Spin susceptibility and magnetic short-range order in the Hubbard model

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The uniform static spin susceptibility in the paraphase of the one-band Hubbard model is calculated within a theory of magnetic short-range order (SRO) which extends the four-field slave-boson functional-integral approach by the transformation to an effective Ising model and the self-consistent incorporation of SRO at the saddle point. This theory describes a transition from the paraphase without SRO for hole dopings $\delta > \delta_{c_2}$ to a paraphase with antiferromagnetic SRO for $\delta_{c_1} < \delta < \delta_{c_2}$. In this region the susceptibility consists of interrelated ''itinerant'' and ''local'' parts and increases upon doping. The zero-temperature susceptibility exhibits a cusp at δ_{c_2} and reduces to the usual slave-boson result for larger dopings. Using the realistic value of the on-site Coulomb repulsion $U=8t$ for $La_{2-\delta}Sr_\delta CuO_4$, the peak position ($\delta_{c_2}=0.26$) as well as the doping dependence reasonably agree with low-temperature susceptibility experiments showing a maximum at a hole doping of about 25%. [S0163-1829(96)05535-X]

Among the most striking features of high-T_c superconductors in the normal state, the unconventional magnetic properties have attracted increasing attention.[1] As revealed by neutron scattering[2] and nuclear magnetic resonance[3] experiments, in the metallic state there exist pronounced antiferromagnetic (AFM) spin correlations which are ascribed to strong Coulomb correlations within the CuO_2 planes. Knight-shift[4] and bulk measurements[4–6] of the spin susceptibility $\chi(T,\delta)$ in $La_{2-\delta}Sr_\delta CuO_4$ show a maximum in the doping dependence as well as, for moderate hole doping ($\delta \leqslant 0.21$), in the temperature dependence, where the temperature of the maximum decreases with increasing doping. Such a behavior, also observed in $YBa_2Cu_3O_{6+y}$ ($y \leqslant 0.92$),[7,8] may be qualitatively understood as an effect of AFM short-range order (SRO) which decreases with increasing doping and temperature.

Up to now there have been only a few attempts, based on one-band[9–12] and three-band[13] correlation models, to describe the unusual doping and temperature dependence of the normal-state susceptibility. In the t-t'-J model, a maximum in χ was obtained for the Pauli susceptibility of a strongly renormalized quasiparticle band[9] or for the random-phase approximation (RPA) slave-boson susceptibility[10] showing a cusp in the temperature dependence at the transition to the singlet resonating valence bond state. In the one-band Hubbard model, a maximum in the doping dependence of χ was found by a semiphenomenological weak-coupling approach[11] or by the composite operator method.[12] The role played by SRO in explaining the normal-state susceptibility was investigated on the basis of the three-band Hubbard model[13] by means of a slave-boson coherent potential approximation theory which, however, is self-consistent only at the single-site level and does not hold at very low temperatures. To improve the treatment of SRO in the paraphase being valid also at $T=0$, in a previous paper,[14] hereafter referred to as I, we have presented the main features of a theory of magnetic SRO in the one-band Hubbard model based on the scalar four-field slave-boson (SB) approach.[15] In I we have focused on the stability of magnetic long-range order (LRO) versus SRO, where magnetic LRO phases are found to make way to a paraphase with SRO in a wide doping region.

In this paper we extend our theory by the inclusion of an external magnetic field h and by the calculation of the uniform static spin susceptibility χ in the paraphase, where special care is taken to the influence of SRO.

Following the lines indicated in I, the action of the SB functional integral for the partition function of the two-dimensional (2D) Hubbard model is expressed in terms of the SB fields m_i, ξ_i, n_i, ν_i, d_i, and d_i^*.[16] To treat the fluctuations of the local magnetizations m_i and the internal magnetic fields ξ_i we write $m_i=\overline{m}_i s_i$, $\xi_i=\overline{\xi}_i s_i$ ($s_i=\pm$) and make the ansatz $b_i \rightarrow b_{s_i}$ for the magnetic amplitudes $b \in \{\overline{m},\overline{\xi}\}$ and the charge degrees of freedom $b \in \{n,\nu,d=d^*\}$. We transform the free-energy functional Ψ to an effective Ising model in the nearest-neighbor pair ($\langle ij\rangle$) approximation and obtain

