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

by

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Abstract

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 \( \delta > \delta_c \) to a paraphase with antiferromagnetic SRO for \( \delta_c < \delta < \delta_{c2} \). In this region the susceptibility consists of interrelated ‘itinerant’ and ‘local’ parts and increases upon doping. The zero–temperature susceptibility exhibits a cusp at \( \delta_{c2} \) and reduces to the usual slave–boson result for larger dopings. Using the realistic value of the on–site Coulomb repulsion \( U = 8t \) for \( \text{La}_2-\delta \text{Sr}_\delta \text{CuO}_4 \), the peak position \( \delta_{c2} = 0.26 \) as well as the doping dependence agree very well with low–temperature susceptibility experiments showing a maximum at a hole doping of about 25%.

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I. INTRODUCTION

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$_{2-x}$Sr$_{x}$CuO$_4$ show a maximum in the doping dependence as well as, for moderate hole doping ($\delta \leq 0.21$), in the temperature dependence, where the temperature of the maximum decreases with increasing doping. Such a behaviour, also observed in YBa$_2$Cu$_3$O$_{6+y}$ ($y \leq 0.92$) [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 $\chi$ was obtained for the Pauli susceptibility of a strongly renormalized quasiparticle band [9] or for the RPA slave–boson susceptibility [11] showing a cusp in the temperature dependence at the transition to the singlet RVB state. In a semi–phenomenological weak–coupling approach to the one–band Hubbard model [12], the zero–temperature susceptibility was found to increase upon doping. 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 CPA 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 communication [14] 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 Ref. [14] 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 and by the calculation of the uniform static spin susceptibility in the parahelix, where special care is taken to the influence of SRO.

The paper is organized as follows. In Sec. II the action of the SB functional integral for the partition function, expressed in terms of fluctuating local magnetizations and internal magnetic fields, is transformed to an effective Ising model. In Sec. III the saddle-point equations are derived, where the SRO is self-consistently incorporated by the Bethe cluster approximation. Sec. IV is devoted to the calculation of the uniform static spin susceptibility. In Sec. V numerical results for the doping dependence of the zero-temperature susceptibility are presented and compared with experiments on high-$T_c$ cuprates. A brief summary of our work can be found in Sec. VI.

II. TRANSFORMATION TO AN EFFECTIVE ISING MODEL

It is widely believed that the essential characteristics of low-energy charge and spin excitations in the CuO$_2$ planes of high-$T_c$ cuprates may be described by effective one-band correlation models on a square lattice [16,17], such as the Hubbard model.

In the scalar four-field SB representation [15] the Fock space at each site is enlarged by introducing the Bose fields $e_i$, $d_i$, and $p_{i\sigma}$ describing projection operators onto empty, doubly and singly occupied states, respectively, and the Hubbard model is expressed as

$$\mathcal{H} = \sum_{ij\sigma} t_{ij} z_{i\sigma} f_{i\sigma}^\dagger f_{j\sigma} z_{j\sigma} + U \sum_i d_i^\dagger d_i + h \sum_{i\sigma} \sigma f_{i\sigma}^\dagger f_{i\sigma} ,$$

where $t_{(ij)} = -t$, $h$ denotes the uniform external magnetic field, and $z_{i\sigma} = z_{i\sigma}(e_i^{(1)}, d_i^{(1)}, p_{i\sigma}^{(1)})$.

To exclude unphysical states in the extended Fock space, the local constraints

$$e_i^\dagger e_i + d_i^\dagger d_i + \sum_{\sigma} p_{i\sigma}^\dagger p_{i\sigma} = 1 \quad \text{(completeness)},$$

$$f_{i\sigma}^\dagger f_{i\sigma} = p_{i\sigma}^\dagger p_{i\sigma} + d_i^\dagger d_i \quad \text{(one-to-one correspondence)}$$

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have to be fulfilled. Expressing the partition function $\mathcal{Z}$ by a coherent–state functional integral over complex Bose and pseudofermionic Grassmann fields, the local constraints are enforced by the time–independent Lagrange multipliers $\lambda_i^{(1)}$ and $\lambda_i^{(2)}$. By a local $U(1)^{\otimes 3}$ gauge transformation, the phases of the Bose fields $\epsilon_i$ and $p_{i\sigma}$ can be removed (radial gauge), where the Lagrange multipliers become time–dependent fields. Integrating out the pseudofermions ($f_{i\sigma}$) and applying the static approximation for the bosons ($p_{i\sigma}$, $d_i$, $\lambda_i^{(2)}$, where the saddle–point approximation for $\lambda_i^{(1)}$ is used to eliminate the integrals over the $\epsilon_i$ fields [18]) we get

$$\mathcal{Z} = \int [Dd][Dd^*][Dn][Dn][D\epsilon][D\lambda] \exp \{-\beta \Psi(\{d, d^*, n, \epsilon, \lambda\})\}, \quad (4)$$

$$\Psi = \sum_i \left(U d_i^* d_i - n_i \epsilon_i + m_i \lambda_i^{(2)}\right) + \frac{1}{\beta} \int d\omega f(\omega - \mu) \text{Im} \text{Tr} \ln \left[-G^{-1}_{ij\sigma}(\omega)\right], \quad (5)$$

$$G^{-1}_{ij\sigma}(\omega) = [\omega - \nu_i + \sigma(\xi_i + \hbar)]\delta_{ij} - z^*_{i\sigma} z_{j\sigma} t_{ij}, \quad (6)$$

where

$$m_i = \sum_{\sigma} \sigma p_{i\sigma}^2, \quad \xi_i = -\frac{1}{2} \sum_{\sigma} \sigma \lambda_i^{(2)}, \quad (7)$$

$$n_i = \sum_{\sigma} p_{i\sigma}^2 + 2d_i^* d_i, \quad \nu_i = \frac{1}{2} \sum_{\sigma} \lambda_i^{(2)}, \quad (8)$$

and

$$z_{i\sigma} = \sqrt{2} \frac{\sqrt{(n_i + \sigma m_i - 2d_i^* d_i)(1 - n_i + d_i^* d_i) + d_i \sqrt{n_i - \sigma m_i - 2d_i^* d_i}}}{\sqrt{(n_i + \sigma m_i)(2 - n_i - \sigma m_i)}}. \quad (9)$$

In eqs. (7) and (8), $m_i$ and $n_i$ are the bosonic representations of the local magnetization and particle number, respectively, defined analogously to its fermionic counterparts $m_i^f = \sum_{\sigma} \sigma f_{i\sigma}^f d_{i\sigma}$ and $n_i^f = \sum_{\sigma} f_{i\sigma}^f f_{i\sigma}^\dagger$. Since $\xi_i$ couples to $m_i$ as a magnetic field we denote $\xi_i$ by 'internal magnetic field'.

