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HALL RESISTIVITY OF HOLE- AND ELECTRON-DOPED HIGH-T_c CUPRATES

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We investigate the doping dependence of the Hall resistivity of high-T_c superconductors in terms of the t-t'-J model using a spin-rotation-invariant slave-boson technique. A second-neighbour hopping t' of different sign is included in order to reproduce the Fermi surfaces of both hole- and electron-doped systems in the noninteracting limit. Correlation effects are responsible for renormalization of the quasiparticle band. The results of our slave-boson calculation are in excellent agreement with experiments on $La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_{6+x}$, and $Nd_{2-x}Ce_xCuO_4$.

As one of the main normal-state puzzles of the CuO_2 based high-T_c superconductors, the anomalous transport properties, in particular the temperature (T) and doping (δ) dependence of the Hall resistivity $R_H(T,\delta)$ [1-4], has been under extensive experimental and theoretical study. Quasiparticle transport measurements suggest a small density of charge carriers and hence a *small* "pocketlike" Fermi surface (FS) [5]. On the other hand, direct (angle-resolved photoemission (ARPES)) probes of the FS [6, 7] yield a *large* FS which satisfies Luttinger's theorem and might be well described by (LDA) band-structure calculations. In principle, this contrasting behaviour is found for hole- ($La_{2-x}Sr_xCuO_4$ [LSCO], $YBa_2Cu_3O_{6+x}$ [YBCO]) and electron-doped ($Nd_{2-x}Ce_xCuO_4$ [NCCO]) copper oxides as well. An important common feature of both types of systems seems to be the strong coupling of spin and charge dynamics, i.e., the antiferromagnetic (AFM) correlations realized in the Cu^{2+}-spin background are clearly manifest in the charge transport [8]. Despite the qualitative similiarity between hole and electron doping, there is an apparent asymmetry regarding the stability of their AFM phases; in LSCO, AFM long-range order disappears at $x \sim 0.02$ whereas in the NCCO system it continues up to $x \sim 0.14$ [9]. This may be in part due to a different microscopic doping mechanism [10] but there is also strong evidence [11-13], that band structure (FS) and correlation effects arising from next nearest-neighbour hopping processes in the CuO_2 plane stabilize the AFM order in the electron-doped systems. An adequate framework to adress these issues from a microscopic point of view seems to be an effective one-band t-t'-J model, that includes apart from the AFM exchange interaction (J) and the nearest-neighbour (NN) transfer t, a direct second-neighbour (NNN) hopping t' [14].

Motivated by these findings, the aim of this communication is to calculate the doping dependence of the Hall resistivity in terms of an extended t-J model, with the Hamiltonian given by

$$\mathcal{H} = \sum_{i,j} t_{ij}\, \Psi_i^\dagger \Psi_j - \frac{J}{4} \sum_{\langle ij \rangle} \left(\Psi^\dagger \underline{\tau}^\mu \Psi \right)_i \left(\Psi^\dagger \underline{\tau}_\mu \Psi \right)_j . \qquad (1)$$

In order to bring out the $SU(2)$ symmetry of the system we use a spinor representation, where the one-row [one-column] matrices $\Psi_i^\dagger = (\tilde{c}_{i\sigma}^\dagger, \tilde{c}_{i-\sigma}^\dagger)$ [Ψ_i] are related to the projected creation [annihilation] operators $\tilde{c}_{i\sigma}^\dagger = c_{i\sigma}^\dagger (1 - c_{i-\sigma}^\dagger c_{i-\sigma})$ [$\tilde{c}_i$] of spin σ electrons at Wannier site i. $\underline{\tau}_\mu$ is the kovariant four-component vector of Pauli matrices (underbars denote a 2×2 matrix in the spin variables).

For quantitative comparisons between low-energy experiments and theory, we first comment on typical parameter values which enter the minimal one-band model (1). Starting from a more realistic three-band Hubbard model for the CuO_2 planes, the NN hopping in (1) mimics the motion of the so-called Zhang-Rice singlet for hole-doped systems whereas it stands for an exchange of the Cu d^{10} state for electron-doped systems. Including NNN hopping processes we obtain an effective tight-binding dispersion relation

$$\varepsilon_{\vec{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y , \qquad (2)$$

