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TRANSPORT AND CHARGE/MAGNETIC ORDER IN THE 2D HOLSTEIN/t–t'–J MODEL

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The magnetic phase diagram of the t-t'-J model is presented, where in the framework of a spin-rotation-invariant slave-boson approach incommensurate magnetic structures are taken into account. Including Gaussian fluctuations, a general expression for the dynamic spin and charge susceptibilities of the t-t'-J model is derived, which goes beyond RPA. The doping dependence of the Hall resistivity is calculated, the results being in accord with experiments on LSCO and YBCO. The commensurate charge/lattice modulations, reported recently for the isostructural nickelates at quarter filling, can be understood in terms of the 2D Holstein-t-J model.

Among the most striking features of the charge-transfer oxides, such as $La_{2-\delta}Sr_\delta CuO_4$ (LSCO), the isostructural $La_{2-\delta}Sr_\delta NiO_4$ (LSNO) or $YBa_2Cu_3O_{6+\delta}$ (YBCO), are the dependence of transport properties (e.g. Hall coefficient R_H) or magnetic, charge and lattice fluctuations on temperature and doping (δ). The strong electronic correlations, which are believed to be responsible for most of the unusual normal-state properties at least in the cuprates, may be described by an effective one-band Hamiltonian $\mathcal{H}_{t-t'-J}$. Here t denotes nearest-neighbor (NN) transfer, while t' corresponds to next NN hopping processes along the diagonal of the square unit cell, i.e., $\varepsilon_{\vec{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$. The reason for this extension of the original t–J model is based on the experimental finding that the wavevector ($\vec{q}$) dependence of spin fluctuations is not universal for the cuprates, i.e. (in)commensurate for the (LSCO-) YBCO-type systems, which may be due to the different shape of the Fermi surfaces in the low doping region. We choose $t' = 0$ ($t' = -0.4t$) for the LSCO (YBCO) family, which is consistent with band structure calculations, and fix the exchange interaction $J/t = 0.4$.

For an adequate description of spin and charge degrees of freedom in $\mathcal{H}_{t-t'-J}$, we make use of the ($SU(2)\otimes U(1)$) spin-rotation-invariant slave-boson (SB) technique[1] by introducing auxiliary boson fields $e_i^{(\dagger)}$ and matrix operators $\underline{p}_i^{(\dagger)}$, representing empty and single occupied sites, respectively. Then $\tilde{c}_{i\sigma} = \sum_\rho z_{i\sigma\rho} f_{i\rho}$ follows, where the ($\underline{z}$)-factors yield a correlation-induced band renormalization. The interaction term is bosonized via $n_i = 2Tr\,\underline{p}_i^\dagger \underline{p}_i$ and $\vec{S}_i = Tr\,\underline{p}_i^\dagger \vec{\tau} \underline{p}_i$. Now the partition function can be expressed as a path integral $\mathcal{Z} = \int \mathcal{D}[\Phi^*, \Phi] \exp\{-\mathcal{S}_{eff}\}$ over bosonic fields $\Phi_i(\tau) = (e_i, p_{io}, \lambda_{io}^{(2)}, \lambda_i^{(1)}; \vec{p}_i, \vec{\lambda}_i^{(2)})$, where in the radial gauge *all* $\Phi_{i\alpha}$ ($\alpha = 1\dots10$) become real. The local constraints are enforced by five Langrange-multiplier fields ($\lambda_i^{(1)}$, $\lambda_{io}^{(2)}$, $\vec{\lambda}_i^{(2)}$).

At saddle-point level, we use the ansatz $\vec{m}_i = (-2p_{io}\vec{p}_i) \propto (\cos\vec{Q}\vec{R}_i, \sin\vec{Q}\vec{R}_i, 0)$ for the local magnetization. The resulting ground-state phase diagram is shown in Fig. 1. The order vector $\vec{Q}$ describes several magnetic phases: PM, FM, AF, as well as incommensurate (1,1)-spiral [$\vec{Q} = (Q, Q)$] and (1,0)-spiral [$\vec{Q} = (Q, \pi)$] states.

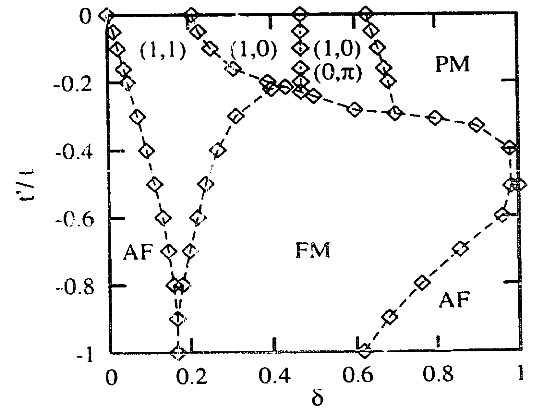

Figure 1. Phase diagram of the t-t'-J model

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Compared to the pure t-J model, the t'-term stabilizes the Néel order in a finite δ-region near half-filling. For $t'/t < -1.4$, we obtain the AF phase $\forall\delta$. Note the differences to the phase diagram obtained within a semiclassical $(1/N)$-expansion[2].

