Magnetic properties of weakly doped antiferromagnets

I. R. Pimentel,* F. Carvalho Dias, and L. M. Martelo
Department of Physics and CFMC, University of Lisbon, 1649 Lisboa, Portugal

R. Orbach
Department of Physics, University of California, Riverside, California
(Received 4 December 1998)

We study the spin excitations and the transverse susceptibility of a two-dimensional antiferromagnet doped with a small concentration of holes in the *t-J* model. The motion of holes generates a renormalization of the magnetic properties. The Green's functions are calculated in the self-consistent Born approximation. It is shown that the long-wavelength spin waves are significantly softened and the shorter-wavelength spin waves become strongly damped as the doping increases. The spin wave velocity is reduced by the coherent motion of holes, and not increased as has been claimed elsewhere. The transverse susceptibility is found to increase considerably with doping, also as a result of coherent hole motion. Our results are in agreement with experimental data for the doped copper oxide superconductors. [S0163-1829(99)07541-4]

I. INTRODUCTION

After the discovery of high-T_c superconductors there has been intensive investigation of the magnetic properties[1] of doped copper oxide materials because of their connection to high temperature superconductivity. The undoped compounds are antiferromagnetic (AF) insulators. Doping introduces holes,[2,3] the charge carriers, in the AF square lattice of the copper oxide planes. The long-range AF order rapidly disappears at low doping, and superconductivity arises upon further doping. Strong two-dimensional AF fluctuations are nevertheless observed[4] even at fairly high doping, suggesting a conducting phase that, in spite of being paramagnetic, exhibits short-range AF order. A striking feature of the copper oxides is the strong sensitivity of their magnetic properties to the hole concentration δ. Experiments have shown important softening and damping in the spin excitations,[5–7] as well as a significant increase in the spin susceptibility,[8–10] for the doped copper oxides. It is therefore important to study the interplay between doping and antiferromagnetism for an understanding of these materials.

It is believed that the essential physics of strong electron correlations in the copper oxide planes is described by the *t-J* model

$$H_{t\text{-}J}=-t\sum_{\langle i,j\rangle,\sigma}(c^{\dagger}_{i\sigma}c_{j\sigma}+\text{H.c.})+J\sum_{\langle i,j\rangle}\left(\mathbf{S}_i\cdot\mathbf{S}_j-\frac{1}{4}n_in_j\right),\quad(1)$$

where $c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$ are creation and annihilation electron operators acting on a reduced Hilbert space with no doubly occupied sites, the spin operator is $S_i^{\mu}=\frac{1}{2}\sum_{\alpha\beta}c^{\dagger}_{i\alpha}\sigma^{\mu}_{\alpha\beta}c_{i\beta}$, $n_i=n_{i\uparrow}+n_{i\downarrow}$ and $n_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$. In the copper oxides, $J\simeq 1500$ K and $t\sim 3J$. For the undoped materials, i.e., at half filling, only the Heisenberg part of the Hamiltonian is relevant and it describes a spin-1/2 AF insulator. With doping, and nearly half-filling, the Hamiltonian describes holes moving in an AF background, the holes strongly interacting with the spin array. The motion of holes tends to disrupt the AF order, because a moving hole leaves behind a string of flipped spins. The charge carriers are then holes dressed by a cloud of spin excitations.

The propagation of a single hole in a two dimensional antiferromagnet has been studied with a variety of approaches. Considering the *t-J* model in a Schwinger boson representation, hole motion was treated within a self-consistent Born approximation (SCBA).[11–15] It was found that a hole can propagate coherently because of its strong coupling to the spin excitations, having a quasiparticle bandwidth $\sim J$ and energy minima at momenta $\mathbf{q}_i=(\pm\pi/2,\pm\pi/2)$. The calculated spectral density shows a quasiparticle peak of intensity $\sim(J/t)^{2/3}$ and a broad incoherent multiple spin wave continuum, of width $\sim 2zt$ (z is the coordination number), that is located at higher energies. These results are in good agreement with those from exact diagonalization of small clusters.[16] The study of hole motion has been extended for a finite concentration of holes, within the SCBA.[17–19] The results obtained show that, to first order in δ, the quasiparticle characteristics remain essentially the same, supporting a description of the quasiholes as noninteracting particles, filling up a Fermi surface consisting of four pockets located at momenta $\mathbf{q}_i$, having an enclosed area proportional to δ. The spectral density for finite doping again contains a coherent and an incoherent part. The role of the coherent motion of holes on the magnetic properties of the copper oxides has been a matter of discussion. Some authors,[17,20] in contradiction to others,[21–23] have claimed that the coherent motion of holes leads to stiffening of the spin excitations, while it is the incoherent motion of holes that generates significant softening, leading to an overall softening.

In this work we study the effects of hole doping on the spin excitations, calculating both the softening and the damping, and determine the doping dependence of the transverse spin susceptibility of a two-dimensional antiferromagnet, discussing in particular the contributions from the coherent and the incoherent motion of holes. Our study starts from the *t-J* model in the Schwinger boson representation and is carried out in the SCBA. It is shown that the magnetic properties are very sensitive to hole doping, as a result of the strong interaction between the hole and spin systems, and that the coherent motion of holes leads in fact to softening of the spin excitations.

