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Dynamical spin susceptibility in weakly doped antiferromagnets

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We study the dynamical spin susceptibility of a two-dimensional antiferromagnet that is weakly doped with mobile holes. The motion of the holes leads to a renormalization of the velocity v and of the linewidth of spin wave excitations. In agreement with inelastic-neutron-scattering experiments for high-T_c superconductors v vanishes at a critical hole concentration δ_c of a few percent. This behavior is mainly due to the low energy or so-called coherent part of the hole motion and not to its incoherent part as was claimed recently. Therefore spin and hole excitations have the same energy scale and adiabatic approximations are not allowed. Moreover, the system undergoes a magnetic phase transition at a critical hole-concentration value δ_c. At δ_c the transverse staggered susceptibility diverges for all wave vectors for which the spin-wave excitations $\omega_{\mathbf{q}}$ are approximately linear in $\mathbf{q}$.

I. INTRODUCTION

It is important to study the interplay between antiferromagnetism and doping for the understanding of high-temperature superconductors, especially since antiferromagnetic fluctuations are known to persist in the superconducting phase. Neutron-scattering experiments[1–3] show that magnetic properties in oxide high-T_c superconductors strongly depend on the hole concentration δ within the CuO_2 planes. The parent compounds, i.e., the systems at half filling, are antiferromagnetic semiconductors. With increasing hole concentration the Néel temperature as well as the staggered magnetization decrease rapidly and vanish at a critical hole concentration δ_c of a few percent before the systems become metallic and superconducting. With respect to dynamical properties one knows from inelastic-neutron-scattering experiments that spin-wave excitations exist for the undoped systems.[1–3] They are well described by conventional two-dimensional spin-wave theory.[4] Upon doping, however, the spin-wave velocity decreases and vanishes approximately at the same hole concentration δ_c at which the Néel temperature vanishes. At the same time the spin waves become overdamped. The main aim of this paper is to discuss the doping dependence of both the spin-wave velocity and of the damping in the antiferromagnetic phase and to ask at which doping concentration δ_c spin-wave excitations cease to exist.

The essential aspects of the electronic structure of the CuO_2 planes in high-T_c superconductors are believed by now to be well described by the two-dimensional t-J model[5,6]

$$H = -t \sum_{\langle i,j\rangle,\sigma} (\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \text{H.c.}) + J \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j . \tag{1}$$

Here $\mathbf{S}_i$ are the electronic spin operators and $\langle ij\rangle$ indicates a sum over all pairs of nearest neighbors. The operators $\hat{c}^{\dagger}_{i,\sigma}$ are defined by $\hat{c}^{\dagger}_{i,\sigma} = c^{\dagger}_{i,\sigma}(1-n_{i,-\sigma})$, where $n_{i,-\sigma}$ is the electron number per site with spin $-\sigma$. Thus hopping onto already occupied sites is forbidden. At half filling the t-J Hamiltonian reduces to the antiferromagnetic Heisenberg model. Note that the standard form of the t-J Hamiltonian used by most people contains on the right-hand side an additional term $-J\sum_{\langle i,j\rangle}(n_i n_j)/4$. We have neglected this term for simplicity because the qualitative behavior of the model will not be affected dramatically by leaving this term out.

II. PROJECTION TECHNIQUE

The inelastic neutron cross section is determined by the imaginary part of the dynamical spin susceptibility $\chi(\mathbf{q},\omega)$. To evaluate $\chi(\mathbf{q},\omega)$ we use a projection technique.[7–9] This method is used to derive equations of motion for a set of relevant variables $\{A_\nu\}$. One starts by introducing a metric in operator space in order to define the projectors $\mathcal{P}$ and $\mathcal{Q} \equiv 1 - \mathcal{P}$ on the operator space formed by the set of relevant variables and on its orthogonal subspace. Often, the so-called Mori metric[7] is used which follows naturally from linear response theory. However, in the present case of a state with broken symmetry, $\langle N_z\rangle \neq 0$, it is advantageous instead to introduce a commutator metric $(A_\nu|A_\mu) = \langle[A^{+}_\nu, A_\mu]\rangle$. This will be explained below in more detail. As our set of relevant variables $\{A_\nu\}$ we now choose as usual the staggered magnetization $A_1 = N_x(\mathbf{q})$ and the total magnetization $A_2 = S_y(\mathbf{q})$ in the x and y directions, respectively. They are defined by

$$\begin{aligned} A_1 &= N_x(\mathbf{q}) = S^{\uparrow}_x(\mathbf{q}) - S^{\downarrow}_x(\mathbf{q}), \\ A_2 &= S_y(\mathbf{q}) = S^{\uparrow}_y(\mathbf{q}) + S^{\downarrow}_y(\mathbf{q}). \end{aligned} \tag{2}$$

