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Magnetic short-range order versus long-range order in the Hubbard model

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A theory of magnetic short-range order in the paraphase of the one-band Hubbard model is presented on the basis of the four-field slave-boson approach. In the functional-integral scheme the bosonized action, expressed in terms of fluctuating local magnetizations and internal magnetic fields, is transformed to an effective Ising model treated in the Bethe-cluster approximation. The theory is evaluated in the saddle-point approximation including short-range-order effects in a fully self-consistent way. Comparing our results with previous approaches, the ground-state phase diagram shows the suppression of antiferromagnetic and incommensurate spiral long-range-ordered phases in the favor of a paraphase with short-range order in a wide doping region. Using realistic values of the on-site Coulomb repulsion for $La_{2-x}Sr_xCuO_4$, $U/t \simeq 8$, the critical doping concentration for the destruction of antiferromagnetism is obtained as 3–4 %, in agreement with experiments.

The unconventional magnetic properties of high-T_c superconductors in the normal state,[1] such as the pronounced antiferromagnetic (AFM) spin correlations probed by neutron scattering[2] and NMR,[3] as well as the maximum in the magnetic susceptibility of $La_{2-x}Sr_xCuO_4$ as a function of doping and temperature,[4] are ascribed to strong Coulomb correlations within the CuO_2 planes. In the slightly doped cuprates, the strong on-site correlation on the Cu sites is believed to result in a considerable AFM short-range order[5,6] (SRO) which decreases with increasing doping and temperature.

The role played by SRO in explaining the normal-state magnetic susceptibility was investigated on the basis of a slave-boson coherent potential approximation (CPA) approach to the three-band Hubbard model.[6] This theory is self-consistent only at the single-site level and does not hold at very low temperatures. Thus, an improved treatment of SRO in the paraphase of itinerant correlation models, which is valid also at $T=0$, is highly desirable. Since the essential features of magnetic correlations in the CuO_2 plane may be described by effective one-band models,[7,8] it is worthwhile to attack the problem of SRO within the two-dimensional (2D) Hubbard model. In spite of the numerous analytical approaches to the description of spin correlations in the Hubbard model, there are only a few methods designed for the investigation of SRO. For example, in previous Hubbard-Stratonovich/CPA theories, the free-energy functional can be transformed to an effective Ising model,[9,10] where the SRO is treated in the Bethe-cluster approximation.[9] At $T=0$, however, those theories reduce to the Hartree-Fock approximation in both the weak- and strong-coupling limits[11] and therefore neglect important correlations. On the other hand, in the scalar[12] and spin-rotation-invariant[13] slave-boson (SB) approaches, an appreciable part of the correlations is taken into account at the saddle point. At this level of approximation, the SB results for local observables,[14] quasiparticle band renormalization,[15] and ground-state energy[16] of various magnetically ordered phases agree surprisingly well with exact diagonalization[16] and quantum Monte Carlo (QMC) (Ref. 17) data. However, as yet all previous SB theories do not take into consideration SRO effects.

In this paper we present a theory of magnetic SRO based on the scalar four-field SB approach[12] to the one-band Hubbard model. The basis feature of our theory is the self-consistent inclusion of SRO in the saddle-point solution. Therefore, we expect to obtain qualitatively new results concerning the stability of magnetic long-range order (LRO) versus SRO, the problem of phase separation, and the doping dependence of the spin susceptibility. Here, we focus on the description of SRO in the paraphase at $T=0$ as a function of doping and on the magnetic phase diagram.

