Estimation of the doping dependence of the Néel temperature in high-T_c copper oxides

J. L. Richard
CNRS, Centre de Physique Theorique, Luminy case 907, F-13288 Marseille, France

V. Yu. Yushankhaï*
CNRS, Centre de Physique Theorique, Luminy case 907, F-13288 Marseille, France
and Dèpartement de Physique, Université de Provence, F-13288 Marseille, France
(Received 16 March 1994)

Using the polaron model as an approximation of the t-J model, we have computed in the two-time Green's-function formalism the spin-wave spectrum and the staggered magnetization at nonzero temperature near the transition to the disordered phase. The incoherent part of the charge spectrum mainly contributes and leads to an estimate of the doping-dependent Néel temperature which turns out to be in fairly good agreement with experiment for high-T_c copper oxides.

I. INTRODUCTION

Magnetic properties of layered copper oxides have been investigated intensively by different methods[1-4] during the last years. It was found that the parent compounds are three-dimensional (3D) long-range ordered antiferromagnets (AFM's) with a well defined spin-wave excitation spectrum and a Néel temperature T_N of a few hundred K. With increasing hole concentration δ within the CuO_2 planes, the staggered magnetization and the spin-wave velocity are strongly reduced and the AFM ordering vanishes at a critical concentration δ_c of a few percent. However, strong AFM correlations still persist in the disordered state ($T > T_N$) due to the large in-plane superexchange interaction between copper magnetic moments.

It is now widely accepted that the t-J model provides an adequate basis for the discussion of the essential physics for layered copper oxide compounds. In the framework of this model there is a strong coupling between charge and spin degrees of freedom and hence a small amount of charges, which are controlled by doping, are expected to modify significantly the magnetic properties of the system. It has been argued in particular that at very small doping the long-range ordered AFM state might be unstable against a spiral phase state.[21] In this paper, we start from a 3D ordered AFM state and study its instability for finite temperature and doping.

Along this direction, the results of several investigations were reported.[5-8] In particular it was shown in Refs. 5 and 6 that the motion of the holes has a pronounced effect on the spin dynamics. More precisely in the framework of the slave fermion Schwinger boson representation for the t-J model and within the Born approximation in a perturbative approach, a strong softening of the long-wavelength spin excitations was found, due to their coupling to "electron-hole" pair excitations. The spin-wave velocity was shown to vanish at a critical hole concentration of δ^* of a few percent, in agreement with experiments.[3,4] These calculations also imply that even at zero temperature there is a finite number of spin-wave excitations produced by the moving holes of the doped system that leads to a reduction of the AFM order parameter. Some arguments have been given in Refs. 6 and 8 that a complete suppression of the order parameter takes place at the critical hole concentration δ_c for which the spin-wave velocity vanishes, i.e., $\delta_c \simeq \delta^*$. However, this point remains to be clarified.

It should also be noted that being restricted to the case of zero temperature the calculations presented in Refs. 5–8 do not give the concentration dependence of the Néel temperature $T_N = T_N(\delta)$. The present paper is motivated by this question. We extend the approach developed in Refs. 5 and 6 and consider the doped AFM state for finite temperatures. We assume that the driving interaction which establishes the 3D AFM ordering at finite temperature is a weak interlayer exchange interaction J'. Starting with the t-J model in a spinless fermion pseudospin representation, we describe the magnetic subsystem in terms of two-time spin Green's functions. As is well known,[9] at zero doping these Green's functions treated within the Tyablikov random-phase approximation provide a spin-wave excitation spectrum which is renormalized by the staggered magnetization σ. In our self-consistent scheme the staggered magnetization depends not only on the temperature but on the hole concentration δ as well, i.e., $\sigma = \sigma(T,\delta)$. To obtain the renormalization of σ and the self-enegy corrections to the spin excitation spectrum due to the interaction of spin waves with moving holes, a standard decoupling procedure for higher-order spin Green's functions is used. This decoupling procedure, which is the second main approximation in our scheme, is equivalent to the Born approximation in the usual diagrammatic approach.

Our paper is organized as follows. In Sec. II, the effective Hamiltonian in a slave-fermion pseudospin representation is derived. In Sec. III, Dyson's equation for the spin two-time Green's function is introduced in the framework of the irreducible Green's function method. The main approximations adopted to solve this equation

are discussed in detail there. In Sec. IV, the self-energy part for the spin Green's function is calculated with a particular choice for a hole spectral function which is valid near the phase transition to a disordered magnetic state. The equation for the magnetic order parameter is analyzed to calculate a doping dependence of the Néel temperature.

II. THE EFFECTIVE HAMILTONIAN

The Hamiltonian of the t-J model can be written as

$$H=\sum_{i,j,\sigma} t_{ij}\tilde{C}^{\dagger}_{i,\sigma}\tilde{C}_{j,\sigma}+\tfrac{1}{2}\sum_{i,j}J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j \tag{1}$$

using the following notations. In the kinetic term, $\tilde{C}^{\dagger}_{i,\sigma}=C^{\dagger}_{i,\sigma}(1-n_{i,-\sigma})$ are electron creation operators and the factor $(1-n_{i,-\sigma})$ enforces the constraint of no double occupancy. The hopping amplitude t_{ij} is nonzero only for nearest-neighbor sites belonging to the same layer, which is a square lattice. In the magnetic term $\mathbf{S}_i$ are electron-spin operators. The exchange integral J_{ij} is also nonzero only for nearest neighbors and is given by a large constant $J\sim 0.1$ eV for the intralayer interaction, and a small constant $J'\sim 10^{-4}\,J$ for the interlayer coupling.[3,4] The hopping parameter t is usually estimated such that $3\le t/J\le 5$.