Here $\mathbf{S}^{\uparrow}(\mathbf{q})$ and $\mathbf{S}^{\downarrow}(\mathbf{q})$ are the two sublattice magnetizations for the up and down sublattice $\mathcal{U}_\uparrow$ and $\mathcal{U}_\downarrow$,

$$\mathbf{S}^{\sigma}(\mathbf{q}) = \frac{1}{\sqrt{N}} \sum_{i\in\mathcal{U}_\sigma} e^{i\mathbf{q}\cdot\mathbf{R}_i}\mathbf{S}_i . \tag{3}$$

The projector on the space formed by the operator set $\{A_\nu\}$ is given by

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$$\mathcal{P} = \sum_{\nu,\mu} |A_\nu) g^{-1}_{\nu,\mu} (A_\mu|. \tag{4}$$

Here $g^{-1}_{\nu,\mu}$ is the inverse matrix of $g_{\nu,\mu}$,

$$g_{\nu,\mu} = \langle [A^\dagger_\nu, A_\mu] \rangle, \tag{5}$$

where $g_{1,1} = g_{2,2} = 0$ and $g_{1,2} = g^*_{2,1} = i\langle N_z \rangle = (i/\sqrt{N})\langle N_z(\mathbf{q}=0)\rangle$. Since the off-diagonal matrix elements $g_{1,2}$ and $g_{2,1}$ are proportional to the order parameter $\langle N_z \rangle \neq 0$, the inverse matrix $g^{-1}_{\nu,\mu}$ and thus the projector $\mathcal{P}$ exists within the whole antiferromagnetic regime. We want to evaluate the dynamical susceptibility for the spin component $S_y(\mathbf{q})$. It is given by

$$\chi_{22}(\mathbf{q},\omega) = \frac{1}{i} \int_0^\infty \langle [A^\dagger_2(\mathbf{q}), A_2(\mathbf{q},-t)] \rangle e^{izt}\, dt, \tag{6}$$

where $z = \omega + i\eta$, $(\eta \to 0)$. Due to the commutator in (6) one can rewrite χ_{22} in terms of the above commutator metric,

$$\chi_{22}(\mathbf{q},\omega) = \left\langle \left[A^\dagger_2(\mathbf{q}), \frac{1}{z-\mathcal{L}} A_2(\mathbf{q}) \right] \right\rangle = \left(A_2(\mathbf{q}) \Big| \frac{1}{z-\mathcal{L}} A_2(\mathbf{q}) \right), \tag{7}$$

so that the projection technique can be applied. Within this formalism coupled equations for the dynamical susceptibilities, $\chi_{\nu\mu}(\mathbf{q},\omega)$, defined for the whole set of relevant variables in analogy to (6), can be derived:

$$\sum_\nu [z\delta_{\eta,\nu} - \Omega_{\eta,\nu}(\mathbf{q}) - \Gamma_{\eta,\nu}(\mathbf{q},\omega)] \chi_{\nu,\mu}(\mathbf{q},\omega) = g_{\eta,\mu}. \tag{8}$$

Here the frequencies $\Omega_{\eta,\nu}(\mathbf{q})$ and self-energies $\Gamma_{\eta,\nu}(\mathbf{q},\omega)$ are defined by

$$\Omega_{\eta,\nu}(\mathbf{q}) = \sum_\mu L_{\eta,\mu}(\mathbf{q}) g^{-1}_{\mu,\nu}, \qquad L_{\eta,\mu}(\mathbf{q}) = (A_\eta | \mathcal{L} A_\mu), \tag{9}$$

$$\Gamma_{\eta,\nu}(\mathbf{q},\omega) = \sum_\mu M_{\eta,\mu}(\mathbf{q},\omega) g^{-1}_{\mu,\nu}, \qquad M_{\eta,\mu}(\mathbf{q},\omega) = \left(A_\eta \Big| \mathcal{L}\mathcal{Q} \frac{1}{z - \mathcal{Q}\mathcal{L}\mathcal{Q}} \mathcal{Q}\mathcal{L} A_\mu \right). \tag{10}$$

From this one easily obtains the following exact representation for $\chi_{22}(\mathbf{q},\omega)$:

$$\chi_{22}(\mathbf{q},\omega) = \frac{-[L_{22}(\mathbf{q}) + M_{22}(\mathbf{q},\omega)]}{\left(z + \frac{iM_{12}(\mathbf{q},\omega)}{\langle N_z\rangle} \right)\left(z - \frac{iM_{21}(\mathbf{q},\omega)}{\langle N_z\rangle} \right) - \left(\frac{L_{11}(\mathbf{q}) + M_{11}(\mathbf{q},\omega)}{\langle N_z\rangle} \right)\left(\frac{L_{22}(\mathbf{q}) + M_{22}(\mathbf{q},\omega)}{\langle N_z\rangle} \right)}. \tag{11}$$

