Theory of magnetic short-range order in the *t*-*J* model

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A spin-rotation-invariant theory of antiferromagnetic short-range order (SRO) in the two-dimensional *t*-*J* model is presented based on the Green's-function projection technique for the dynamic spin susceptibility which is divided into a local and an itinerant contribution. The SRO is incorporated in the local contribution. By a sum-rule-conserving mean-field approximation the two-spin correlation functions of arbitrary range, the staggered magnetization, and the uniform static spin susceptibility are calculated self-consistently over the whole doping and temperature region. A good agreement with available exact diagonalization data at ratios J/t realistic for the cuprates is found. The antiferromagnetic long-range order at $T=0$ is destroyed at the critical doping $\delta_c = 5.9\%$ ($J/t = 0.4$) in favor of a paramagnetic phase with SRO. The maxima in the doping and temperature dependences of the uniform spin susceptibility found in exact diagonalization studies are explained as an effect of antiferromagnetic SRO. Comparing the theory with magnetic susceptibility experiments on $La_{2-\delta}Sr_\delta CuO_4$, a reasonable agreement in the doping dependence is obtained. [S0163-1829(98)06838-6]

I. INTRODUCTION

The pronounced antiferromagnetic (AFM) spin correlations in high-T_c superconductors probed by neutron scattering[1,2] and their unconventional magnetic properties, such as the maximum in the doping and temperature dependences of the normal-state magnetic susceptibility of $La_{2-\delta}Sr_\delta CuO_4$ (LSCO),[3,4] yield a challenge for a microscopic theory of the dynamic spin susceptibility $\chi(\mathbf{q},\omega;T,\delta)$ that takes into account the AFM short-range order (SRO).

To explain the uniform static susceptibility $\chi(T,\delta)$ of LSCO, the concept of magnetic SRO was elaborated in the three-band[5] and one-band Hubbard models,[6] and in the *t*-*J* model.[7–9] In the one-band correlation models, the evaluation of SRO effects within a slave-boson functional-integral scheme at $T=0$ (Refs. 6,7) yields a good agreement with the doping dependence of the low-temperature magnetic susceptibility of LSCO.[3] To calculate the SRO (two-spin correlation functions) in the *t*-*J* model near half-filling, Shimahara and Takada[8,9] proposed a spin-rotation-invariant Green's-function decoupling scheme introducing site-dependent vertex parameters. In Ref. 9 the lowest-order corrections by *t* are considered, so that the maximum in χ as a function of doping is not reproduced. Up to now, there has been no analytical approach to the *t*-*J* model that describes both the doping and temperature dependences of SRO and their effects on the spin susceptibility in accordance with experiments. In a previous paper,[10] hereafter referred to as I, we developed a spin-rotation-invariant theory of SRO in the square-lattice AFM Heisenberg model based on the Green's-function projection technique for the dynamic spin susceptibility, using the decoupling scheme by Shimahara and Takada.[8,9]

In this paper we extend the Green's-function projection approach of I and present a theory of AFM SRO for the *t*-*J* model. We focus on the two-spin correlation functions of arbitrary range and on the uniform static spin susceptibility as functions of doping and temperature over the whole range of variables. In particular, we study the competition between

magnetic long-range order (LRO) and SRO at $T=0$. Our main goals are to compare the theory with available exact diagonalization data and with experiments on LSCO.

II. DYNAMIC SPIN SUSCEPTIBILITY

We start with the *t*-*J* model on the square lattice written in terms of Hubbard operators $X_i^{pq} = |p_i\rangle\langle q_i| [p,q \in (0,\sigma); \sigma = \pm]$ as

$$H = H_t + H_J$$
$$= -t \sum_{\langle i,j \rangle,\sigma} X_i^{\sigma 0} X_j^{0\sigma} + \frac{J}{2} \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \mathbf{S}_j - \frac{1}{4} n_i n_j \right), \quad (1)$$

with $\mathbf{S}_i = \frac{1}{2} \sum_{\sigma,\sigma'} X_i^{\sigma 0} \boldsymbol{\tau}_{\sigma\sigma'} X_i^{0\sigma'}$ and $n_i = \sum_\sigma X_i^{\sigma\sigma}$. For the cuprates, realistic values of J/t are $0.3 \lesssim J/t \lesssim 0.4$.[11]

In the projection method (cf. I), two sets of basis operators, $\mathbf{A} = (A^{(1)}, \ldots, A^{(n)})^T$ and $\mathbf{B} = (B^{(1)}, \ldots, B^{(n)})^T$, are chosen to calculate the two-time retarded matrix Green's function $\mathbf{G}(\omega) = \langle\langle \mathbf{A}; \mathbf{B}^+ \rangle\rangle_\omega$. Neglecting the self-energy defines a generalized mean-field approximation, and we get

$$\mathbf{G}(\omega) = (\omega - \mathbf{M}'\mathbf{M}^{-1})^{-1}\mathbf{M}, \quad (2)$$

with the spectral moments

$$\mathbf{M} = \langle [\mathbf{A}, \mathbf{B}^+] \rangle, \quad \mathbf{M}' = \langle [i\dot{\mathbf{A}}, \mathbf{B}^+] \rangle. \quad (3)$$