As noted by Zhang and Rice,[10] the t-J model describes the low-energy properties of the more general p-d model for copper oxides. A proper reduction procedure from p-d to t-J Hamiltonians was developed later in several papers (see, for instance, Ref. 11). It is worth noting that one may incorporate a weak transverse interlayer exchange interaction ($\sim J'$) into the t-J model. This is quite natural and formally could be done in the same reduction procedure as in Ref. 11. In the present paper we also dropped some more involved structural peculiarities of copper oxides such as, for instance, the bilayer character of Y-Ba-Cu-O compounds. However, that would not significantly change our main conclusions.

In a previous paper,[12] a kind of slave-fermion representation was proposed for the t-J model that can be derived in a few steps. First, to simplify the matter it is convenient to perform a 180° rotation of the spins on the B sublattice which leads to the changes

$$\begin{aligned}&\tilde{C}_{i,\sigma}\to\tilde{C}_{i,-\sigma}\ ,\\ &s_i^{\pm}\to S_i^{+}\ ,\\ &S_i^{z}\to -S_i^{z}\ ,\end{aligned} \tag{2}$$

when $i\in B$. Hence from now on the spin background is effectively a ferromagnetic one, and one should not distinguish between sublattices anymore. Second, we define the action of the operators $\tilde{C}_{i,\sigma},\tilde{C}^{\dagger}_{i,\sigma}$ on an extended quantum space associated with spinless fermions f_i,f_i^{+} and pseudospin operators $\mathbf{s}_i$. To eliminate unphysical states one must introduce projection operators π_i that are equivalent to the familiar constraint reducing the number of states at a given site in the widely used slave-fermion Schwinger boson representation.[13] We then have

$$\tilde{C}_{i\uparrow}=f_i^{+}\pi_i\ , \tag{3a}$$

$$\tilde{C}_{i\downarrow}=f_i^{+}s_i^{+}\ , \tag{3b}$$

$$\mathbf{S}_i=\mathbf{s}_i(1-n_i)\ , \tag{3c}$$

where $n_i=f_i^{+}f_i$ denotes the hole number operator at site i. The projection operators π_i act on the pseudospin system and are given by $\pi_i=\frac{1}{2}+s_i^z$ in the case of $\frac{1}{2}$ spin.

In the above representation, the t-J Hamiltonian $H=H_t+H_J$ reads

$$H_t=\sum_{i,j}t_{ij}f_i^{+}f_j(\pi_i s_j^{-}+\pi_j s_i^{+})\ , \tag{4}$$

$$H_J=\tfrac{1}{2}\sum_{i,j}J_{ij}(1-n_i)(1-n_j)\times\left[-s_i^z s_j^z+\tfrac{1}{2}s_i^{+}s_j^{+}+\tfrac{1}{2}s_i^{-}s_j^{-}\right]\ . \tag{5}$$

As is discussed in Ref. 12, this representation with $\pi_i=\frac{1}{2}+s_i^z$ is rigorously equivalent to the t-J model, and is well adapted to further approximation when considering an AFM spin background. The additional factors $(1-n_i)$ in the H_J term take care of the loss of magnetic energy in the presence of holes. In the mean-field approximation we may replace $(1-n_i)$ by $(1-\delta)$, where δ is the concentration of holes that leads to a renormalization of the exchange constants

$$J_{ij}\to J_{ij}(1-\delta)^2\ . \tag{6}$$

For the sake of shortening the notations, we omit this renormalization for a while, to restore it at the final stage of calculations.

It is possible to generalize representation (3) for an arbitrary spin S in such a way that the constraint imposed by the operators π_i is relaxed in the large-S limit. Indeed, the essence of the projection operator π_i is the following: because of the presence at a given site i of a fermion, one pseudospin state, say, the lowest one at the site, must be forbidden. Then in the large-S limit the operators π_i relax to the identity operators, so that finally the effective Hamiltonian is written as

$$H_t=\sum_{i,j}t_{ij}f_i^{+}f_j[s_j^{-}+s_i^{+}]\ , \tag{7}$$

$$H_J=\tfrac{1}{2}\sum_{i,j}J_{ij}\left[-s_i^z s_j^z+\tfrac{1}{2}s_i^{-}s_j^{-}+\tfrac{1}{2}s_i^{+}s_j^{+}\right]\ . \tag{8}$$

We take this effective Hamiltonian as the basic one for our consideration, without mapping the pseudospin operators onto the boson's ones done in Refs. 5–7.

III. TWO-TIME GREEN'S FUNCTION FOR THE SPIN SYSTEM AND DYSON'S EQUATION

We will study the properties of the magnetic subsystem and its interaction with holes by using a matrix Green's function defined as

$$\langle\langle\mathcal{B}_q(t)|\mathcal{B}_q^{+}(t')\rangle\rangle=-i\theta(t-t')\langle[\mathcal{B}_q(t),\mathcal{B}_q^{+}(t')]\rangle\ , \tag{9}$$

where [ ] stands for the commutator, and

$$\mathcal{B}_q=\begin{bmatrix} s_q^+ \\ s_{-q}^- \end{bmatrix}, \quad \mathcal{B}_q^+=(s_q^-, s_{-q}^+) , \tag{10}$$

with

$$s_q^{\pm}=\frac{1}{\sqrt{N}}\sum_j e^{\pm iqj}s_j^{\pm} . \tag{11}$$

To obtain an equation of motion for the Green's function, one may follow Refs. 15 and 16, differentiating $\langle\langle \mathcal{B}_q(t)|\mathcal{B}_q^+(t')\rangle\rangle$ with respect to both times t and t'. In this way, after performing some algebra one obtains Dyson's equation for the Fourier transform of (9) in the following form

$$\omega\langle\langle \mathcal{B}_q|\mathcal{B}_q^+\rangle\rangle_\omega=\langle[\mathcal{B}_q,\mathcal{B}_q^+]\rangle + [\Omega_q+\Lambda_q(\omega)]\langle\langle \mathcal{B}_q|\mathcal{B}_q^+\rangle\rangle_\omega , \tag{12}$$

