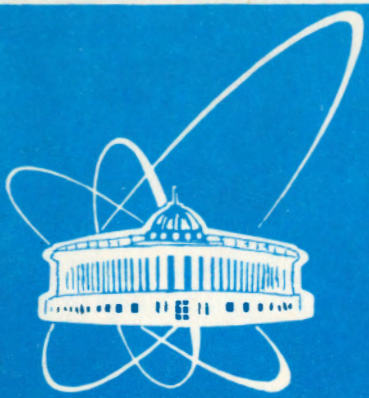

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DOPING DEPENDENCE OF ANTIFERROMAGNETISM IN COPPER OXIDES: AN ESTIMATION OF THE NEEL TEMPERATURE BASED ON THE t-J MODEL

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Зависящий от допирования антиферромагнетизм в медных оксидах: оценка температуры Нееля, основанная на t-J модели

Предложен механизм подавления антиферромагнитного дальнего порядка в слабо допированных медных оксидах. Подавление возникает вследствие распада спиновых волн в парные возбуждения типа "частица—дырка". На основе t-J модели и метода неприводимых функций Грина развито самосогласованное борновское приближение. Получено быстрое уменьшение температуры Нееля с ростом концентрации "дырок", что находится в соответствии с экспериментально наблюдаемым поведением.

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Richard J.L., V.Yu.Yushankhai E17-94-6

Doping Dependence of Antiferromagnetism in Copper Oxides: an Estimation of the Neel Temperature Based on the t-J Model

A mechanism of suppression of the antiferromagnetic long-range order in slightly doped copper oxides is proposed. This suppression is due to a decay of spin waves into particle-hole pair excitations. A self-consistent Born approximation is developed within the t-J model and the irreducible Green's function method. It is shown that the Neel temperature drops shurply with increasing hole concentration in accordance with experiment.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

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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 $3d$ long-range ordered antiferromagnets (AFM) with a well defined spin wave excitation spectrum and a Neel 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 by 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 is controlled by doping, is expected to modify significantly the magnetic properties of the system.

Along this direction, the results of several investigations were reported [5-8]. In particular it was shown in [5,6] 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, it was found a strong softening of the long wave length spin excitations due to their coupling to "electron-hole" pair excitations. The spin wave velocity was shown to vanish at a critical hole concentration δ^* of a few percent in agreement with experiments [3,4]. These calculations imply also 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 [6,8] 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 be noted also that being restricted to the case of zero temperature the calculations presented in [5-8] do not give a concentration dependence of the Neel temperature $T_N = T_N(\delta)$. The present paper is motivated by this question. We extend the approach developed in [5,6] and consider the doped AFM state for finite temperatures. We

assume that the driving interaction which establishes the $3d$ AFM ordering at finite temperatures 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 it 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-energy 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, the 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 details 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 Neel temperature.

II. The Effective Hamiltonian

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

$$H = \sum_{i,j,\sigma} t_{ij} \tilde{C}^{+}_{i,\sigma} \tilde{C}_{j,\sigma} + \frac{1}{2} \sum_{i,j} J_{ij} \vec{S}_i . \vec{S}_j \qquad (1)$$

using the following notations. In the kinetic term, $\tilde{C}^{+}_{i,\sigma} = C^{+}_{i,\sigma}(1-n_{i,-\sigma})$ are electron creation operators and the factor $(1-n_{i,-\sigma})$ enforces the constraint of no double occupancy. The hopping amplitude t_{ij} is non zero only for nearest neighbor sites belonging to the same layer which is a square lattice. In the magnetic term $\vec{S}_i$ are electron spin operators. The exchange integral J_{ij} is also non zero only for nearest neighbors

and is given by a large constant $J \sim 0.1eV$ 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 $3 \leq t/J \leq 5$.