II. THE INTERACTION BETWEEN HOLES AND SPIN WAVES

Our system is described by the *t-J* Hamiltonian (1) on a two-dimensional square lattice. In order to enforce no double occupancy of sites we use the slave-fermion Schwinger Boson representation $c_{i\sigma}=f_i^\dagger b_{i\sigma}$, where the slave-fermion operator $f_i^\dagger$ creates a hole and the boson operator $b_{i\sigma}$ accounts for the spin, subject to the constraint $f_i^\dagger f_i+\Sigma_\sigma b_{i\sigma}^\dagger b_{i\sigma}=2S$.

We consider the low doping regime, $\delta \ll 1$, where the states are close to the pure AF state, and hence exhibit long-range order. The AF state is approximated by the Néel state, which in the Schwinger representation can be interpreted as a condensate of Bose fields $b_{i\uparrow}=\sqrt{2S}$ and $b_{j\downarrow}=\sqrt{2S}$, respectively, in the up and down sublattices, and the bosons $b_{i\downarrow}=b_i$ and $b_{j\uparrow}=b_j$ are then Holstein-Primakov spin-wave operators on the Néel state.

The Hamiltonian (1), with $S=1/2$, then becomes

$$H_{t\text{-}J}=-t\sum_{\langle i,j\rangle}[f_i f_j^\dagger(b_i^\dagger+b_j)+\text{H.c.}]+\frac{J}{2}\sum_{\langle i,j\rangle}(1-f_i^\dagger f_i)\times(1-f_j^\dagger f_j)\left[b_i^\dagger b_i+b_j^\dagger b_j+b_i b_j+b_i^\dagger b_j^\dagger-\frac{1}{2}\right]. \quad (2)$$

The transfer part describes the reversal of spins as the hole moves. In the Heisenberg part, the factor $(1-f_i^\dagger f_i)(1-f_j^\dagger f_j)$ accounts for a loss of magnetic energy due to doping, and for small hole concentrations it may be replaced by $1-f_i^\dagger f_i-f_j^\dagger f_j$.

Applying Fourier transforms and the Bogoliubov-Valatin transformation for the spin variables $b_{-\mathbf{k}}^\dagger=u_\mathbf{k}\beta_{-\mathbf{k}}^\dagger+v_\mathbf{k}\beta_\mathbf{k}$ and $b_\mathbf{k}=v_\mathbf{k}\beta_{-\mathbf{k}}^\dagger+u_\mathbf{k}\beta_\mathbf{k}$, where $u_\mathbf{k}=\{[(1-\gamma_\mathbf{k}^2)^{-1/2}+1]/2\}^{1/2}$, $v_\mathbf{k}=-\text{sgn}(\gamma_\mathbf{k})\{[(1-\gamma_\mathbf{k}^2)^{-1/2}-1]/2\}^{1/2}$, and $\gamma_\mathbf{k}=\frac{1}{2}(\cos k_x+\cos k_y)$, we obtain from Eq. (2) the effective Hamiltonian

$$H=-\frac{1}{\sqrt{N}}\sum_{\mathbf{q},\mathbf{k}}f_\mathbf{q}f_{\mathbf{q}-\mathbf{k}}^\dagger[V(\mathbf{q},-\mathbf{k})\beta_{-\mathbf{k}}+V(\mathbf{q}-\mathbf{k},\mathbf{k})\beta_\mathbf{k}^\dagger]+\sum_\mathbf{k}\omega_\mathbf{k}^0\beta_\mathbf{k}^\dagger\beta_\mathbf{k}. \quad (3)$$

Here, $V(\mathbf{q},\mathbf{k})=zt(\gamma_\mathbf{q}u_\mathbf{k}+\gamma_{\mathbf{q}+\mathbf{k}}v_\mathbf{k})$, $\omega_\mathbf{k}^0=(zJ/2)(1-\gamma_\mathbf{k}^2)^{1/2}$, the coordination number is $z=4$, the sums run over the Brillouin zone for an antiferromagnet on a square lattice, and N is the number of sites in each sublattice. In Eq. (3), the first term represents the interaction between holes and spin waves resulting from the motion of holes with emission and absorption of spin waves, and the second term describes spin waves in a pure antiferromagnet. In writing Eq. (3) we neglected an interaction term involving the scattering of holes by spin-waves, proportional to J, because its effect is small compared to the other term, proportional to t.[17] We note that at the bare level the holes have no dispersion. In fact, they propagate only after being dressed by spin waves. Here we study the renormalization of the magnetic properties induced by the dynamical interaction between the holes and the spin waves.