where the matrix Ω_q reads

$$\Omega_q=\langle[i\dot{\mathcal{B}}_q,\mathcal{B}_q^+]\rangle/\langle[\mathcal{B}_q,\mathcal{B}_q^+]\rangle \tag{13}$$

and describes a free evolution of the system, while the matrix $\Lambda_q(\omega)$ given by

$$\Lambda_q(\omega)=\langle\langle i\dot{\mathcal{B}}_q|-i\dot{\mathcal{B}}_q^+\rangle\rangle_\omega^{(\mathrm{irr})}/\langle[\mathcal{B}_q,\mathcal{B}_q^+]\rangle \tag{14}$$

is the self-energy part accounting for the interaction effects. Here $i\dot{\mathcal{B}}_q=[\mathcal{B}_q,H]$ and $\langle\langle i\dot{\mathcal{B}}_q|-i\dot{\mathcal{B}}_q^+\rangle\rangle_\omega^{(\mathrm{irr})}$ is an irreducible Green's function defined as

$$\begin{aligned}\langle\langle i\dot{\mathcal{B}}_q|-i\dot{\mathcal{B}}_q^+\rangle\rangle_\omega^{(\mathrm{irr})} &= \langle\langle i\dot{\mathcal{B}}_q|-i\dot{\mathcal{B}}_q^+\rangle\rangle_\omega \\ &\quad -\langle\langle i\dot{\mathcal{B}}_q|\mathcal{B}_q^+\rangle\rangle_\omega \\ &\quad \times\frac{1}{\langle\langle \mathcal{B}_q|\mathcal{B}_q^+\rangle\rangle_\omega}\langle\langle \mathcal{B}_q|-i\dot{\mathcal{B}}_q^+\rangle\rangle_\omega ,\end{aligned} \tag{15}$$

which is a higher-order Green's function with respect to $\langle\langle \mathcal{B}_q|\mathcal{B}_q^+\rangle\rangle_\omega$.

Noting also that

$$\langle[\mathcal{B}_q,\mathcal{B}_q^+]\rangle=2\sigma\tau_3 , \tag{16}$$

where $\sigma=\langle s_i^z\rangle$ is the staggered moment and τ_3 is the Pauli z-component matrix, it is useful to rewrite Eq. (12) as

$$\langle\langle \mathcal{B}_q|\mathcal{B}_q^+\rangle\rangle_\omega=2\sigma[\omega-\Omega_q-\Lambda_q(\omega)]^{-1}\tau_3 , \tag{17}$$

where according to definition (9), ω stands for $\omega+i0^+$.

Let us now consider the equation of motion for $s_i^+(t)$, which reads

$$i\dot{s}_i^+=[s_i^+,H]=2\sum_j t_{ij}s_i^z f_j^+ f_i+\sum_j J_{ij}(s_i^+ s_j^z+s_i^z s_j^-) . \tag{18}$$

Let us first discuss a pure magnetic system without doping, in which case the first term in (18) does not contribute. Then Eq. (18) can be linearized by using the Tyablikov approximation.[9] This approximation applied to a magnetically ordered system consists of replacing the z component of the spin operators by its expectation value, $s_i^z\to\langle s_i^z\rangle=\sigma$, which should be evaluated self-consistently as a function of temperature. As is well known,[9] this approach leads to a fairly good extrapolation of the spin-wave dynamics at finite temperatures and provides a reasonable estimate for the AFM (or FM) phase-transition temperature.

In the work that follows, our main goal is to extend the Tyablikov approximation to the cases of a doped AFM state and examine effects of moving holes on the staggered magnetic moment σ. These effects, which are expected to be due mainly to a coupling of spin waves to particle-hole pair excitations, will be examined by estimating the self-energy part in (12) to the lowest order ($\sim t^2$). Of course, the particular character of the energy spectrum of holes in an AFM background[13,14] will be taken into account in the calculations. Hence, after performing Tyablikov linearization, the Fourier-transformed equation (18) reads

$$i\dot{s}_q^+=2\sigma\left\{\frac{1}{\sqrt{N}}\sum_k t(q-k)f_{k-q}^+ f_k+\tfrac{1}{2}J(0)s_q^+ + \tfrac{1}{2}J(q)s_{-q}^-\right\} , \tag{19}$$

where

$$\begin{aligned} t(q)&=\frac{1}{N}\sum_{i,j}e^{-iq(i-j)}t_{ij} , \\ J(q)&=\frac{1}{N}\sum_{i,j}e^{-iq(i-j)}J_{ij} .\end{aligned} \tag{20}$$

Using the definitions of t_{ij} and J_{ij} one obtains

$$t(q)=zt\gamma_q, \quad \gamma_q=\tfrac{1}{2}[\cos q_x+\cos q_y] , \tag{21}$$

$$J(q)=zJ[\gamma_q+\xi\cos q_z], \quad \xi=J'/2J , \tag{22}$$

where $z=4$. The equation for $\mathcal{B}_q(t)$ can be now written as

$$i\dot{\mathcal{B}}_q=2\sigma\lambda_q\mathcal{B}_q+j_q , \tag{23}$$

where λ_q is 2×2 matrix,

$$\lambda_q=\frac{1}{2}\begin{bmatrix} J(0) & J(q) \\ -J(q) & -J(0)\end{bmatrix} , \tag{24}$$

and j_q is the current produced by the presence of the holes. It reads

$$j_q=\frac{2\sigma}{\sqrt{N}}\sum_k\begin{bmatrix} t(k-q)f_{k-q}^+ f_k \\ -t(k+q)f_k^+ f_{k+q}\end{bmatrix} . \tag{25}$$

