

Damping of spin waves for a doped antiferromagnet

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The spin-wave energy, the damping, and the staggered magnetization are calculated for a lightly doped antiferromagnet in the framework of the t - J model. The Dyson equation for the dynamical spin susceptibility is derived and studied at zero temperature. It is shown that the staggered magnetization as well as the spin-wave velocity vanish for some critical hole concentration. The damping of spin waves is computed and found to be very sensitive to the hole doping. The results are in good agreement with experimental data of $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$.

I. INTRODUCTION

The understanding of the transition from the insulating phase to the metallic phase for high- T_c superconductors is a problem of current interest.¹ The undoped parent compounds of high- T_c materials are antiferromagnetic (AFM) insulators. When a small quantity of holes is introduced (a few percent), the long-wavelength spin-wave modes are overdamped and consequently the AFM order disappears.

The magnetic properties of the undoped high- T_c materials are well described by the isotropic spin- $\frac{1}{2}$ Heisenberg model on a square lattice.^{2,3} It is by now widely accepted that when extra holes are introduced, a good candidate for describing the physics of the CuO_2 planes of these high- T_c oxides is the t - J model. It has been argued that in the linear spin-wave approximation this model reduces to the so-called magnetic-polaron model,⁴⁻⁶ with a Hamiltonian given by

$$H = \frac{zt}{\sqrt{N}} \sum_{qk} V(q, k) f_k^\dagger f_{k-q} \alpha_q + \text{H.c.} + \sum_q \omega_q^0 \alpha_q^\dagger \alpha_q, \quad (1)$$

where

$$V(q, k) = u_q \gamma_{k-q} + v_q \gamma_k,$$

$$\omega_q^0 = \frac{1}{2} z J \sqrt{1 - \gamma_q^2}$$

with $\gamma_k = \frac{1}{z} \sum_\tau \exp(i\mathbf{k}\boldsymbol{\tau})$, τ running over the band directions and z is the coordination number of nearest neighbors. N is the total number of sites. The lattice spacing is taken as unity. u_q and v_q are the usual parameters of the Bogoliubov u - v transformation

$$u_q = \left[\frac{1 + \sqrt{1 - \gamma_q^2}}{2\sqrt{1 - \gamma_q^2}} \right]^{\frac{1}{2}},$$

$$v_q = -\text{sgn}(\gamma_q) \left[\frac{1 - \sqrt{1 - \gamma_q^2}}{2\sqrt{1 - \gamma_q^2}} \right]^{\frac{1}{2}}. \quad (2)$$

In the Hamiltonian Eq. (1), f_k and f_k^\dagger are canonical spinless fermion operators. α_q and α_q^\dagger are canonical boson operators.

The softening of spin waves due to the presence of holes was already investigated by several authors^{7-10,6} within the framework of this model. Igarashi and Fulde⁷ have studied the renormalization of spin waves for low dopant concentration δ on the basis of the self-consistent Born approximation. They have calculated the Green's function for the holes to first order in δ and found that the incoherent part of the Green's function for holes gives the main contributions to the renormalization of spin waves. They have found that the spin-wave velocity is strongly renormalized and the reduction rate increases with decreasing ratio J/t . The spin-wave velocity is found to vanish for a density of holes of about 10%. The experimental value is about 2-5%. Pimental and Orbach⁸ have computed the spin self-energy in an approximation where they take into account only the coherent part of the hole Green's function, that is, they consider quasiholes as weakly interacting Fermi gas described by a single-hole dispersion relation. They have found that the spin-wave velocity is renormalized by a factor 0.98 for a hole concentration $\delta = 0.01$ at $t/J = 3$. But the coherent part of the hole Green's function leads to a small renormalization of the AFM-order parameter, as was found by Becker and Muschelknautz.⁹ Recently Khaliullin and Horsch⁶ have calculated the spin-wave velocity and found that it vanishes for the critical hole concentration $\delta^* = 0.04$ for $t/J = 4$. They have also calculated the staggered magnetization using an interpolation formula for spin self-energy based on the approximation of isotropic Fermi gas, since they did not calculate the spin self-energy at large momentum.

In this paper we calculate the spin-wave energy for any momentum, the damping of spin waves, and the staggered magnetization on the basis of double time Green's-function formalism. Dyson's equation for dynamical spin susceptibility is written and analyzed at zero temperature. We found that the spin-wave energy is strongly renormalized due to the presence of holes, and the spin-wave velocity goes to zero for some critical hole concentration. The damping is also found to be very sensitive to increasing hole concentration. At the critical hole

concentration it becomes greater than the spin-wave energy for small momentum, which shows that the long-wavelength spin waves are overdamped. The staggered magnetization also vanishes at this hole concentration.

The paper is organized as follows: in Sec. II, we have derived Dyson's equation for the double-time Green's function following the method of Tserkovnikov.¹¹ In Sec. III, the spin-wave energy and the damping of spin waves is computed. Section IV is devoted to the computation of the staggered magnetization. Finally, in Sec. V, the comparison of our calculation with experimental data is performed.