To describe SRO effects in a wide doping region, the localized-itinerant complementarity must be adequately taken into account, which can be achieved by interpolating between the Heisenberg limit ($\delta = 0$) and the low-density limit (free band electrons). To this end, we exploit the rotational symmetry of the dynamic spin susceptibility $\chi^{+-}(\mathbf{q},\omega) = -\langle\langle S_\mathbf{q}^+; S_{-\mathbf{q}}^- \rangle\rangle_\omega$. Thus, the equation of motion $\omega\langle\langle S_\mathbf{q}^+; S_{-\mathbf{q}}^- \rangle\rangle_\omega = \langle\langle i\dot{S}_\mathbf{q}^+; S_{-\mathbf{q}}^- \rangle\rangle_\omega$ permits us to separate $\chi^{+-}(\mathbf{q},\omega)$ into a local and an itinerant contribution,

$$\chi^{+-}(\mathbf{q},\omega) = \chi_J^{+-}(\mathbf{q},\omega) + \chi_t^{+-}(\mathbf{q},\omega), \quad (4)$$

with

$$\chi_{J,t}^{+-}(\mathbf{q},\omega)=-\frac{1}{\omega}\langle\langle J_{\mathbf{q}}^{J,t};S_{-\mathbf{q}}^{-}\rangle\rangle_{\omega}; \quad J_{\mathbf{q}}^{J,t}=[S_{\mathbf{q}}^{+},H_{J,t}]. \quad (5)$$

The local and itinerant contributions predominate in the Heisenberg and low-density limits, respectively. Both contributions are calculated by the Green's-function projection method employing decoupling procedures adapted to the localized or itinerant characteristics.

First we consider the local contribution $\chi_J^{+-}(\mathbf{q},\omega)$. To calculate the Green's function $\langle\langle J_{\mathbf{q}}^{J};S_{-\mathbf{q}}^{-}\rangle\rangle_{\omega}$ taking into account the AFM SRO, we choose the basis sets

$$\mathbf{A}=(J_{\mathbf{q}}^{J},i\dot{J}_{\mathbf{q}}^{J})^{T}, \quad \mathbf{B}=(S_{\mathbf{q}}^{+},i\dot{S}_{\mathbf{q}}^{+})^{T}. \quad (6)$$

Concerning the spectral moments, we note that neglecting the self-energy (cf. I) corresponds to the approximation

$$-\ddot{S}_{-\mathbf{q}}^{-}=\omega_{\mathbf{q}}^{2}S_{-\mathbf{q}}^{-}, \quad (7)$$

where $\omega_{\mathbf{q}}$ is the spin-excitation spectrum (see below). Then, the second moment is given by

$$M_{\mathbf{q}}^{(2)}=\langle[J_{\mathbf{q}}^{J},-\ddot{S}_{-\mathbf{q}}^{-}]\rangle=\omega_{\mathbf{q}}^{2}M_{\mathbf{q}}^{(0)}, \quad (8)$$

where

$$M_{\mathbf{q}}^{(0)}=\langle[J_{\mathbf{q}}^{J},S_{-\mathbf{q}}^{-}]\rangle=-8JC_{1,0}(1-\gamma_{\mathbf{q}}), \quad (9)$$

and $\gamma_{\mathbf{q}}=\frac{1}{2}(\cos q_x+\cos q_y)$. $C_{\mathbf{R}}\equiv C_{n,m}$ denotes the spin correlation function

$$C_{\mathbf{R}}=\langle S_0^+S_{\mathbf{R}}^-\rangle=\frac{1}{N}\sum_{\mathbf{q}}\langle S_{\mathbf{q}}^+S_{-\mathbf{q}}^-\rangle\cos\mathbf{q}\mathbf{R}, \quad (10)$$

with $\mathbf{R}=n\mathbf{e}_x+m\mathbf{e}_y$. Furthermore, we get $M_{\mathbf{q}}^{(1)}=\langle[i\dot{J}_{\mathbf{q}}^{J},S_{-\mathbf{q}}^{-}]\rangle=0$ and $M_{\mathbf{q}}^{(3)}=\langle[i\dot{J}_{\mathbf{q}}^{J},-\ddot{S}_{-\mathbf{q}}^{-}]\rangle=\omega_{\mathbf{q}}^{2}M_{\mathbf{q}}^{(1)}=0$.

By Eq. (2) and the moments (8) and (9), we obtain the local contribution

$$\chi_J^{+-}(\mathbf{q},\omega)=-\frac{M_{\mathbf{q}}^{(0)}}{2\omega_{\mathbf{q}}}\left(\frac{1}{\omega-\omega_{\mathbf{q}}}-\frac{1}{\omega+\omega_{\mathbf{q}}}\right). \quad (11)$$

Calculating the spectrum $\omega_{\mathbf{q}}$ according to Eq. (7) we take the site representation, where $-\ddot{S}_i^-$ contains products of three spin operators along nearest-neighbor sequences, e.g., $S_i^-S_j^-S_l^+$, and spin-hole interaction terms, e.g., $S_i^-X_j^{-0}X_l^{0-}$ ($j\neq i$, $l\neq i$). To approximate the spin-spin interactions, we apply the decoupling procedure proposed by Shimahara and Takada:[8,9]

$$S_i^-S_j^-S_l^+=\alpha_1\langle S_j^-S_l^+\rangle S_i^-+\alpha_2\langle S_i^-S_l^+\rangle S_j^-, \quad (12)$$

where the vertex parameters α_1 and α_2 are attached to nearest-neighbor and further-distant correlation functions, respectively. Compared to I, we have simplified the site dependence of the vertex parameters ($\alpha_2^I=\alpha_1^I\equiv\alpha_1$, $\alpha_3^I\equiv\alpha_2$).

