



# Theory of magnetic short-range order for high- $T_c$ superconductors

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## Abstract

A theory of magnetic short-range order for high- $T_c$  cuprates is presented on the basis of the one-band  $t$ - $t'$ -Hubbard model combining the four-field slave-boson functional integral technique with the Bethe cluster method. The ground-state phase diagram evaluated self-consistently at the saddle-point and pair-approximation levels shows the experimentally observed suppression of magnetic long-range order in the favour of a paraphase with antiferromagnetic short-range order. In this phase the uniform static spin susceptibility consists of interrelated itinerant and local parts and increases upon doping up to the transition to the Pauli paraphase. Using realistic values of the Hubbard interaction we obtain the cusp position and the doping dependence of the zero-temperature susceptibility in reasonable agreement with experiments on  $\text{La}_{2-\delta}\text{Sr}_\delta\text{CuO}_4$ .

*Keywords:* Hubbard model; Magnetic short-range order; Spin susceptibility

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The spin correlations in high- $T_c$  superconductors probed by neutron and NMR experiments and by the spin susceptibility in the paraphase (showing, for  $\text{La}_{2-\delta}\text{Sr}_\delta\text{CuO}_4$  (LSCO), a maximum in the doping and temperature dependences [1]) are believed to be caused by a strong Coulomb interaction in the  $\text{CuO}_2$  planes which may result in a considerable antiferromagnetic short-range order (SRO). In our previous work [2] the role played by SRO in explaining the unconventional magnetic properties of the cuprates was investigated within the 2D one-band Hubbard model based on the scalar four-field slave-boson (SB) approach [3].

In this paper the SRO concept is further elaborated, where attention is paid to band-structure effects on the stability of magnetic SRO versus long-range order (LRO) and on the doping dependence of the spin susceptibility. In the SB representation the

Hubbard model can be expressed as [3]

$$\mathcal{H} = \sum_{ij\sigma} t_{ij} z_{i\sigma}^\dagger f_{i\sigma}^\dagger f_{j\sigma} z_{j\sigma} + U \sum_i d_i^\dagger d_i. \quad (1)$$

The functional integral for the partition function is calculated in the radial gauge and the static approximation for the SB fields  $p_{i\sigma}$ ,  $d_i$  and the Lagrange multiplier field  $\lambda_{i\sigma}^{(2)}$  (enforcing the constraint  $f_{i\sigma}^\dagger f_{i\sigma} = p_{i\sigma}^\dagger p_{i\sigma} + d_i^\dagger d_i$ ), where the  $e_i$  fields are eliminated by the saddle-point approximation for  $\lambda_{i\sigma}^{(1)}$  (guaranteeing  $e_i^\dagger e_i + d_i^\dagger d_i + \sum_\sigma p_{i\sigma}^\dagger p_{i\sigma} = 1$ ) [3]. Transforming away the SB fluctuations in the transfer term (proportional to the band narrowing  $z_{i\sigma}$ ), we get the free-energy functional

$$\psi = \sum_i (U d_i^\dagger d_i - n_i v_i + m_i \xi_i) - \text{Tr} \ln [-\hat{G}^{-1}], \quad (2)$$

$$\hat{G}_{ij\sigma}^{-1} = \frac{\omega - v_i + \sigma(\xi_i + h)}{|z_{i\sigma}|^2} \delta_{ij} - t_{ij}, \quad (3)$$

where  $m_i = \sum_\sigma \sigma p_{i\sigma}^2$  and  $n_i = \sum_\sigma p_{i\sigma}^2$  are the SB representations of the local magnetization and particle number, respectively,  $\xi_i = \sum_\sigma \sigma \lambda_{i\sigma}^{(2)}$  is the

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internal magnetic field, and  $v_i = \sum_{\sigma} \lambda_{i\sigma}^{(2)}$ . In Eq. (3),  $h$  denotes the uniform external magnetic field.

We incorporate the SRO beyond the PM saddle point by an expansion in terms of the local perturbation

$$V_{i\sigma}(\omega) = -\hat{G}_{ij\sigma}^{-1} + \hat{G}_{ij\sigma}^{\circ-1}. \quad (4)$$

$$\hat{G}_{ij\sigma}^{\circ} = \text{FT} \{ [(\omega - v^{\circ} + \sigma(\xi^{\circ} + h)) / (z_{\sigma}^{\circ})^2 - \varepsilon_{\vec{k}}]^{-1} \}$$

is the PM Green propagator (the superscript “o” denotes the uniform paramagnetic (PM) saddle point), where

$$\varepsilon_{\vec{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y \quad (5)$$