Taking into account that

$$\langle[j_q,\mathcal{B}_q^+]\rangle=0 , \tag{26}$$

for the frequency matrix Ω_q we obtain the result

$$\Omega_q=2\sigma\lambda_q , \tag{27}$$

leading to a usual zero-order AFM spin-wave spectrum renormalized with the magnetization σ: $\omega_q=2\sigma\omega_q^{(0)}$, us-

ing the definition

$$\omega_q^{(0)}=1/2\sqrt{J(0)^2-J(q)^2}\ . \tag{28}$$

To obtain the self-energy part $\Lambda_q(\omega)$ from (14) and (15), one should notice, first, that in Eq. (23) the linear terms in $\mathcal{B}_q$ do not contribute to the irreducible Green's function (15) and, hence, $\Lambda_q(\omega)$ is given by a simple substitution into (15) of j_q, Eq. (25), instead of the full derivative $i\dot{\mathcal{B}}_q$. Second, the lowest-order self-energy contribution is provided by the first term on the right-hand side of expression (15), while the second term gives rise to higher-order corrections. Then, restricting ourselves to lowest order, we have

$$\Lambda_q(\omega)=\frac{1}{2\sigma}\langle\langle j_q|j_q^+\rangle\rangle_\omega\tau_3\ . \tag{29}$$

By substituting j_q from (25) into (29) we explicitly obtain $\Lambda_q(\omega)$ as

$$\Lambda_q(\omega)=2\sigma\frac{1}{N}\sum_{kk'}\chi_{q,k,k'}(\omega)\begin{bmatrix} t(k-q)t(k'-q) & t(k-q)t(k') \\ -t(k)t(k'-q) & -t(k)t(k') \end{bmatrix}, \tag{30}$$

where

$$\chi_{q,k,k'}(\omega)=\langle\langle f_{k-q}^+ f_k|f_{k'}^+ f_{k'-q}\rangle\rangle_\omega\ . \tag{31}$$

Below, we calculate the Green's function (31) with a proper decoupling procedure which is equivalent to the Born approximation in a usual diagrammatic approach.[5,6]

Let us now consider the Green's function $\chi_{q,k,k'}(t)$ which is the Fourier transform of (31). By definition $\chi_{q,k,k'}(t)$ involves two time correlation functions of the form $\langle f_{k-q}^+(t)f_k(t)f_{k'}^+f_{k'-q}\rangle$. We decouple them in the following way:

$$\langle f_{k-q}^+(t)f_k(t)f_{k'}^+f_{k'-q}\rangle \simeq\langle f_{k-q}^+(t)f_{k'-q}\rangle\langle f_k(t)f_{k'-q}^+\rangle\ . \tag{32}$$

Then introducing a one-particle retarded Green's function for holes as $G^{(h)}(k,\omega)=\langle\langle f_k|f_k^+\rangle\rangle_\omega$ and applying the Fourier transform

$$\langle f_k^+ f_{k'}\rangle_\omega=\int_{-\infty}^{+\infty}dt\,e^{-\omega t}\langle f_k^+(t)f_{k'}\rangle\ , \tag{33}$$

one obtains

$$\langle f_k^+ f_{k'}\rangle_\omega=2\pi\delta_{kk'}n(\omega)\rho(\omega+\mu,k)\ . \tag{34}$$

Here $n(\omega)=1/(1+e^{\beta\omega})$ is the Fermi distribution function, and

$$\rho(\omega,k)=-\frac{1}{\pi}\mathrm{Im}\langle\langle f_k|f_k^+\rangle\rangle_{\omega+i0+} \tag{35}$$

is the spectral density of the hole Green's function. The chemical potential μ, which is a function of the hole concentration δ and temperature T, satisfies the self-consistent equation

$$\delta=\frac{1}{N}\sum_k\int_{-\infty}^{+\infty}d\omega\,n(\omega-\mu)\rho(\omega,k)\ . \tag{36}$$

Finally, by making use of the spectral representation for Green's functions, one comes to the result

$$\chi_{q,k,k'}(\omega)=\delta_{kk'}\chi_{q,k}(\omega)\ . \tag{37}$$

The function $\chi_{q,k}(\omega)$ is given by

$$\chi_{q,k}(\omega)=\int_{-\infty}^{+\infty}d\omega_1\int_{-\infty}^{+\infty}d\omega_2\frac{n(\omega_1-\mu)-n(\omega_2-\mu)}{\omega+\omega_1-\omega_2+i0^+}\times\rho(\omega_1,k-q)\rho(\omega_2,k)\ , \tag{38}$$

and corresponds to a simple "bubble" diagram in the conventional approach[5,7] developed for $T=0$. It is worth noting that the factor 2σ entering the self-energy, Eq. (30), may be regarded as a hole-spin vertex correction which is a function of temperature T and hole concentration δ in our consideration. In the following it is convenient to indicate more transparently the explicit dependence of $\Lambda_q(\omega)$ on the staggered moment σ by introducing the notation $\Lambda_q(\omega)=2\sigma\tilde{\Lambda}_q(\omega)$.

It is easy to derive some relations between the matrix elements of the self-energy (30). One obtains

$$\begin{aligned}\Lambda_q^{22}(\omega)&=-\Lambda_{-q}^{11}(-\omega)\ ,\\ \Lambda_q^{21}(\omega)&=-\Lambda_q^{12}(\omega)\ .\end{aligned} \tag{39}$$

Hence the poles of the Green's function (17) are given by the equation

$$[\omega-2\sigma A_q(\omega)]^2-(2\sigma\omega_q^0)^2\left[1+\frac{B_q(\omega)+\tilde{\Lambda}_q^{12}(\omega)}{\frac{1}{2}[J(0)+J(q)]}\right]\times\left[1+\frac{B_q(\omega)-\tilde{\Lambda}_q^{12}(\omega)}{\frac{1}{2}[J(0)-J(q)]}\right]=0, \tag{40}$$

with the following notations:

$$\begin{aligned}A_q(\omega)&=\frac{1}{2}\left[\tilde{\Lambda}_q^{11}(\omega)-\tilde{\Lambda}_{-q}^{11}(-\omega)\right]\ ,\\ B_q(\omega)&=\frac{1}{2}\left[\tilde{\Lambda}_q^{11}(\omega)+\tilde{\Lambda}_{-q}^{11}(-\omega)\right]\ .\end{aligned} \tag{41}$$

One can see that the solutions of Eq. (40) scale with the factor 2σ; therefore, a notation $\omega_q=2\sigma\tilde{\omega}_q$ will also be used.