Decoupling the spin-hole interactions, we introduce a vertex parameter λ as follows:

$$S_i^-X_j^{-0}X_l^{0-}=\lambda\langle X_j^{-0}X_l^{0-}\rangle S_i^-. \quad (13)$$

Following the approximation scheme of Ref. 9, we neglect the cross-correlation terms ($\propto Jt$) and those t^2 terms which would violate the relation (7). Finally, we obtain

$$\omega_{\mathbf{q}}^{2}=(1-\gamma_{\mathbf{q}})(A_1+A_2\gamma_{\mathbf{q}}), \quad (14)$$

with

$$A_1=4J^2\left[\lambda\frac{n}{2}-\alpha_1C_{1,0}+\alpha_2(C_{2,0}+2C_{1,1})\right]$$
$$+8t^2[1-\lambda(n+F_{2,0}+2F_{1,1})], \quad (15)$$

$$A_2=-16J^2\alpha_1C_{1,0}, \quad (16)$$

and the transfer amplitudes $F_{\mathbf{R}}\equiv F_{n,m}$,

$$F_{\mathbf{R}}=\langle X_0^{+0}X_{\mathbf{R}}^{0+}\rangle=\frac{1}{N}\sum_{\mathbf{k}}F_{\mathbf{k}}\cos\mathbf{k}\mathbf{R}, \quad (17)$$

where $F_{\mathbf{k}}=\langle X_{\mathbf{k}}^{+0}X_{\mathbf{k}}^{0+}\rangle$ and $n=\langle n_i\rangle$.

Now we calculate the itinerant contribution $\chi_t^{+-}(\mathbf{q},\omega)$. By Eq. (5) we get

$$\chi_t^{+-}(\mathbf{q},\omega)=-\frac{1}{\omega N}\sum_{\mathbf{k}}(\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}})G_{\mathbf{kq}}(\omega), \quad (18)$$

with $\epsilon_{\mathbf{k}}=-4t\gamma_{\mathbf{k}}$ and the Green's function

$$G_{\mathbf{kq}}(\omega)=\langle\langle A_{\mathbf{kq}};S_{-\mathbf{q}}^{-}\rangle\rangle_{\omega}; \quad A_{\mathbf{kq}}=\sqrt{N}X_{\mathbf{k}}^{+0}X_{\mathbf{k}+\mathbf{q}}^{0-}. \quad (19)$$

To calculate $G_{\mathbf{kq}}(\omega)$ we take the basis $A=A_{\mathbf{kq}}$, $B=S_{\mathbf{q}}^+$ and get

$$G_{\mathbf{kq}}(\omega)=\frac{M_{\mathbf{kq}}^{(0)}}{\omega-\omega_{\mathbf{kq}}}; \quad \omega_{\mathbf{kq}}=\frac{M_{\mathbf{kq}}^{(1)}}{M_{\mathbf{kq}}^{(0)}}, \quad (20)$$

with the moments

$$M_{\mathbf{kq}}^{(0)}=\langle[A_{\mathbf{kq}},S_{-\mathbf{q}}^{-}]\rangle=F_{\mathbf{k}}-F_{\mathbf{k}+\mathbf{q}} \quad (21)$$

and $M_{\mathbf{kq}}^{(1)}=\langle[i\dot{A}_{\mathbf{kq}},S_{-\mathbf{q}}^{-}]\rangle$. Performing a Hartree-Fock decoupling of the spin-hole interaction terms in $i\dot{A}_{\mathbf{kq}}$, we obtain

$$i\dot{A}_{\mathbf{kq}}=(\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}})A_{\mathbf{kq}}+T_{\mathbf{kq}}$$
$$+[\epsilon_{\mathbf{k}}F_{\mathbf{k}}-\epsilon_{\mathbf{k}+\mathbf{q}}F_{\mathbf{k}+\mathbf{q}}+2J\gamma_{\mathbf{q}}(F_{\mathbf{k}}-F_{\mathbf{k}+\mathbf{q}})]S_{\mathbf{q}}^+, \quad (22)$$

with

$$T_{\mathbf{kq}}=-\frac{n}{2}(\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}})A_{\mathbf{kq}}$$
$$+\frac{1}{N}\sum_{\mathbf{k}'}(\epsilon_{\mathbf{k}'+\mathbf{q}}F_{\mathbf{k}}-\epsilon_{\mathbf{k}'}F_{\mathbf{k}+\mathbf{q}})A_{\mathbf{k}'\mathbf{q}}. \quad (23)$$

