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Magnetic short-range order effects in the 2D t–J model

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Abstract

We outline an improved theory of short-range magnetic order for strongly correlated itinerant electron systems, and apply it to the two-dimensional t–J model. Within a spin-rotation-invariant slave-boson functional-integral scheme, the short-range order is incorporated at the saddle-point and pair approximation levels. Comparing our numerical results for the free energy with previous approaches, we observe that long-range-ordered antiferromagnetic and spiral phases are suppressed due to the appearance of a paraphase with pronounced antiferromagnetic short-ranged correlations. In this phase, the presence of well-established local magnetizations is sufficient to describe the increase of the low-temperature susceptibility upon doping, which, e.g., is experimentally observed for the high-T_c material $La_{2-\delta}Sr_{\delta}CuO_4$. © 1998 Elsevier Science B.V. All rights reserved.

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The concept of magnetic short-range order (SRO) has been extremely successful in the modern theory of itinerant electron magnetism. Recently, the role played by SRO in explaining the unconventional magnetic normal-state properties of high-T_c superconductors was emphasized and theoretically investigated on the basis of the Hubbard model [1–3]. In particular, it has been argued that the observed strong temperature and doping dependences of the uniform spin susceptibility of $La_{2-\delta}Sr_{\delta}CuO_4$ [4] may be qualitatively understood as an effect of antiferromagnetic (AFM) SRO which decreases with increasing doping δ and temperature T.

In this paper, our main goal is to generalize the theory developed in our previous work [2, 3] in order to describe short-ranged magnetic correlations in the framework of the 2D t–J model. This requires an improved treatment of SRO preserving the SU(2) symmetry of the system. To tackle the strong Coulomb correlations and Hilbert space projections incorporated in the t–J model we use a spin-rotation-invariant slave-boson technique [5]. Then the partition function can be written as a coherent-state path integral, where the bosonized free-energy functional of the t–J model takes the form $\Psi = \Psi^{(B)} + \Psi^{(F)}$ with

$$\Psi^{(B)} = \sum_i (-\nu_i n_i + \xi_i \boldsymbol{m}_i - h m_{iz}) + \frac{J}{4}\sum_{\langle ij\rangle}(\boldsymbol{m}_i\boldsymbol{m}_j - n_i n_j), \tag{1}$$

$$\Psi^{(F)} = \frac{1}{\pi}\int d\omega\, f(\omega-\mu)\,\mathrm{Im}\,\mathrm{Tr}_{ij,\rho\rho'}\ln[-\underline{\hat{G}}_{ij}^{-1}], \tag{2}$$

$$\underline{\hat{G}}_{ij}^{-1}(\omega) = (\underline{z}_i\underline{z}_j)^{-1}[(\omega-\nu_i)\underline{1} + \xi_i\underline{\sigma}]\delta_{ij} - t_{ij}\underline{1} \tag{3}$$

(underbars denote a 2×2 matrix in spin space). Here J measures the AFM exchange interaction, t_{ij} denotes the transfer integral between nearest-neighbour (NN) sites $\langle ij\rangle$, and h is the external magnetic field. The Shiba-transformed Green's propagator $\underline{\hat{G}}_{ij}$ includes the non-linear bosonic hopping factors $\underline{z}_i$ which yield a correlation-induced band renormalization [2, 3, 5]. In Eq. (1), the original slave-boson fields are expressed in terms of local magnetizations $\boldsymbol{m}_i$, particle densities n_i, and 'internal' magnetic [charge] fields $\xi_i[\nu_i]$. We now (i) apply the static approximation to all bosonic fields, (ii) decompose the vector fields ($\boldsymbol{b} = \boldsymbol{m},\xi$) with respect to their amplitudes and directions $\boldsymbol{b}_i = \bar{b}_i \boldsymbol{s}_i$ ($|\boldsymbol{s}_i| = 1$), and (iii) make for the spatial fluctuations of the scalar fields ($b = n, \nu, \bar{m}, \bar{\xi}$) the Ansatz $b_i = b_{s_i}$.

To incorporate SRO effects, one has to go beyond the homogeneous paramagnetic (PM) saddle-point of the

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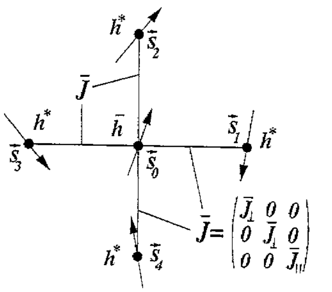

Fig. 1. Bethe cluster, where $\bar{h}$, $h^* \| h = h e_z$.