$$\Psi(\{s_i\})=\overline{\Psi}-\overline{h}\sum_i s_i-\overline{J}\sum_{\langle ij\rangle} s_i s_j , \tag{1}$$

with

$$\begin{aligned}\overline{\Psi}=&-\frac{1}{\beta}\sum_{\mathbf{k}\sigma} \ln[1+\exp\{-\beta[(z_\sigma^o)^2\overline{\epsilon_{\mathbf{k}}}+\nu^o \\ &-\sigma(\xi^o+h)-\mu]\}]+\frac{N}{2}\sum_{\alpha=\pm 1}\Big\{Ud_\alpha^2-n_\alpha\nu_\alpha \\ &+\overline{m}_\alpha\overline{\xi}_\alpha+\sum_\sigma (\Phi_{\alpha\sigma}+\Phi_{\alpha\alpha\sigma}+\Phi_{-\alpha\alpha\sigma})\Big\},\end{aligned} \tag{2}$$

$$\overline{h}=-\frac{1}{2}\sum_{\alpha}\alpha\left[Ud_{\alpha}^{2}-n_{\alpha}\nu_{\alpha}+\overline{m}_{\alpha}\overline{\xi}_{\alpha}+\sum_{\sigma}(\Phi_{\alpha\sigma}+2\Phi_{\alpha\alpha\sigma})\right],\tag{3}$$

$$\overline{J}=-\frac{1}{4}\sum_{\alpha\sigma}(\Phi_{\alpha\alpha\sigma}-\Phi_{-\alpha\alpha\sigma}).\tag{4}$$

The single-site and two-site fluctuation contributions

$$\Phi_{\alpha\sigma}=\Phi_{i\sigma}(\alpha_i)|_{\alpha_i=\alpha}$$

and

$$\Phi_{\alpha\alpha'\sigma}=\Phi_{\langle i\sigma\rangle\sigma}(\alpha_i,\alpha_j)|_{\substack{\alpha_i=\alpha\\ \alpha_j=\alpha'}},$$

respectively, are given by

$$\Phi_{i\sigma}=\frac{1}{\pi}\int d\omega\, f(\omega-\mu)\mathrm{Im}\ln[1-G^{o}_{ii\sigma}V_{i\sigma}(\alpha_i)],\tag{5}$$

$$\Phi_{\langle ij\rangle\sigma}=\frac{1}{\pi}\int d\omega\, f(\omega-\mu)\mathrm{Im}\times\ln[1-G^{o}_{\langle ij\rangle\sigma}T_{j\sigma}(\alpha_j)G^{o}_{\langle ji\rangle\sigma}T_{i\sigma}(\alpha_i)].\tag{6}$$

In (6), $G^{o}_{ij\sigma}(\omega)$ is the uniform paramagnetic (PM) Green propagator, and the scattering matrix $T_{i\sigma}=V_{i\sigma}(1-G^{o}_{ii\sigma}V_{i\sigma})^{-1}$ is expressed in terms of the local perturbation

$$V_{i\sigma}(\alpha_i,\omega)=\frac{1}{(z_{\alpha_i\sigma})^2}\{[(z_{\alpha_i\sigma})^2-(z^{o}_{\sigma})^2][\omega-\nu^{o}+\sigma(\xi^{o}+h)]+(z^{o}_{\sigma})^2[\nu_{\alpha_i}-\nu^{o}-\sigma(\alpha_i\overline{\xi}_{\alpha_i}-\xi^{o})]\},\tag{7}$$

where

$$z_{\alpha_i\sigma}=\left[\frac{2d^2_{\alpha_i}(n_{\alpha_i}-\sigma\alpha_i\overline{m}_{\alpha_i}-2d^2_{\alpha_i})}{(n_{\alpha_i}+\sigma\alpha_i\overline{m}_{\alpha_i})(2-n_{\alpha_i}-\sigma\alpha_i\overline{m}_{\alpha_i})}\right]^{1/2}+\left[\frac{2(n_{\alpha_i}+\sigma\alpha_i\overline{m}_{\alpha_i}-2d^2_{\alpha_i})(1-n_{\alpha_i}+d^2_{\alpha_i})}{(n_{\alpha_i}+\sigma\alpha_i\overline{m}_{\alpha_i})(2-n_{\alpha_i}-\sigma\alpha_i\overline{m}_{\alpha_i})}\right]^{1/2}\tag{8}$$

