Doping dependence of long-range magnetic order in the t-J model

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The renormalization of the staggered-order parameter as a function of hole doping is studied for a two-dimensional doped antiferromagnet in the framework of the t-J model. The self-consistent Born approximation is used to calculate the Green's functions of holes and spin waves. It is shown that magnon softening is mainly due to the incoherent motion of the holes. The staggered-order parameter vanishes at a small critical density of holes δ_c. The calculated value for δ_c as well as the concentration dependence of both the staggered moment and spin-wave velocity are consistent with experimental data for $La_{2-\delta}Ba_\delta CuO_4$ and $YBa_2Cu_3O_{6+x}$.

I. INTRODUCTION

The parent compounds of oxide high-T_c superconductors are antiferromagnetic (AF) semiconductors. The Néel temperature as well as the low-temperature magnetic-order parameter strongly depend upon the hole concentration δ. When δ exceeds some critical value ($\sim$ few percent) the AF long-range order disappears, though the neutron scattering and NMR data has revealed that strong two-dimensional AF fluctuations still persist. Accordingly it is important for an understanding of the electronic properties of these materials to study the interplay between doping and antiferromagnetism. The values of the staggered moment $m=2|\langle S^z\rangle|$ as well as the spin-excitation spectrum of the undoped compounds are well described[1] in the framework of the conventional two-dimensional spin-wave theory.[2] Doping reduces both the spin-wave velocity v and the staggered moment. Both of them have pronounced nonlinear dependencies on hole concentration δ and vanish at critical concentration.[3–6] The calculation of the concentration dependence of the order parameter $m(\delta)$ is the main aim of the present paper.

The suppression of the Néel order parameter as a consequence of hole doping has already been studied by Aharony *et al.*[7] on the basis of a static frustration model and by Lee and Feng[8] in the framework of the t-J model. Lee and Feng considered a variational RVB ground state in the presence of a staggered field and found numerically that the staggered order is strongly affected by the motion of holes and disappears at very low hole concentration which is consistent with experiment.

In this paper we will investigate this problem using a slave-fermion representation of the t-J model. We find that the staggered moment strongly decreases due to the spin disorder introduced by the fast incoherent motion of holes. We show that the magnetic order parameter has a nonlinear concentration dependence and estimate the critical doping concentration

$$\delta_c \simeq (J/zt) \Bigg/ \left[1+\frac{1}{z}\ln(zt/2J)\right] , \qquad (1)$$

at which the long-range order disappears. Here J is the exchange interaction constant, t the hopping integral, and z the number of nearest neighbors.

The slave-fermion formalism has been already used to study the spin dynamics of two-dimensional doped antiferromagnets by Gan, Andrei, and Coleman[9] and by Igarashi and Fulde.[10] Gan *et al.* showed that doping leads to a softening of the long-wavelength spin waves and to a damping of short-wavelength spin waves due to the decay into particle-hole excitations in a coherent band. Igarashi and Fulde[10] took into account the incoherent character of the hole spectrum on the large energy scale $\omega > J$, and pointed out the very important contribution of the incoherent background. Our result for the spin-wave-velocity renormalization is consistent with the numerical result in Ref. 10 at small doping.

Alternatively one may calculate the critical concentration from the condition that the spin-wave velocity tends to zero.[11] We have calculated this concentration δ^* along the lines of Ref. 11. We find that δ^* is very close to the value δ_c obtained from the staggered magnetization (1), and also in agreement with Ref. 11, where a quite different slave-particle representation has been used. Our result for δ^* differs from that obtained in Ref. 9.

The organization of the paper is as follows. The interaction Hamiltonian between spin waves and holes is derived in Sec. II. The Green's functions for the spin waves and holes are obtained in Sec. III within the self-consistent Born approximation. The renormalization of spin-wave velocity and the concentration dependence of the staggered moment are calculated in Sec. IV. Finally, the comparison of theory with experimental data is performed in Sec. V. In the Appendix we present an alternative derivation of the interaction Hamiltonian between spin waves and holes.

II. THE INTERACTION HAMILTONIAN BETWEEN HOLES AND SPIN WAVES

Our theory is based on the t-J model

$$H=-t\sum_{\langle ij\rangle\delta}(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})+J\sum_{\langle ij\rangle}(\bar{S}_i\bar{S}_j)$$
$$=H_t+H_J , \qquad (2)$$

which describes essential aspects of oxide high temperature superconductors (HTSC's) as it is now believed. Here $\bar{S}_i$ is the electronic spin operator and $\langle ij \rangle$ indicates a sum over pairs of nearest neighbors. This Hamiltonian acts on the space with no double occupancy of sites $n_{i,\uparrow}+n_{i,\downarrow} \le 1$. At half filling the model (2) reduces to the $S=\frac{1}{2}$ Heisenberg AF which is expected to show long-range Néel order at zero temperature. The value of the order parameter is considerably reduced by quantum fluctuations. Away from half filling the hole motion introduces further spin disorder. These additional quantum spin fluctuations strongly reduce long-range order.