IV. STAGGERED MAGNETIZATION AND NÉEL TEMPERATURE

Let us recall that the staggered magnetization $\sigma=\langle s_i^z\rangle$ should be obtained self-consistently through the following equation:

$$\sigma=\tfrac{1}{2}-\frac{1}{N}\sum_q\langle s_q^- s_q^+\rangle\ , \tag{42}$$

where

$$\langle s_q^- s_q^+\rangle=\int_{-\infty}^{+\infty}d\omega\frac{-\frac{1}{\pi}\mathrm{Im}\langle\langle \mathcal{B}_q|\mathcal{B}_q^+\rangle\rangle^{11}_{\omega+io+}}{e^{\beta\omega}-1}\ , \tag{43}$$

with the imaginary part of $\langle\langle \mathcal{B}_q|\mathcal{B}_q^+\rangle\rangle^{11}_{\omega}$ being defined from Eq. (17). Equation (42) then becomes

$$\frac{1}{2\sigma}=\frac{1}{N}\sum_q\frac{\frac{1}{2}J(0)+B_q(2\sigma\tilde{\omega}_q)}{\tilde{\omega}_q}\coth(\beta\sigma\tilde{\omega}_q)+\frac{1}{N}\sum_q\frac{A_p(2\sigma\tilde{\omega}_q)}{\tilde{\omega}_q}\ , \tag{44}$$

with the spin excitation spectrum $\omega_q=2\sigma\tilde{\omega}_q$ being a solution of Eq. (40). Below we will solve Eq. (44) for the staggered magnetization σ in the vicinity of the phase transition to a disordered magnetic state when $\sigma\to 0$. Accordingly the quantity $\chi_{q,k}(\omega)$ should be estimated by taking into account a particular character of the hole spectral density $\rho(k,\omega)$ in the AFM spin background near the phase transition.

The Green's function $G^{(h)}(k,\omega)$ for a single hole moving in a 2D square lattice with a quantum Néel background was calculated[13,14] within the self-consistent Born approximation on the basis of Hamiltonians (7) and (8), with spin operators mapped onto boson ones. In this consideration the hopping of a hole is only possible by emitting (or absorbing) a spin-wave excitation that leads to a strong renormalization of the hole propagation properties. When the system approaches an AFM phase transition due to a strong anisotropy of copper oxides a 3D long-range order tends to be broken by losing the interlayer magnetic correlations while strong 2D interlayer spin-spin correlations still persist and survive even in a disordered phase.[3,4] This makes it reasonable to assume that the approach for the one hole motion developed in Refs. 13 and 14 is also applicable near the phase transition. However, the effects of finite hole doping and temperature should be taken into account, and a strong renormalization of the spin-wave excitation spectrum is one of them. Below, we first briefly sketch some results of a calculation of the spectral density function $\rho(k,\omega)$ for a single hole at zero temperature,[13,14] and then estimate how $\rho(k,\omega)$ varies with increasing hole concentration δ and temperature T. In this way some insight is gained about the shape of the spectral density $\rho(k,\omega)$ when the system approaches the AFM phase transition.

First suggested by Schmitt-Rink, Varma, and Ruckenstein[17], and then developed by Kane, Lee, and Reed[13] and Martinez and Horsch,[14] a perturbative approach within a slave-fermion formalism and self-consistent Born approximation proved to be very successful in reproducing the spectral density function $\rho(k,\omega)$ for a single hole obtained by exact diagonalization of small clusters.[18] All of that led to the consensus that the hole spectrum involves a narrow quasiparticle band of coherent states at low energies and a broad continuum of incoherent states above. The corresponding spectral function is then represented as

$$\rho(k,\omega)=\rho^{\mathrm{coh}}(k,\omega)+\rho^{\mathrm{incoh}}(k,\omega)\ , \tag{45}$$

with

$$\rho^{\mathrm{coh}}(k,\omega)=Z_k\delta(\omega-E_k)\ . \tag{46}$$

The quasiparticle (QP) dispersion E_k possesses minima at $k=(\pm\pi/2,\pm\pi/2)$ with the value $E_{\min}(J)=-3.2t+2.9J^{0.7}$ for the relevant values of the exchange constant $0.1<J/t<1$; the QP bandwidth W is estimated to be of order of J, while the residue $Z_k\sim J/t$. Kane, Lee, and Read[13] estimated the incoherent part $\rho(k,\omega)$ of the spectral density to be practically a constant, $\rho(k,\omega)\sim 1/t$, in a wide energy interval above the QP band. Martinez and Horsch[14] calculated this interval to range from $E_{\min}+W$ up to $\Gamma\le zt$, where $z=4$.

Igarashi and Fulde[5] applied the self-consistent Born approximation to calculate $\rho(k,\omega)$ at finite low doping concentration $\delta\ll 1$ and $T=0$. They found that for any particular momentum $\mathbf{k}$ a hole spectral density is redistributed in such a way that an extra incoherent structure appears quite below the QP band. This extra structure, with a spectral weight of the order of δ, provides a fulfilling of a sum rule [Eq. (36) in our notations] with a chemical potential located inside the QP band. Along this way a four-pocket Fermi surface for noninteracting quasiholes was justified within that consideration and used to calculate a renormalization of spin-wave excitations due to their coupling to particle-hole excitations. As a result it was proved that a broad incoherent part of the hole spectrum makes the main contribution to this renormalization. Similar results have been also obtained by Khaliullin and Horsch,[6] who estimated the incoherent part of the hole spectral density as a constant $\rho\sim 1/2\Gamma$, where $\Gamma\lesssim zt$, within proper energy intervals below and above the QP band. They also emphasized that quasiholes produced a minor effect in a spin-wave velocity reduction. That is mainly due to the fact that the QP band is rather narrow and the residue Z_k of a quasihole pole is strongly reduced, i.e., $Z_k\sim(J/t)\ll 1$, in the relevant range of J values.