II. DYSON'S EQUATION FOR RETARDED GREEN'S FUNCTION

In this section we derive the dynamical spin susceptibility using the double-time retarded Green's functions defined by Zubarev:¹²

$$\langle\langle A(t) | B(t') \rangle\rangle = -i\theta(t-t')\langle[A(t), B(t')]\rangle. \quad (3)$$

Its Fourier component with respect to time is

$$\langle\langle A | B \rangle\rangle_\omega = \int dt \langle\langle A(t) | B(0) \rangle\rangle \exp(\omega + i\epsilon)t, \quad (4)$$

where $\langle \dots \rangle$ means averaging over the grand-canonical ensemble and $\theta(t)$ is the usual step function. Let us define the following two-component operators:

$$A_q = \begin{pmatrix} \alpha_q \\ \alpha_{-q}^\dagger \end{pmatrix}, \quad A_q^\dagger = (\alpha_q^\dagger \quad \alpha_{-q}). \quad (5)$$

The different spin-wave Green's functions are contained in the matrix Green's function $\langle\langle A_q | A_q^\dagger \rangle\rangle_\omega$. Using the Tserkovnikov method¹¹ (see Appendix A), we obtain the following equation of motion:

$$\begin{aligned} \omega \langle\langle A_q | A_q^\dagger \rangle\rangle_\omega &= \langle A_q | A_q^\dagger \rangle + \langle\langle A_q | A_q^\dagger \rangle\rangle_\omega \\ &\times \left\{ \langle i\dot{A}_q | A_q^\dagger \rangle \langle A_q | A_q^\dagger \rangle^{-1} \right. \\ &\left. + \langle A_q | A_q^\dagger \rangle \Pi_q(\omega) \right\}, \end{aligned} \quad (6)$$

where the polarization operator is given by

$$\begin{aligned} \Pi_q(\omega) &= \langle A_q | A_q^\dagger \rangle^{-1} \left\{ \langle\langle i\dot{A}_q | -i\dot{A}_q^\dagger \rangle\rangle_\omega - \langle\langle i\dot{A}_q | A_q^\dagger \rangle\rangle_\omega \right. \\ &\left. \times \langle\langle A_q | A_q^\dagger \rangle\rangle_\omega^{-1} \langle\langle A_q | -i\dot{A}_q^\dagger \rangle\rangle_\omega \right\} \langle A_q | A_q^\dagger \rangle^{-1}. \end{aligned} \quad (7)$$

For the Hamiltonian under investigation Eq. (1) we have

$$\langle A_q | A_q^\dagger \rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (8)$$

and

$$\langle i\dot{A}_q | A_q^\dagger \rangle = \omega_q^0 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (9)$$

Then Eq. (6) becomes

$$\begin{pmatrix} \langle\langle \alpha_q | \alpha_q^\dagger \rangle\rangle_\omega & \langle\langle \alpha_q | \alpha_{-q} \rangle\rangle_\omega \\ \langle\langle \alpha_{-q}^\dagger | \alpha_q^\dagger \rangle\rangle_\omega & \langle\langle \alpha_{-q}^\dagger | \alpha_{-q} \rangle\rangle_\omega \end{pmatrix} = \frac{1}{D_q(\omega)} \begin{pmatrix} \omega + \omega_q^0 + \Pi_{22}(q, \omega) & -\Pi_{12}(q, \omega) \\ -\Pi_{21}(q, \omega) & -\{\omega - \omega_q^0 - \Pi_{11}(q, \omega)\} \end{pmatrix}, \quad (10)$$

where

$$D_q(\omega) = [\omega + \omega_q^0 + \Pi_{22}(q, \omega)][\omega - \omega_q^0 - \Pi_{11}(q, \omega)] + \Pi_{12}(q, \omega)\Pi_{21}(q, \omega), \quad (11)$$

and $\Pi_q(\omega)$ is the self-energy matrix. To the lowest order in t , this matrix is given by

$$\Pi_q(\omega) \simeq \begin{pmatrix} \langle\langle b_q | b_q^\dagger \rangle\rangle_\omega & \langle\langle b_q | b_{-q} \rangle\rangle_\omega \\ \langle\langle b_{-q}^\dagger | b_q^\dagger \rangle\rangle_\omega & \langle\langle b_{-q}^\dagger | b_{-q} \rangle\rangle_\omega \end{pmatrix} \quad (12)$$

with $b_q = (zt/\sqrt{N}) \sum_{qk} V(q, k) f_{k-q}^\dagger f_k$. The matrix elements of the self-energy $\Pi_q(\omega)$ contain averages of four fermion operators. To evaluate these quantities we decouple in the following way:

$$\langle f_{k_1-q}^\dagger(t) f_{k_1}(t) f_{k_2-q}^\dagger f_{k_2} \rangle \simeq \delta_{k_1 k_2} \langle f_{k_1-q}^\dagger(t) f_{k_1-q}(t) \rangle \langle f_{k_1}(t) f_{k_1}^\dagger(t) \rangle. \quad (13)$$

