Evolution of antiferromagnetic short-range order with doping in high-T_c superconductors

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Within the framework of the t-J model, the evolution, with hole doping, of the antiferromagnetic (AF) correlation length and the spin correlation function in high-T_c superconductors are studied. The dynamic spin susceptibility has been calculated by using a two-time Green's function method that allows one to take into account both electron and AF spin correlation. A comparison of our results with NMR and neutron scattering data shows that the model is able to reproduce the main features of the temperature and doping dependences of the AF correlation length in both the pure Heisenberg antiferromagnet (e.g., La_2CuO_4) and doped compounds (e.g., $La_{2-x}Sr_xCuO_4$). [S0163-1829(98)07541-9]

I. INTRODUCTION

From an experimental point of view, the magnetic properties of the normal state of high-T_c superconductors (HTSC's) are now relatively well understood. It has been established by neutron scattering[1] that the antiferromagnetic (AF) long-range order of the parent compounds is lost upon doping, but that AF short-range order (SRO) is still present in superconducting compounds. Also, these experiments show that SRO decreases with increasing temperature and doping. Therefore, the understanding of the evolution of the normal state magnetic properties of CuO_2 planes with doping is believed to be a key to elucidate the unusual properties of HTSC's.

The hole dynamics in an AF background is perfectly described by the dynamic spin susceptibility which provides direct information about the low-energy excitation spectrum and its evolution with doping. Much work has been devoted to calculations of the susceptibility. Usually, theories start from the t-J model[2] and make use of various methods like the diagrammatic,[3,4] projection,[5] slave-boson[6,7] or slave-fermion,[8,9] and the extended Dyson representation method.[10] However, in spite of considerable progress, all theories have some disadvantages which are mainly connected with the use of either the mean-field approximation for the local constraints of operators or the random phase approximation (RPA). Therefore, it is tempting to investigate the dynamic spin susceptibility within a constraint-free theory which may be based, as a natural starting point, on the presentation of the t-J model in terms of Hubbard operators. This presentation obeys rotational symmetry of the spin correlation functions and automatically guarantees the exclusion of double occupancy. Moreover, such a technique allows one to take into account the magnetic effects near half-filling of the energy bands where the RPA does not work.[11]

The spin part of the t-J model can be modeled by a spin-1/2 Heisenberg antiferromagnet on a square lattice. The thermodynamic properties of the Heisenberg model have been investigated by analytical methods such as the two-dimensional (2D) quantum nonlinear σ model,[12,13] modified spin-wave theory,[14] Schwinger-boson mean-field theory,[15] isotropic spin-wave theory,[16] and the Green's function method.[17] The first three theories are valid, however, only at sufficiently low temperatures T. For example, the most detailed results for the nonlinear σ model were obtained in the renormalized classical regime where $T \ll 2\pi\rho_S$ (ρ_S is the stiffness). However, in doped HTSC's, ρ_S is likely to be small, thus decreasing the temperature range over which the renormalized classical behavior holds.[18]

In case of the modified spin-wave[14] as well as the Schwinger-boson mean-field[15] theories, the temperature restriction is given by $T < 0.9J$. Moreover, if one extends these theories to doped compounds, the commutation relations between the fermioniclike (holes) and bosoniclike (spins) operators must be obeyed. This can be accomplished only by assuming some kind of mean-field constraints for the operators in the hopping term of the t-J model; this procedure restricts, as mentioned above, the validity of the approach. It is also difficult to extend the isotropic spin-wave theory of Sokol *et al.*[16] to doped antiferromagnets, because it is unclear how to insert the hopping term into the linearization procedure used for the spin operator equations of motion.

On the other hand, the Green's function method is applicable at all temperatures and it naturally allows one to comprise the hopping term since the method uses the Lee algebra for Hubbard operators. The original Green's function method introduced by Tyablikov[19] is very successful in the study of 3D magnetic systems where the decoupling procedure yields a spin-wave spectrum which depends on the spontaneous magnetization, $\langle S_z \rangle$. However, $\langle S_z \rangle$ always vanishes in 1D and also in 2D Heisenberg systems at nonzero temperatures. Therefore, Kondo and Yamaji[17] (KY) proposed a new decoupling scheme which they applied to the study of the spin-1/2 isotropic Heisenberg chains. Their results are consistent with numerical calculations for finite chains.[20] In case of the 2D Heisenberg model, the original KY method was successfully applied by Fukumoto and Oguchi[21] and, with a semiphenomenological improvement, by Shimahara and Takada.[22]

In this paper, we extend, based on the Hubbard-operator presentation, the KY theory to the t-J model. Using the Green's function method we calculate, as a function of doping and temperature, the dynamic spin susceptibility, the spin correlation functions, and the AF correlation length.

The paper is organized as follows. In Sec. II, the Green's function method is applied to calculate the dynamic spin

susceptibility. In Sec. III, we compare our results for the static spin susceptibility, the correlation functions, the internal energy, and the temperature dependence of the AF correlation length with experimental results for La_2CuO_4 and with Monte Carlo calculations. Finally, Sec. IV presents the doping dependence of the AF correlation length together with an investigation of SRO suppression at zero temperature.

II. DERIVATION OF THE SUSCEPTIBILITY

Our starting point is the t-J Hamiltonian written in terms of the Hubbard operators:

$$H_{t\text{-}J}=H_t+H_J=\sum_{i,j,\sigma} t_{ij}X_i^{\sigma 0}X_j^{0\sigma}+\sum_{i>j} J_{ij}\left(\mathbf{S}_i\mathbf{S}_j-\frac{1}{4}n_in_j\right). \tag{1}$$

In Eq. (1), $\mathbf{S}_i$ are spin-1/2 operators at the lattice sites i, J_{ij} is a measure of the AF coupling between nearest-neighbor sites i,j, and $X_i^{\sigma 0}$ are the Hubbard operators that create an electron with spin σ at site i. The hopping integral t_{ij} describes the motion of electrons without causing a change in their spins. The spin and density operators are defined as follows:

$$S_i^{\sigma}=X_i^{\sigma\bar{\sigma}},\quad S_i^z=\frac{1}{2}\sum_{\sigma}\sigma X_i^{\sigma\sigma},$$

$$n_i=\sum_{\sigma} X_i^{\sigma\sigma}\quad(\sigma=-\bar{\sigma}), \tag{2}$$

with the standard normalization $X_i^{00}+X_i^{++}+X_i^{--}=1$. Without loss of generality, we can measure all energies from the center of gravity of the band.