The results outlined above with respect to a hole spectral density function $\rho(k,\omega)$ and its evolution with hole doping were also examined in Ref. 19, and proved to be correct. However, as the system approaches the AFM phase transition a further transformation of $\rho(k,\omega)$ takes place. Actually, in our approach the spin-wave energy $\omega_q=2\sigma\tilde{\omega}_q$ tends to zero as $\sigma\to 0$. It was shown in Refs. 13 and 14 that in the limit $\omega_q\to 0$ the hole spectrum becomes purely incoherent, in close resemblance to that obtained by Brinkman and Rice[21] within the retraceable path approximation (rpa). The rpa predicts a relatively flat k-independent spectral density with rather sharp edges at $\pm 2\sqrt{z-1}t$. This rpa result for the bandwidth $2\Gamma=z\sqrt{z-1}t$ was also reproduced within the refined self-consistent Born approximation in a perturbative approach.[13,14] A physical reason for the disappearance of the QP band in the hole spectrum was pointed out by Kane, Lee, and Read.[13] In fact, the existence of coherent

quasihole states depends crucially on the density of states of low-lying spin-wave excitations. The number of such excitations increases dramatically due to a softening of the spin-wave spectrum near the phase transition.[3,4] In our approach this softening is governed by the staggered magnetization σ. As a result the processes of scattering of a quasihole by spin-wave excitations prove to be dominant, leading to a broadening of the QP peaks. These peaks lose their identity and the entire hole spectrum becomes incoherent.

Hence, to evaluate the function $\chi_{q,k}(\omega)$ [Eq. (38)] near the AFM phase transition, we assume a purely incoherent k-independent hole spectral function

$$\rho(k,\omega)\simeq\rho(\omega)\approx\frac{1}{2\Gamma}\theta(\Gamma-|\omega|)\ , \tag{47}$$

where $2\Gamma=z\sqrt{z-1}t$ in accordance with Refs. 13, 14 and 21.

With this spectral function the quantities $A_q(\omega)$ and $B_q(\omega)$ become q independent. Moreover, note that

$$\begin{aligned}
&A_q(2\sigma\tilde{\omega}_q)=0\ ,\\
&B_q(2\sigma\tilde{\omega}_q)=-\left[\frac{zt}{2}\right]^2\chi(T,\delta)+O[(2\sigma\tilde{\omega}_q)^2]\ ,\\
&B_q(2\sigma\tilde{\omega})\pm\tilde{\Lambda}_q^{12}(2\sigma\tilde{\omega}_q)\\
&\qquad=-\left[\frac{zt}{2}\right]^2(1\pm\gamma_q)\chi(T,\delta)+O[(2\sigma\tilde{\omega}_q)^2]\ ,
\end{aligned} \tag{48}$$

when $2\sigma\tilde{\omega}_q$ tends to zero, and we define $\chi(T,\delta)$ as

$$\chi(T,\delta)=-\int_{-\infty}^{\infty}d\omega_1\int_{-\infty}^{\infty}d\omega_2\frac{n(\omega_1-\mu)-n(\omega_2-\mu)}{\omega_1-\omega_2}\times\rho(\omega_1)\rho(\omega_2)\ . \tag{49}$$

The function $\chi(T,\delta)$ depends on temperature T and doping concentration δ through the chemical potential $\mu=\mu(T,\delta)$ which satisfied Eq. (36). The self-consistent equation (44) for the staggered magnetization σ then becomes

$$\frac{1}{2\sigma}=\frac{1}{N}\sum_q\frac{\frac{1}{2}J(0)-\left[\frac{zt}{2}\right]^2\chi(T,\delta)}{\tilde{\omega}_q}\coth(\beta\sigma\tilde{\omega}_q)\ , \tag{50}$$

and to the lowest order in σ, Eq. (40) leads to the following spin-wave spectrum

$$\omega_q=2\sigma\omega_q^{(0)}\left[1-\frac{zt^2}{2J}\chi(T,\delta)\right]=2\sigma\tilde{\omega}_q\ . \tag{51}$$

Note that we approximated the factors $J(0)\pm J(q)$ in Eq. (40) as the 2D factors $zJ(1\pm\gamma_q)$, while the quantity $\omega_q^{(0)}$ preserves its three-dimensional nature, Eq. (28).

After substituting (51) into (50), we expand the right-hand side of Eq. (50) in terms of σ, which leads to the result

$$\sigma^2=\left[\frac{4}{3T}J\left[1-\frac{zt^2}{2J}\chi(T,\delta)\right]\right]^{-1}\times\left\{1-\frac{T}{T_N(0)}\left[1-\frac{zt^2}{2J}\chi(T,\delta)\right]^{-1}\right\}\ , \tag{52}$$

where the Néel temperature $T_N(0)$ for the undoped case, $\delta=0$, is expressed as follows:

$$T_N(0)=\frac{J}{C_\xi},\quad C_\xi=\frac{1}{N}\sum_q\left[1-\frac{J^2(q)}{J^2(0)}\right]^{-1}\ . \tag{53}$$

When $\xi\to0$ the dominant contribution to the sum in Eq. (53) comes from $\mathbf{q}\simeq0$ leading to a logarithmic divergence, namely, $C_\xi\sim\ln\xi^{-1}$. Hence the Néel temperature vanishes when $\xi\to0$, and the correct thermodynamic behavior is restored in the 2D limit.[9]

From Eq. (53) one can see that at finite doping concentration the staggered magnetization vanishes at a temperature $T_N(\delta)$, which is determined by the equation

$$\frac{T_N(\delta)}{T_N(0)}=1-\frac{zt^2}{2J}\chi(T_N(\delta),\delta)\ . \tag{54}$$

To simplify the matter, let us first rewrite $\chi(T,\delta)$ in the following way:

$$\chi(T,\delta)=-\frac{1}{\Gamma}\int_0^1dx\ n[\Gamma(2x-1)-\mu]\ln\frac{x}{1-x}\ , \tag{55}$$

where the chemical potential $\mu=\mu(T,\delta)$ satisfies Eq. (36). To derive formula (55), the spectral density function $\rho(\omega)$ is taken in the approximate form (47) which is valid near the AFM phase transition. With this constant density, Eq. (36) for the chemical potential μ can easily be solved to give the Fermi distribution function entering in (55) as follows:

$$n[\Gamma(2x-1)-\mu]=\left[1+\frac{\exp[2\beta\Gamma(x-\delta)]}{1-\exp(-2\beta\Gamma\delta)}\right]^{-1}\ , \tag{56}$$

with $\beta=T^{-1}$.