To proceed, we remove the non–diagonal randomness in the transfer term of (6) along the lines indicated by Shiba [19]. Here, we introduce the modified Shiba transformation

$$G_{ij\sigma} \rightarrow \hat{G}_{ij\sigma} = \sum_{lm} \hat{z}^*_{i\sigma} G_{lme} \hat{z}_{m\sigma}, \quad (10)$$
where

\[ \hat{z}_{ij\sigma} = \frac{z_{i\sigma}}{\sqrt{q_{i\sigma}^2}} \delta_{ij}, \quad q_{i\sigma} = |z_{i\sigma}|^2, \]  

(11)

and \( q_{i\sigma}^o \) is the uniform paramagnetic (PM) saddle–point value. Then, under the trace operation in (5), \( G_{ij\sigma}^{-1}(\omega) \) can be replaced exactly by

\[ \hat{G}_{ij\sigma}^{-1}(\omega) = q_{i\sigma}^o \left[ \frac{\omega - \nu_i + \sigma(\xi_i + h)}{q_{i\sigma}} \delta_{ij} - t_{ij} \right]. \]

(12)

Next, we aim to incorporate the SRO by going beyond the PM saddle point. To this end we perform an expansion in terms of the local perturbation

\[ V_{i\sigma} \delta_{ij} = -\hat{G}_{ij\sigma}^{-1} + G_{ij\sigma}^{o-1}, \]

(13)

where \( G_{ij\sigma}^{o-1}(\omega) \) is the inverse PM saddle–point propagator obtained from (12) by replacing \( q_{i\sigma} \rightarrow q_{i\sigma}^o, \nu_i \rightarrow \nu^o \) and \( \xi_i \rightarrow \xi^o \). We have

\[ V_{i\sigma}(\omega) = \frac{q_{i\sigma}^o}{q_{i\sigma}} \left\{ (q_{i\sigma} - q_{i\sigma}^o) \frac{\omega - \nu^o + \sigma(\xi^o + h)}{q_{i\sigma}^o} + \nu_i - \nu^o - \sigma(\xi_i - \xi^o) \right\}. \]

(14)

For further approximations it is convenient to separate \( G_{ij\sigma}^o \) into the diagonal (\( G_{ii\sigma}^o \)) and off-diagonal components (\( G_{ij\sigma}^{o'} \)) given by

\[ G_{ii\sigma}^o(\omega) = \frac{1}{N} \sum_{\vec{k}} \frac{1}{\omega - E_{k\sigma}^o}, \quad G_{ij\sigma}^{o'}(\omega) = \frac{1}{N} \sum_{\vec{k}} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} \frac{\delta_{ij}}{\omega - E_{k\sigma}^o}, \]

(15)

where

\[ E_{k\sigma}^o = q_{i\sigma}^o \epsilon_k + \nu^o - \sigma(\xi^o + h), \]

(16)

and \( \epsilon_k = -2t \sum_{i=1}^{D} \cos k_i \) is the unrenormalized tight–binding band dispersion in D dimensions.

Then, we rewrite

\[ \text{Tr} \ln [\hat{G}_{ij\sigma}^{-1}(\omega)] = \text{Tr} \ln [-G_{ij\sigma}^{o-1}(\omega)] + \text{Tr} \ln [(1 - G_{ii\sigma}^{o}(\omega)V_{i\sigma}(\omega))\delta_{ij}] \]

\[ + \text{Tr} \ln [\delta_{ij} - G_{ij\sigma}^{o'}(\omega)T_{j\sigma}(\omega)] \]

(17)

with the scattering matrix.
\[
T_{i}\sigma(\omega) = \frac{V_{i}\sigma(\omega)}{1 - G_{i}\sigma(\omega)V_{i}\sigma(\omega)}.
\]

The second term on the r.h.s. of (17) yields a single-site fluctuation contribution to the functional (5), whereas the third term describes the coupling between the fluctuations at all sites and is responsible for SRO effects.

Treating the fluctuations of the local magnetizations \(m_i\) and the internal magnetic fields \(\xi_i\) on an equal footing, we express those fields by their amplitude and direction according to

\[
m_i = \bar{m}_i s_i, \quad \xi_i = \bar{\xi}_i s_i, \quad s_i = \pm.
\]

Furthermore, we make the ansatz

\[
b_i \rightarrow b_s, \text{ with } b \in \{\bar{m}, \bar{\xi}, n, \nu, d^*, d\},
\]

which becomes relevant for the calculation of the uniform static spin susceptibility (Sec. IV); for \(h = 0\), we have \(b_s = b\). Then the partition function is given as

\[
Z = \sum_{\{s_i\}} \int [Dd_{s_i}][Dd^*_{s_i}][Dn_{s_i}][D\nu_{s_i}][D\bar{m}_{s_i}][D\bar{\xi}_{s_i}] \exp\{-\beta \Psi(\{s_i\})\}.
\]