A. Evaluation of commutators

Since the dynamic spin susceptibility $\chi_{+-}(\mathbf{q},\omega)$ depending on wave vector $\mathbf{q}$ and frequency ω is given by the two-time retarded Green's function

$$\chi_{+-}(\mathbf{q},\omega)=-g^2\mu_B^2\langle\langle S_q^+|S_{-q}^-\rangle\rangle_{\omega}, \tag{3}$$

it can be calculated by using the Heisenberg equations of motion. Here, S_q^+ is the Fourier transform of $X_i^{+0}X_j^{0-}$:

$$S_q^+=\frac{1}{N}\sum_{\mathbf{k},i,j} X_i^{+0}X_j^{0-}\exp[i(\mathbf{k}+\mathbf{q})\cdot\mathbf{r}_j-i\mathbf{k}\cdot\mathbf{r}_i]. \tag{4}$$

Green's functions satisfy the equation

$$\omega\langle\langle A|B\rangle\rangle_{\omega}=\langle[A,B]\rangle+\langle\langle[A,H]|B\rangle\rangle_{\omega}, \tag{5}$$

where $[A,B]$ denotes the commutator of the two operators A and B. Here H is the Hamiltonian of the system and $\langle\cdots\rangle$ denotes the thermal average:

$$\langle BA\rangle=\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\frac{[\langle\langle A|B\rangle\rangle_{\omega+i\varepsilon}-\langle\langle A|B\rangle\rangle_{\omega-i\varepsilon}]}{\exp(\omega/k_BT)-1}. \tag{6}$$

When evaluating Eq. (3) with the help of Eq. (5), we have to calculate the commutator $[X_i^{+0}X_j^{0-},H]$, with H given by Eq. (1), and the thermal average $\langle[X_i^{+0}X_j^{0-},S_{-q}^-]\rangle$. We get

$$[X_i^{+0}X_j^{0-},H_t]=\sum_s t_{js}[X_i^{+0}X_s^{0-}(1-X_j^{++})+X_i^{+0}X_s^{0+}S_j^+]-\sum_s t_{is}[(1-X_i^{--})X_s^{+0}X_j^{0-}+S_i^+X_s^{-0}X_j^{0-}], \tag{7}$$

$$[X_i^{+0}X_j^{0-},H_J]=\frac{1}{2}\sum_s J_{js}[X_i^{+0}X_j^{0+}S_s^+-X_i^{+0}X_j^{0-}X_s^{++}]-\frac{1}{2}\sum_s J_{is}[S_s^+X_i^{-0}X_j^{0-}-X_s^{--}X_i^{+0}X_j^{0-}], \tag{8}$$

and

$$\langle[X_i^{+0}X_j^{0-},S_{-q}^-]\rangle=\frac{1}{\sqrt{N}}[\langle X_i^{+0}X_j^{0+}\rangle e^{iqr_j}-\langle X_i^{-0}X_j^{0-}\rangle e^{iqr_i}].$$

It should be emphasized that these results are still exact and that they differ from the corresponding expressions in the Stoner theory of metals where one neglects electron correlations. In Eq. (7), terms containing S_j^+ or S_i^+ appear because Hubbard operators do not possess the fermionic commutation relations.

In order to proceed, we employ certain approximations. To evaluate the terms in Eq. (7), we use the decoupling procedure, namely, Hubbard-I, as proposed by Hubbard and Jain.[23] The procedure implies the following substitutions:

$$X_i^{+0}X_s^{0-}X_j^{++}\rightarrow(1-\delta_{ij})\langle X_j^{++}\rangle X_i^{+0}X_s^{0-},\quad X_i^{+0}X_s^{0+}S_j^+\rightarrow\langle X_i^{+0}X_s^{0+}\rangle S_j^+,$$

$$X_i^{--}X_s^{+0}X_j^{0-}\rightarrow(1-\delta_{ij})\langle X_i^{--}\rangle X_s^{+0}X_j^{0-},\quad S_i^+X_s^{-0}X_j^{0-}\rightarrow\langle X_s^{-0}X_j^{0-}\rangle S_i^+. \tag{9}$$

The terms in Eq. (8) can be calculated in the RPA, yielding

$$X_i^{+0}X_j^{0+}S_s^+\rightarrow(1-\delta_{ij})\langle X_i^{+0}X_j^{0+}\rangle S_s^++\delta_{ij}X_i^{++}S_s^+,\quad X_i^{+0}X_j^{0-}X_s^{++}\rightarrow(1-\delta_{ij})\langle X_s^{++}\rangle X_i^{+0}X_j^{0-}+\delta_{ij}S_i^+X_s^{++},$$

$$S_s^+X_i^{-0}X_j^{0-}\rightarrow(1-\delta_{ij})\langle X_i^{-0}X_j^{0-}\rangle S_s^++\delta_{ij}S_s^+X_i^{--},\quad X_s^{--}X_i^{+0}X_j^{0-}\rightarrow(1-\delta_{ij})\langle X_s^{--}\rangle X_i^{+0}X_j^{0-}+\delta_{ij}X_s^{--}S_i^+. \tag{10}$$

In each replacement, the first term on the right-hand side agrees with the usual result of the RPA. The second term, always rejected in the RPA, is responsible for the spin-spin correlations between Cu spins and, hence, becomes very important in the case of the low-dimensional spin systems treated in this work.

We note that, in the absence of long-range order, the average $\langle X_m^{\sigma\sigma}\rangle$ does not depend on the index and, according to Eq. (2), $\langle X^{++}\rangle=\langle X^{--}\rangle=(1-\delta)/2$, where δ is the number of *extra* holes, due to doping, per one planar Cu^{2+}.