Straightforward algebraic calculations lead to

$$\Pi_{11}(q, \omega) = \frac{(zt)^2}{N} \sum_k |V(q, k)|^2 \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 [n(\omega_1)n(-\omega_2) - n(-\omega_1)n(\omega_2)] \frac{\rho_{\omega_1}(k-q)\rho_{\omega_2}(k)}{(\omega + \omega_1 - \omega_2 + i\epsilon)}, \quad (14)$$

$$\Pi_{22}(q, \omega) = \Pi_{11}(-q, -\omega),$$

$$\Pi_{12}(q, \omega) = \frac{(zt)^2}{N} \sum_k V(q, k) V(-q, k - q) \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 [n(\omega_1)n(-\omega_2) - n(-\omega_1)n(\omega_2)] \frac{\rho_{\omega_1}(k - q)\rho_{\omega_2}(k)}{(\omega + \omega_1 - \omega_2 + i\epsilon)} \quad (15)$$

and $\Pi_{21}(q, \omega) = \Pi_{12}(q, \omega)$, with $n(\omega) = 1/[1 + \exp(\beta\omega)]$; β being the inverse of the temperature and $\rho_{\omega}(k) = -\frac{1}{\pi} \text{Im} \langle \langle f_k | f_k^\dagger \rangle \rangle_{\omega+i0^+}$ is the spectral density of holes. The denominator in Eq. (10) can be written as

$$D_q(\omega) = \omega^2 [1 + \lambda_q(\omega)]^2 - (\omega_q^0)^2 [1 - \Pi_q^+(\omega)][1 - \Pi_q^-(\omega)], \quad (16)$$

where $\lambda_q(\omega) = [\Pi_{22}(q, \omega) - \Pi_{11}(q, \omega)]/2\omega$ and $\Pi_q^\pm(\omega) = [\Pi_{11}(q, \omega) + \Pi_{22}(q, \omega) \pm 2\Pi_{12}(q, \omega)]/2\omega_q^0$. Using the expression of u_q and v_q given in Eq. (1), we obtain

$$\lambda_q(\omega) = \frac{(zt)^2}{N} \sum_k (\gamma_{k+q}^2 - \gamma_k^2) \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 n(\omega_1)n(-\omega_2) \frac{\rho_{\omega_1}(k)\rho_{\omega_2}(k+q)}{(\omega + \omega_2 - \omega_1 + i\epsilon)(-\omega + \omega_2 - \omega_1 - i\epsilon)} \quad (17)$$

and

$$\begin{aligned} \Pi_q^\pm(\omega) &= \frac{zt^2}{J} \frac{1}{N} \sum_k \frac{(\gamma_{k+q} \pm \gamma_k)^2}{1 \pm \gamma_q} \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 n(\omega_1)n(-\omega_2) \\ &\quad \times \rho_{\omega_1}(k)\rho_{\omega_2}(k+q) \left\{ \frac{1}{\omega + \omega_2 - \omega_1 + i\epsilon} + \frac{1}{-\omega + \omega_2 - \omega_1 - i\epsilon} \right\}. \end{aligned} \quad (18)$$

Note that knowing the spectral density $\rho_{\omega}(k)$, one can evaluate the renormalized spin-wave energy, the damping, and the staggered magnetization.

III. DAMPING OF SPIN WAVES AT ZERO TEMPERATURE

The spectrum of the spin waves corresponds to the poles of the matrix Green's function $\langle \langle A_q | A_q^\dagger \rangle \rangle_{\omega}$, that is, to the zeros of $D_q(\omega)$. Since $D_q(-\omega) = D_q(\omega)$, if ω_q is a pole, $-\omega_q$ is also a pole. At zero hole concentration the poles reduce to $\pm\omega_q^0$. Then, since we are studying the effect of a small hole density ($\delta \ll 1$) on spin waves, we shall look for poles of the form $\omega_q = \omega_q^0(1 + \delta K_q)$. Moreover, λ_q and Π_q^\pm are proportional to δ . Then, keeping only the first-order correction with respect to δ , $D_q(\omega)$ becomes

$$D_q(\omega) \simeq \omega^2 [1 + \lambda_q(\omega_q^0)]^2 - (\omega_q^0)^2 [1 - \Pi_q^+(\omega_q^0)][1 - \Pi_q^-(\omega_q^0)]. \quad (19)$$

Let us denote by $\omega_q + i\Gamma_q$ the zeros of Eq. (19). ω_q will be the spin-wave energy and Γ_q will be the damping of the spin waves. To the lowest order in δ , one gets

$$\omega_q \simeq \omega_q^0 \sqrt{1 - \text{Re}\Pi_q^-(\omega_q^0) - \text{Re}\Pi_q^+(\omega_q^0) / [1 + \text{Re}\lambda_q(\omega_q^0)]} \quad (20)$$

and

$$\Gamma_q/\omega_q \simeq -\frac{1}{2} \frac{2\text{Im}\lambda_q(\omega_q^0) + \text{Im}\Pi_q^-(\omega_q^0) + \text{Im}\Pi_q^+(\omega_q^0)}{1 - \text{Re}\Pi_q^-(\omega_q^0) - \text{Re}\Pi_q^+(\omega_q^0)}. \quad (21)$$