To avoid a double occupancy of sites we use the slave-fermion parametrization of electron operators[12]

$$c_{i\sigma}=f_i^\dagger b_{i\sigma} , \tag{3}$$

where the Schwinger boson operator $b_{i\sigma}$, $\sigma=\pm\frac{1}{2}$, keeps track of the spins, and the slave fermion $f_i^\dagger$ generates a hole state at site i. This representation is natural for the Néel-ordered state, which can be considered as a condensate of $b_{A\uparrow}(b_{B\downarrow})$ Bose fields in $A\,(B)$ sublattice and uncondensed bosons $b_{A\downarrow}(b_{B\uparrow})$ turn then into spin-wave excitation operators in the Néel background.[13–16]

The replacement (3) transforms the t-J Hamiltonian (1) into

$$H=t\sum_{\langle ij\rangle\sigma} b_{i,\sigma}^\dagger f_j^\dagger b_{j,\sigma} f_i + H_J , \tag{4}$$

together with the local constraint $(f^\dagger f+b_\sigma^\dagger b_\sigma)_i=1$ at each site i. We consider the Néel state at $T=0$ and divide the square lattice into $A\,(\uparrow)$ and $B\,(\downarrow)$ sublattices. Then after substituting

$$\begin{aligned} b_{i\uparrow}&=r_i e^{i\theta_i} , \quad b_{i\downarrow}=b_i e^{i\theta_i} , \quad f_i=h_i e^{i\theta_i}, i\in A , \\ b_{j\downarrow}&=r_j e^{i\theta_j} , \quad b_{j\uparrow}=b_j e^{i\theta_j} , \quad f_j=h_j e^{i\theta_j}, j\in B , \end{aligned} \tag{5}$$

where the r fields are real and $b, b^\dagger$ are simply Holstein-Primakov spin-wave operators, we have

$$H=t\sum_{i\in A}\sum_{j\in B}[(r_i b_j+b_i^\dagger r_j)h_j^\dagger h_i+\text{H.c.}]+H_J , \tag{6}$$

$$r=(1-b^\dagger b-h^\dagger h)^{1/2}\simeq 1-\cdots , \tag{7}$$

Keeping the leading relevant terms for our purpose in the expansion of the r fields in the Hamiltonian (6) we find

$$H=t\sum_{i,j(i)}(b_i+b_j^\dagger)h_i^\dagger h_j+\tfrac{1}{4}J\sum_{i,j(i)}(b_i^\dagger b_i+b_j^\dagger b_j+b_i b_j+b_i^\dagger b_j^\dagger) . \tag{8}$$

The interaction Hamiltonian (8) between spin waves and holes can be derived via a different method based on another representation of the t-J model (see Appendix), which may be particularly useful for the study of the spin-liquid phase.

In Fourier space after Bogolubov $u-v$ transformation $b_q=\cosh\theta_q a_q+\sinh\theta_q a_{-q}^\dagger$, we arrive at

$$\begin{aligned} H_t&-zt\sum_{kq}(\gamma_k\cosh\theta_q+\gamma_{k+q}\sinh\theta_q)h_{k+q}^\dagger h_k a_q+\text{H.c.} , \\ H_J&=\sum_q \omega_q^0 a_q^\dagger a_q , \quad \omega_q=\tfrac{1}{2}zJ(1-\gamma_q^2)^{1/2} . \end{aligned} \tag{9}$$

Here the lattice spacing is taken as unity, and

$$\begin{aligned} \cosh\theta_q&=[1+(1-\gamma_q^2)^{-1/2}]^{1/2}/\sqrt{2} , \\ \sinh\theta_q&=-\text{sign}(\gamma_q)[-1+(1-\gamma_q^2)^{-1/2}]^{1/2}/\sqrt{2} , \\ \gamma_q&=(\cos q_x+\cos q_y)/2 . \end{aligned} \tag{10}$$

The kinetic term of the t-J model now (1) transforms into the coupling term between holes and spin waves. Note that the coupling constant t is large, and therefore the hole motion strongly affects the spin background. The coupling vertex vanishes in the long-wavelength limit $q=0$ as expected for a Goldstone mode.

After $u-v$ transformation, the staggered moment $m(\delta)=1-2\langle b^\dagger b\rangle$ reduces to

$$m(\delta)=m_0[1-\varphi(\delta)] , \tag{11}$$

where

$$m_0=2-\sum_p(1-\gamma_p^2)^{-1/2} \tag{12}$$

is the staggered moment of the two-dimensional Néel AF and

$$\varphi(\delta)=\frac{2}{m_0}\sum_p\langle a_p^\dagger a_p-\gamma_p a_p a_{-p}\rangle/(1-\gamma_p^2)^{1/2} . \tag{13}$$

If there are no holes the expectation values in (13) vanish and the function $\varphi=0$. However, there are a finite number of spin-wave excitations in the doped system even at $T=0$ resulting from the mutual interaction between spin waves due to their coupling to hole-density fluctuations. For the copper oxides t is larger than J and the coupling term in (9) is dominant. Thus the function $\varphi(\delta)$ increases quickly with doping and the Néel-order parameter $m(\delta)$ goes to zero.