III. GREEN'S FUNCTIONS FOR SPIN WAVES AND HOLES

Given the magnitude of the couplings in the copper oxides, we make use of the Green's function formalism at zero temperature. The Green's functions for the spin waves are defined as

$$D^{-+}(\mathbf{k},t-t')=-i\langle\mathcal{T}\beta_\mathbf{k}(t)\beta_\mathbf{k}^\dagger(t')\rangle,$$

$$D^{+-}(\mathbf{k},t-t')=-i\langle\mathcal{T}\beta_{-\mathbf{k}}^\dagger(t)\beta_{-\mathbf{k}}(t')\rangle,$$

$$D^{--}(\mathbf{k},t-t')=-i\langle\mathcal{T}\beta_\mathbf{k}(t)\beta_{-\mathbf{k}}(t')\rangle,$$

$$D^{++}(\mathbf{k},t-t')=-i\langle\mathcal{T}\beta_{-\mathbf{k}}^\dagger(t)\beta_\mathbf{k}^\dagger(t')\rangle,$$

where $\langle\,\rangle$ represents an average over the ground state. Their Fourier transforms satisfy the Dyson equations

$$D^{\mu\nu}(\mathbf{k},\omega)=D_0^{\mu\nu}(\mathbf{k},\omega)+\sum_{\gamma\delta}D_0^{\mu\gamma}(\mathbf{k},\omega)\Pi^{\gamma\delta}(\mathbf{k},\omega)D^{\delta\nu}(\mathbf{k},\omega),$$

where $\mu,\nu=\pm$. The free Green's functions are

$$D_0^{-+}(\mathbf{k},\omega)=(\omega-\omega_\mathbf{k}^0+i\eta)^{-1},$$

$$D_0^{+-}(\mathbf{k},\omega)=(-\omega-\omega_\mathbf{k}^0+i\eta)^{-1},$$

$$D_0^{--}(\mathbf{k},\omega)=D_0^{++}(\mathbf{k},\omega)=0,$$

with $\eta\to 0^+$, and $\Pi^{\gamma\delta}(\mathbf{k},\omega)$ are the self-energies generated by the interaction between holes and spin waves.

We calculate the self-energies in the SCBA, corresponding to only "bubble" diagrams with dressed hole propagators. These diagrams describe the decay of spin waves into "particle-hole" pairs. The approximation neglects corrections to the hole-spin interaction vertex, which have been shown to be unimportant.[12,15,17] The self-energies are given by

$$\Pi^{\gamma\delta}(\mathbf{k},\omega)=-i\frac{1}{N}\sum_\mathbf{q}U^{\gamma\delta}(\mathbf{k},\mathbf{q})\int_{-\infty}^{+\infty}\frac{d\omega_\mathbf{q}}{2\pi}\times G(\mathbf{q},\omega_\mathbf{q})G(\mathbf{q}-\mathbf{k},\omega_\mathbf{q}-\omega), \quad (4)$$

where $G(\mathbf{q},\omega_\mathbf{q})$ is the Fourier transform of the Green's function for the dressed holes, $G(\mathbf{q},t-t')=-i\langle\mathcal{T}f_\mathbf{q}(t)f_\mathbf{q}^\dagger(t')\rangle$, and

$$U^{+-}(\mathbf{k},\mathbf{q})=V(\mathbf{q}-\mathbf{k},\mathbf{k})^2,\quad U^{-+}(\mathbf{k},\mathbf{q})=V(\mathbf{q},-\mathbf{k})^2,$$

$$U^{--}(\mathbf{k},\mathbf{q})=U^{++}(\mathbf{k},\mathbf{q})=V(\mathbf{q},-\mathbf{k})V(\mathbf{q}-\mathbf{k},\mathbf{k}).$$

The relations $\Pi^{-+}(\mathbf{k},\omega)=\Pi^{+-}(-\mathbf{k},-\omega)$ and $\Pi^{--}(\mathbf{k},\omega)=\Pi^{++}(\mathbf{k},\omega)$ are verified.

In the SCBA the holes are dressed by pure AF spin waves. This approach implies a spectral function for the holes that is composed of a coherent quasiparticle peak and an incoherent continuum, with the quasi-holes filling up a Fermi surface that consists of pockets located at $\mathbf{q}_i = (\pm\pi/2, \pm\pi/2)$, as mentioned above. We shall take for the hole spectral function the approximate form

$$\rho(\mathbf{q},\omega) = [\rho^{\mathrm{coh}}(\mathbf{q},\omega) + \rho^{\mathrm{incoh}}(\mathbf{q},\omega)]\mathcal{F}^{\pm}(\mathbf{q})\,\theta(\pm\omega), \quad (5)$$

with, Fermi surface $\mathcal{F}^{-}(\mathbf{q}) = \Sigma_{i=1}^{4}\theta(q_F - |\mathbf{q}-\mathbf{q}_i|)$, $\mathcal{F}^{+}(\mathbf{q}) = 1 - \mathcal{F}^{-}(\mathbf{q})$, Fermi momentum $q_F = \sqrt{\pi\delta}$, and

$$\rho^{\mathrm{coh}}(\mathbf{q},\omega) = a_0\,\delta(\omega - \varepsilon_{\mathbf{q}}),$$

$$\rho^{\mathrm{incoh}}(\mathbf{q},\omega) = h\,\theta(|\omega| - zJ/2)\,\theta(2zt + zJ/2 - |\omega|).$$