B. Fourier transform of Green's function

We substitute Eqs. (7)–(10) into Eq. (5), perform a Fourier transform, and obtain the following:

$$\begin{aligned}(\omega+E_k-E_{k+q})\langle\langle X_k^{+0}X_{k+q}^{0-}|S_q^-\rangle\rangle_\omega &= (n_k-n_{k+q})+\frac{1-\delta}{2}\omega\langle\langle S_q^+|S_{-q}^-\rangle\rangle_\omega \\ &+[(\varepsilon_k+J_q)n_k-(\varepsilon_{k+q}+J_q)n_{k+q}]\langle\langle S_q^+|S_{-q}^-\rangle\rangle_\omega \\ &+\frac{1+\delta}{2}\frac{J}{\sqrt{N}}\sum_{l,\rho}e^{iqr_l}\langle\langle S_l^zS_{l+\rho}^+-S_l^+S_{l+\rho}^z|S_{-q}^-\rangle\rangle_\omega .\end{aligned} \tag{11}$$

Here, E_k is the energy of holes and ε_k is their kinetic energy in the absence of correlations. E_k and ε_k are related to each other by

$$\varepsilon_k=2t(\cos k_x+\cos k_y),\quad E_k=\frac{1+\delta}{2}\varepsilon_k, \tag{12}$$

where t is the hopping integral between *nearest* neighbors; t_{ij} values for hopping to other neighbors have been neglected. Similarly, J_{ij} has been replaced by the nearest-neighbor coupling constant J. We used the abbreviation $J_q=J(\cos q_x+\cos q_y)$.

In Eq. (11), the momentum distribution function $n_k=\langle X_k^{+0}X_k^{0+}\rangle=\langle X_k^{-0}X_k^{0-}\rangle$ is determined by the one-particle Green's function $\langle\langle X_k^{0\sigma}|X_k^{\sigma 0}\rangle\rangle_\omega$, which we calculated in the Hubbard-I decoupling approximation similar to the case described above. We obtain

$$n_k=\frac{1+\delta}{2}(1-f_k^h),$$

where $f_k^h(-E_k+\mu)=[\exp(-E_k+\mu)/k_BT+1]^{-1}$ is the Fermi function of holes and μ is the chemical potential which is related to δ by

$$\frac{2\delta}{1+\delta}=\frac{1}{N}\sum_k f_k^h .$$

For the same reason which we mentioned above [following Eq. (7)], the expression (11) differs from the corresponding result of the Stoner theory insofar as products like $\varepsilon_k\langle\langle S_q^+|S_{-q}^-\rangle\rangle_\omega$ do not appear and the last term of Eq. (11) is absent.

C. Calculation of the spin-spin correlation term

We will now calculate the last term on the right-hand side of Eq. (11); this term describes the correlations between Cu spins. Since the spin Green's function

$$G_q(\omega)=\frac{1}{\sqrt{N}}\sum_{l,\rho}e^{iqr_l}\langle\langle S_l^zS_{l+\rho}^+-S_l^+S_{l+\rho}^z\rangle\rangle_\omega$$

is the same as that for a pure Heisenberg antiferromagnet,[21] it may be derived within the (KY) decoupling procedure.[17] This technique allows one to explain gross features of the magnetic properties of the two-dimensional Heisenberg antiferromagnet, and this for all temperatures.[21] Following Ref. 21, we get

$$\begin{aligned}\omega G_q(\omega)=4(1-\gamma_q)\Bigg[\sum_\rho\langle S_l^zS_{l+\rho}^z\rangle+\frac{z^2}{2}\langle\langle S_q^+|S_{-q}^-\rangle\rangle_\omega\Bigg]+\frac{J}{\sqrt{N}}\sum_{l,\rho\neq\rho'}[\langle\langle S_{l+\rho}^zS_{l+\rho'}^z,S_l^+-S_l^zS_{l+\rho-\rho'}^z,S_{l+\rho}^+|S_{-q}^-\rangle\rangle_\omega \\ -\langle\langle S_l^zS_{l+\rho'}^z,S_{l+\rho}^+-S_l^zS_{l+\rho}^zS_{l+\rho-\rho'}^+|S_{-q}^-\rangle\rangle_\omega+\langle\langle S_l^+S_{l+\rho'}^-,S_{l+\rho}^+-S_l^+S_{l+\rho}^-S_{l+\rho-\rho'}^+|S_{-q}^-\rangle\rangle_\omega/2 \\ -\langle\langle S_{l+\rho}^+,S_l^-S_{l+\rho}^+-S_l^+S_{l+\rho-\rho'}^+,S_{l+\rho}^-|S_{-q}^-\rangle\rangle_\omega/2]e^{iqr_l},\end{aligned} \tag{13}$$

where z is the number of nearest neighbors of spin l and $\gamma_q=(2/z)\Sigma_{\alpha=1}^{z/2}\cos q_\alpha$. Note that the hopping term H_t does not contribute to $G_q(\omega)$ in the Hubbard-I approximation.

Kondo and Yamaji[17] decoupled the higher-order Green's function by using the following scheme:

$$S_l^zS_{l+\rho'}^z,S_{l+\rho}^+\rightarrow\alpha\langle S_l^zS_{l+\rho'}^z\rangle S_{l+\rho}^+,$$

$$S_{l+\rho}^zS_{l+\rho'}^z,S_l^+\rightarrow\beta\langle S_{l+\rho}^zS_{l+\rho'}^z\rangle S_l^+ ,$$

$$S_l^+S_{l+\rho'}^-,S_{l+\rho}^+\rightarrow\alpha\langle S_l^+S_{l+\rho'}^-\rangle S_{l+\rho}^++\beta\langle S_{l+\rho'}^-,S_{l+\rho}^+\rangle S_l^+ ,$$

and similarly for the other Green's functions. While usually, in the decoupling of Green's functions, one sets $\alpha=\beta=1$, Kondo and Yamaji introduced $\alpha,\beta\neq 1$. A value $\alpha\neq 1$ preserves the important property that spin operators obey the relation $\langle\mathbf{S}_i^2\rangle=3/4$ which should hold at all temperatures. The parameter β has been introduced for flexibility reasons; it can be defined in various ways. For simplicity, in Ref. 21 the assumption $\alpha=\beta$ has been made, as in the original work of Kondo and Yamaji.[17] In this case, the theory is completely self-consistent. However, as we shall see below, the condition $\alpha=\beta$ underestimates the role of the next-nearest spin-spin correlations. Therefore, in our theory, β is a variational

parameter whose value is obtained by a comparison with experiment under the assumption that this value does not depend on doping and temperature.