For small wave vectors $\mathbf{q}$ the frequency terms $L_{11}(\mathbf{q})$ and $L_{22}(\mathbf{q})$ are given by

$$L_{11}(\mathbf{q}) = -\frac{4J}{N} \sum_{\langle i,j\rangle} \langle S^y_i S^y_j + S^z_i S^z_j \rangle + \frac{t}{N} \sum_{\langle i,j\rangle,\sigma} \langle \hat{c}^\dagger_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^\dagger_{j,\sigma} \hat{c}_{i,\sigma} \rangle, \tag{12}$$

$$L_{22}(\mathbf{q}) = -\frac{J}{N} q^2 \sum_{\langle i,j\rangle} [\hat{\mathbf{q}} \cdot (\mathbf{R}_i - \mathbf{R}_j)]^2 \langle S^y_i S^y_j + S^z_i S^z_j \rangle + \frac{t}{4N} q^2 \sum_{\langle i,j\rangle,\sigma} [\hat{\mathbf{q}} \cdot (\mathbf{R}_i - \mathbf{R}_j)]^2 \langle \hat{c}^\dagger_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^\dagger_{j,\sigma} \hat{c}_{i,\sigma} \rangle. \tag{13}$$

Note L_{11} is wave vector independent for small $\mathbf{q}$, whereas L_{22} is proportional to q^2. This prefactor follows from the continuity equation, $i\mathcal{L}S^y(\mathbf{q}) = \mathbf{q} \cdot \mathbf{j}_{S^y}(\mathbf{q})$ where $\mathbf{j}_{S^y}(\mathbf{q})$ is the spin current, and from additional inversion symmetry. The continuity equation holds since the total spin $S^y(\mathbf{q})$ is a conserved quantity at $\mathbf{q}=0$.

The expressions for the self-energies $M_{11}(\mathbf{q},\omega)$, $M_{22}(\mathbf{q},\omega)$ read

$$M_{11}(\mathbf{q},\omega) = \left(\dot{N}_x(\mathbf{q}) \Big| \mathcal{Q} \frac{1}{z - \mathcal{Q}\mathcal{L}\mathcal{Q}} \mathcal{Q} \dot{N}_x(\mathbf{q}) \right), \tag{14}$$

$$M_{22}(\mathbf{q},\omega) = q^2 \left(j_{S^y}(\mathbf{q}) \Big| \mathcal{Q} \frac{1}{z - \mathcal{Q}\mathcal{L}\mathcal{Q}} \mathcal{Q} j_{S^y}(\mathbf{q}) \right). \tag{15}$$

The reduction to small wave vectors $\mathbf{q}$ will be done below. The prefactor $\mathbf{q}^2$ in M_{22} again follows from the continuity equation. Note that similar expressions also hold for the off-diagonal self-energies M_{12} and M_{21}. For small $\mathbf{q}$ they are of higher order in $\mathbf{q}$ and do not contribute to the final result. The quantity $\mathcal{L}$ in (14) and (15) denotes the Liouville operator. It acts on operators A of the unitary space according to $\mathcal{L}A = [H, A]$.

Usually one would like to apply the Kubo-Green relation (compare, e.g., Ref. 8) in order to simplify the self-energies for small wave vectors $\mathbf{q}$. In this case the projectors $\mathcal{Q}$ in (14) and (15) could be replaced by 1 so that these expressions would reduce to true dynamical susceptibilities for the quantities $\dot{N}_x = i\mathcal{L}N_x$ and j_{S^y}, respectively. To apply the Kubo-Green relation, the limit $q \to 0$ has to be performed first while keeping ω finite. However, in the present case of a doped antiferromagnet, it turns out that the frequency dependence of the self-energies is crucial. As is shown below quasiparticle-hole excitations from the so-called coherent part of the hole motion are coupled strongly to spin waves via the self-energies. Since these quasiparticle-hole excitations vanish linearly with $\mathbf{q}$ just as the spin-wave excitations, the self-energies are strongly ω dependent for small ω and $\mathbf{q}$. Therefore the Kubo-Green relation cannot be applied. Both types of excitations, i.e., spin-wave and coherent particle-hole excitations, possess the same energy scale so that adiabatic approximations are not allowed.