We start from the Kotliar-Ruckenstein SB representation of the Hubbard model[12]

$$\mathscr{H}=\sum_{ij\sigma} t_{ij} z_{i\sigma}^{\dagger} f_{i\sigma}^{\dagger} f_{j\sigma} z_{j\sigma} + U \sum_i d_i^{\dagger} d_i . \tag{1}$$

In the functional-integral representation of the partition function, the constraints $e_i^{\dagger}e_i + d_i^{\dagger}d_i + \Sigma_{\sigma} p_{i\sigma}^{\dagger} p_{i\sigma} = 1$ and $f_{i\sigma}^{\dagger} f_{i\sigma} = p_{i\sigma}^{\dagger} p_{i\sigma} + d_i^{\dagger} d_i$ are enforced by the Lagrange multipliers $\lambda_i^{(1)}$ and $\lambda_{i\sigma}^{(2)}$, respectively. Integrating out the pseudofermionic fields ($f_{i\sigma}$) and using the radial gauge and the static approximation for the Bose fields [$p_{i\sigma}$, d_i, and $\lambda_{i\sigma}^{(2)}$, where the e_i fields are eliminated by the saddle-point approximation for $\lambda_i^{(1)}$ (Ref. 11)], we get

$$\mathscr{Z}=\int [\mathscr{D}d][\mathscr{D}d^*][\mathscr{D}n][\mathscr{D}\nu][\mathscr{D}m][\mathscr{D}\xi] \times \exp\{-\beta\Psi(\{d,d^*,n,\nu,m,\xi\})\}, \tag{2}$$

$$\Psi=\sum_i (U d_i^* d_i - n_i \nu_i + m_i \xi_i) + \frac{1}{\pi}\int d\omega f(\omega-\mu) \mathrm{Im}\ \mathrm{Tr}\ \ln[-\hat{G}_{ij\sigma}^{-1}(\omega)], \tag{3}$$

$$\hat{G}^{-1}_{ij\sigma}=(z^0)^2\left[\frac{\omega-\nu_i+\sigma\xi_i}{|z_{i\sigma}|^2}\delta_{ij}-t_{ij}\right], \tag{4}$$

where

$$m_i=\sum_\sigma \sigma p^2_{i\sigma}, \quad \xi_i=-\tfrac{1}{2}\sum_\sigma \sigma\lambda^{(2)}_{i\sigma}, \tag{5}$$

$$n_i=\sum_\sigma p^2_{i\sigma}+2d^*_i d_i, \quad \nu_i=\tfrac{1}{2}\sum_\sigma \lambda^{(2)}_{i\sigma}. \tag{6}$$

Here, m_i (n_i) is the bosonic representation of the local magnetization (particle number) defined analogously to its fermionic counterpart. Since ξ_i couples to m_i as a magnetic field, we denote ξ_i by "internal magnetic field." The inverse propagator (4) is introduced by the modified Shiba transformation[18] of $G^{-1}_{ij\sigma}(\omega)=[\omega-\nu_i+\sigma\xi_i]\delta_{ij}-z^*_{i\sigma}z_{j\sigma}t_{ij}$, which is exact under the trace and removes the nondiagonal randomness in the transfer term. Note that $z_{i\sigma}$ is a function of the fields n_i, m_i, and d_i; z^0 denotes the uniform paramagnetic (PM) saddle-point value.

To incorporate the SRO, one has to go beyond the PM saddle point. To this end, we perform an expansion in terms of the perturbation $V_{i\sigma}\delta_{ij}=-\hat{G}^{-1}_{ij\sigma}+G^{0-1}_{ij\sigma}$, where $G^0_{ij\sigma}$ is the PM saddle-point propagator. We describe the fluctuations of the local magnetizations m_i and the internal magnetic fields ξ_i by the ansatz $m_i=\bar{m}s_i$ and $\xi_i=\bar{\xi}s_i$ ($s_i=\pm$) and assume $n_i=n$, $\nu_i=\nu$, and $d_i=d^*_i=d$. Then we transform the free-energy functional Ψ to an effective Ising model along the lines indicated by Kakehashi.[9] In the nearest-neighbor pair approximation, Ψ takes the form

$$\Psi(\{s_i\})=\bar{\Psi}-\bar{J}\sum_{\langle ij\rangle} s_i s_j, \tag{7}$$

where

$$\bar{\Psi}=-\frac{2}{\beta}\sum_{\mathbf{k}} \ln[1+\exp\{-\beta[(z^0)^2\varepsilon_{\mathbf{k}}+\nu^0-\mu]\}]$$
$$+N\left[Ud^2-n\nu+\bar{m}\bar{\xi}+\sum_\eta (\Phi_\eta+\Phi_{\eta\eta}+\Phi_{-\eta\eta})\right], \tag{8}$$