Here the energies are measured with respect to the Fermi level, and the quasiparticle dispersion can, near the minima at $\mathbf{q}_i$, be written as $\varepsilon_{\mathbf{q}} = \varepsilon_{\min} + (\mathbf{q}-\mathbf{q}_i)^2/2m$, with an effective mass $m \simeq 1/J$ (neglecting band anisotropy). The quasiparticle residue is $a_0 \simeq (J/t)^{2/3}$, and the remaining spectral density appears in the incoherent continuum of width $2zt$ and height $h \simeq (1-a_0)/2zt$, satisfying the sum rule $\int d\omega\,\rho(\mathbf{q},\omega) = 1$.

The spin wave self-energies (4) are obtained in terms of the hole spectral function (5) by

$$\Pi^{\gamma\delta}(\mathbf{k},\omega) = \frac{1}{N}\sum_{\mathbf{q}} U^{\gamma\delta}(\mathbf{k},\mathbf{q})[Y(\mathbf{q},-\mathbf{k};\omega) + Y(\mathbf{q}-\mathbf{k},\mathbf{k};-\omega)], \quad (6)$$

with

$$Y(\mathbf{q},-\mathbf{k};\omega) = \int_0^{+\infty} d\omega' \int_{-\infty}^{0} d\omega'' \,\frac{\rho(\mathbf{q},\omega')\rho(\mathbf{q}-\mathbf{k},\omega'')}{\omega + \omega'' - \omega' + i\eta}.$$

From Eqs. (5) and (6) follows that the self-energies will present three contributions

$$\Pi^{\gamma\delta}(\mathbf{k},\omega) = \Pi^{\gamma\delta}_{c,c}(\mathbf{k},\omega) + \Pi^{\gamma\delta}_{c,ic}(\mathbf{k},\omega) + \Pi^{\gamma\delta}_{ic,ic}(\mathbf{k},\omega),$$

corresponding, respectively, to transitions of holes within the coherent band, between the coherent and incoherent bands, and within the incoherent band. We have calculated these different contributions to lowest order in the hole concentration δ. The imaginary parts of these contributions are nonzero only in certain regions of the $(\mathbf{k},\omega)$ space: $\mathrm{Im}\,\Pi_{c,c} \neq 0$ for $[-kq_F/m + k^2/2m] < \omega < [kq_F/m + k^2/2m]$, $\mathrm{Im}\,\Pi_{c,ic} \neq 0$ for $zJ/2 < \omega < zJ/2 + 2zt$, and $\mathrm{Im}\,\Pi_{ic,ic} \neq 0$ for $zJ < \omega < zJ + 4zt$.

IV. MAGNETIC PROPERTIES

We now present the calculation of the effects of hole doping on the magnetic properties. The renormalized spin wave energy $\omega_{\mathbf{k}}$ is given by the poles of the Green's functions $D(\mathbf{k},\omega)$, determined by the condition

$$[(D_0^{-+})^{-1} - \Pi^{+-}][(D_0^{+-})^{-1} - \Pi^{-+}] - \Pi^{++}\Pi^{--} = 0.$$

In the region where $\mathrm{Im}\,\Pi(\mathbf{k},\omega) = 0$, we find to lowest order in δ,

$$\omega_{\mathbf{k}} = \omega^0_{\mathbf{k}} + \mathrm{Re}\,\Pi^{+-}(\mathbf{k},\omega^0_{\mathbf{k}}), \quad (7)$$

leading to

$$\omega_{\mathbf{k}} = \omega^0_{\mathbf{k}}[1 - r(\mathbf{k})], \quad (8)$$

where

$$r(\mathbf{k}) = \delta a_0^2\left(\frac{t}{J}\right)^2 \Bigg\{ \left(\frac{1}{2}\,\frac{k^2}{1-\gamma_{\mathbf{k}}^2}\right)\theta(2q_F - k) + \left(\frac{\sin^2 k_x + \sin^2 k_y}{1-\gamma_{\mathbf{k}}^2}\right)\left(\frac{1-\gamma_{\mathbf{k}}^2 - (k/2)^2}{1-\gamma_{\mathbf{k}}^2 - (k/2)^4}\right)\theta(k - 2q_F)\Bigg\}$$
$$+ \sqrt{\delta}\,\frac{t}{J}\,\frac{(1-a_0)^2}{2}\left[\ln 2 + \frac{a_0}{1-a_0}\ln\left(1 + 4\frac{t}{J}\right)\right] \times \Bigg\{ \frac{1}{2\sqrt{\pi}}\left(\frac{k^3}{1-\gamma^2_{\frac{\mathbf{k}}{2}}}\right)\theta(2q_F - k) + \sqrt{\delta}\left(\frac{\sin^2 k_x + \sin^2 k_y}{1-\gamma_{\mathbf{k}}^2}\right) \times \theta(k - 2q_F)\Bigg\}.$$

In $r(\mathbf{k})$ the first term is generated only by the coherent motion of holes, i.e., $\Pi^{+-}_{c,c}$, whereas the second involves the incoherent motion resulting from the sum $\Pi^{+-}_{c,ic} + \Pi^{+-}_{ic,ic}$. One finds that both the coherent and the incoherent motion of holes generate a reduction of the spin wave energy, and hence give rise to softening of the spin excitations. The fact that the coherent motion of holes leads to softening, even in the regime where the spin wave velocity is larger than the hole Fermi velocity, is explained in detail in the Appendix.