where now the summation in the transfer term is restricted to NN ($\langle i,j \rangle$) and NNN ($\langle\langle i,j \rangle\rangle$) pairs on a square lattice. The importance of the t' term (which can be related to direct oxygen-oxygen overlap in a multi-band description) is suggested by mappings of exact Cu-O cluster diagonalizations onto the t-t'-J Hamiltonian [15]. From (LDA) band-structure theory, a ratio $t'/t = -0.16$ (-0.4) has been found to be appropriate for the hole-doped LSCO (YBCO) family, where the tight-binding parameters t and t' alone are able to reproduce the qualitative features of the FS in the noninteracting limit [6, 16, 17]. In the electron-doped case, the ratio $|t'/t|$ is again on the order of 0.2, however, the signs of t and t' are reversed with respect to the hole-doped case [18]. In fact, the sign of t is of less importance because the transformation $t \to -t$ is equivalent to a phase shift of the hopping term by (π,π). If we use only positive t hereafter, the case $t' > 0$ together with a shift of the momentum $\vec{k} \to \vec{k} + (\pi,\pi)$ implies electron doping in terms of the t-t'-J model [11]. As can be seen from Fig. 1, this convention yields a FS shrinking around the $(0,0)$ or Γ point ((π,π) or M point) with increasing doping in the hole-doped (electron-doped) case, which is also consistent with recent ARPES measurements for YBCO [6] (NCCO [7]). In the following we take $t (= 0.3eV)$ as the energy unit, and fix $J/t = 0.4$ as a realistic value for the exchange interaction [15].

To treat the strong electronic correlations we adopt the $(SU(2) \otimes U(1))$ spin-rotation-invariant slave-boson (SB) scheme [19] to the t-t'-J Hamiltonian (1) with (2). First,

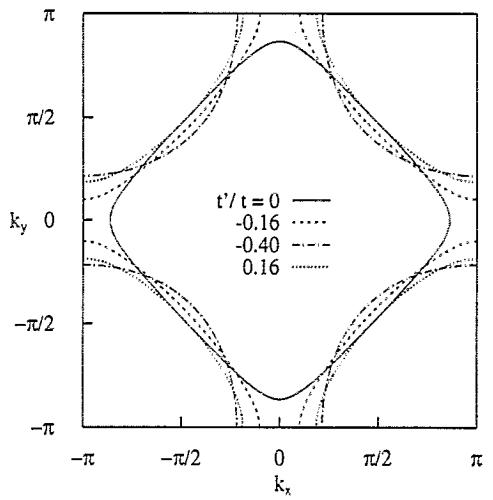

Fig. 1 Fermi surfaces of the noninteracting system for $\delta = \pm 0.1$. The curves with $t'/t = 0, -0.16, -0.4$ and $t'/t = 0.16$ correspond to hole doping ($\delta > 0$) and electron doping ($\delta < 0$), respectively.

we rewrite

$$\Psi = \underline{z}\,\tilde{\Psi}, \tag{3}$$

$$\left(\Psi^\dagger \underline{\tau}_\mu \Psi\right) = 2\,\mathrm{Tr}\,\underline{p}^\dagger \underline{\tau}_\mu \underline{p} \tag{4}$$

in terms of pseudofermionic ($\tilde{\Psi}_i$) and auxiliary bosonic ($e_i^{(\dagger)}$, $\underline{p}_i^{(\dagger)}$) operators, where the SB fields $e_i^{(\dagger)}$ and $\underline{p}_i^{(\dagger)}$ represent empty and single occupied sites, respectively. The nonlinear bosonic hopping operators $\underline{z}_i^{(\dagger)} = \underline{z}_i^{(\dagger)}(e_i, e_i^\dagger, \underline{p}_i, \underline{p}_i^\dagger)$ yield a correlation induced band renormalization. Then, the unphysical states in the extended (bosonic and fermionic) Fock space are eliminated by imposing a set of local constraints:

$$e^\dagger e + 2\,\mathrm{Tr}\,\underline{p}^\dagger \underline{p} - 1 = 0 \quad \text{(completeness)} \tag{5}$$

$$\tilde{\Psi} \otimes \tilde{\Psi}^\dagger + 2\underline{p}^\dagger \underline{p} = 0 \quad \text{(1–1–correspondence)}. \tag{6}$$

Enforcement of the constraints can be achieved via a functional integral representation of the grand canonical partition function by associating (5) and (6) to $5N$ Lagrange multipliers $\lambda_i^{(1)}$, $\underline{\lambda}_i^{(2)}$. Transforming the Lagrange multipliers into Bose fields, we can make use of the $SU(2) \otimes U(1)$ gauge freedom of the action to remove *all* SB phases in the radial gauge [19]. Finally, performing the Gaussian integration over the pseudofermionic fields, we obtain an effective bosonized action which serves as a starting point for approximations.