is the 2D tight-binding dispersion taking into account the transfer integral between nearest ( $t$ ) and next-nearest ( $t'$ ) neighbours. Now we treat the fluctuations of  $m_i = \bar{m}_i s_i$ ,  $\xi_i = \bar{\xi}_i S_i$  ( $s_i = \pm$ ) and of the charge degrees of freedom by the ansatz  $b_i \rightarrow b_{S_i}$ , with  $b \in \{\bar{m}, \bar{\xi}, n, v, d = d^*\}$ . Transforming the functional (2) to an effective Ising model in the nearest-neighbour pair ( $\langle ij \rangle$ ) approximation [4] we obtain

$$\psi(\{s_i\}) = \bar{\psi} - \bar{h} \sum_i s_i - \bar{J} \sum_{\langle ij \rangle} s_i s_j, \quad (6)$$

with

$$\bar{J} = -\frac{1}{4} \sum_{x,\sigma=\pm} (\Phi_{xx\sigma} - \Phi_{-xx\sigma}), \quad (7)$$

where the two-site fluctuation contribution is found to be

$$\Phi_{xx\sigma} = \Phi_{\langle ij \rangle\sigma}(\alpha_i, \alpha_j) \Big|_{\substack{x_i=x \\ x_j=x'}}$$

$$\Phi_{\langle ij \rangle\sigma} = \frac{1}{\pi} \int d\omega f(\omega - \mu)$$

$$\text{Im} \ln [1 - G_{\langle ij \rangle\sigma}^{\circ} T_{j\sigma}(\alpha_j) G_{\langle ji \rangle\sigma}^{\circ} T_{i\sigma}(\alpha_i)], \quad (8)$$

and  $T_{i\sigma} = V_{i\sigma}(1 - G_{ii\sigma}^{\circ} V_{i\sigma})^{-1}$  denotes the scattering matrix. Performing the  $s_i$  sum in the partition function with Eq. (6) we treat the SRO in the Bethe cluster approximation. Thereafter, we determine the saddle point for all Bose fields  $b_x \in \{\bar{m}_x, \bar{\xi}_x, n_x, v_x, d_x\}$ . Correspondingly, in our theory the SRO is self-consistently described at the saddle point and pair approximation levels at each interaction strength  $U$  and hole doping  $\delta = 1 - n$ .

In the  $h = 0$  limit ( $\bar{m}_x = \bar{m}$ ) we obtain two possible paraphases ( $\langle s_i \rangle = 0$ ): (i) the paraphase without SRO (PM;  $\bar{J} = 0, \bar{m} = 0$ ) and (ii) the paraphase

with antiferromagnetic SRO (SRO-PM;  $\bar{J} < 0, \bar{m} > 0$ ). Let us stress that, at  $T = 0$ , the SRO-PM phase must be distinguished from the phase with antiferromagnetic LRO (denoted by AFM) having a finite sublattice magnetization  $m_A = p_{A\uparrow}^2 - p_{A\downarrow}^2 = -m_B$  which is determined from the A-B saddle point [5] and differs from the SRO amplitude  $\bar{m}$ .

In Fig. 1 the ground-state phase diagram is depicted, where only the phases describable by the scalar SB approach are shown and the tight-binding density of states is used (instead of a semielliptic one taken in Ref. [2]). At large enough interaction strengths ( $U/t > 5-6$ ) the antiferromagnetic LRO makes way to antiferromagnetic SRO in a wide doping region, where we obtain an AFM  $\rightleftharpoons$  SRO-PM phase transition of first order at  $\delta_{c_1}$  and a SRO-PM  $\rightleftharpoons$  PM transition of second order at  $\delta_{c_2}$ . For  $U/t = 8$  (being realistic for the cuprates [6]) and  $t' = 0$  we get  $\delta_{c_1} = 0.04$  and  $\delta_{c_2} = 0.26$ . The inclusion of the  $t'$  term in Eq. (5) ( $t'/t = -0.16$  is realistic for LSCO) extends the stability region of the SRO-PM phase, since hopping processes along the lattice diagonals favour antiferromagnetic correlations.

Within our theory, the suppression of magnetic LRO at  $\delta_{c_1} \simeq 4\%$  ( $U/t \simeq 8$ ) observed in LSCO may be related to the persistence of SRO in the paraphase. The SRO breaks down at  $\delta_{c_2} \simeq 30\%$ . Note