Now we transform the free-energy functional \(\Psi\) to an effective Ising model along the lines indicated by Kakehashi [20]. By the identity

\[
\Psi(\{s_i\}) = \sum_{\{\alpha_i = \pm\}} \left( \prod_i \frac{1 + s_i \alpha_i}{2} \right) \Psi(\{\alpha_i\})
\]

we get

\[
\Psi(\{s_i\}) = \bar{\Psi} - \sum_i \bar{h}_i s_i - \sum_{(ij)} \bar{J}_{ij} s_i s_j - \sum_{(ijk)} \ldots
\]

with

\[
\bar{\Psi} = \left(\frac{1}{2}\right)^N \sum_{\{\alpha_i\}} \Psi(\{\alpha_i\}),
\]

\[
\bar{h}_i = -\left(\frac{1}{2}\right)^N \sum_{\{\alpha_i\}} \alpha_i \Psi(\{\alpha_i\}),
\]

\[
\bar{J}_{ij} = -\left(\frac{1}{2}\right)^N \sum_{\{\alpha_i\}} \alpha_i \alpha_j \Psi(\{\alpha_i\}).
\]

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In the pair approximation, all terms of (17) involving more than two sites are neglected so that

$$\text{Tr} \ln \left[ \delta_{ij} - G_{ij \sigma}^\sigma T_{ij \sigma}(\alpha_j) \right] = \sum_{(ij)\sigma} \ln \left[ 1 - G_{ij \sigma}^\sigma T_{ij \sigma}(\alpha_j) G_{ji \sigma}^\sigma T_{ji \sigma}(\alpha_i) \right],$$

(27)

and the higher-order terms in (23) vanish. Restricting ourselves to nearest-neighbour pairs \((ij)\) only, the functional \(\Psi\) takes the form

$$\Psi(\{s_i\}) = \bar{\Psi} - \tilde{h} \sum_i s_i - J \sum_{(ij)} s_i s_j,$$

(28)

with

$$\bar{\Psi} = -\frac{1}{\beta} \sum_{k\sigma} \ln \left[ 1 + e^{-\beta \left( E_{k\sigma} + \nu_{\sigma} \right)} \right],$$

$$+ \frac{N}{2} \sum_\alpha \left\{ U d_\alpha^* d_\alpha - n_\alpha \nu_\alpha + m_\alpha \bar{\xi}_\alpha + \sum_{\sigma} \left[ \Phi_{\alpha\sigma} + \frac{\xi}{4} \left( \Phi_{\alpha\alpha\sigma} + \Phi_{-\alpha\alpha\sigma} \right) \right] \right\},$$

(29)

$$\tilde{h} = -\frac{1}{2} \sum_\alpha \left[ U d_\alpha^* d_\alpha - n_\alpha \nu_\alpha + m_\alpha \bar{\xi}_\alpha + \sum_{\sigma} \left( \Phi_{\alpha\alpha\sigma} + \frac{\xi}{2} \Phi_{-\alpha\alpha\sigma} \right) \right],$$

(30)

$$\tilde{J} = \frac{1}{4} \sum_{\alpha\sigma} (\Phi_{\alpha\alpha\sigma} - \Phi_{-\alpha\alpha\sigma}),$$

(31)

where \(\Phi_{\alpha\sigma} = \Phi_{i\sigma}(\alpha_i)|_{\alpha_i = \alpha}\) and \(\Phi_{\alpha\alpha'\sigma} = \Phi_{(ij)\sigma}(\alpha_i, \alpha_j)|_{\alpha_j = \alpha', \alpha_i = \alpha}\), and

$$\Phi_{i\sigma} = \frac{1}{\tau} \int d\omega f(\omega - \mu) \text{Im} \ln \left[ 1 - G_{i\sigma}^\sigma V_{i\sigma}(\alpha_i) \right],$$

(32)

$$\Phi_{(ij)\sigma} = \frac{1}{\tau} \int d\omega f(\omega - \mu) \text{Im} \ln \left[ 1 - G_{(ij)\sigma}^\sigma T_{ij \sigma}(\alpha_j) G_{(ji)\sigma}^\sigma T_{ji \sigma}(\alpha_i) \right],$$

(33)

\((z)\) is the coordination number). Let us emphasize that the parameters of the effective Ising model (28), in particular the Ising-exchange integral \(\tilde{J}\), are complicated functions of all SB fields and have to be determined self-consistently at each interaction strength \(U\) and hole doping \(\delta = 1 - n\).

III. SADDLE POINT WITH SHORT-RANGE ORDER

To calculate the partition function (21) with the functional (28) in the saddle-point approximation incorporating SRO, we proceed in two steps. First, we perform the \(s_i\)-sum
by means of the Bethe cluster approximation, i.e., we take into account only the nearest-neighbour SRO. Thereafter, we adopt the saddle-point approximation for all Bose fields \( b_o \) (eq.(20)). Correspondingly, contrary to CPA approaches [13,20], our theory incorporates SRO at the saddle-point in a fully self-consistent way at the pair approximation level.

In the Bethe approximation, the lattice is divided into \( N/2 \) clusters consisting of a central site \( s_0 \) and its \( z \) nearest neighbours \( s_l \) which also belong to the surrounding clusters. Accordingly, the external-field term in (28) is weighted by a factor of \( z^{-1} \). The Ising coupling to the neighbouring clusters is approximately taken into account by the effective Bethe field \( h^* \). Thus, we have

\[
\Psi = \bar{\Psi} + \frac{N}{2} \left( -\bar{h} s_0 - \left( \frac{1}{z} \bar{h} + h^* \right) \sum_{l=1}^{z} s_l - J \sum_{l=1}^{z} s_0 s_l \right). \tag{34}
\]