At the saddle-point level, we look for an extremum of the grand canonical potential with respect to the Bose fields using the ansatz $\vec{m}_i = m\vec{n}_i$ with $\vec{n}_i = (\cos\vec{Q}\vec{R}_i, \sin\vec{Q}\vec{R}_i, 0)$ [20] for the local magnetization $\vec{m}_i = -2p_{io}\vec{p}_i$, i.e., all scalar bosons become homogeneous and the vector fields exhibit the same spatial variation as the magnetization ($\vec{p}_i = p\vec{n}_i$, $\vec{\lambda}_i^{(2)} = \lambda^{(2)}\vec{n}_i$; note the $SU(2) \leftrightarrow SO(3)$ homomorphism). Here the order vector $\vec{Q}$ plays the role of a new "variational" parameter that corresponds to several magnetic phases: para-, ferro-, and antiferromagnetic, as well as incommensurate (1,1)-$[\vec{Q} = (Q, Q)]$, (1,π)-$[\vec{Q} = (Q, \pi)]$ and (0,1)-spiral $[\vec{Q} = (0, Q)]$ states. Taking into account all these phases, the quasiparticle energies can be expressed as

$$E_{\tilde{k}\pm} = \delta(1+\delta)(\varepsilon_{\tilde{k}} + \varepsilon_{\tilde{k}-\vec{Q}})/y - \tilde{\mu} \pm \left[\delta^2(\varepsilon_{\tilde{k}} - \varepsilon_{\tilde{k}-\vec{Q}})^2/y + [m\delta(\varepsilon_{\tilde{k}} + \varepsilon_{\tilde{k}-\vec{Q}})/y + \lambda^{(2)}]^2\right]^{1/2} \tag{7}$$

where $\tilde{\mu} = \mu - \lambda_o^{(2)}$ is the chemical potential, and $y = (1+\delta)^2 - m^2$. Note that the renormalized quasiparticle band $E_{\tilde{k}\nu}$ has to be determined in a self-consistent way at each doping level $\delta = 1 - n$ ($\leftrightarrow \tilde{\mu}$) by an iterative solution of the remaining nonlinear stationary equations for m, $\lambda^{(2)}$ and $\vec{Q}$. This should be contrasted to the SB mean field approach of Chi and Nagi [21], where, in the $J \to 0$ limit, the calculation of transport properties is based on the simple replacement $\varepsilon_{\tilde{k}} \to \tilde{\varepsilon}_{\tilde{k}} = -2t\delta\,[(\cos k_x + \cos k_y) + 2t'/t\,\cos k_x \cos k_y]$ of the noninteracting band dispersion (2).

Once the quasiparticle band $E_{\tilde{k}\nu}$ has been obtained, the Hall resistivity

$$R_H = \sigma_{xyz}/\sigma_{xx}\sigma_{yy} \tag{8}$$

can be calculated in the relaxation-time approximation, using standard formulas for the transport coefficients $\sigma_{\alpha\beta}$ and $\sigma_{\alpha\beta\gamma}$:

$$\sigma_{\alpha\beta} = -\frac{e^2\tau}{\hbar^2 V}\sum_{\tilde{k}\nu} v_{\alpha;\tilde{k}\nu} v_{\beta;\tilde{k}\nu} \frac{\partial f}{\partial E_{\tilde{k}\nu}}, \tag{9}$$

$$\sigma_{\alpha\beta\gamma} = -\frac{e^3\tau^2}{\hbar^4 c V}\sum_{\tilde{k}\nu} v_{\alpha;\tilde{k}\nu}\epsilon_{\lambda\kappa\gamma} v_{\lambda;\tilde{k}\nu} \frac{\partial v_{\beta;\tilde{k}\nu}}{\partial k_\kappa}\frac{\partial f}{\partial E_{\tilde{k}\nu}}. \tag{10}$$

Here $f = [\exp(E_{\tilde{k}\nu}) + 1]^{-1}$ is the Fermi function, V denotes the volume of the unit cell, $\epsilon_{\lambda\kappa\gamma}$ is the completely antisymmetric tensor, and $v_{\alpha;\tilde{k}\nu} = \partial E_{\tilde{k}\nu}/\partial k_\alpha$. The $\tilde{k}$ summations are done numerically over the full Brillouin zone of the square lattice, using a 1000×1000 grid. Note that R_H does not depend on the relaxation time τ.