To evaluate λ_q and Π_q^\pm we shall use the result of the one hole problem as an ansatz for the spectral density of

holes $\rho_{\omega}(k)$. The motion of a single hole in an AFM-spin background has been studied by several authors using the model under investigation.^{4,5,13} It is by now widely accepted that the motion of a hole perturbs the magnetic background, but quantum spin fluctuations restore it, leading to a coherent motion of the hole. Then it is natural to take for the spectral hole density $\rho_{\omega}(k)$ a δ function in the range of energy where the motion is supposed to be coherent, which corresponds to a quasi-particlelike behavior and to take the constant density of states approximation for the broad incoherent part of the motion. This picture was found to be quite valid by recent numerical calculation for finite hole concentration on clusters.^{14,15} Then we write

$$\rho_{\omega}(k) = \rho_{\omega}^{\text{coh}}(k) + \rho_{\omega}^{\text{incoh}}(k)$$

with

$$\rho_{\omega}^{\text{coh}}(k) = Z_0 \delta(\omega - E_k), \quad (22)$$

$$\rho_{\omega}^{\text{incoh}}(k) = \frac{1}{2W} \theta(\omega - J) \theta(2W - \omega),$$

where $2W$ is the bandwidth and E_k is the energy of the quasihole. E_k reaches its minimum at momenta $(\pm\pi/2, \pm\pi/2)$. Moreover, we suppose that near the minimum E_k is isotropic and can be written as $E_k \approx k^2/2m$, where m is the effective mass of the quasihole. ω is measured from the minimum of the quasihole energy. The residue of the quasihole Z_0 is determined by the sum rule $\int_{-\infty}^{\infty} d\omega \rho_{\omega}(k) = 1$, which gives $Z_0 = J/2W$. To introduce the chemical potential μ in Eq. (22) one has simply to make the following change $\omega \rightarrow \omega + \mu$.¹⁶ At zero tem-

perature and for small hole density μ will lie near the bottom of the spectrum, that is, in the coherent band. The chemical potential is adjusted in such a way as to give the correct density of holes δ . We have

$$\delta = \frac{1}{N} \sum_{\mathbf{k}} \int_{-\infty}^{\infty} d\omega \rho_{\omega+\mu}(\mathbf{k}) n(\omega).$$

For $T = 0$, $n(\omega) = \theta(-\omega)$, and therefore one gets for μ

$$\mu = \delta \frac{\pi W}{mJ}. \quad (23)$$

It was already noticed by Igarashi and Fulde⁷ that the magnon softening is due to the existence of the incoherent background; that is, the incoherent part of the Green's

function gives rise to the main renormalization. The calculation performed by Khaliullin and Horsch⁶ is an indication that the contribution coming from purely coherent motion is negligible in comparison to that one due to the incoherent background. In what follows we will neglect this purely coherent contribution and will take into account only the coherent-incoherent contribution. The incoherent-incoherent part is strictly zero in our approximation, since we suppose that $\mu < J$. This assumption is compatible with Eq.(23), taking $m = 2J^{-1}$ and δ is a few percent. This value of the effective mass of the quasihole is suggested by the estimation made by Kane, Lee, and Read.⁴ This is a discrepancy between our calculation and that one performed by Khaliullin and Horsch,⁶ since they have an incoherent-incoherent contribution for the renormalization of the spin waves. In this approximation we obtain to first order in δ for the spin-wave energy and the damping the following expressions:

$$\omega_q \simeq \omega_q^0 \sqrt{1 - 2\delta \frac{t^2}{JW} \frac{1 - \gamma_{2q}}{1 - \gamma_q^2} I_1(\omega_q^0)} \left/ \left[1 + \delta \frac{t^2}{JW} \frac{1 - \gamma_{2q}}{\sqrt{1 - \gamma_q^2}} I_0(\omega_q^0) \right] \right. \quad (24)$$

and

$$\Gamma_q/\omega_q \simeq \pi \delta \frac{t^2}{JW} (1 - \gamma_{2q}) \Upsilon(\omega_q^0) \left[\frac{1}{\sqrt{1 - \gamma_q^2}} + \frac{1}{1 - \gamma_q^2} \right] \left/ \left[1 - 2\delta \frac{t^2}{JW} \frac{1 - \gamma_{2q}}{1 - \gamma_q^2} I_1(\omega_q^0) \right] \right., \quad (25)$$

where $I_0(\omega_q^0)$, $I_1(\omega_q^0)$, and $\Upsilon(\omega_q^0)$ are given in Appendix B.

At small momenta, we deduce the spin-wave velocity v from Eq. (24). We have

$$v = v_0 \sqrt{1 - \delta/\delta_c}, \quad (26)$$

where $v_0 = \sqrt{2J}$ is the unrenormalized spin-wave velocity, and δ_c is the critical hole density at which the spin-wave velocity goes to zero. It is given by

$$\delta_c \simeq \frac{(JW/2zt^2)}{\ln(2W/J)}. \quad (27)$$

We notice that at first order in δ , the spin-wave velocity is independent of the effective mass of the quasihole. For the bandwidth $2W = 2zt$ and $t/J = 5$ we have $\delta_c = 0.027$, which is very close to the experimental value for the $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ material.^{17,18}

From Eq. (24), we have plotted in Fig. 1 the momentum dependence of the spin-wave energy for different values of the hole density. We see clearly that a small number of holes strongly renormalize the spin-wave excitation spectrum. We emphasize here that we have obtained a wave-vector-dependent renormalization of the spin-wave

energy in agreement with the results of Rossat-Mignod *et al.*^{18,19} Our result differs from that one of Ko,²⁰ since he had studied the disruption of the spin excitations due to finite-hole doping by considering only the effect of static holes in the t - J model and found that the spin-wave en-

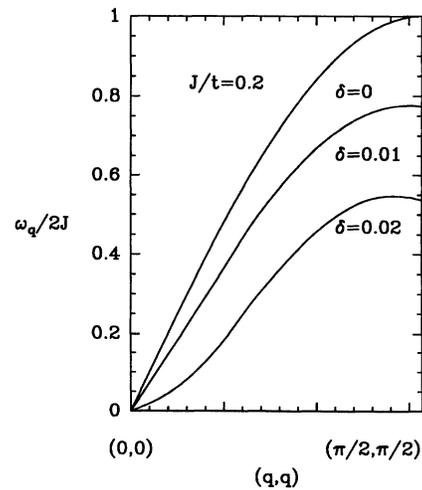


FIG. 1. Spin-wave energy along $\mathbf{q} = (q, q)$ for different hole densities.