From the probability \( W_\alpha \) for the Ising spin \( \alpha \) at the central site,

\[
W_\alpha = \frac{1}{Z_c} e^{\alpha \bar{h} \psi} \left\{ 2 \cosh \left[ \beta \left( \frac{1}{z} \bar{h} + h^* + \alpha J \right) \right] \right\}^{\bar{s}}, \tag{35}
\]

where \( \sum_\alpha W_\alpha = 1 \) and \( Z_c \) is the cluster partition function, the Ising spin averages \( \langle \ldots \rangle \) can be calculated. The field \( h^* \) is determined from the Bethe condition

\[
\langle s_0 \rangle = \langle s_l \rangle, \tag{36}
\]

where \( \langle s_0 \rangle = (z \beta Z_c)^{-1} \partial Z_c / \partial h^* \), which yields the self-consistency equation

\[
h^* = \frac{z-1}{z} \bar{h} + \frac{z-1}{z} \ln \left\{ \frac{\cosh \left[ \beta \left( \frac{1}{z} \bar{h} + h^* + \bar{J} \right) \right]}{\cosh \left[ \beta \left( \frac{1}{z} \bar{h} + h^* - \bar{J} \right) \right]} \right\}. \tag{37}
\]

For the Ising-spin correlation function we get

\[
\langle s_0 s_l \rangle = \sum_\alpha \alpha W_\alpha \tanh \left[ \beta \left( \frac{1}{z} \bar{h} + h^* + \alpha \bar{J} \right) \right]. \tag{38}
\]

Finally, the effective bosonic action is given by

\[
S = \beta \bar{\Psi} - \frac{N}{2} \ln Z_c. \tag{39}
\]

Note that for the square lattice \((z = 4)\) one can also use the exact paramagnetic Onsager solution [21], where it turns out that the nearest-neighbour correlation function in the Bethe approximation (eq.(38)) is exact at \( T = 0 \).
Only just now, we calculate the free energy in the saddle-point approximation for the Bose fields \( b_\alpha = \{ \bar{m}_\alpha, \xi_\alpha, n_\alpha, \nu_\alpha, d_\alpha \} \), where we take the saddle-point solution \( d_\alpha^* = d_\alpha \).

From \( \partial S / \partial b_\alpha = 0 \) and the dependences on \( b_\alpha \) of \( \bar{J}, \bar{h}, \) and \( h^* \) we obtain the self-consistency equations determining the saddle point with SRO, which can be cast to the form

\[
\bar{m}_\alpha = \alpha \sum_\sigma n^{f}_{\alpha\sigma}, \quad \xi_\alpha = -\sum_\sigma Q^f_{\alpha\sigma} \frac{\partial \eta_{\alpha\sigma}}{\partial \bar{m}_\alpha}, \tag{40}
\]

\[
n_\alpha = \sum_\sigma n^{f}_{\alpha\sigma}, \quad \nu_\alpha = \sum_\sigma Q^f_{\alpha\sigma} \frac{\partial \eta_{\alpha\sigma}}{\partial n_\alpha}, \tag{41}
\]

\[
U = -\sum_\sigma Q^f_{\alpha\sigma} \frac{\partial \eta_{\alpha\sigma}}{\partial d^2_\alpha}. \tag{42}
\]

Here, \( n^{f}_{\alpha\sigma} \) is the pseudo-fermionic expression for the particle density given by

\[
n^{f}_{\alpha\sigma} = \frac{1}{1 + \alpha K_h} \sum_{\sigma'} \left\{ \left( 1 + \alpha' K_h \right) \frac{\partial \Phi_{\alpha'\sigma'}}{\partial \lambda^{(2)}_{\alpha\sigma}} \right. \\
- \frac{\partial \Phi_{\alpha'\sigma'}}{\partial \lambda^{(2)}_{\alpha\sigma}} + \frac{\partial \Phi_{\sigma'\sigma}}{\partial \lambda^{(2)}_{\alpha\sigma}} \right\}, \tag{43}
\]

where

\[
K_h = \frac{\langle s_\alpha \rangle}{2} \frac{z + 1 - (z - 1) L_h}{1 - (z - 1) L_h}, \tag{44}
\]

\[
K_J = \langle s_\alpha s_\alpha \rangle + \frac{(z - 1) L_J}{1 - (z - 1) L_h} \langle s_\alpha \rangle, \tag{45}
\]

\[
L_h = \frac{1}{2} \sum_\alpha \alpha \tanh \left[ \beta \left( \frac{1}{z} h^* + \alpha \bar{J} \right) \right], \tag{46}
\]

\[
L_J = \frac{1}{2} \sum_\alpha \tanh \left[ \beta \left( \frac{1}{z} h + h^* + \alpha \bar{J} \right) \right], \tag{47}
\]

and \( \lambda^{(2)}_{\alpha\sigma} = \nu_\alpha - \alpha \sigma \xi_\alpha \). In eqs. (40) to (42), \( Q^f_{\alpha\sigma} \) is given by (43) with \( \partial \lambda^{(2)}_{\alpha\sigma} \) replaced by \( \partial \eta_{\alpha\sigma} \). The chemical potential is determined from the number condition \( n = \sum_\alpha W_\alpha n_\alpha \) with \( n_\alpha \) given by (41). At the saddle point, we have \( n^{f}_{\alpha\sigma} = n_{\alpha\sigma} = (n_\alpha + \alpha \sigma \bar{m}_\alpha)/2 \), where \( n_{\alpha\sigma} \) is the bosonic expression, and the free energy per site is given by

\[
f = \frac{1}{N} \bar{\Psi} - \frac{1}{2g} \left[ \ln \mathcal{Z}_c - (z + 1) \ln 2 \right] + \mu n.
\]

For vanishing local magnetization, \( \bar{m}_\alpha = 0 \), we have \( V_{\alpha\sigma} = 0 \) and (by (31) and (33)) \( \bar{J} = 0 \) so that there is no SRO, and the PM saddle point (with the external field \( h \) is
recovered from (40) to (42). Accordingly, there are two possible paraphrases defined, for
\( h = 0 \), by

\[
\begin{align*}
\text{PM} & : \langle s_i \rangle = 0, \langle s_i s_j \rangle = 0; \ \bar{m} = 0 (J = 0), \\
\text{SRO-PM} & : \langle s_i \rangle = 0, \langle s_i s_j \rangle \neq 0; \ \bar{m} > 0 (J \neq 0),
\end{align*}
\]

(48)

where \( i \) and \( j \) are nearest-neighbour sites. In our previous paper [14] we have investigated
the stability regions of the PM and SRO-PM phases in the \( U/t-\delta \) plane, where also various
magnetic LRO phases are taken into consideration. At \( T = 0 \), the paraphase with antiferro-
magnetic (ferromagnetic) SRO has to be distinguished from the corresponding AFM (FM)
LRO phases [14].