Evaluation of Eq. (13) then yields

$$\omega G_q(\omega)=4zc_1(1-\gamma_q)+\frac{\omega_q^2}{J}\langle\langle S_q^+|S_q^-\rangle\rangle_\omega . \tag{14}$$

Here, ω_q is the energy of the magnetic excitations,

$$\omega_q^2=\frac{J^2zg_-}{2}(1-\gamma_q)(g_++\gamma_q), \tag{15}$$

g_+, g_- are abbreviations which stand for

$$g_+=[1+4(z-1)\beta c_2+4\alpha|c_1|]/g_-, \quad g_-=4\alpha z|c_1|, \tag{16}$$

and c_1, c_2 denote the nearest and next-nearest spin-spin correlation function, respectively, of Cu spins:

$$c_1=\frac{1}{z}\sum_\rho \langle S_i^zS_{i+\rho}^z\rangle, \quad c_2=\frac{1}{z(z-1)}\sum_{\rho\neq\rho'}\langle S_i^zS_{i+\rho-\rho'}^z\rangle. \tag{17}$$

Thus, the essential parameters of $\omega G_q(\omega)$ are α, β, c_1, and c_2.

D. Final result

Inserting Eq. (14) into Eq. (11) and taking into account the relation $S_q^+=\Sigma_k X_k^{+0}X_{k+q}^{0-}/N$, which follows from Eq. (4), our result for the dynamic spin susceptibility becomes

$$\chi_{+-}(\mathbf{q},\omega)=\frac{\omega\chi_0(\mathbf{q},\omega)+4Jzc_1(1-\gamma_q)Z(\mathbf{q},\omega)}{\omega\chi_1(\mathbf{q},\omega)+(\omega^2-\omega_q^2)Z(\mathbf{q},\omega)}, \tag{18}$$

where

$$\chi_0(\mathbf{q},\omega)=\sum_k \frac{f_k^h-f_{k+q}^h}{\omega+E_k-E_{k+q}},$$

$$\chi_1(\mathbf{q},\omega)=J_q\chi_0(\mathbf{q},\omega)+\sum_k \frac{\varepsilon_k f_k^h-\varepsilon_{k+q}f_{k+q}^h}{\omega+E_k-E_{k+q}},$$

$$Z(\mathbf{q},\omega)=\sum_k \frac{1}{\omega+E_k-E_{k+q}}.$$

$\chi_0(\mathbf{q},\omega)$ denotes the dynamic susceptibility of free holes. $\chi_1(\mathbf{q},\omega)$ has a similar meaning as the exchange enhancement factor in the RPA, where, however, the second term of $\chi_1(\mathbf{q},\omega)$ is equal to 1. In our theory, this second term is due to the strong electron correlations and provides the correct concentration behavior of $\chi_{+-}(\mathbf{q},\omega)$ at half-filling ($\delta=0$).[23] $Z(\mathbf{q},\omega)$ is a convenient abbreviation.

Our result for $\chi_{+-}(\mathbf{q},\omega)$ agrees with special cases treated in the literature. If $J=0$, we have agreement with the relation derived by Hubbard and Jain.[23] For $J\neq 0$ but without AF correlations, our result is consistent with results of Refs. 24 and 25.

Finally, we have to determine self-consistent equations for the parameters c_1, c_2, and α. We can express these parameters in terms of $\chi_{+-}(\mathbf{q},\omega)$ by using the relation $2\langle S_l^zS_m^z\rangle=\langle S_l^+S_m^-\rangle$, which holds for the isotropic Heisenberg term in Eq. (1), and the thermal average definition of Eq. (6). When taking the average, we have replaced the integration over ω by summation over Matsubara's frequencies, $\omega_m=2\pi mT$, where $m=-\infty,\ldots,-1,0,1,\ldots,\infty$. We get

$$\frac{1}{2}=k_BT\sum_{q,m}\chi_{+-}(\mathbf{q},i\omega_m), \tag{19}$$

$$2c_1=k_BT\sum_{q,m}\gamma_q\chi_{+-}(\mathbf{q},i\omega_m), \tag{20}$$

$$2(z-1)c_2=k_BT\sum_{q,m}(z\gamma_q^2-1)\chi_{+-}(\mathbf{q},i\omega_m). \tag{21}$$

We conclude this section by addressing the relation between the width of the conduction band, E_k, and the hopping integral t. The width, as given by Eq. (12), is doping dependent, where the reduction factor $(1+\delta)/2$ is due to the strong electron correlations. However, this reduction is not sufficient to reconcile results of experiments and Monte Carlo (MC) calculations.[26] The origin of this discrepancy arises from the fact that the AF spin correlations reduce the width of the conduction band.

The reduction effect cannot be treated in the Hubbard-I approximation we used above. Roth[27] improved the Hubbard-I approximation by introducing the nonperturbative two-pole ansatz for the one-particle spectrum. It can be shown that this ansatz is essentially equivalent to the Mori-Zwanzig projection technique[28,29] and is strongly related to the moments method.[30] Since then, this new approach has been studied by many authors,[24,29,31–33] and became a general method to treat approximately, with no need for a small parameter,[34] the quasiparticle spectrum and the spectral density in an interacting system. The reliability of the method has been demonstrated by comparison with exact diagonalization results.[33]

Using the Roth method, one finds[32] that the hopping integral t is reduced by AF correlations, resulting in an effective value

$$t_{eff}=t\left(1+\frac{4\langle S_iS_j\rangle_1}{(1+\delta)^2}\right),$$

where $\langle S_iS_j\rangle_1=3c_1$ is the nearest-neighbor spin correlation function. This effect, which has recently been discussed in Refs. 35 and 36, is easily understood because a hole when moving through the Cu lattice retains its spin orientation. From now on we replace t by t_{eff}.

III. CORRELATION LENGTH IN THE 2D HEISENBERG ANTIFERROMAGNET

In order to check our theory, we consider the case of the two-dimensional Heisenberg antiferromagnet (with $z=4$) where numerical results for the relevant parameters are already known. Since now $f_k^h=0$, the low-energy excitations predicted by the t-J model are spin waves with energies ω_q. In the limit of $T=0$, the self-consistent equations (19)–(21) can be solved exactly. With the help of Eqs. (16) and (17), we obtain

$$c_2=\frac{16|c_1|-1}{12},\quad g_-=\frac{4}{3}(1+12c_2\beta),\quad g_+=1, \quad (22)$$

and c_1 is determined from the equation

$$\beta(16|c_1|-1)=\frac{96c_1^2I^2}{(1-4|c_1|)^2}-1, \quad (23)$$

where $I=(8/\pi^2)E^2(1/\sqrt{2})-(2/\pi)=0.842$ and $E(x)$ is a complete elliptic integral.