The theoretical Hall resistivity $R_H(T, \delta)$ as a function of δ is depicted in Fig. 2 in comparison to experiments on LSCO [1], YBCO [2] and NCCO [3, 4]. In the LSCO and NCCO systems, the concentration of chemically doped charge carriers in the CuO_2 planes (δ) definitely agrees with the composition (x) of the substitutes Sr and Ce. This simple relation, however, no longer holds for YBCO, i.e., the amount of "holes" transferred into the planes does not increase linearly with the oxygen content. Indeed, the magnetic properties indicate $\delta \simeq 0$ up to $x = 0.2$ [22]. In order to compare our theoretical model with the $R_H(x)$ data found on oxygen doped YBCO, we use the relation $\delta = (x - 0.2)/2$ (also, using (9) and (10), it has to be kept in mind that YBCO has two CuO_2 layers per unit cell). Figure 2 clearly demonstrates the importance of the NNN transfer term t' for a consistent theoretical description of the experimental Hall data. For $J/t = 0.4$, a surprisingly good agreement with experiments on LSCO and NCCO, including the sign change of $R_H(\delta)$ at a very similar value, can be achieved using the parameter values $t'/t = 0$ and $t'/t = 0.16$, respectively. It should be noted that in the case of LSCO we obtain $t'/t = 0$ from $R_H(\delta)$ while LDA calculations yield a ratio $t'/t = -0.16$ [16, 17]. For $YBa_2Cu_3O_{6+x}$, where the experiments [2] give $R_H > 0$ up to $x = 1$, a negative t'-term suffices to give the correct tendency to $R_H(\delta)$. Using $t'/t = -0.4$, our theory yields a sign change of R_H at $\delta \sim 0.7$. The discontinuities, occuring in the theoretical curves at various δ, are related to changes of the magnetic structure of the ground state (cf. the magnetic phase diagram of the t-t'-J model [13]). The strong increase (decrease) of the positive (negative) Hall coefficient as $\delta \to 0$ can be attributed to the formation of small hole (electron) pockets in the FS (see below). Obviously, this is a correlation effect. A

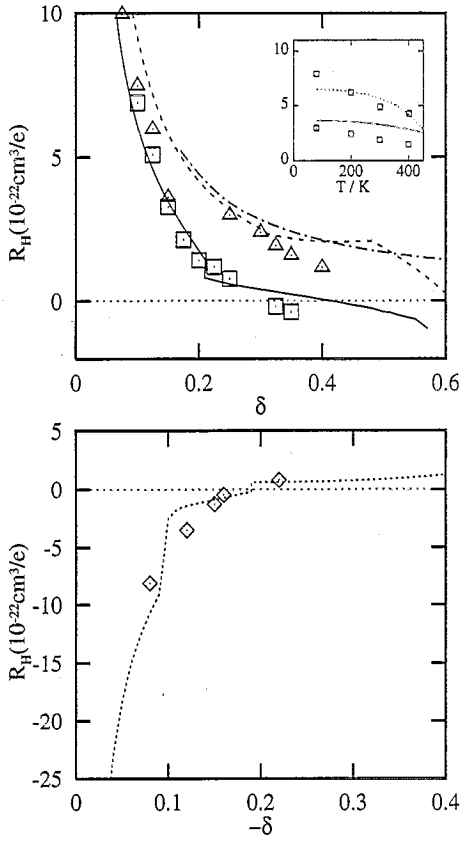

Fig. 2 Doping dependence of the Hall resitivity for hole- (upper panel) and electron-doped (lower panel) systems. The slave-boson results for $J/t = 0.4$ and different ratios $t'/t = 0$ (solid), -0.16 (dashed), -0.4 (chain dotted) and $t'/t = 0.16$ (dotted) are compared with experiments on LSCO (□) [1] [at 80 K], YBCO (△) [2] [at 100 K] and NCCO (◇) [3,4] [at 80 K], respectively. The inset shows the temperature dependence of R_H for $t'/t = 0$ at $\delta = 0.1$ (short dashed) and $\delta = 0.15$ (dotted).

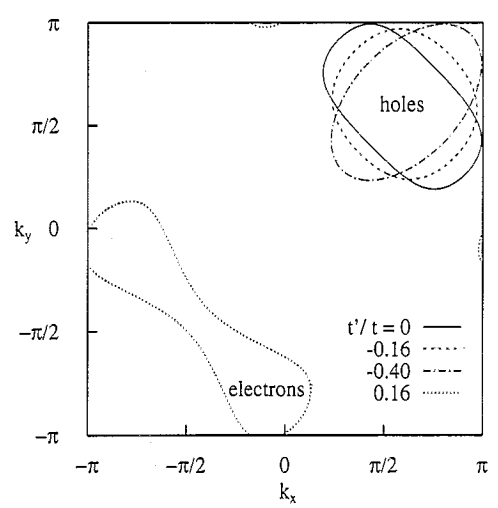

Fig. 3 Quasiparticle Fermi surface in the (1,1)-spiral phase at $J/t = 0.4$ for $\delta = 0.1$ (hole-doped system) and $\delta = -0.1$ (electron-doped system).