In the long-wavelength limit, $k \ll 1$, one has

$$\omega_{\mathbf{k}} = ck, \quad (9)$$

with

$$c = Z_c c_0, \quad (10)$$

where $c_0 = zJ/(2\sqrt{2})$ is the spin wave velocity for a pure antiferromagnet, and the renormalization factor is

$$Z_c = 1 - \delta a_0^2\left(\frac{t}{J}\right)^2. \quad (11)$$

For finite hole concentrations one has $Z_c < 1$, which implies a reduction of the spin wave velocity with doping. This effect is generated only by the coherent motion of the holes, as can be seen from Eq. (8).

In the region where the spin wave dispersion crosses the pair excitation continuum, defined as the region where $\mathrm{Im}\,\Pi(\mathbf{k},\omega) \neq 0$, one finds, to lowest order in δ, that the spin excitations become damped, acquiring an inverse lifetime given by

$$\Gamma(\mathbf{k}) = -2\,\mathrm{Im}\,\Pi^{+-}(\mathbf{k},\omega_{\mathbf{k}}). \quad (12)$$

One finds that the damping is determined only by the coherent motion of holes, i.e., $\mathrm{Im}\,\Pi^{+-}_{c,c}$, because the contributions involving the incoherent motion, $\mathrm{Im}\,\Pi^{+-}_{c,ic}$ and $\mathrm{Im}\,\Pi^{+-}_{ic,ic}$, vanish in the relevant region of the $(\mathbf{k},\omega)$ space. Hence we have

$$\Gamma(\mathbf{k})=zJ\sqrt{\delta}a_0^2\left(\frac{t}{J}\right)^2\frac{1}{\sqrt{\pi}k(1-\gamma_{\mathbf{k}}^2)^{1/2}}F^{+-}(\mathbf{k})\times\{\sqrt{1-s^2(g_{\mathbf{k}})}\,\theta(1-|s(g_{\mathbf{k}})|)-\sqrt{1-s^2(-g_{\mathbf{k}})}\,\theta(1-|s(-g_{\mathbf{k}})|)\},\tag{13}$$

with

$$F^{+-}(\mathbf{k})=(\cos k_y-\cos k_x)[\cos(g_{\mathbf{k}}k_x)-\cos(g_{\mathbf{k}}k_y)]-2(1-\gamma_{\mathbf{k}}^2)^{1/2}[\sin k_x\sin(g_{\mathbf{k}}k_x)+\sin k_y\sin(g_{\mathbf{k}}k_y)]+4(1-\gamma_{\mathbf{k}}^2),$$

where $s(g_{\mathbf{k}})=(1-g_{\mathbf{k}})k/2q_F$, $g_{\mathbf{k}}=(2\omega_{\mathbf{k}}/J)/k^2$, and $\omega_{\mathbf{k}}$ is given by Eq. (8). We note the strong doping dependence of the damping $\sim\sqrt{\delta}$, as compared to that of the reduction of the spin wave velocity $(Z_c-1)\sim\delta$, $\delta\ll 1$.

From Eq. (13) one has that for sufficiently small doping, long-wavelength spin waves remain well defined, whereas the shorter wavelength spin waves are damped, decaying into ''particle-hole'' pairs. As the doping increases more spin waves, in the shorter wavelength side, dive into the pair excitation continuum, and become damped. For hole concentrations above a certain threshold δ^*, such that the spin wave velocity equals the Fermi velocity, $Z_c^*c_0/(k_F^*/m)=1$, the spin wave dispersion lies entirely in the pair excitation continuum, and then even the long-wavelength spin waves are damped. In the limit $k\ll 1$ one has $\Gamma\sim k$, which implies that the spin waves are overdamped.

