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 $\delta > \delta_2$ to a paraphase with antiferromagnetic SRO for $\delta_1 < \delta < \delta_2$. In this region the susceptibility consists of interrelated ‘itinerant’ and ‘local’ parts and increases upon doping. The zero–temperature susceptibility exhibits a cusp at $\delta_2$ 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$_{2–x}$Sr$_x$CuO$_4$, the peak position ($\delta_2 = 0.26$) as well as the doping dependence reasonably agree with low–temperature susceptibility experiments showing a maximum at a hole doping of about 25%.

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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 models, to describe the unusual doping and temperature dependence of the normal–state susceptibility. In the t–t’–J model as an effect of AFM short–range order (SRO) which decreases with increasing doping and temperature.

In this Brief Report we extend our theory by the inclusion of an external magnetic field $h$ and by the calculation of the uniform static spin susceptibility $\chi$ 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 2D Hubbard model is expressed in terms of the SB fields $m_i, \xi_i, n_i, \nu_i, d_i$ and $d_\ast$ [16]. To treat the fluctuations of the local magnetizations $m_i$ and the internal magnetic fields $\xi_i$ we write $m_i = \bar{m}_i \xi_i$, $\xi_i = \xi_i s_i$ ($s_i = \pm 1$) and make the ansatz $b_i \to \bar{b}_i$ for the magnetic amplitudes $b \in \{\bar{m}, \xi\}$ and the charge degrees of freedom $b \in \{n, \nu, d = d_\ast\}$. We transform the free–energy functional $\Psi$ to an effective Ising model in the nearest–neighbour pair ($\langle ij \rangle$) approximation and obtain

$$\Psi(\{s_i\}) = \Psi - \bar{h} \sum_i s_i - \bar{J} \sum_{\langle ij \rangle} s_is_j,$$

(1)
with
\[ \bar{\psi} = -\frac{i}{\beta} \sum_{\sigma} \ln \left[ 1 + \exp \left\{ \beta \left( \frac{1}{2} \left[ z_{\sigma}^2 \xi_k^2 + \nu^o - \sigma (\xi^o + h) - \mu \right] \right) \right\} \right] \]
\[ + \frac{N}{2} \sum_{\alpha = \pm 1} \left\{ U d_{\alpha}^2 - n_{\alpha} \nu_{\alpha} + \bar{m}_{\alpha} \xi_{\alpha} + \sum_{\sigma} (\Phi_{\alpha \sigma} + \Phi_{\alpha \sigma} + \Phi_{-\alpha \sigma}) \right\} , \] \[ \bar{h} = -\frac{i}{\beta} \sum_{\alpha} \left[ U d_{\alpha}^2 - n_{\alpha} \nu_{\alpha} + \bar{m}_{\alpha} \xi_{\alpha} + \sum_{\sigma} (\Phi_{\alpha \sigma} + 2\Phi_{\alpha \sigma}) \right] , \] \[ \bar{J} = -\frac{i}{2} \sum_{\alpha \sigma} (\Phi_{\alpha \sigma} - \Phi_{-\alpha \sigma}) . \] (2)

The single–site and two–site fluctuation contributions \( \Phi_{\alpha \sigma} = \Phi_{\alpha i}(\alpha_i)|_{\alpha_i = \alpha} \) and \( \Phi_{\alpha \sigma} = \Phi_{\alpha i}(\alpha_i, \alpha_j)|_{\alpha_j = \alpha} \), respectively, are given by
\[ \Phi_{\alpha i} = \frac{1}{\beta} \int d\omega f(\omega - \mu) \Im \ln |1 - G_{\alpha i}^o(\omega)| , \] \[ \Phi_{\alpha i}(\alpha_j) = \frac{1}{\beta} \int d\omega f(\omega - \mu) \Im \ln \left[ 1 - G_{\alpha j}^o(\omega) G_{\alpha i}^o(\omega) T_{\alpha j}(\alpha_j) \right] . \] (5)

In (4), \( G_{\alpha i}(\omega) \) is the uniform paramagnetic (PM) Green propagator, and the scattering matrix \( T_{\alpha j}(\alpha_j) = V_{\alpha j} (1 - G_{\alpha i}^o V_{\alpha j})^{-1} \) is expressed in terms of the local perturbation
\[ V_{\alpha i}(\alpha, \omega) = \frac{1}{\omega - \mu^o + \sigma (\xi^o + h)} \left( \frac{z_{\alpha \sigma}^o}{(z_{\sigma}^o)^2} - \frac{(z_{\sigma}^o)^2}{[\omega - \nu^o + \sigma (\xi^o + h)]} \right) \] \[ + \frac{\rho(\alpha, h) \mu^o}{(z_{\sigma}^o)^2} \left( \frac{1}{\omega - \mu^o + \sigma (\xi^o + h)} + \frac{1}{\omega - \nu^o - \sigma (\xi^o - \xi^o)} \right) \]
\[ \bar{\xi} = \frac{\sqrt{2}}{\sqrt{(n_{\alpha} + \sigma \alpha n_{\alpha} + 2d_{\alpha}) (1 - n_{\alpha} + d_{\alpha}) + d_{\alpha} \sqrt{n_{\alpha} - \sigma \alpha n_{\alpha} - 2d_{\alpha}}} \] \[ \sqrt{(n_{\alpha} + \sigma \alpha n_{\alpha}) (2 - n_{\alpha} - \sigma \alpha m_{\alpha})} \] \[ \sqrt{(n_{\alpha} + \sigma \alpha m_{\alpha}) (2 - n_{\alpha} - \sigma \alpha m_{\alpha})} \] \[ \end{document} \]
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$_{2-x}$Sr$_x$CuO$_4$ at $T = 50$ K [5,6].

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 [7]. As stated in I, in the region $6 < U/t < 12$, there occurs a first-order (1,1)-spiral$\Rightarrow$SRO–PM transition at $\delta_c^1$ and a SRO–PM$\Rightarrow$PM transition of second order at $\delta_c^2$. 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 $\delta_c^2$ a cusp in $\chi(0, \delta)$ appears. Since, for $\delta_c^1 < \delta < \delta_c^2$, $|J|$ decreases with increasing $\delta$ [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$\Rightarrow$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$\Rightarrow$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$_{2-x}$Sr$_x$CuO$_4$ at 50 K.
obtained from the experimental data on the total susceptibility 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. 18, can be taken to be 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 δc2 = 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 La2−xSrxCuO4. Especially, concerning the low–doping limit δ → δc1 = 0.04, the theoretical susceptibility is much too low as compared with experiments. This deficiency may be explained as follows. For δ = 0 and large U/t values, the Hubbard model is equivalent to the Heisenberg antiferromagnet with the exchange interaction J = 4t2/U. In this model, the spin susceptibility at T = 0 has a finite value proportional to J−2/2 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 and resulting in an effective Heisenberg–model functional may improve the results in 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 QMC data 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–Tc 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 probing the AFM correlation length over several lattice spacings, the effects of a longer than nearest–neighbour ranged SRO (which may be described beyond the nearest–neighbour pair approximation) should be investigated.

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