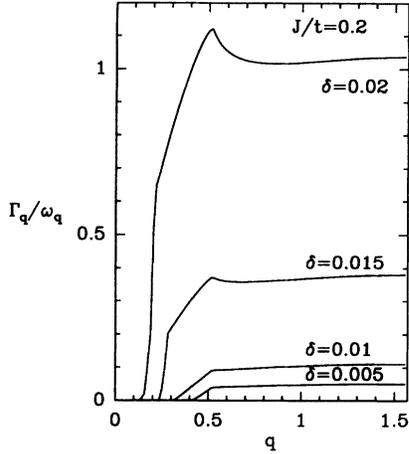


FIG. 2. Ratio of the spin-wave damping to the spin-wave energy Γ_q/ω_q along $\mathbf{q} = (q, q)$ for different hole densities.

ergy collapses for some critical δ about 0.1. This shows that the hole motion produces the main disruption to the spin excitations.

The momentum dependence of the damping Γ_q for different values of the hole density is represented in Fig. 2. It shows that the doping leads to a heavy damping of the long-wavelength spin waves due to their decay into particle-hole pairs. The damping of the spin waves occurs when the spin-wave spectrum crosses the pair excitation continuum, defined as the region where $\text{Im}\Pi(q, \omega) \neq 0$.²¹ For a very small hole concentration such that the spin-wave velocity v is still larger than the Fermi velocity v_F , long-wavelength spin waves remain well defined, because they cannot decay into particle-hole pairs while the short wavelength spin waves are damped, which is shown in Fig. 2 for $\delta = 0.01$. When the hole density increases the spin-wave velocity decreases and becomes smaller than the Fermi velocity and therefore the spin-wave spectrum lies entirely in the pair excitation continuum and even the long-wavelength spin waves are overdamped.

IV. STAGGERED MAGNETIZATION

Khaliullin and Horsch in Ref. 6, calculated the self-energy of spin excitations for a small wave-vector only. Then they estimated the staggered magnetization by making an interpolation formula for the self-energy, based on the approximation of two-dimensional (2D) isotropic Fermi gas. In our calculation we get the self-energy at any momentum and therefore can compute, without further assumption, the staggered magnetization for different values of the hole concentration.

In the model under investigation the magnetization is given by

$$M = M_0 - \frac{1}{2N} \sum_q \frac{\langle \alpha_q^\dagger \alpha_q \rangle - \gamma_q \langle \alpha_{-q} \alpha_q \rangle}{\sqrt{1 - \gamma_q^2}}, \quad (28)$$

where M_0 is the staggered magnetization at zero hole density. It is given by

$$M_0 = 1 - \frac{1}{2N} \sum_q \frac{1}{\sqrt{1 - \gamma_q^2}}. \quad (29)$$

The quantities $\langle \alpha_q^\dagger \alpha_q \rangle$ and $\langle \alpha_{-q} \alpha_q \rangle$ are related to the imaginary part of the Green's functions $\langle \langle \alpha_q | \alpha_q^\dagger \rangle \rangle_\omega$ and $\langle \langle \alpha_q | \alpha_{-q} \rangle \rangle_\omega$, respectively, by the fluctuation-dissipation theorem. From Eq. (10), we have

$$\langle \langle \alpha_q | \alpha_q^\dagger \rangle \rangle_\omega = \frac{\omega + \omega_q^0 + \Pi_{22}(q, \omega)}{D_q(\omega)} \quad (30)$$

and

$$\langle \langle \alpha_q | \alpha_{-q} \rangle \rangle_\omega = -\frac{\Pi_{12}(q, \omega)}{D_q(\omega)}. \quad (31)$$

For a small hole concentration δ , we can neglect the damping and get to first order in δ

$$-\frac{1}{\pi} \text{Im} \langle \langle \alpha_q | \alpha_q^\dagger \rangle \rangle_{\omega+i0^+} = \frac{\omega + \omega_q^0 + \text{Re}\Pi_{22}(q, \omega_q^0)}{2\omega_q [1 + 2 \text{Re}\lambda_q(\omega_q^0)]} \times [\delta(\omega - \omega_q) - \delta(\omega + \omega_q)] \quad (32)$$

and

$$-\frac{1}{\pi} \text{Im} \langle \langle \alpha_q | \alpha_{-q} \rangle \rangle_{\omega+i0^+} = -\frac{\text{Re}\Pi_{12}(q, \omega_q^0)}{2\omega_q [1 + 2 \text{Re}\lambda_q(\omega_q^0)]} \times [\delta(\omega - \omega_q) - \delta(\omega + \omega_q)]. \quad (33)$$