To calculate $\varphi(\delta)$ and the staggered moment (11) we need the Green's functions $D_\tau(p)=\langle -T_\tau a_p a_p^\dagger(\tau)\rangle$ and $F_\tau(p)=\langle -T_\tau a_{-p} a_p(\tau)\rangle$ which will be considered in the following section.

III. GREEN'S FUNCTIONS FOR SPIN WAVES AND HOLES

The equations for spin-wave Green's functions in Born approximation are as follows:[9,10]

$$\begin{aligned} (i\nu-\omega_p^0)D_\nu(p)&=1+\Sigma_{11}(i\nu,p)D_\nu(p)+\Sigma_{12}(i\nu,p)F_\nu(p) , \\ -(i\nu+\omega_p^0)F_\nu(p)&=\Sigma_{21}(i\nu,p)D_\nu(p)+\Sigma_{22}(i\nu,p)F_\nu(p) . \end{aligned} \tag{14}$$

The self-energy diagrams for $\Sigma_{11}(i\nu,p)=\Sigma_{22}(-i\nu,-p)$ and $\Sigma_{12}=\Sigma_{21}$ are shown in Fig. 1. Equations (14) lead to

$$\begin{aligned} D_\nu(p)-\gamma_p F_\nu(p)=[&i\nu-A(i\nu,p)+\omega_p^0+B(i\nu,p) \\ &+\gamma_p\Sigma_{12}(i\nu,p)]/d(i\nu,p) , \end{aligned} \tag{15}$$

where

$$\begin{aligned} d(i\nu,p)=&[i\nu-A(i\nu,p)]^2 \\ &-[\omega_p^0+B(i\nu,p)+\Sigma_{12}(i\nu,p)] \\ &\times[\omega_p^0+B(i\nu,p)-\Sigma_{12}(i\nu,p)] \end{aligned} \tag{16}$$

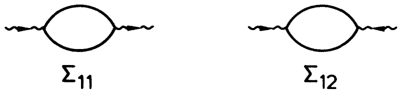

FIG. 1. Feynman diagrams for spin-wave self-energy from particle-hole excitations.

and

$$A(i\nu,p)=\tfrac{1}{2}[\Sigma_{11}(i\nu,p)-\Sigma_{11}(-i\nu,-p)]\,,$$
$$B(i\nu,p)=\tfrac{1}{2}[\Sigma_{11}(i\nu,p)+\Sigma_{11}(-i\nu,-p)]\,. \tag{17}$$

The renormalized spin-wave energy $\omega=\omega_p$ is determined by Equation $d(\omega,p)=0$ and the function (15) gives the expectation value $\langle a^\dagger a-\gamma\rangle$ in (13). Straightforward algebraic calculations lead to

$$A(\omega,p)=-\tfrac{1}{2}(zt)^2\sum_k(\gamma_{k+p}^2-\gamma_k^2)\chi_\omega^-(k,p)\,, \tag{18}$$

$$(B\pm\Sigma_{12})_{\omega,p}=-\omega_p^0(zt^2/J)\sum_k\frac{(\gamma_{k+p}\pm\gamma_k)^2}{1\pm\gamma_p}\chi_\omega^+(k,p)\,, \tag{19}$$

$$(B+\gamma\Sigma_{12})_{\omega,p}=-\omega_p^0(zt^2/J)\sum_k(\gamma_{k+p}^2+\gamma_k^2)\chi_\omega^+(k,p)\,. \tag{20}$$

Here $\omega_p^0\simeq v_0p$ is the unrenormalized spin-wave energy and the function $\chi_\omega^\pm(k,p)$ is determined by the polarizability due to the holes (bubble in Fig. 1):

$$\chi_\omega^\pm(k,p)=\chi_\omega(k,p)\pm\chi_{-\omega}(k,p)\,,$$
$$\chi_\omega(k,p)=\int_{-\infty}^0 dx\int_0^\infty dy\frac{\rho_x(k)\rho_y(k+p)}{\omega+y-x+i\epsilon} \tag{21}$$

The function χ_ω (21) depends on the spectral density $\rho_x(k)$ of the hole Green's function. It is well known[16–18] that the quasiparticle spectrum of holes in quantum AF has minima at four points $k_{\min}^i=(\pm\pi/2,\pm\pi/2)$, i.e., there are small hole pockets around $k_{\min}^i$. The summation over the filled states $\bar{k}=\bar{k}_{\min}^i+\bar{k}'$ in (18)–(20) can be rewritten as

$$\sum_k f(\bar{k})\simeq\sum_i\sum_{\bar{k}'}f(\bar{k}_{\min}^i+\bar{k}')\,. \tag{22}$$