As it was first 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 the $p-d$ to the $t-J$ Hamiltonians was developed later in several papers (see, for instance [11]). It is worth noting that one may incorporate in the $t-J$ model a weak transverse interlayer exchange interaction ($\sim J'$). This is quite natural and formally could be done in the same reduction procedure as in [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. That however would not change significantly 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

$$\begin{aligned} &\tilde{C}_{i,\sigma} \rightarrow \tilde{C}_{i,-\sigma} \\ &S^{\pm}_i \rightarrow S^{\mp}_i \\ &S^{z}_i \rightarrow -S^{z}_i \end{aligned} \qquad (2)$$

when $i \in B$. Hence from now on the spin background is effectively a ferromagnetic one and one should not distinguish between sublattices anymore. Secondly we define the action of the operators $\tilde{C}_{i,\sigma}, \tilde{C}^{+}_{i,\sigma}$ on an extended quantum space associated with spinless fermions f_i, f^{+}_i and pseudospin operators $\vec{s}_i$. To eliminate unphysical states one must introduce projection operators π_i that is 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

$$\tilde{C}_{i\uparrow} = f^{+}_i \pi_i \qquad (3a)$$

$$\tilde{C}_{i\downarrow} = f^{+}_i s^{+}_i \qquad (3b)$$

$$\vec{S}_i = \vec{s}_i (1-n_i) \qquad (3c)$$

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 $\pi_i = 1/2 + s^{z}_i$ in the case of $1/2$ spin.

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

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

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

As it is discussed in [12] this representation with $\pi_i = 1/2 + s_i^z$ 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 H_J term take care of the loss of magnetic energy in the presence of holes. In 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 for a while this renormalization to restore it at the final stage of calculations.

It is possible to generalize the 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 that 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

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

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

We fix this effective Hamiltonian as a basic one for our consideration without mapping the pseudospin operators onto boson's ones as it done in [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

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

where $[\ ,\ ]$ stands for the commutator and

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

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.[15,16] differentiating $\ll \mathcal{B}_q(t) | \mathcal{B}_q^+(t') \gg$ with respect to both times t and t'. In this way, after performing some algebra one gets the Dyson's equation for the Fourier transform of (9) in the following form

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

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

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

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

$$\ll i\dot{\mathcal{B}}_q | - i\dot{\mathcal{B}}_q^+ \gg_\omega^{(irr)} = \ll i\dot{\mathcal{B}}_q | - i\dot{\mathcal{B}}_q^+ \gg_\omega - \\ - \ll i\dot{\mathcal{B}}_q | \mathcal{B}_q^+ \gg_\omega \frac{1}{\ll \mathcal{B}_q | \mathcal{B}_q^+ \gg_\omega} \ll \mathcal{B}_q | - i\dot{\mathcal{B}}_q^+ \gg_\omega \tag{15}$$

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

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 Eqn.(12) as

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

where according to the 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 the equation (18) can be linearized by using the Tyablikov approximation [9]. This approximation applied to a magnetically ordered system consists in 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 it 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 case of a doped-AFM state and examine effects of moving holes on the staggered magnetic moment σ. These effects which are expected to be mainly due to a coupling of spin waves to particle-hole pair excitations will be examined by calculation the self-energy part in (12) to the lowest ($\sim t^2$) order. 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

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

where

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

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

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

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

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

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

where λ_q is 2×2 matrix

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

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

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

Taking into account that

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

we obtain for the frequency matrix Ω_q 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 : $\omega_q = 2\sigma\omega_q^{(0)}$, here we use 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 the equation (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, Eqn.(25), instead of the full derivative $i\dot{\mathcal{B}}_q$. Secondly, the lowest order self-energy contribution is provided by the first term in the right hand side of the expression

(15), while the second term gives rise to higher order corrections. Then, restricting ourselves to the lowest order we have

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

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

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

where

$$\chi_{q,k,k'}(\omega) = \ll f_{k-q}^+ f_k | f_{k'}^+ f_{k'-q} \gg_\omega \tag{31}$$

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 consider now a 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 $G^{(h)}(k,\omega) = = \ll f_k | f_k^+ \gg_\omega$ and applying the Fourier transform

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

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

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

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

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

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 in the self energy, Eqn. (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 $\Lambda_q(\omega) = 2\sigma\widetilde{\Lambda}_q(\omega)$.