At zero temperature, we have

$$\langle \alpha_q^\dagger \alpha_q \rangle \simeq \frac{-\omega_q + \omega_q^0 + \text{Re}\Pi_{22}(q, \omega_q^0)}{2\omega_q [1 + 2 \text{Re}\lambda_q(\omega_q^0)]} \quad (34)$$

and

$$\langle \alpha_{-q} \alpha_q \rangle \simeq \frac{-\text{Re}\Pi_{12}(q, \omega_q^0)}{2\omega_q [1 + 2 \text{Re}\lambda_q(\omega_q^0)]} \quad (35)$$

the self-energies $\text{Re}\Pi_{22}$ and $\text{Re}\Pi_{12}$ being given by

$$\text{Re}\Pi_{22}(q, \omega_q^0) \simeq -\delta \frac{t^2}{W} (1 - \gamma_{2q}) \times \left[\frac{1}{\sqrt{1 - \gamma_q^2}} I_1(\omega_q^0) + I_0(\omega_q^0) \right] \quad (36)$$

and

$$\text{Re}\Pi_{12}(q, \omega_q^0) \simeq \delta \frac{t^2}{W} \frac{1 - \gamma_{2q}}{\sqrt{1 - \gamma_q^2}} \gamma_q I_1(\omega_q^0). \quad (37)$$

For δ in the neighborhood of δ_c and for small q , $\Gamma_q \gg \omega_q$ so that we neglect ω_q in front of Γ_q . We obtain then

$$\langle \alpha_q^\dagger \alpha_q \rangle \simeq \frac{\omega_q^0 + \text{Re}\Pi_{22}(q, \omega_q^0)}{2\omega_q [1 + 2 \text{Re}\lambda_q(\omega_q^0)]}$$

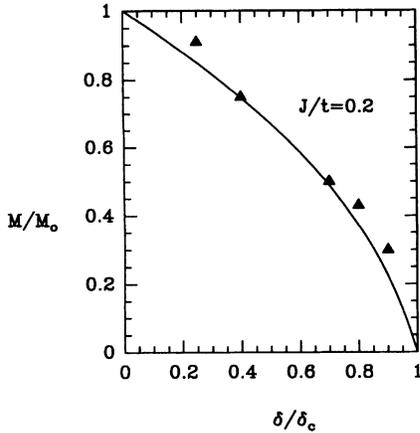


FIG. 3. Data of the normalized staggered magnetization M/M_0 as a function of the normalized hole density δ/δ_c : Theory for $J/t = 0.2$ and $m = 2J^{-1}$ (solid curve); measurement of ordered moment for $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ (solid triangles) (Ref. 18).

and

$$\langle \alpha_{-q} \alpha_q \rangle \simeq \frac{-\text{Re} \Pi_{12}(q, \omega_q^0)}{2\omega_q [1 + 2 \text{Re} \lambda_q(\omega_q^0)]}.$$

Having the quantities $\langle \alpha_q^\dagger \alpha_q \rangle$ and $\langle \alpha_{-q} \alpha_q \rangle$, we integrate numerically over q in Eq. (28) for different values of hole density to obtain the staggered magnetization. The dependence of the reduced magnetization on hole density $M(\delta)/M_0$ is plotted in Fig. 3 for the physical ratio $t/J = 5$ and $m = 2J^{-1}$. We see that the staggered magnetization goes to zero for the critical hole concentration δ_c .

V. CONCLUSION

The aim of this work was to study the magnetic properties of the t - J model, and especially the transition from the insulating phase to the metallic phase. We have presented the results of calculations of the spin-wave energy, the damping of spin waves and the staggered magnetization to first order in δ . Let us notice that the actual expansion parameter appears to be $t\sqrt{\delta}/\sqrt{JW}$ [see, for example, Eqs. (24) and (25)], which is very small for the range of δ we considered. In fact $t\sqrt{\delta}/\sqrt{JW} \leq 0.16$ for $t/J = 5$ and $W = zt$. These results may be compared to the experimental data for high- T_c superconductors. We have found that the spin-wave energy is strongly renormalized by a small hole doping (Fig. 1). The spin-wave velocity has a square-root concentration dependence and vanishes for the critical hole concentration $\delta_c = 2.7\%$ (for $t/J = 5$). The value of δ_c depends only on the ratio t/J . This value is very close to the experimental value ($\sim 2\%$) for $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$.^{18,19} We have also computed the damping of the spin waves and found that it is very sensitive to the hole doping (Fig. 2). For the critical hole concentration not only the short-wavelength spin waves

but also the long-wavelength spin waves are overdamped due to their decay into electron-hole pairs. The damping of the spin waves leads to the disappearance of the AFM order. Figure 3 shows the dependence of the staggered magnetization on the hole density. The available experimental data for $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ gives the dependence of the AFM order on the oxygen content x , but there is no trivial linear relationship between x and the hole concentration δ . Then to make the comparison between our result and the experimental data for $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$, we have used the relation between δ and x given by Uimin and Rossat-Mignod.²² According to their results, we see in Fig. 3 that our theory is in good quantitative agreement with experimental data for $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$.^{18,19}

Our calculation is based on the polaron model for which an antiferromagnetic background is assumed. However, it has been noticed by Shraiman and Siggia²³ that an AFM state is always unstable against a spiral state as soon as the density of holes is nonzero. According to Igarashi and Fulde,²⁴ the corresponding Hamiltonian can be decomposed into the polaron Hamiltonian, Eq. (1), and an extra term containing only charge operators. So the equation of motion for the susceptibility remain the same. The spectral hole density $\rho_\omega(k)$ will change. If we assume, however, that the picture of a small coherent spectrum and a large incoherent one, is not modified, the main effect will be contained only in a renormalized effective mass, the inverse of which is shifted by a term proportional to δ . But we have noticed in Appendix B that the critical hole density is independent of the effective mass in our lowest order calculation. Therefore, we expect that the spiral state will manifest itself only when computing second-order corrections.