One can see that $\chi(T,\delta)$ is a rather complicated function of T and δ. Then we estimate $\chi(T,\delta)$ and solve Eq. (54) in two limiting cases. In both cases Eq. (54) leads to qualitatively close results, and describes a sharp drop of the Néel temperature with increasing doping concentration.

First we estimate the quantity $\chi(T,\delta)$ at an extremely low hole concentration, and high enough temperatures $\beta\sim T_N^{-1}(0)$ such that

$$2\beta\Gamma\delta\ll1\ . \tag{57}$$

In this case, from Eq. (56) one obtains

$$n[\Gamma(2x-1)-\mu]\simeq2\beta\Gamma\delta e^{-2\beta\Gamma x}\quad(0\le x\le1)\ . \tag{58}$$

This Boltzmann-type form of the distribution function arises due to a strong renormalization of the chemical potential μ, Eq. (36). Such behavior resembles a low-density Fermi gas in a strongly nondegenerate limit. However, it is only a formal analogy, because there are no well-defined quasiparticles in our consideration. Inserting (58)

into (55), we obtain

$$\chi(T,\delta)=2\beta\delta F(2\beta\Gamma)\ , \tag{59}$$

with

$$F(2\beta\Gamma)=\int_0^1 dx\, e^{-2\beta\Gamma x}\ln\frac{1-x}{x}\ . \tag{60}$$

Typical values for $2\beta\Gamma\sim t/T_N(0)$ are quite large. Therefore an asymptotic expression for $F(2\beta\Gamma)$ can be used that yields the following estimate:

$$F(2\beta\Gamma)=\frac{1}{2\beta\Gamma}\left[\ln 2\beta\Gamma+\mathcal{C}+0\left[\frac{1}{2\beta\Gamma}\right]\right]\ , \tag{61}$$

where $\mathcal{C}$ is the Euler constant ($\mathcal{C}\sim 0.6$). Hence Eq. (54) reads

$$\delta=\frac{J\Gamma}{2t^2}\frac{1-\tau}{\mathcal{C}+\ln\frac{2\Gamma}{T_N(0)}-\ln\tau}\ , \tag{62}$$

where $\tau(\delta)=T_N(\delta)/T_N(0)$ denotes the reduced Néel temperature. We have plotted the corresponding curve $\tau(\delta)$ in Fig. 1 with $t=0.5$ eV, $J/t=0.2$, and $\Gamma=2\sqrt{3}t$, and with the Néel temperature $T_N(0)=J/3$ (~ 300 °K) which is typical for the undoped copper oxides.

From Fig. 1 one can see that being valid at extremely low hole concentration, $\delta<0.01$ and temperatures $\tau\lesssim 1$, Eq. (62) describes a sharp decrease of $T_N(\delta)$ in the upper part of the magnetic phase diagram. Being formally extended to lower temperatures and higher concentrations δ, the curve $\tau(\delta)$ crosses the temperature axis at $\delta^*\simeq 0.04$ i.e., $\tau(\delta^*)=0$, that is in a good agreement with an experimental value $\delta_c\sim 0.03$.[3,4]

An extrapolation of Eq. (62) to the region of higher values of δ and lower temperature still remains questionable. Therefore, let us return to the basic equation (54) and examine the other limit,

$$2\beta\Gamma\delta\gg 1\ , \tag{63}$$

in which case Eq. (54) can also be treated analytically. The Fermi distribution function (56) then becomes

$$n[\Gamma(2x-1)-\mu]\simeq[1+e^{2\beta\Gamma(x-\delta)}]^{-1}\ . \tag{64}$$

In comparison with the case we considered above, Eqs. (57) and (58), the values of the parameter $2\beta\Gamma\sim t/T_n(\delta)$ is now strongly enhanced due to a strong reduction of the Néel temperature $T_N(\delta)$ at finite hole concentration δ. This allows us to approximate further Eq. (64) with a familiar step function. Then a straightforward algebraic calculation of $\chi(T,\delta)$ leads to the following result:

$$\tau(\delta)=1-\frac{zt^2}{2\Gamma J(1-\delta)^2}|\delta\ln\delta-(1-\delta)\ln(1-\delta)|\ , \tag{65}$$

where a mean-field renormalization of the exchange constant $J\to J(1-\delta)^2$ is also taken into account in accordance with (6). With the same values for the parameters as above, we found that $\tau(\delta^*)=0$ at $\delta^*\simeq 0.08$. It is worth noting that in our calculations the chosen bandwidth value $2\Gamma=4\sqrt{3}t$ differs only slightly from the maximum given by the free band value $8t$. It can easily be seen, for instance, from Eq. (65) that a smaller bandwidth 2Γ would lead to a lower critical concentration δ^*.

Finally, we solved Eq. (54) in two limiting cases. The first solution (62) is applicable at an extremely low hole concentration, and the second one (65) is for somewhat higher values of δ. Both solutions reveal a strong decrease of the Néel temperature at a very small doping level, that is consistent with the experimentally observed behavior of $T_N(\delta)$ in copper oxides.