Expanding the matrix elements in (18)–(20) for small momentum p and $|\bar{k}'|\sim k_0\sim\sqrt{\delta}$, where k_0 is the Fermi momentum, one finds

$$A(\omega,p)\simeq-\tfrac{1}{8}(zt)^2\sum_{i,\bar{k}'}p^2\chi_\omega^-(\bar{k}_{\min}^i+\bar{k}',\bar{p})\,, \tag{23}$$

$$(B+\Sigma_{12})_{\omega,p}=-\omega_p^0(zt^2/2J)\sum_{i\bar{k}'}[(k')^2+p^2/4]\chi_\omega^+(\bar{k}_{\min}^i+\bar{k}',\bar{p})\,, \tag{24}$$

$$(B-\Sigma_{12})_{\omega,p}=-\omega_p^0(zt^2/J)\sum_{i,\bar{k}'}\chi_\omega^+(\bar{k}_{\min}^i+\bar{k}',\bar{p})\,, \tag{25}$$

$$(B+\gamma\Sigma_{12})_{\omega,p}=-\omega_p^0\left[\frac{zt^2}{2J}\right]\sum_{i,\bar{k}'}\left[(k')^2+\frac{p^2}{2}\right]\times\chi_\omega^+(\bar{k}_{\min}^i+\bar{k}',\bar{p})\,. \tag{26}$$

If we keep in (15) and (16) the leading terms in spin-wave momentum p and hole density δ only, we may then neglect $(B+\Sigma)$ (24) and $B+\gamma\Sigma$ (26), since the function $\chi_\omega\sim\delta$. Only the combination $B-\Sigma\sim p\delta$ (25) is considerable at small p due to the factor $1-\gamma_p$ in the denominator of Eq. (19). In this approximation Eq. (16) for the renormalized spin-wave energy ω_p reads as

$$\omega_p=\omega_p^0(1-\kappa_p)^{1/2}/(1+\lambda_p)\,, \tag{27}$$

with

$$\kappa_p=(zt^2/J)\Pi_p\,,$$
$$\Pi_p=2\sum_k\int_{-\infty}^0 dx\int_0^\infty dy\,\rho_x(\bar{k})\rho_y(\bar{k}+\bar{p})\frac{y-x}{(y-x)^2-\omega_p^2} \tag{28}$$

and

$$\lambda_p=\sum_k\int_{-\infty}^0 dx\int_0^\infty dy\,\rho_x(\bar{k})\rho_y(\bar{k}+\bar{p})\frac{(ztp/2)^2}{\omega_p^2-(y-x)^2}\,. \tag{29}$$

For the function $\varphi(\delta)$ (13) we arrive at

$$\varphi(\delta)=m_0^{-1}\sum_p\frac{(1-\kappa_p)^{-1/2}-1}{(1+\lambda_p)(1-\gamma_p^2)^{1/2}}\,. \tag{30}$$

The spectral density $\rho_\omega(\bar{k})$ in (28) and (29) can be estimated following Kane, Lee, and Read.[14] In Born approximation the hole self-energy is given by

$$\Sigma_\omega(k)=(zt)^2\sum_p\int dx\,\rho_x(\bar{k}+\bar{p})\left[\frac{\alpha^+(k,p)\theta(-x)}{\omega+|x|+\omega_p+i\epsilon}+\frac{\alpha^-(k,p)\theta(x)}{\omega-(x+\omega_p)+i\epsilon}\right]\,, \tag{31}$$

where $\theta(x)$ is the step function and

$$\alpha^\pm(k,p)=(\gamma_k^2+\gamma_{k+p}^2-2\gamma_k\gamma_{k+p}\gamma_p)(1-\gamma_p^2)^{-1/2}\pm(\gamma_k^2-\gamma_{k+p}^2)\,. \tag{32}$$

Note that $\alpha^\pm\sim p$ at small p so the coupling to the short-wavelength spin waves is important.

It is well known[14,16] that the spectral density $\rho_\omega(k)$ has quasiparticle-like behavior $Z_k\delta(\omega-\xi_k)$ at small $|\omega|\leq J$. Since the quasiparticle weight $Z_k\sim J/t$ is small, it is clear however that the main contributions to the polarizability stem from the incoherent part of the spectrum due to the motion of the hole inside a "spin-polaron." To estimate the incoherent part of the hole spectrum ρ_{incoh}, we use a dominant-pole approximation

$$\rho_\omega(k)=\rho_{\rm coh}+\rho_{\rm incoh} \;,$$
$$\rho_{\rm coh}=Z_k\delta(\omega-\xi_k)\theta(J-|\xi_k|) \;, \tag{33}$$
$$\rho_{\rm incoh}=\frac{1}{2\Gamma}\theta(|\omega|-J)\theta(2\Gamma-\omega) \;,$$

with

$$Z_k=(1-\partial\Sigma_\omega(k)/\partial\omega)^{-1}_{\xi\kappa} \;,$$
$$\xi_k=Z_0[\Sigma_0(k)-\Sigma_0(k_0)] \;, \tag{34}$$
$$\Gamma={\rm Im}\Sigma_{\omega\gg J}(0) \;.$$

Inserting (33) into (31) and performing calculations as in Ref. 14 one obtains the incoherent bandwidth $2\Gamma\sim 2zt$, the quasiparticle residue $Z_0\simeq J/t$, and the effective mass $m_{\rm eff}^{-1}\simeq J$ for quasiparticles in a narrow coherent band. The strong renormalization of the quasiparticle band has its origin in a retardation effect, since the time scale $(\tau_s\sim J^{-1})$ for spins to relax is larger than the time scale $(\tau_h\sim t^{-1})$ for a hole to hop. The contribution $\rho_{\rm incoh}\simeq 1/2zt$ to the density of states is provided by incoherent motion of the "bare" hole inside the "spin polaron" due to the local "string" potential.