and the superscript o refers to PM saddle-point values. By the functional (1) we determine the saddle point for all Bose fields $b_{\alpha}=\{\overline{m}_{\alpha},\xi_{\alpha},n_{\alpha},\nu_{\alpha},d_{\alpha}\}$ in the external field h, where, in the spirit of I, the SRO is self-consistently incorporated within the Bethe cluster approximation (taking into account only the nearest-neighbor SRO). As found in I, in the $h=0$ limit ($\overline{m}_{\alpha}=\overline{m}$) the self-consistent calculation of the effective Ising-exchange integral J as function of the interaction strength U and the hole doping $\delta=1-n$ yields two possible paraphases ($\langle s_i\rangle=0$): (i) the paraphase without SRO (PM; $J=0$, $\overline{m}=0$) and (ii) the paraphase with antiferromagnetic SRO (SRO-PM; $J<0$, $\overline{m}>0$).

The uniform static spin susceptibility $\chi(T,\delta)$ has to be calculated according to

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

where $m_{\alpha}=\overline{m}_{\alpha}\alpha$, $W_{\alpha}=W_{\alpha}(\overline{h},h^*,\overline{J})$ is the probability for the Ising spin projection α 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 χ. The second term describes directional fluctuations of the local magnetizations and is called the ''local'' contribution being finite only in the SRO-PM phase. Note that the itinerant and local properties are interrelated and determine *both* contributions to the spin susceptibility. In the PM and SRO-PM phases we have calculated the doping dependence of the zero-temperature susceptibility in the 2D Hubbard model (being finite in contrast to the theory of Ref. 13) in a completely self-consistent way, where in the tedious numerical evaluation of the integrals (5) and (6) and of their derivatives particular attention has to be paid to the analytical behavior of the complex logarithm.

Figure 1 shows our result without any fit procedure using the commonly accepted value $U/t=8$ for the Hubbard model applied to high-T_c cuprates.[17] As stated in I, in the region $6<U/t<12$, there occurs a first-order (1,1)-spiral$\rightleftharpoons$SRO-PM transition at δ_{c_1} and a SRO-PM$\rightleftharpoons$PM transition of second order at δ_{c_2}. In the PM phase ($\delta>\delta_{c_2}$) the SB band-renormalized Pauli susceptibility has a pronounced doping dependence in two dimensions and agrees with the static and uniform limit of the dynamic spin susceptibility derived, within the spin-rotation-invariant SB scheme,[18] from the Gaussian fluctuation matrix at the PM saddle point.[19] In the SRO-PM phase ($\delta_{c_1}<\delta<\delta_{c_2}$), 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 δ_{c_2} a cusp in $\chi(0,\delta)$ appears. Since, for $\delta_{c_1}<\delta<\delta_{c_2}$, $|\overline{J}|$ decreases with increasing δ,[14] the susceptibility increases upon doping.

The peak in $\chi(0,\delta)$ only appears at sufficiently high ratios $U/t>6$, for which a SRO-PM$\rightleftharpoons$PM transition may occur. According to the phase diagram, given in Fig. 2 of I, in the region $6<U/t<12$ the SRO-PM$\rightleftharpoons$PM transition shifts to higher doping values with increasing U/t. Correspondingly, the peak position in $\chi(0,\delta)$ reveals the same U/t dependence.