IV. SPIN SUSCEPTIBILITY

The uniform static spin susceptibility \( \chi(T, \delta) \) is of particular interest in the investigation
of magnetic correlation effects. It is defined as

\[
\chi = \lim_{h \to 0} \frac{d m}{d h} \quad \text{with} \quad m = \sum_{o} W_{o} m_{o},
\]

(49)

where \( m = \langle m_{s_{i}} \rangle \) \( (m_{s_{i}} = m_{s_{i}} s_{i} \) according to (19), (20); \( s_{i} \to \alpha_{i} \)) is the averaged magnetization, and \( W_{o} \) is given by (35). Thus, we have

\[
\chi = \lim_{h \to 0} \sum_{o} \left( W_{o} \frac{d m_{o}}{d h} + m_{o} \frac{d W_{o}}{d h} \right).
\]

(50)

The first term in (50) 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 and is called the ‘local’ contribution being
finite only in the presence of SRO. Note that the ‘itinerant’ and ‘local’ properties are inter-
related and determine both contributions to the spin susceptibility. By \( W_{o} = W_{o}(h, h^{*}, \bar{J}) \)
we obtain

\[
\frac{d W_{o}}{d h} = \frac{\alpha \beta d \bar{h}}{\Theta_{l} d h}
\]

(51)
with

\[ \Theta_1 = z \exp \{-2\beta \bar{J}\} - z + 2. \]  

(52)

The structure of (51), for \( z = 4 \), coincides with that derived by Baumgärtel et al. [13]. Calculating \( d\bar{h}/dh \) we take care of the dependence \( \bar{h} = \bar{h}(\{\bar{m}_\alpha\}, \{\xi_\alpha\}, m^o, \xi^o, h) \) which differs from that in the CPA approach of Ref. [13], where instead of \( m^o \) and \( \xi^o \), \( W_o \) appears. Moreover, we take into account the symmetry relations in the paraphrase, \( \frac{d\bar{m}_+}{dh} \bigg|_{h=0} \equiv \bar{m}_+ = -\bar{m}_- \), \( \frac{d\xi_+}{dh} \bigg|_{h=0} \equiv \bar{\xi}_+ = -\bar{\xi}_- \), and \( \frac{dW_+}{dh} \bigg|_{h=0} \equiv W_+ = -W_- \). According to the saddle-point equations (40) for \( \bar{m}_+ \) and \( \bar{\xi}_+ \), resulting from \( \partial S/\partial \bar{\xi}_+ = 0 \) and \( \partial S/\partial \bar{m}_+ = 0 \), respectively, we have \( \bar{m}_+ = \bar{m}_+(\{\bar{m}_\alpha\}, \{\xi_\alpha\}, m^o, \xi^o, h) \) and the analogous dependence of \( \bar{\xi}_+ \). Taking into consideration the full dependence on the external field \( h \) of \( W_+, \bar{m}_+, \bar{\xi}_+, m^o, \) and \( \xi^o \), for the derivatives of those quantities in the limit \( h \to 0 \) we obtain the linear system of equations

\[
\begin{pmatrix}
\frac{1}{\beta} \Theta_1 & -\bar{h}_{\bar{m}_{[+,-1]}} & -\bar{h}_{\bar{\xi}_{[+,-1]}} & -\bar{h}_{m^o} & -\bar{h}_{\xi^o} \\
S_{W_{[+,-1]}\bar{\xi}_+} & S_{\bar{m}_{[+,-1]}\bar{\xi}_+} & S_{\bar{\xi}_{[+,-1]}\bar{\xi}_+} & S_{m^o\bar{\xi}_+} & S_{\xi^o\bar{\xi}_+} \\
S_{W_{[+,-1]}\bar{m}_+} & S_{\bar{m}_{[+,-1]}\bar{m}_+} & S_{\bar{\xi}_{[+,-1]}\bar{m}_+} & S_{m^o\bar{m}_+} & S_{\xi^o\bar{m}_+} \\
0 & 0 & 0 & S_{m^o\xi^o} & S_{\xi^o\xi^o} \\
0 & 0 & 0 & S_{m^o\xi^o} & S_{\xi^o\xi^o}
\end{pmatrix}
= 
\begin{pmatrix}
\bar{W}_+ \\
\bar{m}_+ \\
\bar{\xi}_+ \\
m^o \\
\xi^o
\end{pmatrix}
= 
\begin{pmatrix}
\bar{h} \\
-S_{h\bar{\xi}_+} \\
-S_{h\bar{m}_+} \\
-S_{h^2} \\
-S_{h^2}
\end{pmatrix},
\]  

(53)

where

\[
X_y = \frac{\partial X}{\partial y}, \quad X_{x_{[+,-1]}} = \left( \frac{\partial}{\partial x_+} - \frac{\partial}{\partial x_-} \right) X, \quad X_{xy} = \frac{\partial^2 X}{\partial x \partial y},
\]  

(54)

and \( S^o \) denotes the action at the PM saddle point. In the paraphrase without SRO, from the lower block of (53), the susceptibility is obtained as

\[
\chi^o = m^o_h = \frac{\chi^o_0}{1 + A \chi^o_0 + B \chi^o_1 + \frac{1}{4} B^2 (\chi^o_1 - \chi^o_0 \chi^o_2)}
\]  

(55)

with

\[
A = \sum_{o} \frac{\partial^2 q^o}{\partial m^o}, \quad B = \frac{1}{2} \sum_{o} \sigma \frac{\partial q^o}{\partial m^o},
\]  

(56)
\[ \chi_n = -\frac{1}{N} \sum_{k\sigma} (2\varepsilon_{k})^{n} \frac{\partial f(E_{k\sigma}^{n} - \mu)}{\partial E_{k\sigma}^{n}} . \]  

(57)

Let us point out that our result for the spin susceptibility \( \chi^{c} \) agrees with the static and uniform limit of the dynamic spin susceptibility derived, within the spin–rotation–invariant SB scheme [22], from the Gaussian fluctuation matrix at the PM saddle point [23]. Contrary, the uniform static spin susceptibility given in Ref. [24] within the scalar four–field SB approach disagrees with the result of Li et al. [23] away from half-filling.