In conclusion we have shown that the motion of holes strongly modifies the spin dynamics: the low-energy part of the spectrum is strongly renormalized and the damping of spin waves becomes very important, and consequently the long-range magnetic order is destroyed.

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APPENDIX A: TSERKOVNIKOV METHOD

The equation of motion of $\langle\langle A_q | A_q^\dagger \rangle\rangle_\omega$ is given by

$$\omega \langle\langle A_q | A_q^\dagger \rangle\rangle_\omega = \langle A_q | A_q^\dagger \rangle + \langle\langle i\dot{A}_q | A_q^\dagger \rangle\rangle_\omega, \quad (\text{A1})$$

where $i\dot{A}_q$ is the Fourier transform of

$$i \frac{d}{dt} A_q(t) = [A_q, H](t) \quad (\text{A2})$$

and $\langle A_q | A_q^\dagger \rangle = \langle [A_q, A_q^\dagger] \rangle$. The operator $i\dot{A}_q(t)$ can be separated into a linear part proportional to $A_q(t)$ and the remaining orthogonal part, that is

$$i\dot{A}_q(t) = C_q A_q(t) + B_q(t), \quad (\text{A3})$$

where the irreducible part $B_q(t)$ is defined to be orthogonal to $A_q(t)$, that is

$$\langle [B_q, A_q^\dagger] \rangle = 0 \quad (\text{A4})$$

the matrix C_q being given by

$$C_q = \langle i\dot{A}_q | A_q^\dagger \rangle \langle A_q | A_q^\dagger \rangle^{-1}. \quad (\text{A5})$$

Taking into account Eqs. (A3) and (A5), the equation of motion (A1) becomes

$$\omega \langle \langle A_q | A_q^\dagger \rangle \rangle_\omega = \langle A_q | A_q^\dagger \rangle + \langle i\dot{A}_q | A_q^\dagger \rangle \langle A_q | A_q^\dagger \rangle^{-1} \langle \langle A_q | A_q^\dagger \rangle \rangle_\omega + \langle \langle B_q | A_q^\dagger \rangle \rangle_\omega. \quad (\text{A6})$$

Defining the polarization operator by

$$\Pi_q(\omega) = \langle A_q | A_q^\dagger \rangle^{-1} \langle \langle B_q | A_q^\dagger \rangle \rangle_\omega \langle \langle A_q | A_q^\dagger \rangle \rangle_\omega^{-1}. \quad (\text{A7})$$

Equation (A6) becomes

$$\omega \langle \langle A_q | A_q^\dagger \rangle \rangle_\omega = \langle A_q | A_q^\dagger \rangle + \langle \langle A_q | A_q^\dagger \rangle \rangle_\omega \left\{ \langle i\dot{A}_q | A_q^\dagger \rangle \langle A_q | A_q^\dagger \rangle^{-1} + \langle A_q | A_q^\dagger \rangle \Pi_q(\omega) \right\}. \quad (\text{A8})$$

Now we shall write explicitly the polarization operator $\Pi_q(\omega)$ in terms of the following Green's functions: $\langle \langle i\dot{A}_q | A_q^\dagger \rangle \rangle_\omega$, $\langle \langle A_q | -i\dot{A}_q^\dagger \rangle \rangle_\omega$, and $\langle \langle i\dot{A}_q | -i\dot{A}_q^\dagger \rangle \rangle_\omega$. To do this we write the equation of motion for $\langle \langle A_q | A_q^\dagger \rangle \rangle_\omega$ by deriving with respect to the right time argument

$$\omega \langle \langle A_q | A_q^\dagger \rangle \rangle_\omega = \langle A_q | A_q^\dagger \rangle + \langle \langle A_q | -i\dot{A}_q^\dagger \rangle \rangle_\omega \quad (\text{A9})$$

which is written as

$$\langle \langle A_q | A_q^\dagger \rangle \rangle_\omega^{-1} = \left\{ \omega - \langle \langle A_q | A_q^\dagger \rangle \rangle_\omega^{-1} \langle \langle A_q | -i\dot{A}_q^\dagger \rangle \rangle_\omega \right\} \langle A_q | A_q^\dagger \rangle^{-1}. \quad (\text{A10})$$

We also write the equation of motion of $\langle \langle i\dot{A}_q | A_q^\dagger \rangle \rangle_\omega$:

$$\omega \langle \langle i\dot{A}_q | A_q^\dagger \rangle \rangle_\omega = \langle i\dot{A}_q | A_q^\dagger \rangle + \langle \langle i\dot{A}_q | -i\dot{A}_q^\dagger \rangle \rangle_\omega. \quad (\text{A11})$$

