qualitatively reproduced using the same method [1]. In Fig. 3 we present the results for $R_H(n_l)$ as they develop with the attractive potential $V > 0$, already in the presence of small stabilizing $h = 0.1t$. From results it is evident that for $V \gg 0$ Hall constant is suppressed $|R_H| \ll R_H^*$ for $n_l = 1/2$ but as well in a wider range of stripe filling $n_l \sim 1/2$. On the other hand, at lowest doping $n_h = 1/N$ we find large $|R_H| \gg 1$ (even changing the sign) which is an indication that the system is close to an insulator with small $D_{xx} \propto E^0_{\theta \theta}$ and consequently very sensitive $R_H$ due to Eq. (5). Results in Fig. 4 show the effect of $h$ on $R_H$ for fixed $n_l = 1/2$. We observe a systematic decrease of $R_H$ with $h$, and consequently $R_H \sim 0 \ll R_H^*$ even at quite modest $V/t$.

Similar conclusions can be reached following $D(n_l)$ for the same $6 \times 3$ system, as presented in Fig. 5 for $h = 0.4t$. $D$ develops from quite monotonously increasing function of doping (with some finite-size even-odd effect in $N_h$) at $V \sim 0$, $h \sim 0$ to a dependence with a broad maximum around $n_l \sim 1/2$ for larger $V$ and $h$, as seen in Fig. 5, consistent with the vanishing of $R_H$ through Eq. (5). Such a broad maximum is also in accord with results on the $4 \times 4$ system in Fig. 1.

Let us return in conclusion to the relevance of above results to the physics of LNSCO. Our calculations confirm that stripe structures with filling $n_l = 1/2$ indeed have $R_H \sim 0$, due to a maximum $D_{xx}$ closely related to minimum hole kinetic energy in such configurations. Such a result should be directly relevant to the commensurate case, e.g., $x = 1/8$ with the inter-stripe distance $d_0 = 4$ in LNSCO. In our study we however evaluate only $R_H$ and $D(n_h)$ imposing static stripes corresponding to
fixed $d_0$ between stripes, so we can only conjecture the behavior in the regime around the commensurate values of $x$. Going beyond $x > 1/8$ in LNSCO the stripes are not static (and finally disappear above the LTT-LTO transition) so our assumption of the broken symmetry is not justified any more. One can argue that the loss of the (nearly) long range stripe order leads to the situation closer to normal phase, i.e., to an increasing $D(n_h)$ and hence to $R_H > 0$ approaching the behavior $R_H \sim R_H^*$ in the reference LSCO. In fact already our results in Fig. 3 indicate that $R_H > 0$ for $n_l > 1/2$. On the other hand, for $x < 1/8$ experiments reveal quite static stripes with an incommensurate spin density modulation corresponding to $d_0 = 2/x$. Following our results and arguments at fixed $d_0$ and for the spin ordering induced by the staggered field $h$ we would again expect maximum $D(n_h)$ and consequently $R_H \sim 0$ at the specific stripe filling $n_l = 1/2$. Therefore one can speculate that $R_H \sim 0$ persists in the whole regime of static stripes. This would be definitely a very peculiar and striking novel phenomenon, to be resolved by experiments which have so far not been performed in LNSCO well below $x < 0.12$.

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