To keep the calculations tractable, the Fock term in $T_{\mathbf{kq}}$ is taken into account effectively by the approximation

$$T_{\mathbf{kq}}=-\eta\frac{n}{2}(\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}})A_{\mathbf{kq}}, \quad (24)$$

where we have introduced the decoupling parameter η. Then we have

$$\omega_{\mathbf{kq}} = \left(1 - \eta\frac{n}{2}\right)(\epsilon_{\mathbf{k+q}} - \epsilon_{\mathbf{k}}). \qquad (25)$$

By Eqs. (18), (20), and (25) we obtain the itinerant contribution

$$\chi_t^{+-}(\mathbf{q},\omega) = \frac{1}{\left(1-\eta\dfrac{n}{2}\right)N} \sum_{\mathbf{k}} \frac{F_{\mathbf{k+q}} - F_{\mathbf{k}}}{\omega - \omega_{\mathbf{kq}}}. \qquad (26)$$

To determine the distribution function $F_{\mathbf{k}}$, occurring in the local and itinerant contributions [see Eqs. (15), (17), and (26)], from the Green's function $\langle\langle X_{\mathbf{k}}^{0+}; X_{\mathbf{k}}^{+0}\rangle\rangle_\omega$, we use the Hubbard I approximation[12] and get

$$F_{\mathbf{k}} = \left(1 - \frac{n}{2}\right) f(E_{\mathbf{k}}) \qquad (27)$$

with

$$E_{\mathbf{k}} = \left(1 - \frac{n}{2}\right)\epsilon_{\mathbf{k}} - Jn, \qquad (28)$$

where $f(\omega) = (e^{(\omega-\mu)/T} + 1)^{-1}$. The chemical potential μ is given by the number condition

$$n = \frac{2}{N} \sum_{\mathbf{k}} F_{\mathbf{k}}. \qquad (29)$$

Note that the itinerant contribution (26) vanishes in the limit $n=1$ ($\lim_{n\to 1} F_{\mathbf{k}} = \frac{1}{2}$) and becomes the familiar Lindhard function for $n\to 0$.

For both the local and itinerant contributions, we have checked that our scheme preserves the spin-rotation invariance, i.e., for the total susceptibility we have $\chi(\mathbf{q},\omega) \equiv \chi^{zz}(\mathbf{q},\omega) = \frac{1}{2}\chi^{+-}(\mathbf{q},\omega)$. From Eqs. (4), (11), (9), and (26) we get the static spin susceptibility

$$\chi(\mathbf{q}) = -\frac{8JC_{1,0}}{\omega_{\mathbf{q}}^2}(1-\gamma_{\mathbf{q}}) + \frac{1}{\left(1-\eta\dfrac{n}{2}\right)^2 N}\sum_{\mathbf{k}} \frac{F_{\mathbf{k}} - F_{\mathbf{k+q}}}{\epsilon_{\mathbf{k+q}} - \epsilon_{\mathbf{k}}}, \qquad (30)$$

and the two-spin correlation function

$$\langle S_{\mathbf{q}}^+ S_{-\mathbf{q}}^- \rangle = -\frac{4JC_{1,0}}{\omega_{\mathbf{q}}}(1-\gamma_{\mathbf{q}})[1 + 2n_B(\omega_{\mathbf{q}})]$$
$$+ \frac{1}{\left(1-\eta\dfrac{n}{2}\right)N}\sum_{\mathbf{k}}(F_{\mathbf{k}} - F_{\mathbf{k+q}})n_B(\omega_{\mathbf{kq}}), \qquad (31)$$

where $n_B(\omega) = (e^{\omega/T} - 1)^{-1}$. By Eqs. (10), (14) to (16), and (31), the correlation functions $C_{n,m}$ are evaluated self-consistently.

For the determination of the decoupling parameter η and the vertex parameters α_1, α_2, and λ we employ the sum rule

$$C_{0,0} = \langle S_0^+ S_0^- \rangle = \frac{n}{2}. \qquad (32)$$

Due to the mean-field approximations made to obtain the excitation spectra (14) and (25), it is inappropriate to con-

sider higher-order sum rules involving higher correlation functions. Therefore, we treat only one parameter as doping dependent.

The parameters α_1 and α_2 cannot be used to satisfy the sum rule (32) with Eq. (31) at high hole densities because for $t\gtrsim J$ the t^2 term in Eq. (15) will dominate the J^2 term at high enough doping levels. Therefore, the influence of $\alpha_{1,2}$ on the local contribution to $\langle S_{\mathbf{q}}^+ S_{-\mathbf{q}}^- \rangle$ rapidly weakens with increasing doping. Similarly, the parameter η in the itinerant contribution of Eq. (31) does not allow to satisfy the sum rule at small doping levels, since the local contribution dominates the itinerant one there. The vertex parameter λ, however, which describes the coupling between the spin and hole degrees of freedom, is suitable to satisfy the sum rule (32) over the whole density region. As a consequence, we fix the parameters $\alpha_{1,2}$ and η at their values in the limits $n=1$ and $n\to 0$, respectively, and take λ as doping dependent.