Using Eqs. (A7), (A10), (A11), and (A3) we can write the polarization operator as

$$\Pi_q(\omega) = \langle A_q | A_q^\dagger \rangle^{-1} \left\{ \langle \langle i\dot{A}_q | -i\dot{A}_q^\dagger \rangle \rangle_\omega - \langle \langle i\dot{A}_q | A_q^\dagger \rangle \rangle_\omega \langle \langle A_q | A_q^\dagger \rangle \rangle_\omega^{-1} \langle \langle A_q | -i\dot{A}_q^\dagger \rangle \rangle_\omega \right\} \langle A_q | A_q^\dagger \rangle^{-1}. \quad (\text{A12})$$

To see that Eq. (A8) can be written as the usual Dyson's equation, $G = G^0 + G^0 \Pi G$, we define the "zero-order" Green's function by

$$\omega \langle \langle A_q | A_q^\dagger \rangle \rangle_\omega^{(0)} = \langle A_q | A_q^\dagger \rangle + \langle i\dot{A}_q | A_q^\dagger \rangle \langle A_q | A_q^\dagger \rangle^{-1} \langle \langle A_q | A_q^\dagger \rangle \rangle_\omega^{(0)} \quad (\text{A13})$$

and get

$$\langle \langle A_q | A_q^\dagger \rangle \rangle_\omega = \langle \langle A_q | A_q^\dagger \rangle \rangle_\omega^{(0)} + \langle \langle A_q | A_q^\dagger \rangle \rangle_\omega^{(0)} \Pi_q(\omega) \langle \langle A_q | A_q^\dagger \rangle \rangle_\omega. \quad (\text{A14})$$

APPENDIX B: THE RENORMALIZED PARAMETERS

To first order in δ , straightforward algebraic calculation leads to

$$\begin{aligned} \operatorname{Re}\lambda_q(\omega_q^0) &\simeq \delta \frac{t^2}{JW} \frac{1 - \gamma_{2q}}{\sqrt{1 - \gamma_q^2}} I_0(\omega_q^0), \\ \operatorname{Re}\Pi_q^\pm(\omega_q^0) &\simeq \delta \frac{t^2}{JW} \frac{1 - \gamma_{2q}}{1 \pm \gamma_q} I_1(\omega_q^0), \\ \operatorname{Im}\lambda_q(\omega_q^0) &\simeq -\pi\delta \frac{t^2}{JW} \frac{1 - \gamma_{2q}}{\sqrt{1 - \gamma_q^2}} \Upsilon(\omega_q^0), \\ \operatorname{Im}\Pi_q^\pm(\omega_q^0) &\simeq -\pi\delta \frac{t^2}{JW} \frac{1 - \gamma_{2q}}{1 \pm \gamma_q} \Upsilon(\omega_q^0) \end{aligned} \quad (\text{B1})$$

with

$$\begin{aligned} I_0(\omega_q^0) &= \left(1 - \frac{J + \omega_q^0}{\mu}\right) \ln \left|1 - \frac{J + \omega_q^0}{\mu}\right| - \left(1 - \frac{J - \omega_q^0}{\mu}\right) \ln \left|1 - \frac{J - \omega_q^0}{\mu}\right| \\ &\quad + \left(\frac{J + \omega_q^0}{\mu}\right) \ln \left(\frac{J + \omega_q^0}{\mu}\right) - \left(\frac{J - \omega_q^0}{\mu}\right) \ln \left|\frac{J - \omega_q^0}{\mu}\right|, \end{aligned} \quad (\text{B2})$$

$$\begin{aligned} I_1(\omega_q^0) &= 2 \left[1 + \ln \left(\frac{2W}{\mu}\right)\right] - \left(1 - \frac{J + \omega_q^0}{\mu}\right) \ln \left|1 - \frac{J + \omega_q^0}{\mu}\right| - \left(1 - \frac{J - \omega_q^0}{\mu}\right) \ln \left|1 - \frac{J - \omega_q^0}{\mu}\right| \\ &\quad - \left(\frac{J + \omega_q^0}{\mu}\right) \ln \left(\frac{J + \omega_q^0}{\mu}\right) - \left(\frac{J - \omega_q^0}{\mu}\right) \ln \left|\frac{J - \omega_q^0}{\mu}\right|, \end{aligned} \quad (\text{B3})$$

and

$$\Upsilon(\omega_q^0) = \theta(\omega_q^0 - J) + \left(1 - \frac{J - \omega_q^0}{\mu}\right) \theta \left(1 - \frac{J - \omega_q^0}{\mu}\right) \theta(J - \omega_q^0). \quad (\text{B4})$$

For $q \rightarrow 0$, $I_0(\omega_q^0) \rightarrow 0$ and

$$I_1(\omega_q^0) \rightarrow 2 \left\{1 + \ln \left(\frac{2W}{J}\right) - \ln \left|1 - \frac{\mu}{J}\right| + \frac{J}{\mu} \ln \left|1 - \frac{\mu}{J}\right|\right\}, \quad (\text{B5})$$

and for $\mu/J \ll 1$ we obtain

$$I_1(\omega_q^0 \rightarrow 0) \simeq 2 \ln \left(\frac{2W}{J}\right) + \frac{\mu}{J}. \quad (\text{B6})$$

Since the renormalized parameters are proportional to δ , the term μ/J should be dropped. As a consequence, we see that, up to first order in δ , the spin-wave velocity and the critical hole concentration δ_c are independent of the effective mass of the quasiparticle.

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