The transverse spin susceptibility is defined by

$$\chi_\perp=\chi_\perp(\mathbf{k}=0,\omega=0),\tag{14}$$

where the dynamical susceptibility is given by

$$\chi_\perp(\mathbf{k},\omega)=i\int_0^\infty dte^{i\omega t}\langle[S^x(\mathbf{k},t),S^x(-\mathbf{k},0)]\rangle.$$

Writing the spin operator in terms of the electron creation and annihilation operators, $S_i^x=(S_i^++S_i^-)/2$ with $S_i^+=c^\dagger_{i\uparrow}c_{i\downarrow}$ and $S_i^-=c^\dagger_{i\downarrow}c_{i\uparrow}$, using the Schwinger boson representation with the bose condensation associated with the Néel state, and performing the Bogoliubov-Valatin transformation, one finds that the susceptibility can be expressed in terms of the spin wave Green's functions by

$$\chi_\perp=-\lim_{\mathbf{k}\to 0}\left(\frac{1-\gamma_{\mathbf{k}}}{1+\gamma_{\mathbf{k}}}\right)^{1/2}[\mathrm{Re}\,D^{+-}(\mathbf{k},0)+\mathrm{Re}\,D^{++}(\mathbf{k},0)].\tag{15}$$

In Eq. (15) we have approximated $\langle f_i^\dagger f_i b_i^\dagger\rangle\simeq\delta\langle b_i^\dagger\rangle$, and neglected a prefactor $(1-\delta)^2$ which is caused by dilution of the spin lattice by holes. To lowest order in δ, the transverse susceptibility is given by

$$\chi_\perp=\lim_{\mathbf{k}\to 0}\frac{1}{zJ(1+\gamma_{\mathbf{k}})}\left[1-\frac{2}{zJ(1-\gamma_{\mathbf{k}}^2)^{1/2}}\times[\mathrm{Re}\,\Pi^{+-}(\mathbf{k},0)+\mathrm{Re}\,\Pi^{++}(\mathbf{k},0)]\right].\tag{16}$$

One finds that only the coherent motion, i.e., $\Pi^{+\pm}_{c,c}$, contributes to the susceptibility in Eq. (16), because the contributions involving the incoherent motion, $\Pi^{+\pm}_{c,i}$ and $\Pi^{+\pm}_{i,i}$, vanish in the limit $\mathbf{k}\to 0$. We then obtain

$$\chi_\perp=Z_\chi\chi_\perp^0,\tag{17}$$

where $\chi_\perp^0=1/(2zJ)$ is the transverse susceptibility for a pure Heisenberg antiferromagnet, and the renormalization factor is given by

$$Z_\chi=1+4\delta a_0^2\left(\frac{t}{J}\right)^2.\tag{18}$$

From Eq. (18) one sees that the transverse susceptibility increases with hole doping, this effect being determined by the coherent motion of holes.

V. RESULTS AND DISCUSSION

We have considered a two-dimensional antiferromagnet doped with a small concentration of mobile holes and calculated the renormalization of magnetic properties induced by hole motion. In our calculation it is assumed that there is long-range AF order in the system. In real materials true long-range AF order disappears at rather low concentrations, e.g., $\delta_c\simeq 0.02$ for $La_{2-\delta}Sr_\delta CuO_4$. However, experiments have revealed that above such concentrations, there are large AF correlated regions in the system corresponding to the size of the magnetic correlation length ξ, scaling as $\xi\sim 1/\sqrt{\delta}$.[24] Those regions can in particular sustain spin excitations with wavelengths up to the region size. One expects that the results that we derived when there is long-range order, still describe the physics on length scales less than ξ, with ξ large, when long range order is broken.

We find that the spin excitations are very sensitive to doping, with significant softening and damping occurring as a result of hole motion. In the low momenta region, the reduction of the spin wave energy is mainly determined by the coherent motion of holes, while the contribution from the incoherent motion becomes more significant with increasing momenta. The spin wave velocity decreases due to the coherent motion of holes, which for $t/J=3$ and a concentration $\delta=0.02$ produces a renormalization factor $Z_c=0.96$, while a concentration $\delta=0.05$ leads to $Z_c=0.90$. However, for momenta k around q_F, the slope of the spin dispersion shows a much higher reduction, by a factor 0.91 for a concentration $\delta\simeq 0.02$, and a factor 0.78 for a concentration $\delta\simeq 0.05$, as a result of the coherent plus the incoherent motion of holes. For $\delta\simeq 0.02$ there is little damping since only spin waves near the upper end of the spin wave spectrum lie inside the pair excitation continuum. For $\delta\simeq 0.05$ the spin dispersion dives partially into the pair excitation continuum, so that excitations with $k>2q_F$ are strongly damped. For concentrations above the threshold $\delta^*\simeq 0.17$, where the spin wave velocity equals the Fermi velocity, all the spin waves lie in the pair excitation continuum, and therefore are completely damped. This occurs at a concentration well below the value for which the spin wave velocity would vanish. One expects that long-range order will collapse at a concentration $\delta_c < \delta^*$, implying a small value for the critical concentration, in agreement with experimental data. The disappearence of the long-range magnetic order with doping will be discussed elsewhere.[25] Aeppli *et al.*[5] and Hayden *et al.*[6] investigated the spin dynamics of pure and doped $La_{2-\delta}Sr_{\delta}CuO_4$, with $\delta=0.05$, and found that spin excitations within the AF correlated regions in the doped material show softening and damping with respect to the corresponding excitations in the pure material. Aeppli *et al.* found that the spin wave velocity in the doped material is renormalized by a factor $0.74(\pm 0.08)$, while Hayden *et al.* found a renormalization factor 0.60. These values are to be compared with the renormalization factor for the slope of the spin dispersion around q_F, the momenta range associated to the AF correlated regions, therefore our result, 0.78 for $\delta=0.05$, is in good agreement with experimental data. Experiments[7] at a much higher concentration, $\delta=0.14$, have also revealed a large broadening of the spin excitations with doping.