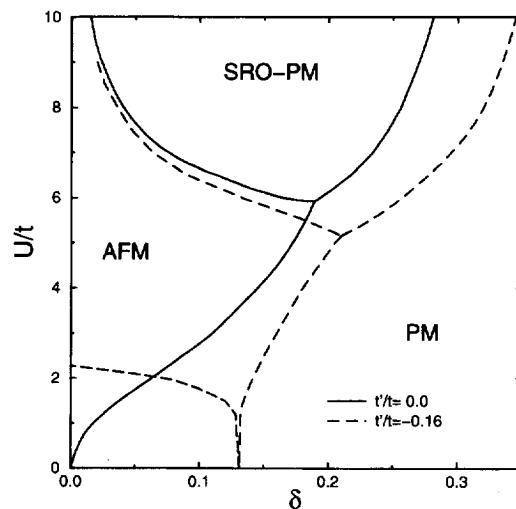


Fig. 1. Ground-state phase diagram.

that just at this doping the superconductivity in LSCO disappears. Correspondingly, the unconventional behaviour of high- $T_c$  cuprates may be due to the presence of magnetic SRO which we suggest from our results to play also a role in the pairing mechanism.

The uniform static spin susceptibility  $\chi$  has to be calculated according to

$$\chi = \lim_{h \rightarrow 0} \sum_{\alpha} \left( W_{\alpha} \frac{dm_{\alpha}}{dh} + m_{\alpha} \frac{dW_{\alpha}}{dh} \right), \quad (9)$$

where  $m_{\alpha} = \bar{m}_{\alpha} \alpha$ ,  $W_{\alpha}(\bar{h}, h^*, \bar{J})$  is the probability for the Ising spin projection  $\alpha$  at the central site of the Bethe cluster, and  $h^*$  is the effective Bethe field. The first term in Eq. (9) describes the change of the magnetization amplitude with the applied magnetic field and gives mainly the ‘itinerant’ contribution to  $\chi$ . The second term describes directional fluctuations of the local magnetizations (‘local’ contribution) and is finite only in the SRO-PM phase. Note that the ‘itinerant’ and ‘local’ properties are interrelated and determine *both* contributions to the spin susceptibility.

Fig. 2 shows our results for the doping dependence of the zero-temperature susceptibility  $\chi(\delta)$ . In the PM phase ( $\delta > \delta_{c2}$ ) the SB band-renormalized Pauli susceptibility has a pronounced doping dependence in two dimensions which is strongly affected by  $t'$ . In the SRO-PM phase ( $\delta_{c1} < \delta < \delta_{c2}$ ), the Pauli susceptibility is suppressed due to the SRO-induced spin stiffness against the orientation of the local magnetizations along the homogeneous external field. Accordingly, at  $\delta_{c2}$  a cusp in  $\chi(\delta)$  appears, where the  $U/t$  and  $t'$  dependences of the peak-position emerge from Fig. 1. Since, for  $\delta_{c1} < \delta < \delta_{c2}$ ,  $|\bar{J}|$  decreases with increasing  $\delta$ , the susceptibility increases upon doping.

In Fig. 2 we have also depicted the spin contribution to the magnetic susceptibility of LSCO at 50 K obtained from the experimental data on the total susceptibility by subtracting the diamagnetic core ( $-9.9 \times 10^{-5}$  emu/mol) and Van Vleck ( $2.4 \times 10^{-5}$  emu/mol) contributions which can be taken as independent of doping and temperature over the limited parameter region studied here [1]. The experimentally observed pronounced maximum at a hole doping of about 25% and the qualitative

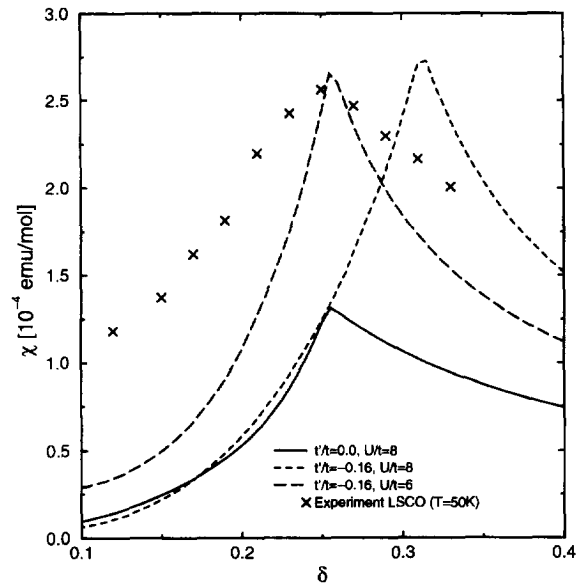


Fig. 2. Uniform static spin susceptibility at  $T = 0$  (taking the realistic value  $t = 0.3$  eV).

doping dependence of  $\chi$  are reproduced rather well by our theory without any fit procedure.

From our results we conclude that the concept of magnetic SRO in strong-correlation models may play the basic role in the explanation of many unconventional properties of high- $T_c$  compounds. As motivated by neutron scattering probing the correlation length over several lattice spacings, our theory should be extended by the description of a larger than nearest-neighbour ranged SRO.

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