IV. SPIN-WAVE VELOCITY AND STAGGERED MOMENT

The approximation (33) for the density of states $\rho_\omega(k)$ leads to three different contributions to the parameters κ (28) and λ (29) describing the spin-wave renormalization. The first contribution is due to the transitions within the narrow quasiparticle band, when both ρ_x and ρ_y in (28) are replaced by $\rho_{\rm coh}$. The remaining two contributions are provided by the transitions between the incoherent background and the quasiparticle band, and the transitions within the incoherent band.

After integration in (28) with $\rho=\rho_{\rm coh}$ one can obtain for small momentum p

$$\Pi_p({\rm coh})=-Z_0^2\delta/J^2m_{\rm eff}\simeq-(J/t^2)\delta \;. \tag{35}$$

The unusual minus sign of the fermion polarizability is due to the fact that the Fermi velocity $v_F=k_0/m_{\rm eff}\sim J\sqrt{\pi\delta}$ of a quasiparticle is smaller than the spin-wave velocity, hence the denominator of the integrand in (28) has a minus sign. Thus the transitions within the narrow quasiparticle band actually lead to a stiffening of the spin-wave dispersion. In other words, the particle-hole excitation energy $\epsilon_p(p-h)$ in an intermediate state (Fig. 1) is smaller than the initial spin-wave energy and the second-order correction to the magnon energy $\delta\omega_p\sim V^2/[\omega_p^0-\epsilon_p(p-h)]$ has positive sign.

The magnon softening is provided by large energy $\epsilon(p-h)\sim t$ transitions due to the existence of the incoherent background $\rho_{\rm incoh}$ as was already noticed by Igarashi and Fulde.[10]

Taking into account the sum rule

$$\sum_k\int_{-\infty}^0 dx\,\rho_x(k)=\delta \;, \tag{36}$$

which provides the negative energy cutoff of $\rho_{\rm incoh}$ in Eq. (33), one can estimate the integral (28) at small p:

$$\Pi_p({\rm incoh;coh})=\delta/t \;,$$
$$\Pi_p({\rm incoh;incoh})=(\delta/zt)\ln(zt/2J) \;. \tag{37}$$

The renormalization constant κ_p then reads as

$$\kappa_p=[-z+(zt/J)+(t/J)\ln(zt/2J)]\delta=\delta/\delta^* \;, \tag{38}$$

where

$$\delta^*\simeq(J/zt)\Big/\left[1+\frac{1}{z}\ln(zt/2J)\right] . \tag{39}$$

The renormalization constant λ_p (29) gives a negligible contribution at small momentum due to the factor $(\gamma_{k+p}^2-\gamma_k^2)$ in (18):

$$\lambda_p\simeq(1-4tp^2/J)\delta\ll 1 \;. \tag{40}$$

The square-root concentration dependence of the spin-wave velocity follows from (27):

$$v=v_0(1-\delta/\delta^*)^{1/2} \;. \tag{41}$$

The spin-wave velocity vanishes at the threshold concentration δ^* (39) and the long-range AF order disappears. We will see below that δ^* is very close to the concentration δ_c where the staggered moment becomes zero. The value δ^* depends only on the ratio t/J; e.g., for $t/J=4$ we obtain $\delta^*\sim 0.04$.

Our result (41) is in agreement with numerical calculations of Ref. 10 for small $\delta\ll\delta^*$, i.e., when Eq. (41) can be expanded. However, there is a discrepancy between (39) and the estimation $\delta^*\sim(J/t)^2$ obtained in Ref. 9. As the renormalization in Ref. 9 is due to the particle-hole excitations within the coherent narrow band only, this result is surprising in view of the fact that the Fermi velocity is smaller than the spin-wave velocity. Kuboki and Yoshioka[19] investigated the destruction of Néel order in the so-called t'-J model, where $t'\sim J$ describes hopping between next-nearest neighbors. Implicit to their calculation is also the neglect of the essential incoherent scattering on scale t. The critical concentration obtained for this model is therefore much larger than for the t-J model even after inclusion of gauge fluctuations.[19]

To calculate a staggered moment we need the momentum dependence of the spin-wave renormalization constant κ_p (28) at large p. For an estimate we may approximate each hole pocket by a 2D isotropic Fermi gas. The polarizability of the low-density fermion gas usually decreases as $(2k_0/p)^2$ for $p>2k_0\sim\sqrt{\delta}$, or in other words at distances shorter than the average distance between fermions.