To calculate the influence of SRO on the spin susceptibility in the SRO–PM phase, we insert the solutions for \( m_h^{c} \) and \( \xi_h^{c} \) into the system (53), where the corresponding terms appear in the inhomogeneities of the equations for \( W_{+h}^{c}, \bar{m}_{+h}, \) and \( \bar{\xi}_{+h}^{c} \). From the solution of (53), we finally obtain the spin susceptibility as

\[ \chi = \frac{\Theta_{I} \chi_{1} + \chi_{II}}{\Theta_{I} + \Theta_{II}} \]  

(58)

with

\[ \chi_{1} = \Delta \left[ \Xi S_{m_{+}^{c} \xi_{+}^{c}} - \Lambda S_{\bar{\xi}_{+}^{c} \xi_{+}^{c}} \right] , \]  

(59)

\[ \chi_{II} = 2\beta \bar{m}_{+} \Gamma + \beta \Delta \left\{ 2\bar{m}_{+} \left( \Xi \bar{h}_{m_{+}^{c} \xi_{+}^{c}} + \Lambda \bar{\xi}_{+}^{c} \right) - \Gamma S_{W_{+}^{c} \xi_{+}^{c}} \right\} S_{m_{+}^{c} \xi_{+}^{c}} \]

\[ -\bar{\xi}_{+}^{c} \left( \Lambda S_{W_{+}^{c} \xi_{+}^{c}} - \Xi S_{W_{+}^{c} \bar{m}_{+}^{c}} \right) - 2\bar{m}_{+} \Xi \bar{\xi}_{+}^{c} S_{m_{+}^{c} \bar{m}_{+}^{c}} \]

\[ + \left( \Gamma S_{W_{+}^{c} \bar{m}_{+}^{c}} - 2\bar{m}_{+} \Lambda \bar{\xi}_{+}^{c} \right) S_{\bar{\xi}_{+}^{c} \bar{\xi}_{+}^{c}} \],

(60)

and

\[ \Theta_{II} = \beta \Delta \left[ \left( S_{W_{+}^{c} \xi_{+}^{c}} \bar{h}_{m_{+}^{c} \xi_{+}^{c}} + S_{W_{+}^{c} \bar{m}_{+}^{c} \bar{\xi}_{+}^{c}} \right) S_{m_{+}^{c} \xi_{+}^{c}} \right. \]

\[ -\bar{h}_{\bar{\xi}_{+}^{c}} S_{W_{+}^{c} \bar{\xi}_{+}^{c}} S_{m_{+}^{c} \bar{m}_{+}^{c}} - \bar{h}_{m_{+}^{c} \xi_{+}^{c}} S_{\bar{\xi}_{+}^{c} \bar{\xi}_{+}^{c}} \],

(61)

where

\[ \Delta = \left[ S_{m_{+}^{c} \xi_{+}^{c}}^{2} - S_{m_{+}^{c} \xi_{+}^{c}} S_{m_{+}^{c} \bar{m}_{+}^{c}} \right]^{-1} \]  

(62)

\[ \Xi = -S_{h_{\xi_{+}^{c}}} - S_{m_{+}^{c} \xi_{+}^{c}} \bar{m}_{+}^{c} - S_{\xi_{+}^{c} \xi_{+}^{c}} \bar{\xi}_{+}^{c} \]  

(63)
\[ A = -S_{mn} - S_{m^*n^*} m^*_h - S_{n^*n^*} n^*_h, \]  
\[ \Gamma = \tilde{h}_h + \tilde{h}_m m^*_h + \tilde{h}_n n^*_h. \]  
(64)  
(65)

In this paper we are primarily interested in the zero-temperature susceptibility. Equations (58) to (61) then lead to

\[ \lim_{T \to 0} \chi = \begin{cases} 
\chi_1 & \text{for antiferromagnetic SRO (} \bar{J} < 0 \text{)} \\
\frac{\chi_{11}}{\Theta_{11}} & \text{for ferromagnetic SRO (} \bar{J} > 0 \text{)}.
\end{cases} \]  
(66)

Let us emphasize that, in contrast to the theory by Baumgärtel et al. [13], we get a finite susceptibility at \( T = 0 \).

Hereafter we consider the case of antiferromagnetic SRO at \( T = 0 \) (ferromagnetic SRO can be realized only at large values of \( U/t \) being unrealistic for the cuprates). For this case, the coefficients \( S_{xy} \) in (53) occurring in \( \chi_1 \) become

\[ S_{n^*n^*} = S_{n^*n^*} = 1 + \sum_{\eta} q^{-1} n_{\eta} q_{\eta} \left\{ n_{\eta} - a_{\eta}^2 \Phi^{(0,2)}_{1,\eta} + a_{\eta} b_{\eta} \Phi^{(0,2)}_{0,\eta} - z \left[ a_{\eta}^2 \Phi^{(0,1,1)}_{1,-\eta} + a_{\eta} b_{\eta} \Phi^{(0,0,2)}_{1,-\eta} - a_{\eta} b_{\eta} \Phi^{(0,0,2)}_{0,-\eta} \right] \right\}, \]  
(67)

\[ S_{n^*n^*} = \sum_{\eta} q^{-1} \left\{ a_{\eta} \Phi^{(0,2)}_{0,\eta} + z \left( a_{\eta} \Phi^{(0,1,1)}_{0,-\eta} + a_{\eta} \Phi^{(0,0,2)}_{0,-\eta} \right) \right\}, \]  
(68)