Numerical values of these parameters may be compared with data of the literature by considering the static susceptibility χ_S and the magnetic excitation spectrum ω_q. Here χ_S is equal to $(1/2)\chi_{+-}(0,0)$.[11] Then, Eq. (18) becomes

$$\chi_S=\frac{2|c_1|}{Jg_-}.$$

We take $\beta=2.5$, because this value, as we shall see below, provides the best fit of our calculated AF correlation length to experimental data. Then, Eqs. (22) and (23) yield $c_1=-0.115$, $c_2=0.07$, $g_-=4.133$, and $\chi_S=0.055/J$.

These results agree quite well with those of various other theories. (i) The values of c_1, c_2, and χ_S agree remarkably well with those of a modified spin-wave theory,[14] namely, $c_1^{SW}=-0.112$, $c_2^{SW}=0.068$, and $\chi_S^{SW}=0.045/J$. (ii) Our χ_S value is compatible with the results $\chi_S=0.043/J$ and $\chi_S=0.06/J$ of the nonlinear σ model[12] and isotropic spin-wave theory,[16] respectively. (iii) The original KY procedure, with $\alpha=\beta$, gives $c_1^{KY}=-0.104$, $c_2^{KY}=0.055$, $g_-^{KY}=2.82$, and $\chi_S^{KY}=0.073/J$ which all are close to our result. (iv) Finally, our results for χ_S, c_1, and the internal energy $u=6c_1=-0.69$ agree quite well with Monte Carlo data: $\chi_S^{MC}=0.0446/J$,[37] $c_1^{MC}=-0.112$, and $u^{MC}=-0.6693$.[38]

According to Eq. (15), the excitation spectrum becomes, for $T=0$, $\omega_q=2JZ_c(1-\gamma_q^2)^{1/2}$ with $Z_c=\sqrt{g_-/2}=1.44$. The structure of ω_q agrees with the result of many other theories for antiferromagnets and our value for Z_c is consistent with $Z_c=1.36$ obtained by Sokol *et al.*[16] using the isotropic spin-wave model.

Having established the basic reliability of our model, we will now evaluate the AF correlation length. Let us consider the spin-spin correlation function $\langle \mathbf{S}(\mathbf{0})\cdot\mathbf{S}(\mathbf{r})\rangle$ for spins residing, for example, along the x axis of a square lattice. Utilizing the relation $\langle S_l^xS_m^x\rangle=\langle S_l^yS_m^y\rangle=\langle S_l^zS_m^z\rangle$ and Eqs. (6) and (18), we have

$$\langle \mathbf{S}(\mathbf{0})\cdot\mathbf{S}(\mathbf{r})\rangle=\frac{6J|c_1|}{N}\sum_q\frac{(1-\gamma_q)\cos q_x r}{\omega_q}\coth\frac{\omega_q}{2k_BT}. \quad (24)$$

Since the main contribution to the sum arises from $\mathbf{q}$ values which are close to the AF wave vector $\mathbf{Q}=(\pi/a,\pi/a)$, we can replace this sum by an integral over vectors $\mathbf{q}-\mathbf{Q}$ and Eq. (24) reduces to

$$\langle \mathbf{S}(\mathbf{0})\cdot\mathbf{S}(\mathbf{r})\rangle=(-1)^r\frac{24|c_1|k_BT}{Jg_-\pi}K_0(2\sqrt{(g_+-1)}r/a),$$

where a is the lattice period and $K_0(x)$ is the modified Bessel function. In the limit of large separations x, where $K_0(x)\sim\exp(-x)/\sqrt{x}$, we get

$$\langle \mathbf{S}(\mathbf{0})\cdot\mathbf{S}(\mathbf{r})\rangle\sim(-1)^r\sqrt{\frac{\xi}{r}}\exp(-r/\xi),$$

where ξ is the AF correlation length and given by

$$\xi=\frac{a}{2\sqrt{g_+-1}}. \quad (25)$$

Our correlation function has a distance dependence which is of the same shape as that given by the nonlinear σ model.[12]

We will now investigate the temperature dependence of the correlation length for a temperature range where the inequality $a^2/\xi^2\ll 1$ holds; this even refers to temperatures around 500 K as the numerical result will show. Substituting g_+, as taken from Eq. (25), into Eqs. (19) and (21), we solve these equations for ξ:

$$\frac{\xi}{a}\sim\frac{J\sqrt{g_-}}{k_BT}\exp(2\pi\rho_s/k_BT). \quad (26)$$

The temperature dependence of ξ, expressed by the exponential and the preexponential factor $1/T$, again agrees with the result of the spin-wave (SW) theory. The appearance of the factor $1/T$ in our and in the KY and SW theories is an artifact of the mean-field approach. Chakravarty *et al.*[12] eliminated this artifact by taking into account two-loop renormalization-group corrections.

In Eq. (26), ρ_s is called the stiffness; it is given by

$$\rho_s=\frac{Jg_-}{64|c_1|}[1-32|c_1|K^2(1/\sqrt{2})\sqrt{2/\pi^4g_-}], \quad (27)$$

where $K(x)$ is a complete elliptic integral.

We now determine numerical values for the temperature dependence of ξ in La_2CuO_4 using the experimental values $J=0.12$ eV (Ref. 39) and $a=3.79$ Å, and treating β as the only adjustable parameter. The best fit to the experimental data (see Fig. 1), which were deduced from neutron scattering,[40] was obtained with $\beta=2.5$. Obviously, the inequality $a^2/\xi^2\ll 1$ is fulfilled.

For comparison, we have also calculated ξ by using the original KY procedure when $\alpha=\beta$ (dashed line in Fig. 1). Although this procedure is capable of reproducing the temperature dependence, it fails to give the absolute value of ξ; at low temperatures the discrepancy is a factor of 10. This failure is connected, as we mentioned above, with underestimating, in the original KY theory, the role of the next-nearest spin-spin correlations. Indeed, an increase of the value of these correlations (expressed by c_2) causes an extension of the AF short-range order and, consequently, an enhancement of ξ. Since, in our theory, β enters in the combination βc_2, we can realize the ξ enhancement, even at fixed J, by increasing the value of β.