First, we consider the undoped case, $n=1$. In this limit, the kinetic term H_t of Eq. (1) has no influence on physical quantities and therefore the theory may not depend on t. By this condition, as can be seen from Eq. (15) and $F_{\mathbf{R}}=0$ for $\mathbf{R}\neq 0$, we have to choose $\lambda(n=1)=1$. Thus, the $n=1$ limit becomes the Heisenberg limit, and Eqs. (14) to (16) agree with the result of I. To determine the parameters α_1 and α_2 in this limit, we use the sum rule and get $\alpha_1 = \alpha_1(T)$. To obtain $\alpha_2(T)$, we take the Monte Carlo value of the ground-state energy [$3C_{1,0} = -0.6693J$ (Ref. 13)] and, following Ref. 8, assume the ratio $[\alpha_2(T)-1]/[\alpha_1(T)-1] = 0.8530$ as temperature independent.

Considering the limit $n\to 0$, the parameter η is calculated by a low-density expansion which, for $T=0$, is detailed in the next section. Thereby, $\eta(T)$ turns out to be independent of the vertex parameters.

III. MAGNETIC LONG-RANGE ORDER VERSUS SHORT-RANGE ORDER

The critical behavior of the t-J model is reflected in our approach by the divergence of the local contribution to $\chi(\mathbf{q})$ at $\mathbf{Q}=(\pi,\pi)$ as $T\to 0$, i.e., by $\omega_{\mathbf{Q}}(T=0)=0$ [cf. Eq. (30)]. Accordingly, in the phase with AFM LRO which may occur at $T=0$ only (in agreement with the Mermin-Wagner theorem) we get the condition $A_1 = A_2$ [cf. Eq. (14)] and the spin-wave spectrum

$$\omega_{\mathbf{q}}^2 = -16J^2\alpha_1 C_{1,0}(1-\gamma_{\mathbf{q}}^2). \qquad (33)$$

To calculate the correlation functions (10) with Eq. (31) in the LRO phase, we separate the condensation part C, arising from $\omega_{\mathbf{Q}}=0$, as follows:

$$C_{\mathbf{R}} = \sqrt{-\frac{C_{1,0}}{\alpha_1}}\, I_{\mathbf{R}} + C\cos\mathbf{QR} + C_{\mathbf{R}}^t, \qquad (34)$$

where

$$I_{\mathbf{R}} = \frac{1}{N}\sum_{\mathbf{q}}\sqrt{\frac{1-\gamma_{\mathbf{q}}}{1+\gamma_{\mathbf{q}}}}\cos\mathbf{qR}, \qquad (35)$$

with $I_{0,0} = 1.393$ and $I_{1,0} = -0.551$. $C_{\mathbf{R}}^t$ is the itinerant contribution which results from Eq. (31) in the $T=0$ limit making use of $\omega_{\mathbf{kq}} \propto E_{\mathbf{k+q}} - E_{\mathbf{k}}$ and of the identity $[f(\omega) - f(\omega')]n_B(\omega'-\omega) = f(\omega')[1-f(\omega)]$,
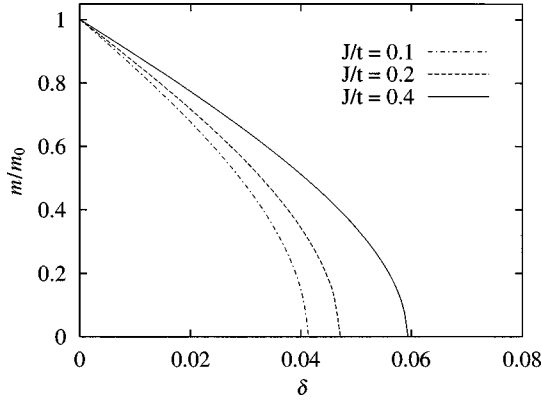
FIG. 1. Staggered magnetization as a function of hole doping for different values of J/t.

$$C_{\mathbf{R}}^t = F_{\mathbf{R}} \frac{\delta_{\mathbf{R},0} - (1 + \delta_{\mathbf{R},0})F_{\mathbf{R}}}{\left(1 - \eta\frac{n}{2}\right)\left(1 - \frac{n}{2}\right)}. \quad (36)$$

By Eq. (34) with $\mathbf{R} = (0,0)$ and $\mathbf{R} = (1,0)$ we get the nearest-neighbor correlation function

$$C_{1,0} = -\left(\sqrt{\frac{I^2}{4\alpha_1} + \frac{n}{2} - C_{0,0}^t - C_{1,0}^t} - \frac{I}{2\sqrt{\alpha_1}}\right)^2, \quad (37)$$

where $I = I_{0,0} + I_{1,0}$, and the condensation part

$$C = \frac{n}{2} - C_{0,0}^t - \sqrt{-\frac{C_{1,0}}{\alpha_1}} I_{0,0}. \quad (38)$$

The staggered magnetization m is calculated from Eq. (34) according to

$$m^2 = \lim_{|\mathbf{R}| \to \infty} \langle \mathbf{S}_0 \mathbf{S}_{\mathbf{R}} \rangle \cos \mathbf{Q}\mathbf{R} = \frac{3}{2}C. \quad (39)$$