For the transverse spin susceptibility we find a significant increase with doping, having for $t/J=3$ a renormalization factor $Z_\chi=1.17$ for $\delta=0.02$, and $Z_\chi=1.42$ for $\delta=0.05$. This effect is also due to the coherent motion of holes. When long-range order is broken and the magnetic correlation length diverges, the susceptibility of the system should be essentialy given by $\chi_\perp$. An increase in the spin susceptibility with doping has in fact been observed experimentally,[8–10] in agreement with our results. Above the critical doping a gap gradually opens in the spin excitation spectrum, and one may expect the magnetic correlation length in that regime to be determined by the imaginary part of the spin dispersion. According to our results this implies an inverse correlation length proportional to $\mathrm{Im}\,\Pi^{+-}_{c,c}$ and therefore $\xi \sim 1/\sqrt{\delta}$, precisely the scaling found experimentally.[24]

Spin excitations of a weakly doped antiferromagnet have been investigated elsewhere in the SCBA. In Ref. 21, the present authors considered the effect of the coherent motion of holes only, and showed that it generates spin wave softening, in agreement with the results in the present work. Other authors[17,20] claimed, however, that the coherent motion of holes leads instead to stiffening of spin waves. This contradicts our results, and may arise from approximations made in Refs. 17 and 20. The renormalization of the spin excitations has also been calculated by another group,[23] but their calculation contains a self-energy independent of δ, a result difficult to understand. Becker and Mushelknautz in Ref. 22 also studied the effects of hole doping on the spin excitations, but using a different technique. They found softening and damping of the spin excitations, due to both the coherent and the incoherent motion of holes, in agreement with our results. In conclusion, we have shown that the magnetic properties of a two-dimensional antiferromagnet are very sensitive to doping due to the strong interaction between holes and spin waves, the coherent motion of holes leading to softening of the spin excitations, similar to the incoherent motion.

APPENDIX

The contribution of the coherent motion of holes for the renormalization of the spin waves excitations is given by $\mathrm{Re}\,\Pi^{+-}_{c,c}(\mathbf{k},\omega^0_{\mathbf{k}})$. From Eqs. (5) and (6) one has

$$\mathrm{Re}\,\Pi^{+-}_{c,c}(\mathbf{k},\omega^0_{\mathbf{k}}) = a_0^2 \frac{1}{2N}\sum_{\mathbf{q}} \theta(|\mathbf{q}-\mathbf{k}|-q_F)\,\theta(q_F-|\mathbf{q}|) \times \sum_{i=1}^{4}\left[\frac{U^{+-}(\mathbf{k},\mathbf{k}-\mathbf{q}-\mathbf{q}_i)}{\omega^0_{\mathbf{k}}-(\varepsilon_{\mathbf{q}-\mathbf{k}}-\varepsilon_{\mathbf{q}})} - \frac{U^{+-}(\mathbf{k},\mathbf{q}+\mathbf{q}_i)}{\omega^0_{\mathbf{k}}+(\varepsilon_{\mathbf{q}-\mathbf{k}}-\varepsilon_{\mathbf{q}})}\right],$$

where $\varepsilon_{\mathbf{q}}=\mathbf{q}^2/2m$. Given that

$$\sum_{i=1}^{4} U^{+-}(\mathbf{k},\mathbf{k}-\mathbf{q}+\mathbf{q}_i) = \sum_{i=1}^{4} U^{+-}(\mathbf{k},\mathbf{q}+\mathbf{q}_i) - (zt)^2 \times \sum_{i=1}^{4}(\gamma^2_{\mathbf{q}-\mathbf{k}+\mathbf{q}_i}-\gamma^2_{\mathbf{q}+\mathbf{q}_i}),$$

one has

$$\mathrm{Re}\,\Pi^{+-}_{c,c}(\mathbf{k},\omega^0_{\mathbf{k}}) = a_0^2 \frac{1}{N}\sum_{\mathbf{q}} \theta(|\mathbf{q}-\mathbf{k}|-q_F)\,\theta(q_F-|\mathbf{q}|) \times [A(\mathbf{k},\mathbf{q})-B(\mathbf{k},\mathbf{q})],$$

where

$$A(\mathbf{k},\mathbf{q}) = \sum_{i=1}^{4} U^{+-}(\mathbf{k},\mathbf{q}+\mathbf{q}_i)\frac{2(\varepsilon_{\mathbf{q}-\mathbf{k}}-\varepsilon_{\mathbf{q}})}{[(\omega^0_{\mathbf{k}})^2-(\varepsilon_{\mathbf{q}-\mathbf{k}}-\varepsilon_{\mathbf{q}})^2]}$$

and

$$B(\mathbf{k},\mathbf{q}) = (zt)^2\sum_{i=1}^{4}(\gamma^2_{\mathbf{q}-\mathbf{k}+\mathbf{q}_i}-\gamma^2_{\mathbf{q}+\mathbf{q}_i})\frac{1}{[\omega^0_{\mathbf{k}}-(\varepsilon_{\mathbf{q}-\mathbf{k}}-\varepsilon_{\mathbf{q}})]}.$$