In Fig. 1 we have also depicted the spin contribution to the magnetic susceptibility of $La_{2-\delta}Sr_{\delta}CuO_4$ at 50 K ob-

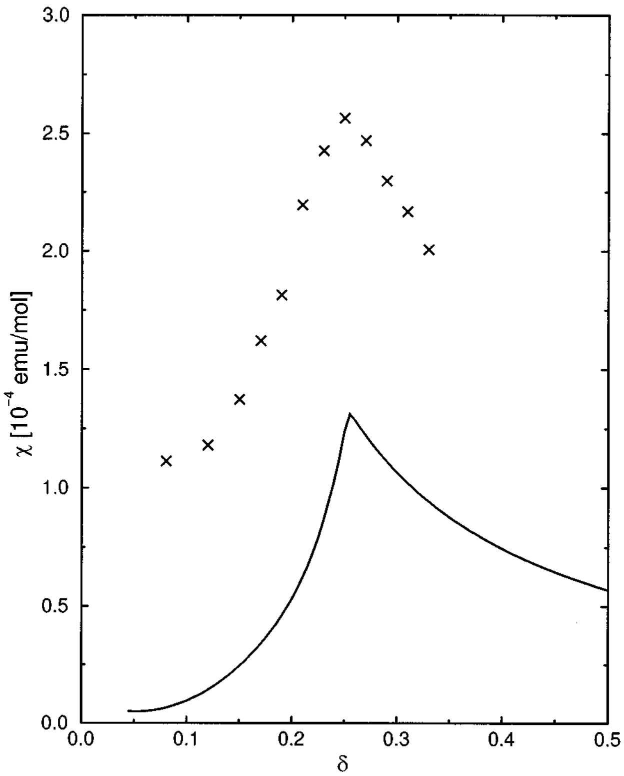

FIG. 1. Uniform static spin susceptibility as a function of doping at $T=0$. The theoretical result obtained for the 2D Hubbard model at $U/t=8$ and $t=0.3$ eV (solid) is compared with the spin contribution ($\times$) to the (corrected) experimental susceptibility on $La_{2-\delta}Sr_{\delta}CuO_4$ at $T=50$ K (Refs. 5 and 6).

tained from the experimental data on the total susceptibility[5] by subtracting the diamagnetic core (-9.9×10^{-5} emu/mol) and Van Vleck (2.4×10^{-5} emu/mol) contributions which, according to Ref. 6, can be taken as independent of doping and temperature over the limited parameter region studied here. As Fig. 1 shows, the experimentally observed pronounced maximum at a hole doping of about 25% is reproduced very well by our theory yielding the peak position at $\delta_{c_2}=0.26$ ($U/t=8$). Moreover, the qualitative doping dependence of χ reasonably agrees with experiments. Of course, it could not be expected that our approach based on the simple (single-band) Hubbard model yields the correct magnitude of χ for $La_{2-\delta}Sr_{\delta}CuO_4$. Especially, concerning the low-doping limit $\delta\rightarrow\delta_{c_1}=0.04$, the theoretical susceptibility is much too low as compared with experiments. This deficiency may be explained as follows. For $\delta=0$ and large U/t values, the Hubbard model is equivalent to the Heisenberg antiferromagnet with the exchange interaction $J=4t^2/U$. In this model, the spin susceptibility at $T=0$ has a finite value proportional to J^{-1} (Ref. 20) which is due to the existence of transverse spin fluctuations. However, our *scalar* four-field SB approach to the spin susceptibility in the presence of SRO implies the transformation of the free-energy functional to an effective Ising model describing longitudinal fluctuations only. Since the local contribution to χ is of Ising-type, we get a too small susceptibility in the low-doping limit which, however, is finite due to the interrelation to the itinerant contribution to χ. Therefore, we suggest that a theory of SRO based on the spin-rotation-invariant SB scheme[18] and resulting in an effective Heisenberg-model functional may improve the results on the magnitude of χ, in particular at low doping levels.

Finally, we notice that the increase of the susceptibility upon doping obtained within our theory for moderate Coulomb repulsions ($U/t>6$) is in qualitative accord with recent quantum Monte Carlo data[21] and with the approaches of Refs. 11 and 12. However, in those works a maximum in the spin susceptibility was found even at a smaller coupling ($U/t=4$).

From our results we conclude that the concept of magnetic SRO in strong-correlation models may play the key role in the explanation of many unconventional properties of high-T_c compounds. The theory may be extended in several directions. As discussed above, a spin-rotation-invariant theory of SRO may improve the agreement of the spin susceptibility with experiments. Furthermore, as motivated by neutron scattering experiments[2] probing the AFM correlation length over several lattice spacings, the effects of a longer than nearest-neighbor ranged SRO (which may be described beyond the nearest-neighbor pair approximation) should be investigated.

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