\[ S_{m^*\xi} = -\sum_{\eta} q^{-1} \left\{ a_{\eta} \Phi^{(0,2)}_{1,\eta} - a_{\eta} \Phi^{(0,0,2)}_{1,\eta} + z \left[ a_{\eta} \Phi^{(1,0,1)}_{1,-\eta} - a_{\eta} \Phi^{(0,1,1)}_{1,-\eta} - a_{\eta} \Phi^{(0,0,2)}_{1,-\eta} \right] \right\}, \]  
(69)

\[ S_{\xi^*} = S_{\tilde{h}^*} - S_{\xi^* \tilde{h}^*}, \]  
(70)

\[ S_{\tilde{h}^*} = \sum_{\eta} a_{\eta} \left\{ \Phi^{(0,1,1)}_{0,\eta} + z \Phi^{(1,0,1)}_{0,-\eta} \right\}, \]  
(71)

\[ S_{n^*n^*} = \sum_{\eta} q^{-1} \left\{ \left[ q_{\eta} - 2q_{\eta} \left( q_{\eta} \right)^2 \right] \Phi^{(0,2)}_{1,\eta} + q_{\eta} - q_{\eta} \left( q_{\eta} \right)^2 \right\}, \]  
(72)

\[ + a_{\eta} b_{\eta} \Phi^{(0,2)}_{0,\eta} + z \left[ a_{\eta} \Phi^{(0,1,1)}_{1,-\eta} + a_{\eta} \Phi^{(0,0,2)}_{1,-\eta} - a_{\eta} b_{\eta} \Phi^{(0,0,2)}_{0,-\eta} \right] \} \]
\[ S_{m,m_0} = \sum_{\eta} q_{\eta}^{-1} q_{\eta}^{(m)} q^{(m)} \left\{ z \left[ a_{\eta} \left( 2\Phi_{1,-\eta,0}^{(0,2)} + q^{0}\Phi_{2,-\eta,0}^{(1,0,1)} - a_{\eta}\Phi_{2,-\eta,1}^{(1,0,1)} - a_{\eta}\Phi_{2,-\eta,2}^{(0,0,2)} \right) \\
+ b_{\eta} \left( \Phi_{0,-\eta,0}^{(0,0,1)} + \Phi_{0,-\eta,1}^{(0,1,0)} - a_{\eta}\Phi_{0,-\eta,2}^{(0,0,2)} - a_{\eta}\Phi_{0,-\eta,2}^{(0,0,2)} \right) \\
+ a_{\eta} \left( 2\Phi_{1,-\eta,1}^{(0,1)} + q^{0}\Phi_{2,-\eta,0}^{(1,1,1)} - a_{\eta}\Phi_{2,-\eta,2}^{(0,2)} \right) - b_{\eta} \left( \Phi_{0,-\eta,1}^{(0,1)} + \Phi_{0,-\eta,2}^{(1,1,1)} - a_{\eta}\Phi_{0,-\eta,2}^{(0,2)} \right) \right\} , \] (73)

\[ S_{m,m_0} = S_{h,m_0} - \sum_{\eta} q_{\eta}^{-1} q_{\eta}^{(m)} \left\{ a_{\eta} \left( \Phi_{0,0,1}^{(0,1)} - a_{\eta}\Phi_{0,1,0}^{(1,0,2)} + b_{\eta} \left( \Phi_{0,0,1}^{(0,1)} + \Phi_{0,1,0}^{(1,0,2)} \right) + z \left[ a_{\eta}\Phi_{1,0,1}^{(1,1)} - b_{\eta}\Phi_{0,0,1}^{(1,1)} + z \left[ a_{\eta}\Phi_{1,0,1}^{(1,1)} - b_{\eta}\Phi_{0,0,1}^{(1,1)} \right] \right\} , \] (74)

\[ S_{h,m_0} = - \sum_{\eta} a_{\eta} q_{\eta}^{(m)} \left\{ a_{\eta}\Phi_{1,0,1}^{(1,1)} - b_{\eta}\Phi_{0,0,1}^{(1,1)} + z \left[ a_{\eta}\Phi_{1,0,1}^{(1,1)} - b_{\eta}\Phi_{0,0,1}^{(1,1)} \right] \right\} , \] (75)

with the abbreviations:

\[ q^{(m)} = \sigma \frac{\partial q_{\sigma}}{\partial m} \bigg|_{m=0} , \quad q_{\eta}^{(m)} = \eta \frac{\partial q_{\eta}}{\partial \eta} , \quad q_{\eta}^{(m^2)} = \frac{\partial^2 q_{\eta}}{\partial \eta^2} , \] (76)

\[ \Phi_{n,\eta}^{(k,l,m)} = \frac{\partial^{k+l}\Phi_{n,\eta}^{(k,l,m)}}{\partial \eta^k \partial \lambda_{\eta}^{(2)l} \partial \lambda_{\eta}^{(2)m}} , \quad \Phi_{n,\eta,\eta'}^{(k,l,m)} = \frac{\partial^{k+l+m}\Phi_{n,\eta,\eta'}^{(k,l,m)}}{\partial \eta^k \partial \lambda_{\eta}^{(2)l} \partial \lambda_{\eta'}^{(2)m}} , \] (77)

\[ \Phi_{n,\eta} = \frac{1}{\tau} \int d\omega \omega^n f(\omega - \mu) \text{Im} \ln \left[ 1 - G^0 V_n \right] , \] (78)

\[ \Phi_{n,\eta,\eta'} = \frac{1}{\tau} \int d\omega \omega^n f(\omega - \mu) \text{Im} \ln \left[ 1 - G^0 T_n G^0 T_{\eta'} \right] , \] (79)

and $a_{\eta} = \frac{\xi_{\eta}}{q_{\eta}}, b_{\eta} = \frac{\lambda_{\eta}^{(2)} - \lambda_{\eta}}{q_{\eta}},$ where $\eta = \alpha \sigma = \pm$.