For sufficiently small doping the spin wave velocity is larger than the Fermi velocity, and therefore $A(\mathbf{k},\mathbf{q})\,\theta(|\mathbf{q}-\mathbf{k}|-q_F)\,\theta(q_F-|\mathbf{q}|)>0$. However, one has that $B(\mathbf{k},\mathbf{q})>A(\mathbf{k},\mathbf{q})$, even in the long-wavelength limit, $\mathbf{k}\ll 1$, where $B(\mathbf{k},\mathbf{q})\sim 2A(\mathbf{k},\mathbf{q})$. This implies that $\mathrm{Re}\,\Pi^{+-}_{c,c}(\mathbf{k},\omega^0_{\mathbf{k}})<0$, and therefore softening of the spin excitations, as given in Eq. (7). The inclusion of band anisotropy does not qualitatively change our results.

*Electronic address: iveta@alf1.cii.fc.ul.pt

[1] A. P. Kampf, Phys. Rep. **249**, 219 (1994).

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

[3] L. H. Tjeng, B. Sinkovic, N. B. Brookes, J. B. Goedkoop, R. Hesper, E. Pellegrin, F. M. F. de Groot, S. Altieri, S. L. Hulbert, E. Shekel, and G. A. Sawatzky, Phys. Rev. Lett. **78**, 1126 (1997).

[4] R. J. Birgeneau and G. Shirane, in *Physical Properties of High Temperature Superconductors*, edited by D. M. Ginzberg (World Scientific, Singapore, 1990).

[5] G. Aeppli, S. M. Hayden, H. A. Mook, Z. Fisk, S.-W. Cheong, D. Rytz, J. P. Remeika, G. P. Espinosa, and A. S. Cooper, Phys. Rev. Lett. **62**, 2052 (1989).
[6] S. M. Hayden, G. Aeppli, H. Mook, D. Rytz, M. F. Hundley, and Z. Fisk, Phys. Rev. Lett. **66**, 821 (1991).
[7] S. M. Hayden, G. Aeppli, H. A. Mook, T. G. Perring, T. E. Mason, S.-W. Cheong, and Z. Fisk, Phys. Rev. Lett. **76**, 1344 (1996).
[8] Y.-Q. Song, M. A. Kennard, K. R. Poppelmeier, and W. P. Halperin, Phys. Rev. Lett. **70**, 3131 (1993).
[9] T. Nakano, M. Oda, C. Manabe, N. Momono, Y. Miura, and M. Ido, Phys. Rev. B **49**, 16 000 (1994).
[10] S. Ohsugi, Y. Kitaoka, and K. Asayama, Physica C **282-287**, 1373 (1997).
[11] S. Schmitt-Rink, C. M. Varma, and A. E. Ruckenstein, Phys. Rev. Lett. **60**, 2793 (1988).
[12] C. L. Kane, P. A. Lee, and N. Read, Phys. Rev. B **39**, 6880 (1989).
[13] G. Martinez and P. Horsch, Phys. Rev. B **44**, 317 (1991).
[14] F. Marsiglio, A. E. Ruckenstein, S. Schmitt-Rink, and C. M. Varma, Phys. Rev. B **43**, 10 882 (1991).
[15] Z. Liu and E. Manousakis, Phys. Rev. B **45**, 2425 (1992).
[16] E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994).
[17] J. Igarashi and P. Fulde, Phys. Rev. B **45**, 12 357 (1992).
[18] N. M. Plakida, V. S. Oudovenko, and V. Yushanhai, Phys. Rev. B **50**, 6431 (1994).
[19] B. Kyung and S. Mukhin, Phys. Rev. B **55**, 3886 (1997).
[20] G. Khaliullin and P. Horsch, Phys. Rev. B **47**, 463 (1993).
[21] I. R. Pimentel and R. Orbach, Phys. Rev. B **46**, 2920 (1992).
[22] K. W. Becker and M. Muschelknautz, Phys. Rev. B **48**, 13 826 (1993).
[23] D. W. Murray and O. P. Suskov, Physica C **258**, 389 (1996).
[24] R. J. Birgeneau, D. R. Gabbe, H. P. Jenssen, M. A. Kastner, P. J. Picone, T. R. Thurston, G. Shirane, Y. Endoh, M. Sato, K. Yamada, Y. Hidaka, M. Oda, Y. Enomoto, M. Suzuki, and T. Murakami, Phys. Rev. B **38**, 6614 (1988).
[25] F. Carvalho Dias, I. R. Pimentel, and R. Orbach (unpublished).