By solving Eqs. (22) and (23) and using Eq. (27), we determined, for $T=0$, how $2\pi\rho_S/J$ depends on the anisotropy $1-\alpha/\beta$ (see Fig. 2) and how the ratio α/β varies with β (inset in Fig. 2). While α/β depends only very weakly on

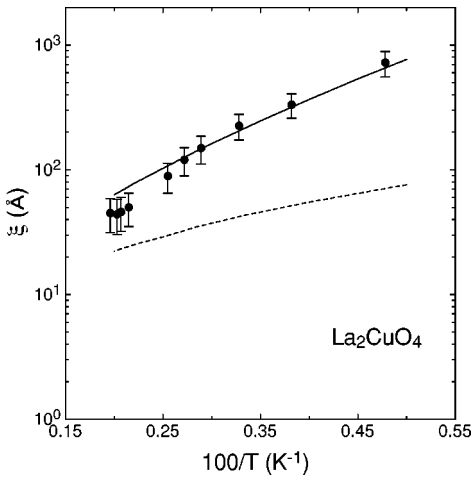

FIG. 1. The calculated temperature dependence (solid line) of the antiferromagnetic correlation length ξ compared with experimental data (solid circles) (Ref. 40) for La_2CuO_4 and with the result (dashed line) following from the original Kondo-Yamaji procedure (Ref. 17).

β, the stiffness is very sensitive to β. In case of the KY procedure, where $\alpha=\beta=1+1/2I^2=1.705$, the stiffness becomes

$$\frac{2\pi\rho_S^{KY}}{J}=\frac{\pi}{4I^2}\left(1+2I^2-\frac{8}{\pi^2}K^2(1/\sqrt{2})I\right)=0.0797,$$

which is an extremely small value. However, in our model, β is a parameter fixed to the value 2.5 by the fit to experimental data, resulting in a stiffness (see Fig. 2) which is 4.8 times larger than the KY value. This strong dependence of the stiffness and hence the even stronger dependence of ξ on the α/β anisotropy explains why our model fits the correlation length data better than the KY procedure does.

In Fig. 3, we compare our correlation length results with numerical MC data.[41] The agreement is fairly well except for a range around $T=0.5J$. In principle, the agreement between theory and MC calculations can be improved by making β temperature dependent as done by Winterfeldt and Ihle[42] who extracted $\beta(T)$ values from MC data in their treatment

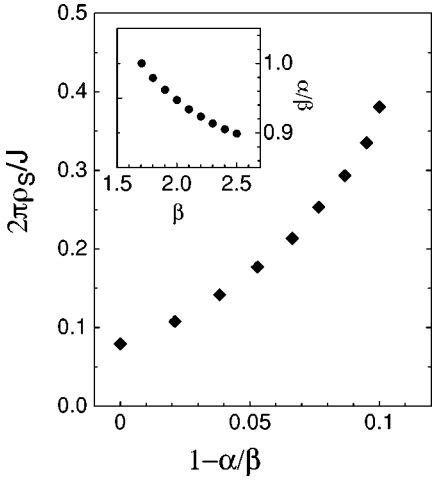

FIG. 2. The calculated dependence of the stiffness $2\pi\rho_S/J$ on the anisotropy $1-\alpha/\beta$. Inset: α/β as a function of β.

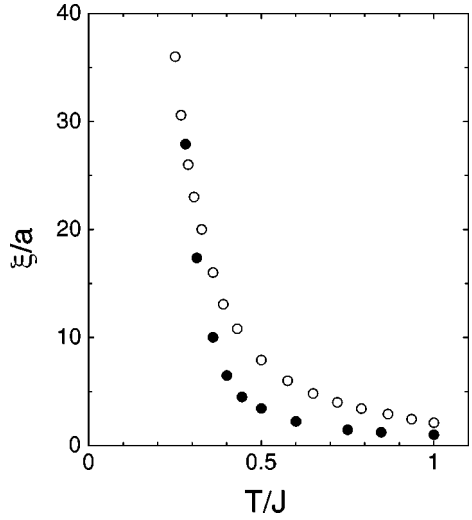

FIG. 3. The calculated temperature dependence of the AF correlation length (open circles) compared with MC data (solid circles) (Ref. 41).

of the 2D Heisenberg model. However, the improvements became noticeable only above 600 K which is a temperature range beyond our present interest.

IV. CORRELATION LENGTH AT FINITE DOPING

We turn now to the calculation of the temperature and concentration dependence of the correlation length ξ for finite doping. We first note that this can be accomplished by again using Eq. (25), and this for the following reason. Instead of obtaining ξ from the exponentional decay of the spin-spin correlation function at large separations, it may be derived from the expansion of the static susceptibility $\chi_{+-}(q)$ taken around the AF wave vector $\mathbf{Q}$.[43] For this case, Eq. (18) becomes

$$\chi_{+-}(\mathbf{Q}-\mathbf{q})=\frac{32|c_1|}{Jg_-[4(g_+-1)+q^2a^2]}.$$

According to Ref. 43, the quantity $4(g_+-1)+q^2a^2$ is equal to $a^2/\xi^2+q^2a^2$ and, therefore, we find $\xi^2=a^2/4(g_+-1)$ which is identical to Eq. (25). Again, g_+ should be derived from the self-consistent equations (19)–(21), however taking into account now the hole subsystem's contribution to $\chi_{+-}(\mathbf{q},\omega)$.