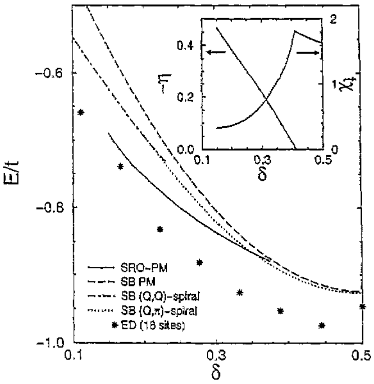

Fig. 2. Ground-state energy E, SRO parameter η and uniform static spin susceptibility χ (inset) as functions of doping obtained for the 2D t–J model with $J/t = 0.4$ at $T = 0$. The energy of the SRO–PM phase is compared with various slave-boson (SB) and exact diagonalization (ED) results.

functional Ψ. Thus, we perform an expansion of the *nonlocal* 'fermionic' part $\Psi^{(F)}$ in terms of the *local* perturbation $\underline{V}_i\delta_{ij} = -\underline{\hat{G}}_{ij}^{-1} + \underline{\hat{G}}_{ij}^{o\,-1}$, where $\hat{G}^o$ is the PM saddle-point propagator. Using spherical harmonics we are able to transform the free-energy functional to that of an *effective* classical anisotropic Heisenberg model at the NN pair-approximation level (ϑ: azimuthal angle with respect to $\boldsymbol{h}$):

$$\Psi[\{b(\vartheta)\},\{s_i\}] = \bar{\Psi} - \bar{h}\sum_i s_{iz} - \sum_{\langle ij \rangle} s_i \bar{J} s_j. \tag{4}$$

Let us emphasize that both the local field $\bar{h}$ and the Heisenberg exchange integrals $\bar{J}_{\perp,\parallel}$ are complicated functions of the slave-boson fields and have to be determined self-consistently at each J and δ. The next step is to integrate out the classical spin degrees of freedom in the partition function of the model (4). This we do by employing the standard Bethe–Peierls–Weiss approximation which introduces a Bethe field h^* determined by the condition $\langle s_{0z} \rangle = \langle s_{1z} \rangle$. The resulting functional $\Psi[\{b(\vartheta)\},h^*,\langle s_0 s_1 \rangle,\langle s_{0z} \rangle]$ may now be used to derive the saddle-point equations for the Bose fields $b(\vartheta)$, where NN SRO effects ($\propto \eta = \langle \boldsymbol{m}_0 \boldsymbol{m}_1 \rangle$) are taken into account within the Bethe cluster sketched in Fig. 1. Then the free energy per site $f(\delta,h,T) = [\Psi/N + \mu(1-\delta)]_{\mathrm{SP}}$ is calculated from the extremal functional Ψ_{SP} in the paraphases with ($\eta < 0$; SRO-PM) and without ($\eta = 0$; PM) AFM SRO.

Finally, using the solutions of the saddle-point and Bethe field equations, the uniform static spin susceptibility can be obtained from

$$\chi = \lim_{h\to 0} \int \mathrm{d}[\cos\vartheta] \frac{\mathrm{d}[W_0(\vartheta) m_{0z}(\vartheta)]}{\mathrm{d}h}, \tag{5}$$

where $W_0(\vartheta)$ is the probability that the central spin s_0 points in directions parametrized by ϑ. Our expression for χ clearly indicates the interrelation of mainly 'local' and 'itinerant' contributions given by the change of the direction ($W_0(\vartheta)$) and the amplitude ($\bar{m}_0(\vartheta)$) of the local magnetization with the applied field, respectively.

From our numerical results shown in Fig. 2 we conclude: (i) The AFM and incommensurate spiral long-range-ordered phases obtained within previous approaches make way to a paramagnetic phase with strong antiferromagnetic SRO ($\eta < 0$) in a wide doping region. [Of course, we cannot rule out that other *spin* and/or *charge* modulated structures, e.g., stripe phases, may yield lower energy than the phases studied.] (ii) The increase and maximum of the spin susceptibility of $La_{2-\delta}Sr_{\delta}CuO_4$ upon doping, which is difficult to reconcile with the standard Fermi-liquid picture, may be explained by our theory as an SRO effect of local magnetic moments in the paramagnetic phase.

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