$$\bar{J}=-\tfrac{1}{2}\sum_\eta (\Phi_{\eta\eta}-\Phi_{-\eta\eta}). \tag{9}$$

In (8), the single-site fluctuation contribution is given by

$$\Phi_\eta=\int d\omega f(\omega-\mu)\frac{1}{\pi}\text{Im}\ \ln[1-G^0V_\eta], \tag{10}$$

with $\eta_i=\sigma s_i=\pm$. The two-site contributions

$$\Phi_{\eta\eta'}=\int d\omega f(\omega-\mu)\frac{1}{\pi}\text{Im}\ \ln[1-G^{0'}T_\eta G^{0'}T_{\eta'}] \tag{11}$$

couple fluctuations between nearest-neighbor pairs and are responsible for SRO effects. Here, $T_\eta=V_\eta(1-G^0V_\eta)^{-1}$ is the scattering matrix, and G^0 ($G^{0'}$) denotes the diagonal (off-diagonal) components of G^0_{ij}. Let us emphasize that the effective Ising-exchange integral $\bar{J}$ is a complicated function of all SB fields and has to be determined self-consistently at each interaction strength U and hole doping $\delta=1-n$. Performing the s_i sum in the partition function with the functional (7) we treat the SRO in the Bethe-cluster approximation, i.e., only nearest-neighbor correlations are taken into account. Only just now, we adopt the saddle-point approximation for all Bose fields ($\bar{m},\bar{\xi},n,\nu,d$). Then we obtain the free-energy functional,

$$f=\frac{\bar{\Psi}}{N}-\frac{1}{2\beta}\{4\ \ln[\cosh(\beta\bar{J})]-(\delta_{\bar{J},0}-1)\ln 2\}+\mu n, \tag{12}$$

which has to be minimized with respect to the Bose fields, yielding a coupled system of self-consistency equations. Correspondingly, our theory incorporates SRO at the saddle point in a fully self-consistent way at the pair approximation level. For vanishing local magnetization, $\bar{m}=0$, we have $V_\eta=0$ and [by (9) and (11)] $\bar{J}=0$ so that there is no SRO, and the PM saddle point[12] is recovered. Accordingly, we have two possible paraphases defined by

$$\text{PM:}\ \langle s_i\rangle=0,\ \langle s_is_j\rangle=0;\ \bar{m}=0\ (\bar{J}=0),$$

$$\text{SRO-PM:}\ \langle s_i\rangle=0,\ \langle s_is_j\rangle\neq 0;\ \bar{m}>0\ (\bar{J}\neq 0), \tag{13}$$

where i and j are nearest-neighbor sites. At $T=0$, the paraphase with antiferromagnetic (ferromagnetic) SRO has to be distinguished from the corresponding LRO phases, which are denoted by AFM (FM): $\langle s_i\rangle=-\langle s_j\rangle=1$, $\langle s_is_j\rangle=-1$, $\bar{J}<0$ ($\langle s_i\rangle=\langle s_j\rangle=1$, $\langle s_is_j\rangle=1$, $\bar{J}>0$). In the AFM phase there is a *finite* sublattice magnetization ($m_A=p^2_{A\uparrow}-p^2_{A\downarrow}=-m_B$) obtained from the A-B saddle-point solution.[14,15] Of course, the local-magnetization amplitude $\bar{m}$ of the SRO-PM phase differs from m_A; in particular, we found $\bar{m}\neq 0$ in parameter regions, where $m_A=0$ (see below, Fig. 2). Let us further stress that the characteristics of $\bar{J}$ have to be contrasted from the effective Ising-exchange energy $\bar{J}$ occurring in previous Hubbard-Stratonovich/CPA approaches,[9,10] where $\bar{J}$ couples thermally induced local moments and is finite also in the paraphase without SRO.