Our approximation (33) for the incoherent part of spectral density $\rho_{\rm incoh}\sim$const prevents us from calculating the momentum dependence of κ_p and ω_p explicitly. We believe even though the low-energy spin waves change drastically with doping, the short-range order should be a smooth function of doping, and large-momentum spin excitations should be scaled by J as in the undoped case. Indeed, it was revealed by neutron scattering experiments[4–6] that the spin-wave renormalization is p dependent and decreases at large p. The doping is expected to lead only to damping of the short-wavelength spin waves due to their decay into particle-hole pairs when the spin-excitation spectrum at large $p \sim 1$ enters into the incoherent particle-hole spectrum. One can estimate this damping $\gamma \sim t\delta$ from the imaginary part of (27) and (28). Such damping of short-range spin waves without an essential change of their energy has been seen, e.g., in two-magnon Raman-scattering experiments.[20] To estimate the function (30) we assume the following interpolation formula for the momentum dependence of the hole polarizability:

$$\Pi(p)/\Pi(0)=1/[1+(p/2k_0)^2] \qquad (42)$$

which decreases as p^{-2} at large momentum as for a free fermion gas.

In the approximation (42) the staggered moment reads as

$$m=m_0(1-\varphi)\,,$$
$$\varphi=\frac{k}{m_0}(8\delta^*/\pi)^{1/2}(K_k-E_k)\,,\quad k^2=\delta/\delta^*\,, \qquad (43)$$

where K_k and E_k are complete elliptic integrals. At small doping

$$\varphi(\delta \ll \delta^*) \simeq \frac{1}{m_0}(\pi\delta^*/2)^{1/2}(\delta/\delta^*)^{3/2}\,. \qquad (44)$$

The staggered moment $m(\delta)$ (43) vanishes at the critical concentration

$$\delta_c \simeq \delta^* - \delta^* \exp(-m_0\sqrt{\pi/2\delta^*})\,, \qquad (45)$$

which differs only slightly from δ^* (39). This exponentially small difference is an artifact of our theory based on the linear spin-wave description and the approximation (42). The staggered moment (43) is in qualitative agreement with the numerical results obtained by Lee and Feng[8] for a staggered RVB-type wave function.

V. COMPARISON WITH EXPERIMENT

The dependences of spin-wave velocity (41) and ordered moment (43) on the hole density and the value of critical concentration (39) are the main predictions of our theory and may be compared with experimental results.

$(La_{1-x}Ba_x)_2CuO_4$: The internal magnetic field (which is just proportional to the staggered moment) was measured by NQR method.[3] The theoretical formula (43) calculated at $t/J=4$ gives a reasonable agreement with experiment (Fig. 2). At $t/J=4$ we have $\delta^*=0.04$ which is comparable with the experimental value $\delta^*=0.05$.[3]

$YBa_2Cu_3O_{6+x}$: According to experiment the AF ordering is not affected by doping at $x \leq 0.2$, since there are no holes in Cu(2) planes at small x.[4–6] We assume the value $x=0.15$ corresponds to $\delta=0$ and $x=0.41$ (where AF state breaks down) to $\delta=\delta^*$. Using this scale we have good agreement of our theory with experiment (Fig. 2) and the hole density $\delta^*=0.04$ in Cu(2) planes at $x=0.41$. The reduced value of spin-wave velocity $v=0.45$ eV Å in the doped compound ($x=0.37$) (Refs. 5 and 6) is also well explained theoretically (Fig. 2).

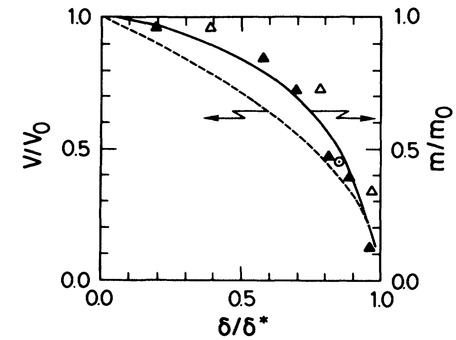

FIG. 2. Data of the ratio v/v_0 and m/m_0 as a function of the normalized hole concentration: theory for $t/J=4$ (dashed and solid curves); internal field measurement (Ref. 3) of $(La_{1-x}Ba_x)_2CuO_4$ (open triangles); ordered moment (Ref. 4) (solid triangles) and spin-wave velocity (Refs. 5 and 6) (circle) for $YBa_2Cu_3O_{6+x}$ (see text).

It should be noticed, however, that the hole states do not actually have extended character in the vicinity of the Fermi level due to Anderson localization in a random impurity potential in the semiconducting phase. Our implicit assumption is that the localization length is larger than the average distance between holes (doping impurities). Good agreement of theory with experiment probably indicates that this assumption is rather reasonable in $La_{2-x}Ba_xCuO_4$ and $YBa_2Cu_3O_{6+x}$ while our theory is not applicable to $Nd_{2-x}Ce_xCuO_4$ perhaps due to a reduced localization length.

In conclusion we have shown that the strong coupling of spin waves to charge fluctuations destroys long-range magnetic order at very small doping levels. The main source of spin disorder is the fast incoherent motion of holes inside the "spin polaron" while the coherent low-energy motion is less important. The analytical expressions for the concentration dependence of the staggered moment as well as the value of critical concentration obtained in this paper seem to give a favorable description of the experimental data for hole-doped HTSC's.