Including Gaussian fluctuations $\Phi_i = \bar{\Phi} + \delta\Phi_i$ (at the PM saddle-point $\bar{\Phi}$), the spin and charge susceptibilities can be expressed via $\chi_{s,c}(q) \propto \langle\delta\Phi_{e,p_z}(-q)\ \delta\Phi_{e,p_z}(q)\rangle$ in terms of the inverse fluctuation propagator matrix[5]. From here we may derive the following general expression for both the dynamic spin and charge susceptibility $\chi_\nu(q=(\vec{q},\omega_m))$ $[\nu = s, c]$ of the t-t'-J model:

$$\chi_\nu(q) = \frac{\overline{\chi}_o(q)}{1 + C_\nu(\vec{q})\overline{\chi}_o(q) + \mathcal{K}_\nu(q)}, \quad (1)$$

$\mathcal{K}_\nu = f_\nu(\delta)\overline{\chi}_1(q) + f_\nu^2(\delta)\,[\overline{\chi}_1^2(q) - \overline{\chi}_o(q)\overline{\chi}_2(q)]\,/4$, and $\overline{\chi}_n(q) = -\frac{2}{N}\sum_k(\varepsilon_{\vec{k}} + \varepsilon_{\vec{k}+\vec{q}})^n G(k)G(k+q)$. The coefficients $C_\nu(\vec{q})$ are functions of δ, $J(\vec{q})$, and $\tilde{\varepsilon}(\vec{q};\delta,\mu)$. The saddle-point phase boundary PM $\rightleftharpoons$ (1,1)/(0,π)-spiral (cf. Fig. 1) coincides with a divergency (pole structure) in $\chi_s(\vec{q},0)$, proving the consistency of both approaches.

In a next step, we calculate the Hall resistivity $R_H = \sigma_{xyz}/\sigma_{xx}\sigma_{yy}$ within the relaxation time approximation using the SB quasiparticle band. The SB results agree surprisingly well with experiments on LSCO[3] (see Fig. 2) For YBCO, it seems to be more difficult to extract the number of holes contained in the CuO_2 planes from the experimental data[4]. Nevertheless, the t'-term suffices to give the correct tendency to $R_H(\delta)$.

To incorporate the influence of electron-phonon coupling, which is observed to be more important in the nickelates LSNO[6], we add to $\mathcal{H}_{t-J}$ an (adiabatic) Holstein term

$$\mathcal{H}_{el-ph} = -\sum_i \Delta_i n_i + \frac{1}{4\varepsilon_p}\sum_i \Delta_i^2. \quad (2)$$

Here $\Delta_i \propto (\Delta_i^x - \Delta_{i-(1,0)}^x + \Delta_i^y - \Delta_{i-(0,1)}^y)$ corresponds to bond-parallel oxygen lattice displacements, i.e. $\Delta_i = (-1)^i\Delta$ describes an in-plane oxygen breathing mode. Adapting the frozen phonon approach to the quarter-filled case, our results for the static charge susceptibility $\chi_c(\pi,\pi)$ (with C_c replaced by $C_c - 2\varepsilon_p$ in (1)) and the order parameter Δ resembles the observed 2D ordering of self-trapped "polarons"[6] above a critical electron-phonon coupling strength ε_p.

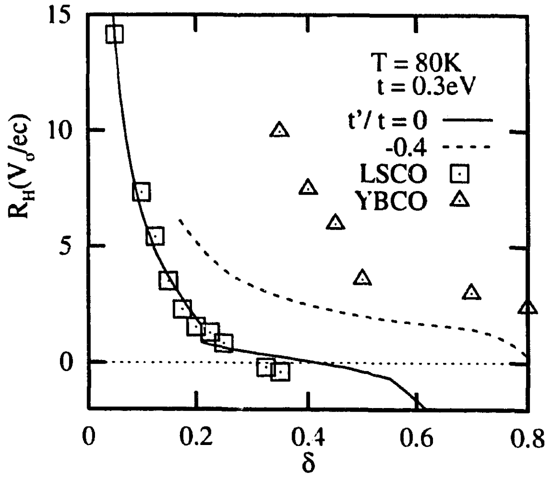

Figure 2. Hall resistivity R_H *vs* doping δ.

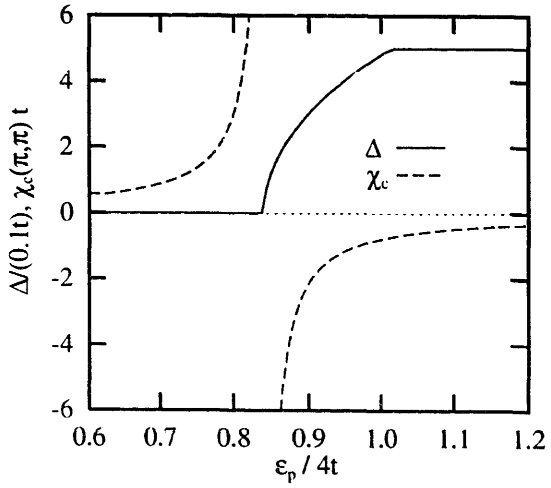

Figure 3. Order parameter and charge susceptibility of the 2D Holstein-t-J model at $\delta = 0.5$.

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