In Fig. 1 the ground-state energies of various phases are plotted as functions of δ at $U/t=8$, where the 2D tight-binding unperturbed density of states is used. For comparison, we have also depicted the results obtained by the spin-rotation-invariant SB saddle-point solution for incommensurate spiral LRO states[13] and by exact diagonalizations on a 4×4 lattice.[16] Most notably, in the doping region $0.045\lesssim\delta\lesssim 0.21$ the ground-state energy of the SRO-PM phase is lower than that of the spiral phases and, moreover, lies very close to the exact data. At very small and higher dopings, where the (1,1) and $(1,\pi)$ spirals become the ground state, respectively, our PM-SRO solution behaves less favorably. We suggest that the inclusion of spiral SRO within a spin-rotation-invariant SB theory may further improve the results in both doping regions.

Next, let us discuss the stability of the PM, SRO-PM, and AFM phases in more detail. As shown in Fig. 1, for $U/t=8$ we obtain an AFM$\rightleftharpoons$SRO-PM phase transition of first order at the critical hole doping $\delta_{c_1}\simeq 0.04$ and a SRO-PM$\rightleftharpoons$PM

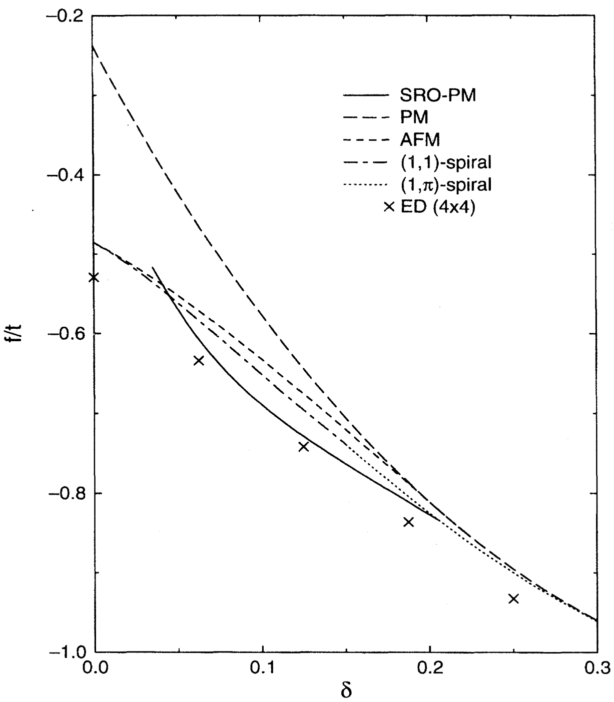

FIG. 1. Ground-state energies of the 2D Hubbard model as functions of doping at $U/t=8$. The energy of the SRO-PM phase is compared with SB (Ref. 13) and exact diagonalization (ED) (Ref. 16) results.

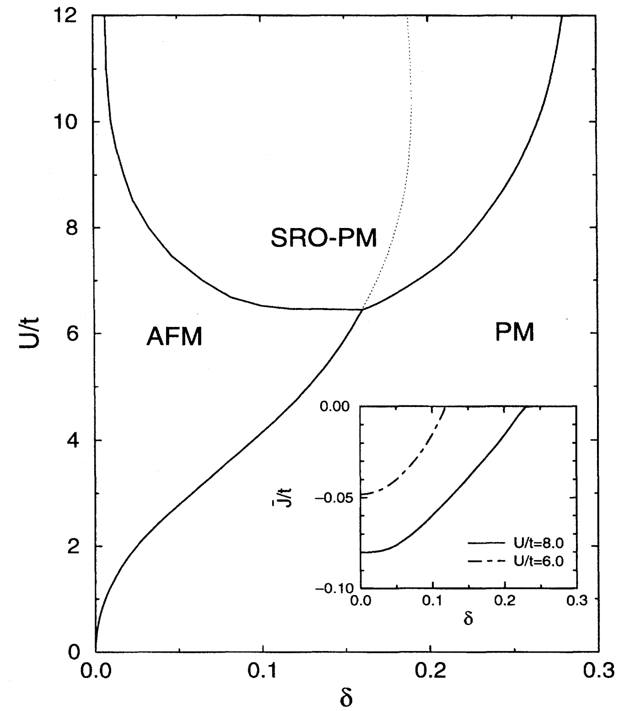

FIG. 2. Ground-state phase diagram of the Hubbard model, where AFM, PM, and SRO-PM denote the antiferromagnetic LRO phase, the paraphase without SRO, and the paraphase with SRO, respectively. The dotted line marks the well-known AFM⇌PM transition (Refs. 2,14,22) which is suppressed by the SRO-PM phase. The effective antiferromagnetic exchange interaction ($\bar{J}<0$) is shown in the inset.