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

$$\Lambda_q^{22}(\omega) = -\Lambda_{-q}^{11}(-\omega) \\ \Lambda_q^{21}(\omega) = -\Lambda_q^{12}(\omega) \tag{39}$$

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

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

with the following notations

$$A_q(\omega) = \frac{1}{2}\left[\widetilde{\Lambda}^{11}_q(\omega) - \widetilde{\Lambda}^{11}_{-q}(-\omega)\right]$$
$$B_q(\omega) = \frac{1}{2}\left[\widetilde{\Lambda}^{11}_q(\omega) + \widetilde{\Lambda}^{11}_{-q}(-\omega)\right] \qquad (41)$$

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

IV. Staggered magnetization and Neel temperature

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

$$\sigma = \frac{1}{2} - \frac{1}{N}\sum_q \langle s^-_q s^+_q \rangle \qquad (42)$$

where

$$\langle s^-_q s^+_q \rangle = \int_{-\infty}^{+\infty} d\omega \frac{-\frac{1}{\pi}\mathrm{Im} \ll B_q | B^+_q \gg^{11}_{\omega+i0+}}{e^{\beta\omega}-1} \qquad (43)$$

with the imaginary part of $\ll B_q | B^+_q \gg^{11}_{\omega}$ being defined from the equation (17). The equation (42) then becomes

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

with the spin excitation spectrum $\omega_q = 2\sigma\widetilde{\omega}_q$ being a solution of the Eqn.(40). Below we will solve the Eqn.(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 Neel background was calculated [13,14] within the self-consistent Born approximation on the basis of the Hamiltonian (7),(8) with spin's operators mapped onto boson's ones. In this

consideration a hopping of a hole is only possible by emitting (or absorbing) of 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 $2d$ intralayer spin-spin correlations still persist and survive even in a disordered phase [3,4]. This makes reasonable an assumption that the approach to a hole motion developed in [13,14] is also applicable near the phase transition. However, effects of a finite hole doping and of temperature should be taken into account and a strong renormalization of spin-wave excitation spectrum is one of them.Below we first briefly sketch some results of 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 the spectral density $\rho(k,\omega)$ tends to when the system approaches the AFM phase transition.

Being 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

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

with

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

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 band width W is estimated to be of order of J, while the residue $Z_k \sim J/t$. Kane et al.[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 $\Gamma \leq zt$, where $z = 4$.

Igarashi and Fulde [5] applied the self-consistent Born approximation to calculate $\rho(k,\omega)$ at finite low dopant concentration $\delta << 1$ and $T = 0$. They found that for any particular momentum $\vec{k}$ a hole spectral density is redistributed in such a way that a new incoherent extra structure appears quite below the QP band. This extra structure with a spectral weight of order of δ provides a fulfilling of a sum rule (Eqn.(36) in our notations) with a chemical potential located inside the QP band. Along this way a four-pocket Fermi surface for non-interacting 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, however, that a broad incoherent part of the hole spectrum gives 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 $\rho \sim \frac{1}{2\Gamma}$, where $\Gamma \lesssim zt$, within proper energy intervals below and above the QP band. They also emphasized that quasiholes produce 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. $Z_k \sim \frac{J}{t} << 1$, 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 [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, as it was pointed out by Kane et al.[13] 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 stuggered magnetization σ. As a result the processes of scattering of a quasihole by spin-wave excitations turn to be dominant, that lead to a broadening of the QP peaks. These peaks lose their identity and the entire hole spectrum becomes incoherent.

Hence, to evaluate the function $\chi_{q,k}(\omega)$, Eqn.(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 $\Gamma \lesssim zt$.

So taking into account the incoherent part only, it is easy to check that the quantities $A_q(\omega)$ and $B_q(\omega)$ become q-independent. Moreover, note that

$$A_q(2\sigma\tilde{\omega}_q) = 0$$

$$B_q(2\sigma\tilde{\omega}_q) = -\left(\frac{zt}{2}\right)^2 \chi(T,\delta) + O[(2\sigma\tilde{\omega}_q)^2]$$

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

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

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

The function $\chi(T,\delta)$ depends on temperature T and dopant concentration δ through the chemical potential $\mu = \mu(T,\delta)$ which satisfies the Eqn.(36). The self-consistent equation (44) for the stuggered 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 the Eqn.(40) leads to the following spin-wave spectrum

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

Note that we approximated the factors $J(0) \pm J(q)$ in Eqn. (40) as the $2d$ factors $zJ(1 \pm \gamma_q)$ while the quantity $\omega_q^{(0)}$ preserves its 3-dimensional nature, Eqn.(28).