The doping dependence of the stiffness constant and related problems are presently also under investigation by applying projection techniques.[21]

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APPENDIX

The spinless hole-spin wave Hamiltonian (8) can be derived in a quite different way using the following representation of the t-J model:[11]

$$H=\sum_{\langle ij\rangle}\left[t(h_i^\dagger h_j+h_j^\dagger h_i)(2\bar{S}_i\bar{S}_j+\tfrac{1}{2})\right.$$
$$\left.+J(\bar{S}_i\bar{S}_j)(1-n_i)(1-n_j)\right] . \quad \text{(A1)}$$

Here $n_i=h_i^\dagger h_i$, $h_i^\dagger$ is the spinless fermion operator which creates a hole, and $\bar{S}_i$ is the local pseudospin $\frac{1}{2}$. The fermions in (A1) describe the charge degree of freedom while the physical spin at the singly occupied sites is expressed in terms of the pseudospin as $\bar{S}_i(1-n_i)$. The factor $(2\bar{S}_i\bar{S}_j+\frac{1}{2})$ in the hopping terms is nothing but Dirac's spin permutation operator, so that the hole hopping in (A1) is carried out in a manner which conserves the projection of the physical spin as in the original model. The spinless fermion-pseudospin representation (A1) introduces, however, the unphysical pseudospin degeneracy at sites occupied by holes. In the single-hole problem[16] this extra degeneracy does not matter as the pseudospin at the hole site does not interact with others. Hence the Hamiltonian (A1) has the same partition sum as the original t-J model: $Z(T)\equiv 2Z_{\rm ph}(T)$. However, some kinematic interaction may emerge between holes at finite hole density due to this unphysical degeneracy. It is plausible, however, that the inaccuracy is not so large at small hole density $\delta \ll 1$.

There is the following correspondence:

$$\sum_\sigma c_{i\sigma}^\dagger c_{j\sigma}=(1-\tfrac{1}{2}\delta_{ij})(2\bar{S}_i\bar{S}_j+\tfrac{1}{2})h_i h_j^\dagger ,$$
$$c_{i\uparrow}^\dagger c_{j\uparrow}=(1-\tfrac{1}{2}\delta_{ij})[S_i^+S_j^-+(\tfrac{1}{2}+S_i^z)(\tfrac{1}{2}+S_j^z)]h_i h_j^\dagger , \quad \text{(A2)}$$
$$c_{i\downarrow}^\dagger c_{j\downarrow}=(1-\tfrac{1}{2}\delta_{ij})[S_i^-S_j^+ +(\tfrac{1}{2}-S_i^z)(\tfrac{1}{2}-S_j^z)]h_i h_j^\dagger .$$

The momentum distribution function for physical electrons $n_k=\langle n_\uparrow(k)+n_\downarrow(k)\rangle/2$ then reads as

$$n_k=\tfrac{1}{2}(1-\delta)-\sum_{R\neq 0} e^{ikR}\langle(\bar{S}_0\bar{S}_R+\tfrac{1}{4})h_R^\dagger h_0\rangle . \quad \text{(A3)}$$

It is easy to check that

$$\langle(\bar{S}_i\bar{S}_j+\tfrac{1}{4})h_j^\dagger h_i\rangle=\langle h_j^\dagger h_i\rangle , \quad \text{(A4)}$$

as the Hamiltonian (A1) has the global SU(2) invariance in the pseudospin as well as in the physical spin subspaces:

$$\left[H,\sum_i \bar{S}_i n_i\right]=\left[H,\sum_i \bar{S}_i(1-n_i)\right]=0 . \quad \text{(A5)}$$

Indeed the unitary transformation

$$U=\Pi_i u_i , \quad u_i=(1-n_i)+g({\rm SU(2)})n_i , \quad \text{(A6)}$$

leaves H invariant. Performing this transformation with $g=\sigma^z$ and $g=\sigma^+ +\sigma^-$ in the expression

$$\langle h_j^\dagger h_i\rangle=\frac{1}{Z}\,{\rm Sp}\{e^{-\beta H}Uh_j^\dagger h_i U^{-1}\} \quad \text{(A7)}$$

one can find the equality (A4). The following relation between n_k and spinless hole momentum distribution function n_k^h is then obtained:

$$n_k=(1+\delta)/2-n_k^h . \quad \text{(A8)}$$

The relation between the Green's functions for physical electrons $G^{\rm ph}$ and fermions G^h in (A1) can be found also by similar arguments. In the spin-disordered state with $G^\sigma=G^{-\sigma}=G$,

$$G^{\rm ph}(R,\tau)=-(1-\tfrac{1}{2}\delta_{R,0})G^h(-R,-\tau) , \quad \text{(A9)}$$

and in momentum space

$$G^{\rm ph}(k,\epsilon)=\tfrac{1}{2}\sum_p G^h(p,-\epsilon)-G^h(-k,-\epsilon) . \quad \text{(A10)}$$

It should be stressed that (A9) and (A10) are only true in the spin-disordered phase while the expression (A8) still remains valid in the ordered state.