transition of second order at $\delta_{c_2}\simeq 0.26$. We would like to point out that in the SRO-PM phase the energy is a convex function of the particle density, so that this phase is locally stable against phase separation. There is much controversy about the problem of phase separation in the Hubbard model, as well as in cuprate superconductors.[19–21] Whereas exact diagonalization[16] (see Fig. 1) and QMC studies[17] do not yield evidence of phase separation, in mean-field-like theories[13,22,23] the lowest-energy state has a negative compressibility over a wide doping region ($\delta\lesssim 0.15$; see also Fig. 1). In contrast, our SRO-PM state has a positive compressibility also at very low dopings ($\delta>\delta_{c_1}\simeq 0.04$). For $\delta\lesssim\delta_{c_1}$, both the AFM and (1,1) spiral phases are locally unstable. Correspondingly, the existence of phase separation for $\delta\rightarrow 0$ remains an open problem. However, from our results we argue that an extended SRO theory which, e.g., includes a longer than nearest-neighbor ranged SRO may yield a convex energy for all δ.

Having established the quality of our method, in Fig. 2 the ground-state phase diagram is mapped out, where for numerical simplification we have used a semielliptic unperturbed density of states. Note that for $U/t=8$, the critical dopings at the phase transitions, $\delta_{c_1}\simeq 0.03$ and $\delta_{c_2}\simeq 0.23$, nearly coincide with those given above. At large enough U/t ratios, the LRO is strongly suppressed in favor of SRO. For values of U/t being realistic for high-T_c cuprates [$U/t\simeq 8$ (Ref. 8)], the AFM phase is destroyed at the critical hole doping $\delta_{c_1}\simeq 0.03$, which agrees with the experimentally observed value in $La_{2-x}Sr_xCuO_4$. Thus, the rapid disappearance of antiferromagnetism in high-T_c cuprates at very low hole dopings may be related to the persistence of a pronounced SRO in the paraphase. Obviously, the stability region of the SRO-PM phase at $U/t\simeq 8$, $0.03\lesssim\delta\lesssim 0.23$, nearly coincides with the doping regime of $La_{2-x}Sr_xCuO_4$ compounds, where, above T_c, the so-called "strange metal" phase occurs. Correspondingly, the unconventional normal-state behavior of high-T_c cuprates may be due to the presence of a considerable degree of SRO. The effective Ising-exchange integral $\bar{J}(\delta,U)$, shown in the inset of Fig. 2, is intimately related to the existence of SRO and reflects the interplay of local and itinerant magnetic behavior. With decreasing magnetic correlations, i.e., with increasing δ and decreasing U/t, $|\bar{J}|$ decreases, as expected.

To conclude, the main result of our theory concerning the ground-state properties of the Hubbard model is that the magnetic LRO phases make way to a paraphase with SRO in a wide doping region. This SRO-PM phase is locally stable against phase separation. Besides the advantage of our method to treat the SRO at $T=0$ (contrary to CPA-based schemes[6,9,24]), the self-consistent incorporation of SRO at the saddle point gives a conceptually clear starting point for the consideration of Gaussian fluctuations around the saddle point with SRO. Although those results are interesting in themselves, we emphasize that the concept of SRO in strong-correlation models may give a clue to a better understanding of the unconventional normal-state properties of high-T_c compounds. In particular, the SRO effects on the uniform static susceptibility have to be explored, where a maximum in the doping dependence, as observed in $La_{2-x}Sr_xCuO_4$, is expected. This will be left for further study.

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