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

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

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

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

When $\xi \to 0$ the dominant contribution to the sum in Eqn.(53) originates from the neighborhood of $\vec{q} = 0$ that leads to a singular dependence as $C_\xi \sim ln\xi^{-1}$. Hence, the Neel temperature tends to zero with $\xi \to 0$ and the correct thermodynamic behavior is restored in $2d$ limit [9].

From the Eqn.(53) one can see that at finite dopant concentration the stuggered magnetization vanishes at 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

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

where the chemical potential $\mu = \mu(T, \delta)$ satisfies the Eqn.(36). To derive the 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 the Eqn.(36) for the chemical potential μ can be easily solved to give the Fermi distribution function entering in (55) as follows

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

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

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

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

$$2\beta\Gamma\delta << 1. \tag{57}$$

In this case one obtains from Eqn.(56)

$$n\left[\Gamma(2x-1) - \mu\right] \simeq 2\beta\Gamma\delta e^{-2\beta\Gamma x}, \qquad (0 \le x \le 1). \tag{58}$$

This Boltzmann–type form of the distribution function arises due to a strong renormalization of the chemical potential μ, Eqn.(36). Such a 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 Euler constant ($\mathcal{C} \sim 0.6$). Hence Eqn. (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 Neel temperature. We have plotted the corresponding curve $\tau(\delta)$ in Fig. 1 with $t = 0.5\text{eV}$, $J/t = 0.2$, $\Gamma = 2\sqrt{3}t$ and with the Neel temperature $T_N(0) = J/3$ ($\sim 300°\text{K}$) 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 $\tau \lesssim 1$, the Eqn.(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 the Eqn.(62) to the region of higher values of δ and more lower temperature still remains questionable. Therefore, let us return to the basic equation (54) and examine the other limit

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

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

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

In comparison with the case we considered above, Eqns.(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 Neel temperature $T_N(\delta)$ at finite hole concentration δ. This allows us to approximate further the Eqn.(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 $\delta^* \simeq 0.08$.

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

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 the results of previous studies as a background we argued in favour of a broad structureless shape for $\rho(k,\omega)$. In this approximation an equation for the magnetic order parameter is analyzed to obtain the Neel temperature dependence on hole concentration. Analytical estimations carried out in the final stage shown clearly a sharp decrease of the Neel temperature with doping. Just this behavior was observed in copper oxides.

The scheme developed in the present paper could be considered as a preliminary step to start accomplishing a more tendentious program. Actually, 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 by 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 in progress now and the results of numerical computations will be presented elsewhere.

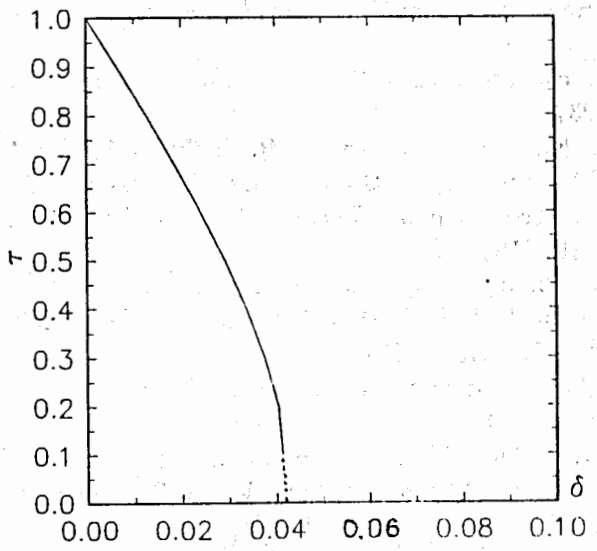

Fig. 1 The reduced Neel temperature dependence on hole concentration as following from Eqn.(62). The parameters are defined in the text.

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