Other spinless fermion pseudospin representations for the t-J model were proposed by Richard and Yushankhai[22] and by Krier.[23] While all approaches agree for the antiferromagnetic ordered phase they lead to distinct formulations for the spin-liquid regime. The question which formulation is superior in the latter regime still deserves further investigation.

To introduce the spin-wave language in the AF state we should, however, not apply naively the Holstein-Primakov transformation to the Hamiltonian (A1) as in Ref. 11. If one nevertheless does it, the hopping term in (A1) leads to the interaction of holes with two magnons, yet one of the magnons is due to the existence of a nonphysical pseudospin at the hole site. Such an inconsistency may lead to unphysical exponents for the damping rate of the quasiparticles at small $\omega<J$, i.e., ω^3 instead of ω^2. At first glance it seems surprising that the critical concentration δ^* obtained in Ref. 11 is very close to our present result. Actually it is quite natural since δ^* mainly depends on the incoherent background of the hole spectrum on scale t, which is insensitive to details of the interaction.

One possible way to obtain the correct interaction between holes and spin waves is to perform the unitary transformation of the Hamiltonian (A1) on the B sublattice:[22]

$$u_j=g(1-n_j)+n_j,\quad g+\exp(i\pi\sigma_x/2) , \quad j\in B . \quad \text{(A11)}$$

Then

$$H_{\rm AF}=t\sum_{i,j(i)} h_i^\dagger h_j[(\tfrac{1}{2}+S_j^z)S_i^+ +(\tfrac{1}{2}+S_i^z)S_j^-$$
$$+(\tfrac{1}{2}-S_j^z)S_i^- +(\tfrac{1}{2}-S_i^z)S_j^+]$$
$$+\frac{J}{2}\sum_{i,j(i)}[-S_i^zS_j^z+\tfrac{1}{2}(S_i^+S_j^+ +S_i^-S_j^-)] \quad \text{(A12)}$$
$$\times(i-n_i)(1-n_j) .$$

In linear spin-wave approximation $S_z=\frac{1}{2}-b^+b$, $S^+=b$ the Hamiltonian (A12) becomes just the same as (8) because now the extra magnon has been eliminated by the transformation (A11).

One can obtain also the physical Green's functions in

AF state. In the linear spin-wave approximation

$$G^{\uparrow}_{AA}(R,\tau)=G^{\downarrow}_{BB}(R,\tau)\simeq -G^{h}(-R,-\tau)\ ,$$
$$G^{\downarrow}_{AA}=G^{\uparrow}_{BB}\simeq 0\ . \tag{A13}$$

The same relations were obtained in Ref. 16. Therefore the representation (A1) leads to the same physical picture in the AF phase as the slave-fermion description. One can hope it can be useful in the spin-liquid phase due to the absence of a local constraint at least at low hole doping.

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[1]S. M. Hayden *et al.*, Phys. Rev. Lett. **67**, 3622 (1991).
[2]For a review, see E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991).
[3]Y. Kitaoka *et al.*, Physica C **153-155**, 733 (1988).
[4]M. J. Jurgens *et al.*, Physica B **156-157**, 846 (1989).
[5]J. Rossat-Mignod *et al.*, Physica B **169**, 58 (1991).
[6]J. Rossat-Mignod *et al.*, in *Dynamics of Magnetic Fluctuations in High T_c Materials,* edited by G. Reiter, P. Horsch, and G. Psaltakis (Plenum, New York, 1991).
[7]A. Aharony *et al.*, Phys. Rev. Lett. **60**, 1330 (1988).
[8]T. K. Lee and Shiping Feng, Phys. Rev. B **38**, 11 809 (1988).
[9]J. Gan, N. Andrei, and P. Coleman, J. Phys. Condens. Matter **3**, 3537 (1991).
[10]J. Igarashi and P. Fulde, Phys. Rev. B **45**, 12 357 (1991).
[11]G. Khaliullin, Pis'ma Zh. Eksp. Teor. Fiz. **52**, 999 (1990) [JETP Lett. **52**, 389 (1990)].
[12]D. Yoshioka, J. Phys. Soc. Jpn. **58**, 1516 (1989); C. Jayaprakash, H. R. Krishnamurthy, and S. Sarker, Phys. Rev. B **40**, 2610 (1989).
[13]D. P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988).
[14]C. L. Kane, P. A. Lee, and N. Read, Phys. Rev. B **39**, 6880 (1989).
[15]S. Schmitt-Rink, C. M. Varma, and A. E. Ruckenstein, Phys. Rev. Lett. **60**, 2793 (1988).
[16]G. Martinez and P. Horsch, Phys. Rev. B **44**, 317 (1991).
[17]S. A. Trugman, Phys. Rev. B **37**, 1579 (1988).
[18]S. Sachdev, Phys. Rev. B **39**, 12 232 (1989).
[19]K. Kuboki and D. Yoshioka, J. Phys. Soc. Jpn. **61**, 621 (1992).
[20]P. Knoll (private communication).
[21]U. Muschelknautz and K. W. Becker (unpublished).
[22]J. L. Richard and V. Yu. Yushankhai (unpublished).
[23]G. Krier, Diploma Thesis, University of Saarbrücken, 1991 (unpublished).