A. Derivation of the correlation length formula

In Eq. (19), $\chi_{+-}(\mathbf{q},i\omega_m)$ is given by Eq. (18). Since $\chi_{+-}(\mathbf{q},i\omega_m)$ itself strongly peaks at $\mathbf{q}=\mathbf{Q}$, we replace $\mathbf{q}$ by $\mathbf{Q}$ in the functions $\chi_0(\mathbf{q},i\omega_m)$, $\chi_1(\mathbf{q},i\omega_m)$, and $Z(\mathbf{q},i\omega_m)$, since they vary weakly with $\mathbf{q}$ near $\mathbf{Q}$ as we have shown by numerical calculations (not reproduced here). In order to calculate $\chi_0(\mathbf{Q},i\omega_m)$, $\chi_1(\mathbf{Q},i\omega_m)$, and $Z(\mathbf{Q},i\omega_m)$, we define, for the conduction band E_k, the density of states function in the following way:

$$w(E)=\frac{1}{N}\sum_k \delta(E-E_k).$$

For $N\to\infty$, $w(E)$ becomes

$$w(E)=\frac{1}{2\tilde{t}\pi^2}K(\sqrt{1-E^2/16\tilde{t}^2}),\quad -4\tilde{t}\leq E\leq 4\tilde{t},$$

with the abbreviation $\tilde{t}=t_{eff}(1+\delta)/2$. Then, substituting $w(E)$ into Eq. (19) and performing the integration over E, we find

$$\frac{1}{2}=\frac{16|c_1|k_BT}{Jg_+g_-\pi}K(1/g_+)+2k_BT\sum_{q,m=1}^{\infty}\frac{\upsilon_m+16J|c_1|(1-\gamma_q)}{\theta_m^2+\omega_m^2+\omega_q^2},\qquad(28)$$

where

$$\upsilon_m=\frac{8t_{eff}(1+\delta)}{\pi}\int_{-1}^{1}d\gamma\frac{\gamma K(\sqrt{1-\gamma^2})f_\gamma^h}{\gamma^2+\tilde{\omega}_m^2}\frac{\tilde{\omega}_m\sqrt{1+\tilde{\omega}_m^2}}{K(1/\sqrt{1+\tilde{\omega}_m^2})},$$

$$\tilde{\omega}_m=\frac{\omega_m}{8\tilde{t}},\qquad(29)$$

and

$$\theta_m^2=\frac{32t_{eff}^2(1+\delta)}{\pi}\int_{-1}^{1}d\gamma\frac{\gamma^2K(\sqrt{1-\gamma^2})f_\gamma^h}{\gamma^2+\tilde{\omega}_m^2}\times\frac{\tilde{\omega}_m\sqrt{1+\tilde{\omega}_m^2}}{K(1/\sqrt{1+\tilde{\omega}_m^2})}-2J\upsilon_m,\qquad(30)$$

with $f_\gamma^h=[\exp(-4\tilde{t}\gamma+\mu)/k_BT+1]^{-1}$ being the Fermi function of holes. At small hole concentrations δ, Eqs. (29) and (30) become

$$\upsilon_m=\frac{8\pi t_{eff}\delta}{K(1/\sqrt{1+\tilde{\omega}_m^2})}\frac{\tilde{\omega}_m}{\sqrt{1+\tilde{\omega}_m^2}}+O(\delta^2),$$

$$\theta_m^2=2(2t_{eff}-J)\upsilon_m.\qquad(31)$$

For δ values up to 0.1, $O(\delta^2)$ is at most 15% of the total result. The elliptic integral in the expression for υ_m appears because of the Van Hove singularity in the density of states of the conduction band E_k.

Equation (28) is the starting point for the calculation of ξ. First, we rewrite part of the sum on the right-hand side in the following way:

$$2k_BT\sum_{q,m=1}^{\infty}\frac{16J|c_1|(1-\gamma_q)}{\theta_m^2+\omega_m^2+\omega_q^2}=2k_BT\sum_{q,m=1}^{\infty}\frac{16J|c_1|(1-\gamma_q)}{\theta_1^2+\omega_m^2+\omega_q^2}-S_1,\qquad(32)$$

where

$$S_1=2k_BT\sum_{q,m=1}^{\infty}\frac{16J|c_1|(1-\gamma_q)(\theta_m^2-\theta_1^2)}{(\theta_m^2+\omega_m^2+\omega_q^2)(\theta_1^2+\omega_m^2+\omega_q^2)}.$$

The summation over m in the first term on the right-hand side of Eq. (32) is performed exactly. Inserting the results into Eq. (28), we arrive at

$$\frac{1}{2}=\frac{16k_BT|c_1|}{Jg_+g_-\pi}K(1/g_+)+S_2-S_1+16J|c_1|\sum_q(1-\gamma_q)\times\left[\frac{\coth[(\sqrt{\omega_q^2+\theta_1^2})/2k_BT]}{2\sqrt{\omega_q^2+\theta_1^2}}-\frac{k_BT}{\omega_q^2+\theta_1^2}\right],\qquad(33)$$

with

$$S_2=2k_BT\sum_{q,m=1}^{\infty}\frac{\upsilon_m}{\theta_m^2+\omega_m^2+\omega_q^2}.$$

To calculate the sum over $\mathbf{q}$ in Eq. (33), we expand all ω_q^2 around the AF vector $\mathbf{Q}$ and make the expansions

$$\coth x=1+2\sum_{m=1}^{\infty}\exp(-2mx),$$

$$K(1/g_+)=\ln(4g_+/\sqrt{g_+^2-1})+O(g_+^2-1).$$

Then, our result for the correlation length in doped samples becomes

$$\frac{\xi}{a}=\frac{J\sqrt{g_-}}{\theta_1}[1-\exp(-\theta_1/k_BT)]\exp(2\pi\tilde{\rho}_s/k_BT),\qquad(34)$$

where θ_1 is obtained from Eq. (30) for $m=1$.

For small δ values up to 0.1 [see note below Eq. (31)], θ_1^2 reduces to

$$\theta_1^2=\frac{8\pi^2\delta}{(1+\delta)}\frac{k_BT}{\sqrt{1+\tilde{\omega}_1{}^2}}\frac{2t_{eff}-J}{K(1/\sqrt{1+\tilde{\omega}_1{}^2})}$$

and the stiffness $\tilde{\rho}_s$ becomes

$$\tilde{\rho}_s=\rho_s-Jg_-(S_2-S_1)/32|c_1|,$$

where

$$\rho_s=\frac{Jg_-}{64|c_1|}\left[1-\frac{32\sqrt{2}|c_1|}{\sqrt{2+\lambda^2}}\times K^2(\sqrt{1-\lambda/\sqrt{2+\lambda^2}}/\sqrt{2})\sqrt{2/\pi^4g_-}\right],$$

$$\lambda=\frac{\theta_1}{J\sqrt{g_-}}.$$

Similar to Eqs. (22) and (23), we can calculate the correlation functions c_1 and c_2 in doped samples for $T=0$. Solving Eqs. (19) and (21) leads to

$$c_2=\frac{16|c_1|-1}{12}+\frac{2}{3}\tilde{S}_2, \quad g_-=\frac{4}{3}(1+12c_2\beta), \quad g_+=1, \tag{35}$$