It remains to discuss the particular form chosen for the hole spectral density. A purely incoherent k-independent and relatively flat character of the hole spectral function $\rho(k,\omega)$ near the phase transition was argued above. The obvious advantage of the specific rectangular shape [Eq. (47)] is in its simplicity, allowing us to perform analytical calculations. However, assuming that the shape for $\rho(k,\omega)$ is not strongly different from Eq. (47), but a ω-dependent one, we inferred a minor importance of the details of the chosen shape. Actually, in Eqs. (38) and (49) an integrated area of the spectral density function contributes to the χ function. This contribution is determined mainly by the magnitude of the chemical potential μ. Being calculated at a particular δ, the magnitude of μ itself does not depend significantly on fine details of the spectral density. Hence we expect our results to be at least qualitatively independent of the choice of $\rho(k,\omega)$.

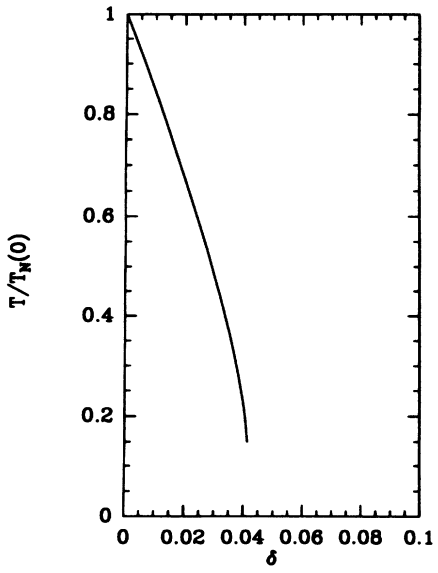

FIG. 1. The reduced Néel temperature dependence on hole concentration as follows from Eq. (62). The parameters are defined in the text.

V. CONCLUSION

Based on the t-J model in a slave-fermion pseudospin representation, we have studied a mechanism of magnetic phase transition for a doped antiferromagnet. Not only thermally excited spin fluctuations, but also processes of decay of spin waves into particle-hole pair excitations lead together to a strong suppression of AFM long-range

order. The self-energy corrections to the spin Green's function are calculated in the self-consistent Born approximation with a particular form for a hole spectral function $\rho(k,\omega)$ which is valid near the phase transition to a magnetically disordered phase. By using results of previous studies as a background, we argued in favor of a broad structureless shape for $\rho(k,\omega)$. In this approximation an equation for the magnetic order parameter is analyzed to obtain the Néel temperature dependence on the hole concentration. Analytical estimations carried out in the final stage clearly show a sharp decrease of the Néel temperature with doping. This same behavior was observed in copper oxides.

The scheme developed in the present paper could be considered a preliminary step to start accomplishing a more tendentious program. Actually, a more accurate description could be done within complete self-consistent calculations when both systems, holes and magnetic excitations, are treated on an equal footing. This program is clearly formulated using the Born approximation both for the spin Green's function and for the hole Green's function.[20] That leads to a set of self-consistent equations for these Green's functions which should be solved numerically. This work is now in progress, and the results of the numerical computations will be presented elsewhere.

---

*Permanent address: Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, 141980 Dubna, Russia.

[1]H. Alloul, Physica B **169**, 51 (1991).

[2]J. I. Budnick *et al.*, in *Proceedings of the International Seminar on High-T_c Superconductivity, Dubna, 1989,* edited by V. L. Aksenov, N. N. Bogolubov, and N. M. Plakida (World Scientific, Singapore, 1990), p. 172.

[3]G. Shirane, Physica C **185-189**, 80 (1991).

[4]J. Rossat-Mignot *et al.*, Physica C **185-189**, 86 (1991).

[5]J. Igarashi and P. Fulde, Phys. Rev. B **45**, 12 357 (1992).

[6]G. Khaliullin and P. Horsch, Phys. Rev. B **47**, 463 (1993).

[7]I. R. Pimental and R. Orbach, Phys. Rev. B **46**, 2920 (1992).

[8]K. Becker and U. Muschelknautz (unpublished).

[9]S. V. Tyablikov, *Methods in the Quantum Theory of Magnetism* (Plenum, New York, 1967). Recent results of applying the Tyablikov RPA among other approximations to examine highly anisotropic antiferromagnets were presented N. Majlis, S. Selzer, and G. C. Strinati, Phys. Rev. B **45**, 7872 (1992).

[10]F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).

[11]S. V. Lovtsov and V. Yu. Yushankhai, Physica C **179**, 159 (1991); R. Hayn, V. Yushankhai, and S. Lovtsov, Phys. Rev. B **47**, 5253 (1993); J. H. Jefferson, H. Eskes, and L. F. Freiner, *ibid.* **45**, 7959 (1992); H.-B. Schüttler and A. J. Fedro, *ibid.* **45**, 7588 (1992); C. D. Batista and A. A. Aligia, *ibid.* **47**, 8929 (1993).

[12]J. L. Richard and V. Yu. Yushankhai, Phys. Rev. B **47**, 1103 (1993).

[13]C. L. Kane, P. A. Lee, and N. Read, Phys. Rev. B **39**, 6880 (1989).

[14]G. Martinez and P. Horsch, Phys. Rev. B **44**, 317 (1991).

[15]Yu. A. Tserkovnikov, Theor. Matem. Fiz **7**, 250 (1971); *ibid.* **49**, 219 (1981) (in Russian).

[16]N. M. Plakida, Phys. Lett. A **43**, 481 (1973).

[17]S. Schmitt-Rink, C. M. Varma, and A. E. Ruckenstein, Phys. Rev. Lett. **60**, 2793 (1988).

[18]See, for instance, the review by E. Dagatto, in Int. J. Mod. Phys. **5B**, 77 (1991).

[19]N. M. Plakida, V. S. Udovenko, and V. Yu. Yushankhai (unpublished).

[20]Such a formulation of the problem at $T=0$ was presented (but was not solved to the end) in 5.

[21]A. Auerbach and B. E. Larson, Phys. Rev. B **43**, 7800 (1991).