recent analysis of resistivity saturation in LSCO [5], based on Boltzmann transport, has been taken as an indication of a small FS as well, however, the existence of a pocket-like FS is still a subtle and unresolved issue. We found that the temperature dependence of $R_H(\delta, T)$ is at least in qualitative agreement with experiments on LSCO (see inset Fig. 2 (upper panel)). Note that the quasiparticle dispersion $E_{\vec{k}\pm}$ exhibits extremely *flat* minima implying the presence of a new small energy scale Δ. Therefore, when the temperature becomes comparable to Δ the hole pockets are washed out and sign change of R_H occurs (cf. Fig. 2 at fixed δ(inset)).

The FS of the interacting system (1) are shown in Fig. 3 for the same typical ratios t'/t as in Fig. 1 at $J/t = 0.4$ and $\delta = \pm 0.1$, where the diagonal (1,1)-spiral phase becomes lowest in energy. As observed for t-J and Hubbard models as well [23], we obtain small hole (or electron) pockets with a volume $\propto |\delta|$. The calculated FS are very anisotopic. As $|\delta|$ increases, the pockets grow, until the FS topology changes completely at a critical doping value δ_c ($R_H(\delta_c) = 0$; cf. Fig 2), reflecting the transition from hole to electron carriers for $t'/t < 0$ and vice versa for $t'/t > 0$.

To illustrate the $\vec{k}$-dependence of the SB quasiparticle dispersion relation, e.g. for the electron-doped system, in more detail, in Fig. 4 the $E_{\vec{k}-}$-contour is shown at 10 % doping in the (1,1)-spiral state. We point out here that $E_{\vec{k}-}$ corresponds to the *upper* quasiparticle band (in electron notation). At $J/t = 0.4$ and $\delta = -0.1$, we have $\tilde{\mu} = 0.309$, $\lambda^{(2)} = -0.667$, $m = 0.757$ and $\vec{Q} = (-2.789, -2, 789)$. In contrast to the hole-doped case, $E_{\vec{k}-}$ exhibits two minima. We stress that at still lower doping level ($|\delta| \leq 0.02$), where the ground state is antiferromagnetically ordered [13], the minima of $E_{\vec{k}-}$ are located around $(\pm\pi, 0)$ and $(0, \pm\pi)$ ((0,0) and $(\pm\pi, \pm\pi)$) in the case of electron doping [$t'/t > 0$] (hole doping [$t' \leq 0$]). The renormalization of the quasiparticle band strongly depends on both electronic correlation (J) and doping level (δ), which, in fact, calls the frequently used rigid-band approximation into question. Obviously, due to the strong coupling of spin and charge dynamics the characteristic energy scale for the coherent motion of the charge carriers is J and not t (provided $t > J$).

In conclusion, we have shown that our calculation of the Hall resistivity in the relaxation-time approximation, combined with a SB based treatment of strong electronic

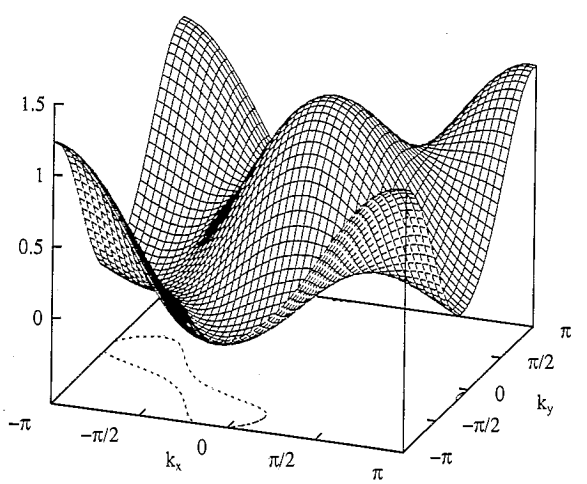

Fig. 4 Quasiparticle band structure $E_{\vec{k}-}$ for $\delta = -0.1$ and $J/t = 0.4$ (see text for further explanation).

correlations and band structure effects in terms of the t–t'–J model, provides a reasonable explanation of the experimentally observed doping dependence of R_H on both hole– ($La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_{6+x}$) and electron–doped ($Nd_{2-x}Ce_xCuO_4$) copper oxides.

Note added in proof. We recently learned of a related exact diagonalization study of Dagotto, Nazarenko, and Bonsinsegni, where, similar in conclusion, the doping and temperature dependence of R_H was calculated using a strongly renormalized *flat* quasiparticle dispersion [24].

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