V. NUMERICAL RESULTS

To evaluate the doping dependence of the uniform static spin susceptibility at $T = 0$, all quantities (eqs. (55) to (57), (59), and (67) to (75)) have to be calculated in the $h = 0$ limit from the solution of the self-consistency equations (40) to (47) [14]. In the tedious numerical evaluation of the integrals (32) and (33) and of their derivatives (77), particular attention has to be paid to the analytical behaviour of the complex logarithm.

Figure 1 shows the doping dependence of the zero–temperature susceptibility for the 2D Hubbard model, where the realistic values $U/t = 8$ and $t = 0.3$ eV for La$_{2-\delta}$Sr$_\delta$CuO$_4$ [17]
are used. As stated in our previous paper [14], for $U/t = 8$ there occurs a first-order $(1,1)$-spiral$\Rightarrow$SRO$\Rightarrow$PM transition at $\delta_{c_1} = 0.04$ and a SRO$\Rightarrow$PM$\Rightarrow$PM transition of second order at $\delta_{c_2} = 0.26$. In the PM phase ($\delta > \delta_{c_2}$) the SB band-renormalized Pauli susceptibility (55) has a pronounced doping dependence in two dimensions. In the SRO$\Rightarrow$PM phase ($\delta_{c_1} < \delta < \delta_{c_2}$), where the finite local-magnetization amplitude $\bar{m}$ results in an effective Ising-exchange interaction $\bar{J} < 0$ and antiferromagnetic SRO, the Pauli susceptibility is suppressed due to the SRO-induced spin stiffness against the orientation along the homogeneous external field. Accordingly, at $\delta_{c_2} = 0.26$ a cusp in $\chi(0,\delta)$ appears. Since, for $\delta_{c_1} < \delta < \delta_{c_2}$, $|\bar{J}|$ decreases with increasing $\delta$ [14], the susceptibility increases upon doping.

The peak in $\chi(0,\delta)$ only appears at sufficiently high ratios $U/t$ ($U/t > 6$ [14]), for which a SRO$\Rightarrow$PM$\Rightarrow$PM transition may occur. According to the phase diagram, given in Fig. 2 of Ref. [14], in the region $6 < U/t < 12$ the SRO$\Rightarrow$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 experimental data on La$_{2-x}$Sr$_x$CuO$_4$ at 50 K [5] showing a pronounced maximum at a hole doping of about 25%. Let us underline that we have not performed any fit procedure of our $T = 0$ results. That means, using the commonly accepted value $U/t = 8$ for the Hubbard model applied to high-$T_c$ cuprates, we obtain an excellent agreement between theory and experiment, in particular as the peak position and the doping dependence of $\chi$ are concerned.

To give more insight into the appearance of SRO resulting in the increase of the susceptibility with doping, in Fig. 2 the doping dependences of the local-magnetization amplitude $\bar{m}$ and of the local magnetic moment $m_{loc} = \frac{3}{4}(n - 2d^2)$ are shown at $U/t = 8$. Obviously, $\bar{m}$ plays the role of an order parameter characterizing the SRO$\Rightarrow$PM phase, whereas $m_{loc}$ is a measure of the ‘localization’ of the electron spin. The local moment increases with the correlation strength, i.e., with decreasing $\delta$ and increasing $U/t$, as known from the theory of itinerant magnetism. Contrary to $\bar{m}$, $m_{loc}$ is finite in the PM phase as well. If the local-moment behaviour is sufficiently pronounced as compared with the itinerant behaviour, the
formation of magnetic SRO becomes energetically favourable \((\delta < \delta_c)\). Once the SRO has been established, \(m_{loc}\) is enhanced with respect to its value in the PM state (cf. Fig. 2).

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 [25] and with a semi–phenomenological and non–selfconsistent approach to the Hubbard model [12]. However, in those works a maximum in the spin susceptibility was found even at a smaller coupling \((U/t = 4)\).

**VI. SUMMARY**

The main results of this paper are summarized as follows.

(i) Our theory of magnetic SRO in the one–band Hubbard model including an external magnetic field extends the four–field SB approach by the self–consistent incorporation of SRO at the saddle point and improves the previous CPA approaches \([13,20]\) to the problem of SRO. In particular, we are able to describe SRO effects at \(T = 0\), e.g., the suppression of LRO in favour of a paraphase with SRO in a wide doping region.

(ii) The uniform static spin susceptibility \(\chi(T, \delta)\) in the paraphase consisting of interrelated 'itinerant' and 'local' parts is calculated in a completely self–consistent way, where the influence of SRO is determined.

(iii) The numerical evaluation of the zero–temperature susceptibility for \(U/t > 6\) shows a cusp at the transition from the paraphase without SRO \((\delta > \delta_c)\) to the paraphase with antiferromagnetic SRO \((\delta_c < \delta < \delta_c)\). In the SRO–PM phase, \(\chi(0, \delta)\) increases upon doping. Using the realistic value \(U/t = 8\) for \(La_{2-x}Sr_xCuO_4\), the peak position and the doping dependence of \(\chi(0, \delta)\) agree very well with low–temperature experiments.

From the results we conclude that the concept of magnetic SRO in strong–correlation models may play the key role in the explanation of many unconventional normal–state properties of high–\(T_c\) compounds. The theory may be extended in several directions. In particular, as
motivated by neutron scattering experiments [2] 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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REFERENCES


FIGURES

Fig. 1: Uniform static spin susceptibility as a function of doping. The theoretical result obtained for the 2D Hubbard model at $U/t = 8$, $t = 0.3$ eV, and $T = 0$ K, is compared with experiments (×) on La$_{2-x}$Sr$_x$CuO$_4$ at $T = 50$ K [5].

Fig. 2: Amplitude of the local magnetization $\tilde{m}$ (solid curve) compared with the local magnetic moment $m_{loc}$ in the PM (dashed line) and SRO–PM (chain–dashed line) phases.