and

$$\beta(16|c_1|-1+8\tilde{S}_2)=\frac{96c_1^2(I-\sqrt{2g_-}\tilde{S}_1/8)^2}{(1-4|c_1|-2S_2)^2}-1, \tag{36}$$

where

$$\tilde{S}_1=2k_BT\sum_{q,m=1}^{\infty}\frac{16J(1-\gamma_q^2)(\theta_m^2-\theta_1^2)}{(\theta_m^2+\omega_m^2+\omega_q^2)(\theta_1^2+\omega_m^2+\omega_q^2)},$$

$$\tilde{S}_2=2k_BT\sum_{q,m=1}^{\infty}\frac{\nu_m\gamma_q^2}{\theta_m^2+\omega_m^2+\omega_q^2},$$

to be taken in the limit $T\to 0$. Equations (35) and (36) reduce, as they should, to Eqs. (22) and (23) when δ approaches zero, because both ν_m and θ_m are $\sim\delta$ in this limit; see Eq. (31).

B. Discussion and comparison with experiments

We solved Eqs. (35) and (36) numerically for $La_{1.86}Sr_{0.14}CuO_4$, using the parameters $\delta=0.14$, $J=0.12$ eV, and $J/t=0.3$, which is reasonable for the t-J model.[44] Our result is $c_1=-0.066$, $c_2=0.043$, and $g_-=3.03$. Compared to the pure Heisenberg antiferromagnet, the spin correlation functions are now reduced by a factor ~ 2 and the stiffness $\tilde{\rho}_S$, which is now $0.11\rho_S^{AF}$, can be regarded as negligible at a hole concentration of ~ 0.14. For t_{eff}, we obtain 0.156 eV; hence, the conduction band is 4.5 times narrower than in the noninteracting case, in agreement with MC calculations.[45]

We will now discuss the doping and temperature dependence of the correlation length as given by Eq. (34). We first note that, for $\delta\to 0$, its solution smoothly goes over into the result for the Heisenberg antiferromagnet, that is, Eq. (26). Next, we remark that for all realistic temperatures and already small hole concentrations, the inequality $\exp(-\theta_1/k_BT)\ll 1$ is fulfilled. For larger doping, the inequality holds even better. For example, let us take $\delta=0.04$, $J=0.12$ eV, $T=1000$ K, and $t_{eff}=0.1$ eV which corresponds to a width of the conduction band of ~ 0.4 eV as observed experimentally in HTSC's and confirmed by MC calculations within the t-J model.[26] This then leads to $\exp(-\theta_1/k_BT)\sim 0.3$ and Eq. (34) becomes

$$\frac{\xi}{a}=\frac{J\sqrt{g_-}}{\theta_1}\exp(2\pi\tilde{\rho}_s/k_BT). \tag{37}$$

Thus, ξ turns out to be proportional to $1/\sqrt{\delta}$ in good agreement with neutron scattering experiments[46] and Monte Carlo calculations.[26] Equation (34) is more complex than the ''simpler'' relation $\xi=a/\sqrt{\delta}$ used in fitting the neutron scattering data.[46] It should be stressed that the origin of the proportionality $\xi\propto 1/\sqrt{\delta}$, in our model, arises from strong electron correlations.

The temperature dependence of the correlation length has been a controversial topic. In Eq. (37), the temperature appears not only in the exponential function but also in the parameter θ_1 which is essentially proportional to $\sqrt{T}$. It is satisfying that this temperature dependence of the preexponential factor agrees with the result of scaling theories.[47,48]

Thus, our theory predicts a temperature-*dependent* behavior of ξ even in doped samples. This conclusion is consistent with recent neutron scattering and NMR and nuclear quadrupole resonance (NQR) experiments. In neutron experiments with $La_{1.86}Sr_{0.14}CuO_4$ single crystals,[49] the authors discovered ''that the normal state magnetic response is characterized by nearly diverging amplitude and length scales.'' Indeed, ξ displays a noticeable temperature dependence: when increasing the temperature from $T_c=35$ K to 300 K, ξ decreases by a factor of 4.8 which is close to the ratio $\xi(35\ \text{K})/\xi(300\ \text{K})\sim 3.6$ we calculated by setting $\xi=J\sqrt{g_-}a/\theta_1$ and thus neglecting the stiffness. Moreover, our results agree even quantitatively with experiment. For example, our values of $\xi(35\ \text{K})=8.10a$ and $\xi(300\ \text{K})=2.23a$ are in good agreement with $\xi(35\ \text{K})=7.7a$ and $\xi(300\ \text{K})=1.6a$ found in neutron scattering.[49] A NMR-NQR detection of a temperature-dependent ξ has been reported by Curro *et al.*[50] who investigated $YBa_2Cu_4O_8$ and applied the scaling hypothesis of Barzykin and Pines.[51]

Finally, we comment on a special consequence of our approximate decoupling procedure. According to Eq. (34), ξ diverges at $T=0$ even in doped compounds, and this disagrees with experimental facts.[46] The origin of this disagreement is connected with using the KY decoupling procedure which, probably, overestimates the role of AF correlations at low temperatures. Indeed, according to Eq. (18), there is no contribution from the hole subsystem to $\chi_{+-}(\mathbf{q},\omega)$ at $\omega=0$, and hence, the AF long-range order persists at $T=0$ for any hole concentration. Thus, further improvement of our theory in this temperature limit can be achieved by taking into account higher orders of the equation of motion for the Green's functions, where nonzero weight of the hole spectral function at $\omega=0$ is expected.

V. CONCLUSION

Using the two-time Green's functions method within the framework of the t-J model, we have calculated the dynamic spin susceptibility of CuO_2 planes in high-temperature superconductors by taking into account both electron and antiferromagnetic spin correlations. The strong electron correlations modify the results of the RPA and hence the susceptibility and thus provide the correct susceptibility behavior at half-filling. The effects of AF correlations were considered within a short-range order theory which provides a systematic treatment of spin correlations in terms of two-spin correlation functions of arbitrary range. It was found that the hole dynamics rapidly suppresses the short-range

order, and this suppression is reflected in the reduction of the stiffness of the system. We have further shown that our model is able to reproduce the main features of the temperature and doping dependences of the antiferromagnetic correlation length in both the pure Heisenberg antiferromagnet and doped compounds.

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