Finally, let us determine the parameter η at $T = 0$ in the low-density limit. There the magnetization m vanishes. By Eqs. (14) to (16) we have $\omega_{\mathbf{q}}^2 = 8t^2(1 - \gamma_{\mathbf{q}})$ at $n = 0$, and $F_{\mathbf{R}}$ is given by $F_{\mathbf{R}} = n/2 + O(\mathbf{R}^2 n^2)$. Using Eqs. (10), (31) and (36), we expand $C_{\mathbf{R}}$ up to the second order of n:

$$C_{\mathbf{R}} = -\frac{J}{t}C_{1,0}K_{\mathbf{R}} + \delta_{\mathbf{R},0}\frac{n}{2} + (\eta\delta_{\mathbf{R},0} - 1)\frac{n^2}{4} + O(n^3), \quad (40)$$

with

$$K_{\mathbf{R}} = \frac{1}{N} \sum_{\mathbf{q}} \sqrt{2(1 - \gamma_{\mathbf{q}})} \cos \mathbf{q}\mathbf{R}. \quad (41)$$

By Eq. (40) with $\mathbf{R} = (0,0)$ and $\mathbf{R} = (1,0)$ we get

$$\eta = 1 - \frac{K_{0,0}J/t}{1 + K_{1,0}J/t}, \quad (42)$$

where $K_{0,0} = 1.355$ and $K_{1,0} = -0.198$.

In Fig. 1 our results for m as a function of the hole doping $\delta = 1 - n$ are shown ($m_0 = 0.253$). We obtain a strong suppression of the staggered magnetization with increasing doping due to spin-hole interactions, where at the critical value $\delta_c(J/t)$ there is a transition from the LRO phase to a paramagnetic phase with AFM SRO. At the ratio $J/t = 0.4$ we get $\delta_c = 5.9\%$, which agrees quantitatively with the value found
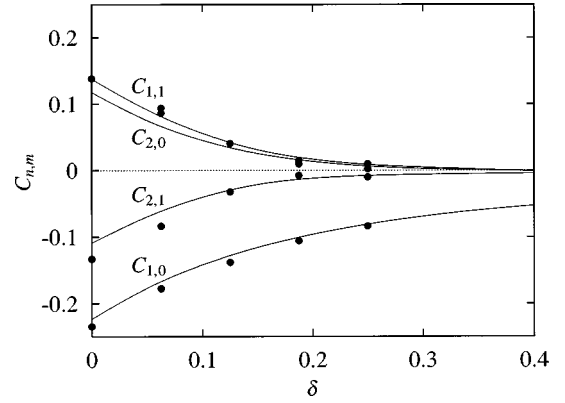
by a recent cumulant approach.[14] With decreasing ratios J/t, the LRO is destroyed more rapidly upon doping, where our δ_c values [$\delta_c(J/t = 0.2) = 4.7\%$] start to deviate from those given in Ref. 14 [$\delta_c(J/t = 0.2) = 3.2\%$]; for more discussion of those results, see the following section.

IV. COMPARISON WITH EXACT DIAGONALIZATION AND EXPERIMENTAL DATA

Let us first test the validity region of the theory by comparing our results for the spin correlation functions and the uniform static spin susceptibility $\chi(T,\delta)$ with exact diagonalization (ED) data.[15–17]

In Fig. 2 the doping dependence of the correlation functions $C_{n,m}$ [Eqs. (10) and (31)] at $T = 0$ and $J/t = 0.4$ is depicted showing a good agreement with the ED results of Ref. 15. The sign changes in $C_{n,m}$ reflect the AFM SRO. With increasing hole doping the SRO, i.e., $|C_{n,m}|$, gradually decreases, and for $\delta \gtrsim 0.25$ only nearest-neighbor spin correlations survive.

Figure 3 shows the dependence of $C_{n,m}$ at $\delta = 0.25$ on the ratio J/t at $T = 0$. Below the physically relevant parameter range $J/t \simeq 0.3 - 0.4$, our results considerably deviate from the ED data, especially the functions $C_{1,0}$ and $C_{1,1}$. In particular, at low doping our theory does not yield ferromagnetic SRO ($C_{1,0} > 0$) observed in ED for $J/t < 0.1$ and $\delta = 0.125$.[16] These discrepancies are likely caused by our
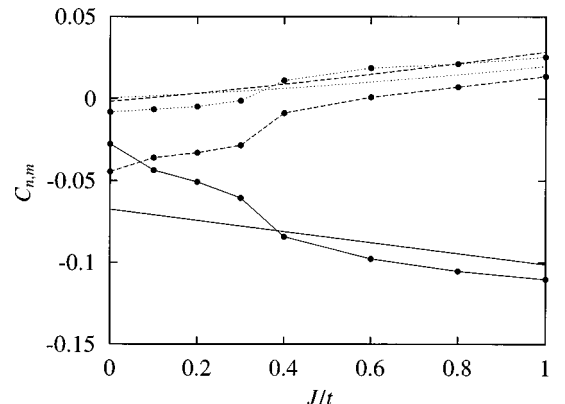

FIG. 2. Spin correlation functions vs doping at $T = 0$ and $J/t = 0.4$ compared with ED data ($\bullet$, Ref. 15).

