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Part S4 - LT Properties of Solids 1: Magnetism (theory)

Theory of short-range magnetic order for the t-J model

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We present a self-consistent theory of magnetic short-range order based on a spin-rotation-invariant slave-boson representation of the 2D t-J model. In the functional-integral scheme, at the nearest-neighbour pair-approximation level, the bosonized t-J Lagrangian is transformed to a classical Heisenberg model with an effective (doping-dependent) exchange interaction which takes into account the interrelation of "itinerant" and "localized" magnetic behaviour. Evaluating the theory in the saddle-point approximation, we find a suppression of antiferromagnetic and incommensurate spiral long-range-ordered phases in the favour of a paramagnetic phase with pronounced antiferromagnetic short-range correlations.

Experimental evidence has been accumulating that high-T_c superconductivity in the perovskite copper oxides develops in the presence of strong antiferromagnetic (AFM) spin correlations, which may have important implications for the pairing mechanism. The interesting low-temperature magnetic behaviour comes predominantly from the complicated interplay between *itinerant* charge carriers (holes) and *localized* spins (Cu^{2+}) within the CuO_2 planes. Hole doping rapidly destroys the AFM long-range order (LRO), but pronounced *short-range order* (SRO) is retained and may account for the unusual normal-state properties of the cuprates, such as the behaviour of the uniform magnetic susceptibility as a function of doping and temperature [1].

Motivated by this situation, in this article we outline a theory of magnetic SRO for strongly correlated electron systems described by the 2D t-J model

$$\mathcal{H} = -t \sum_{\langle ij\rangle\sigma} \left(\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma} + \text{H.c.}\right) + J \sum_{\langle ij\rangle} \left(\vec{S}_i\vec{S}_j - \frac{1}{4}\tilde{n}_i\tilde{n}_j\right). \quad (1)$$

Applying a spin-rotation-invariant slave-boson (SB) technique within the functional-integral representation of the partition function [2], the bosonized free-energy functional of the t-J model takes the form

$$\Psi = \sum_i(-\nu_i n_i + \vec{\xi}_i\vec{m}_i) - \frac{1}{\beta}\mathrm{Tr}_{\substack{ij,n\\ \rho\rho'}} \ln[-\hat{G}^{-1}] + \frac{J}{4}\sum_{\langle ij\rangle}(\vec{m}_i\vec{m}_j - n_i n_j) \quad (2)$$

with the transformed inverse propagator (cf. Ref. [3])

$$\underline{\hat{G}}^{-1}_{ijn} = (\underline{z}_i\underline{z}_j)^{-1}[(-i\omega_n - \nu_i)\underline{1} + \vec{\xi}_i\vec{\underline{\sigma}}]\delta_{ij} - t_{ij}\underline{1}. \quad (3)$$

(underbars denote a 2×2 matrix in spin space). Here, the local magnetization [particle number] operators are given by $\vec{m}_i = 2p_{io}\vec{p}_i$ $[n_i = p_{io}^2 + \vec{p}_i^{\,2}]$, $\vec{\xi}_i$ $[\nu_i]$ refer to the "internal" magnetic [charge] fields, and the nonlinear ($\underline{z}_i$)-factors, which depend only on the single-occupancy matrix operators $\underline{p}_i = \frac{1}{2}(\underline{1}p_{io} + \vec{\underline{\sigma}}\vec{p}_i)$, yield a correlation-induced band renormalization [2]. For simplicity, we describe the fluctuations of the bosonic fields by the Ansatz ($|\vec{s}_i| = 1$):

$$n_i = n \qquad \vec{m}_i = \bar{m}\,\vec{s}_i \quad (4)$$

$$\nu_i = \nu \qquad \vec{\xi}_i = \bar{\xi}\,\vec{s}_i\,, \quad (5)$$

i.e., we assume that the charge fields as well as the amplitudes of the spin components are site independent. Moreover, since the flipping time of the local magnetizations is supposed to be long compared to the electronic hopping time all bosonic degrees of freedom are treated in the static approximation.

To incorporate SRO effects, one has to go beyond the homogeneous paramagnetic (PM) saddle-point. Therefore we perform an expansion in terms of the local perturbation $\underline{V}_i\delta_{ij} = -\underline{\hat{G}}^{-1}_{ij} + \underline{\hat{G}}^{o\,-1}_{ij}$, where the PM propagator $\underline{\hat{G}}^{o\,-1}_{ij}$, with the diagonal [off-diagonal] components $\hat{G}^o_0 \equiv \hat{G}^o_{ii}$ $[\hat{G}^o_1 \equiv \hat{G}^o_{\langle ij\rangle}]$, arises out of (3) by setting $\vec{\xi}_i = 0$ and replacing $\underline{z}_i \to z^o$, $\nu_i \to \nu^o$.