FIG. 3. Spin correlation functions $C_{1,0}$ (solid), $C_{1,1}$ (dashed), and $C_{2,0}$ (dotted) vs J/t at $T = 0$ and $\delta = 0.25$ compared with the ED results ($\bullet$) of Ref. 15 (joined by the corresponding line style).
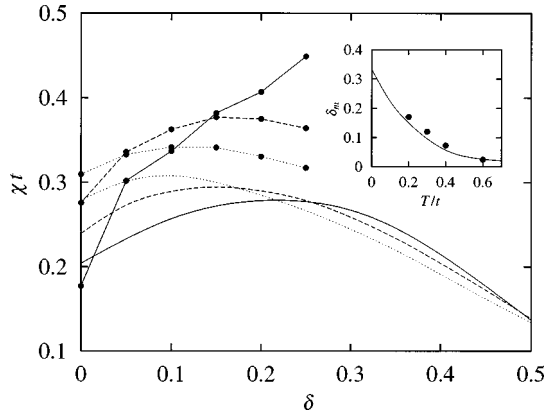
FIG. 4. Uniform static spin susceptibility vs doping at $J/t = 0.3$ and different temperatures ($T/t = 0.1$: solid, $T/t = 0.2$: dashed, $T/t = 0.3$: dotted) compared with the ED data (●) of Ref. 17 (joined by the same line style). The inset shows the position δ_m of the maximum in χ vs T together with the ED data (●, Ref. 17).

rough approximations made in the calculation of the itinerant properties. This may also explain the deviation of our results for the staggered magnetization with decreasing $J/t < 0.4$ from those of Ref. 14. However, in the physical range of J/t our theory provides a good description of SRO.

Next, we compare the spin susceptibility $\chi(T, \delta)$ with the ED data of Ref. 17, available for $T/t \gtrsim 0.1$. As shown in Fig. 4, the doping dependence of χ at $J/t = 0.3$ and different temperatures is correctly reproduced but for the magnitude of χ. In our approach the increase of χ upon doping is caused by the decrease of AFM SRO (cf. Fig. 2), i.e., of the spin stiffness against orientation along a homogeneous external magnetic field, where the itinerant contribution to χ gradually wins over the local one. At large enough doping, the decrease of χ with increasing δ is due to the Paulilike itinerant contribution. The smooth crossover from local to itinerant behavior and the resulting SRO-induced maximum of χ at $\delta_m(T)$ shifts to lower dopings with increasing temperature, since SRO effects are less pronounced at higher T (cf. I). Correspondingly, the maximum position decreases with increasing temperature, as shown in the inset of Fig. 4, in good agreement with the ED results. Note that the $\delta_m(T)$ curve at $J/t = 0.4$ (which is not shown) nearly coincides with that at $J/t = 0.3$. At $T = 0$, we get $\delta_m(0) = 0.33$, being close to the value $\delta_m(0) \simeq 0.4$ found in the slave-boson theory of SRO.[7] However, contrary to Ref. 7, a weak nearest-neighbor SRO persists for $\delta > \delta_m$ (cf. Fig. 2). For comparison we note that the slave-boson theory of SRO for the single-band Hubbard model[6] yields $\delta_m(0) = 0.26$ at $U/t = 8$.

In Fig. 5 the temperature dependence of χ at fixed doping is plotted. The maximum at $T_m(\delta)$ and the crossover to the high-temperature Curie-Weiss behavior can be understood as a SRO effect, in analogy to the explanation of the doping dependence. In particular, the maximum shifts from $T_m(0) \simeq J$ in the Heisenberg limit to lower temperatures with increasing doping, since the SRO is less pronounced at higher doping levels.

Finally, we compare our theory with experiments on $La_{2-\delta}Sr_\delta CuO_4$. First, we consider the Heisenberg model which describes the undoped compound La_2CuO_4. Determining the exchange energy, as in I, by a least-squares fit to
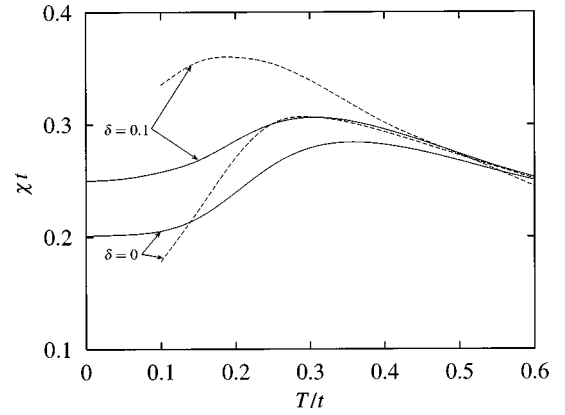
the neutron-scattering data for the AFM correlation length,[2] we obtain for our choice of the vertex parameters α_1 and α_2 the realistic value $J = 117$ meV.

As revealed by neutron-scattering experiments,[1] the (commensurate) AFM LRO is lost at $\delta_c \simeq 2\%$, qualitatively agreeing with our results shown in Fig. 1.

The experimental doping dependence of the magnetic susceptibility exhibits a maximum at $\delta_m \simeq 0.25$ over the whole accessible temperature region, 50 K $\leqslant T \leqslant$ 400 K.[3] Figure 6 compares our result for $\chi(T, \delta)$ at 400 K and $J/t = 0.3$ (corresponding to $t = 0.39$ eV and $T/t = 0.088$) and the ED data at $T/t = 0.1$ (Ref. 17) with the spin contribution to the magnetic susceptibility of LSCO at 400 K. The spin contribution is obtained from the measured total susceptibility[3] by subtracting the diamagnetic core (-9.9×10^{-5} emu/mol) and Van Vleck (2.4×10^{-5} emu/mol) contributions, which can be taken as independent of doping and temperature.[4] The observed maximum position is well reproduced by our theory, which gives $\delta_m(400$ K$) = 0.22$. Note that choosing $J/t = 0.4$ ($t = 0.29$ eV, $T/t = 0.12$) does not significantly change the δ dependence of χ. Concerning the magnitude of χ, the theoretical susceptibility is too low as compared with

FIG. 5. Uniform static spin susceptibility vs T at $J/t = 0.3$ for different dopings (solid) compared with the ED results (dashed) of Ref. 17.
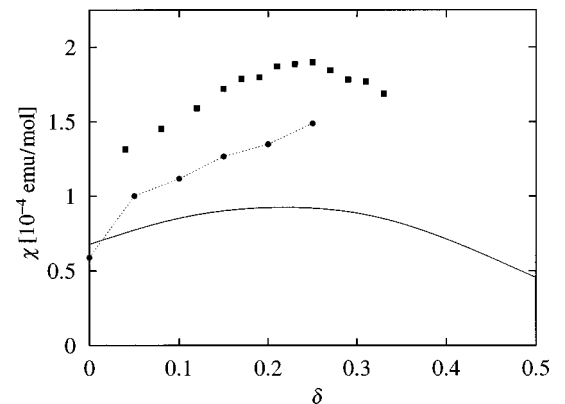

FIG. 6. Uniform static spin susceptibility as a function of doping at $T = 400$ K. The theoretical result obtained at $J/t = 0.3$ and $t = 0.39$ eV (solid) is compared with the ED data at $T/t = 0.1$ (●, dotted line) from Ref. 17 and with the spin contribution (■) to the (corrected) experimental susceptibility of $La_{2-\delta}Sr_\delta CuO_4$ (Refs. 3 and 4).

experiments, whereas the ED result lies in between. From this we conclude that part of the discrepancy in the magnitude of the spin susceptibility may be due to the use of the (single-band) t-J model.

Regarding the doping dependence of $\chi(T,\delta)$ below 400 K ($T/t<0.1$), the theory yields a shift of the maximum position $\delta_m(T)$ towards higher values (cf. Fig. 4), which is ascribed to the doping and temperature dependences of SRO. However, such a shift was not observed experimentally.[3]

The observed temperature dependence of the magnetic susceptibility shows (for $\delta\lesssim0.21$) a maximum, where the temperature of the maximum decreases with increasing doping.[3] This behavior may be qualitatively explained as a SRO effect, as discussed above (Fig. 5).

V. SUMMARY

In this paper we have developed a spin-rotation-invariant theory of antiferromagnetic short-range order in the two-dimensional t-J model. The basic characteristics of our theory are the following.

(i) The dynamic spin susceptibility is divided, by the equation of motion, into a local and an itinerant contribution.

(ii) Both contributions are treated by the Green's-function projection technique and a generalized mean-field approximation. For the local contribution, we choose a two-operator basis to take SRO into account.

(iii) The SRO is described in terms of two-spin correlation functions of arbitrary range over the whole doping and temperature region.

(iv) The parameters introduced at the decoupling of the higher spectral moments are determined from the sum rule and the ground-state energy of the Heisenberg model.

Our approach provides a suitable description of pair-correlation functions and of the uniform static susceptibility $\chi(T,\delta)$. The main results are summarized as follows.

(i) The comparison of the two-spin correlation functions with exact diagonalization data yields a good agreement but for small ratios $J/t(\lesssim0.3)$.

(ii) At $T=0$, the antiferromagnetic long-range order is rapidly destroyed upon doping, where for $\delta>5.9\%$ ($J/t=0.4$) a paraphase with SRO appears.

(iii) The maxima in the doping and temperature dependences of $\chi(T,\delta)$ as compared with exact diagonalization data are well reproduced and explained as SRO effects.

(iv) Comparing the theory with magnetic susceptibility experiments on $La_{2-\delta}Sr_\delta CuO_4$, a reasonable agreement is found, in particular, as the doping dependence is concerned.

From the agreement of our theory with experiments we conclude that the concept of magnetic SRO may be decisive in explaining the unconventional properties of the cuprates and the superconducting pairing mechanism. Thus, our results support the conclusions drawn in Refs. 6 and 7. It is promising to extend the Green's-function projection theory by the inclusion of self-energy effects to describe adequately the spin dynamics in the presence of SRO.

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