Using spherical harmonics we are able to transform $\Psi(\{\vec{s}_i\})$ [3] to an *effective* classical Heisenberg model (within the nearest-neighbour pair approximation):

$$\Psi = \bar{\Psi} - \bar{J}\sum_{\langle ij\rangle} \vec{s}_i\vec{s}_j\,, \tag{6}$$

where

$$\bar{\Psi}/N = \Psi^o/N - \nu n + \bar{\xi}\bar{m} - \frac{Jn^2}{2} \tag{7}$$

$$+\sum_\zeta \left[\Phi_{0\zeta} + \int_{-1}^{1} dx\, \Phi_{1\zeta}(x)\right], \tag{8}$$

$$\bar{J} = -\frac{J\bar{m}^2}{4} - \frac{3}{2}\sum_\zeta \int_{-1}^{1} dx\, x\, \Phi_{1\zeta}(x), \tag{9}$$

$$\Psi^o = -\frac{2}{\beta}\sum_{\vec{k}} \ln\left[1 + e^{-\beta\{(z^o)^2\epsilon_{\vec{k}} + \nu^o - \mu\}}\right], \tag{10}$$

$$\Phi_{0\zeta} = \mathrm{Tr}_n \ln\left[1 - \hat{G}_0^o V_\zeta\right], \tag{11}$$

$$\Phi_{1\zeta} = \mathrm{Tr}_n \ln\left[1 - (\hat{G}_1^o)^2 T_\zeta^{(2)}(x)\right], \tag{12}$$

$x = \vec{s}_0\vec{s}_1$, $\underline{T}_i = \underline{V}_i(\underline{1} - \hat{G}_0^o\underline{V}_i)^{-1}$, and V_ζ and $T_\zeta^{(2)}(x)$ are the eigenvalues of $V_{i\rho\rho'}$ and $(\underline{T}(\vec{s}_0)\underline{T}(\vec{s}_1))_{\rho\rho'}$, respectively. Note that the effective Heisenberg-exchange integral $\bar{J}$ has to be determined self-consistently at each given interaction strength J and hole doping $\delta = 1 - n$. Evaluating the trace over the $\vec{s}_i$-variables in the partition function [4] and hereafter adopting the saddle-point approximation to the resulting *nonlocal* Heisenberg free-energy functional,

$$\Psi = \bar{\Psi} - \frac{2N}{\beta}\ln\left[4\pi\frac{\sinh(\beta\bar{J})}{\beta\bar{J}}\right], \tag{13}$$

the extremal Bose fields are obtained from

$$n = \sum_\zeta n_\zeta^f \qquad \nu = \sum_\zeta b_\zeta^f \frac{\partial[z^2]_\zeta}{\partial n} - Jn \tag{14}$$

$$\bar{m} = \sum_\zeta \zeta n_\zeta^f \qquad \bar{\xi} = -\sum_\zeta b_\zeta^f \frac{\partial[z^2]_\zeta}{\partial\bar{m}} - \eta\frac{J}{\bar{m}} \tag{15}$$

with $x_\zeta^f = \frac{\partial\phi_{0\zeta}}{\partial(y_\zeta)} + \sum_{\zeta'}\int dx\,\left[1+\eta\frac{3x}{\bar{m}^2}\right]\frac{\partial\phi_{1\zeta'}(x)}{\partial(y_\zeta)}$, where $y_\zeta \equiv (\nu - \zeta\bar{\xi})$ $[y_\zeta \equiv (z^2)_\zeta]$ if $x \leftrightarrow n$ $[x \leftrightarrow b]$, and we have introduced the SRO parameter

$$\eta \equiv \langle\vec{m}_i\vec{m}_j\rangle = \bar{m}^2\mathrm{L}(\beta\bar{J}) \tag{16}$$

with the Langevin function $\mathrm{L}(z) = \coth z - z^{-1}$. For vanishing $\bar{m}$, we have $\bar{J} = 0$, and the PM saddle-point is recovered, i.e., our theory adequately describes paraphases without and with SRO ($\bar{m} = \langle\vec{m}_i\rangle$):

$$\begin{array}{lll} \text{PM} : & \bar{m} = 0\,, & \eta = 0 \\ \text{SRO-PM} : & \bar{m} = 0\,, & \eta \neq 0\,. \end{array} \tag{17}$$

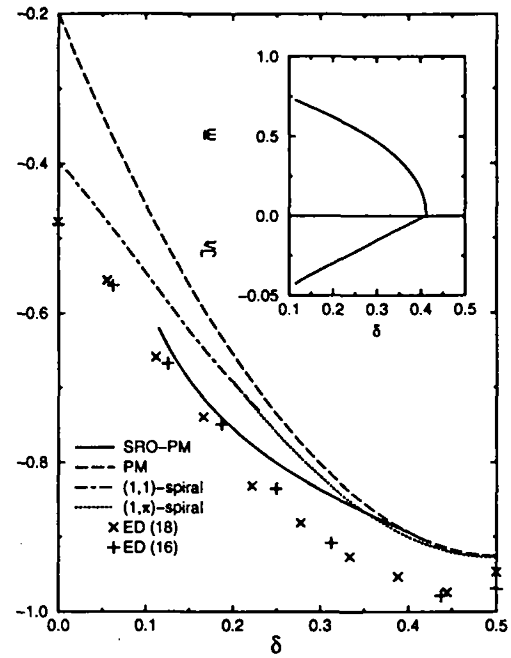

Figure 1: Ground-state energies of the 2D t-J model as functions of doping at $J/t = 0.4$. The energy of the (scalar) SRO-PM phase is compared with SB results for the PM and different spiral states as well as with exact diagonalization (ED) data obtained for the 16- and 18-site lattices. The corresponding local magnetization $\bar{m}$ and effective AFM exchange coupling $\bar{J}$ are shown in the inset.

To illustrate the quality of our approach, some representative numerical results are depicted in Fig. 1. Obviously, in the physically most interesting doping region the ground-state energy of the SRO-PM phase is lower than that of the frequently discussed spiral phases and lies close to the exact data. Thus upon doping magnetic LRO make way to SRO. Note that the SRO-PM phase is locally stable against phase separation. The interplay of local and itinerant magnetic behaviour, which is self-consistently incorporated in our theory, results in strong doping (and temperature) dependences of both $\bar{m}$ and $\bar{J}$.

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