Before we continue let us first discuss in some detail the result for the half-filled case where the Kubo-Green relation holds. Moving holes are absent for half filling and therefore low-energy particle-hole excitations do not exist. First note that usual spin-wave theory for the Heisenberg antiferromagnet is easily recovered. Moreover, a well-known expression for the adiabatic spin stiffness constant ρ_s is found from (11). This quantity is usually defined by the increase of the free energy due to an imposed q-dependent twist in spin space on the system.[10–12] To deduce ρ_s from (11) note that the static transverse spin susceptibility is given by

$$\chi_{22} = \lim_{\omega\to 0}\lim_{\mathbf{q}\to\mathbf{0}} \frac{\langle N_z\rangle^2}{L_{11}(\mathbf{q}) + M_{11}(\mathbf{q},\omega)}. \tag{16}$$

The order of the two limits follows from the assumption that the Kubo-Green relation holds. By comparison with $v^2 = \rho_s/\chi_{22}$, i.e., the hydrodynamic relation between the adiabatic spin stiffness constant ρ_s and the spin-wave velocity v, one easily finds from (11)

$$\rho_s = \lim_{\omega\to 0}\lim_{\mathbf{q}\to\mathbf{0}} \frac{1}{q^2}[L_{22}(\mathbf{q}) + M_{22}(\mathbf{q},\omega)], \tag{17}$$

where M_{22} is given by (15) with $\mathcal{Q}$ replaced by 1. This is exactly the result which is given in the literature (see for instance Refs. 10–12). From (15) one may show that the second term in (17) is always less than or equal to zero. Therefore, the quantity $\lim_{\mathbf{q}\to\mathbf{0}}(1/q^2)L_{22}(\mathbf{q})$ is an upper bound for ρ_s, i.e.,

$$\rho_s \leq \lim_{\mathbf{q}\to\mathbf{0}} \frac{1}{q^2} L_{22}(\mathbf{q}). \tag{18}$$

This result is usually derived by use of the Bogoliubov inequality (compare for the pure[8] and for the doped[13] antiferromagnet).

Also the dynamical susceptibility $\chi_{11}(\mathbf{q},\omega)$ of the staggered magnetization $N_x(\mathbf{q})$ can be derived within the projection formalism. It is given by (11) with the numerator replaced by $-[L_{11} + M_{11}(\omega)]$. For $\omega \to 0$ this reduces to the expression

$$\chi_{11}^{is}(\mathbf{q}) = \frac{\langle N_z\rangle^2}{L_{22}(\mathbf{q}) + M_{22}(\mathbf{q},\omega\to 0)}, \tag{19}$$

which diverges for $q \to 0$ as $1/q^2$. The reason for this divergence is that the quantity $N_x(\mathbf{q})$ tries to restore the broken symmetry of the antiferromagnetic phase.[8] Equation (19) also demonstrates the advantage of the commutator metric used here as compared to the usual Mori metric where only a lower bound $\sim 1/q^2$ for $\chi_{11}(\mathbf{q})$ is found.

III. EVALUATION OF EXPECTATION VALUES

Let us proceed to the case of finite doping where the Kubo-Green relation no longer applies. To evaluate the various quantities in (11) in the presence of a finite hole concentration δ, let us make an ansatz for the ground state $|\Psi_g\rangle$ and assume that it is formed by a Fermi state of independent "quasiparticles":

$$|\Psi_g\rangle = \prod_{\sigma,\mathbf{k}\in\mathrm{FS}} \phi(\mathbf{k},\sigma)|\Psi_{\mathrm{AF}}\rangle. \tag{20}$$

Here $|\Psi_{\mathrm{AF}}\rangle$ is the ground state of the system at half filling, i.e., the ground state of the Heisenberg antiferromagnet which we henceforth approximate by the Néel state. The quasiparticles $\phi(\mathbf{k},\sigma)$ are determined by the motion of independent single holes in the system at half filling. As is well known, by moving through the antiferromagnetic spin background holes leave behind strings of spin defects, i.e., strings of overturned spins.[14,15] These strings can be described by local operators $A_n^\sigma(i)$. When the hole is created on site i on sublattice $\mathcal{U}_\uparrow$, they are defined by

$$\begin{aligned} A_0^\uparrow(i) &= \hat{c}_{i\uparrow}, \\ A_1^\uparrow(i) &= (-1)\sum_j \hat{c}_{j\downarrow} S_i^- \tilde{R}_{ji}, \\ A_2^\uparrow(i) &= \sum_{lj} \hat{c}_{l\uparrow} S_j^+ S_i^- R_{lj}^{(i)} \tilde{R}_{ji}\ , \quad \dots . \end{aligned} \tag{21}$$

Here n denotes the number of steps away from the site i by which the hopping hole has created the string, $\tilde{R}_{ji} = 1$ for the $z_0 = 4$ nearest neighbors j of i and zero elsewhere, whereas $R_{jl}^{(i)} = 1$ for the $z_0 - 1 = 3$ nearest neighbors l of j with l different from i and zero elsewhere. The quasiparticles $\phi(\mathbf{k},\sigma)$ are linear combinations over the $A_n(i)$'s,[16,17]

$$\begin{aligned} \phi(\mathbf{k},\sigma) &= \frac{1}{\sqrt{N/2}} \sum_{i\in U_\sigma} e^{i\mathbf{k}\cdot R_i} \phi^\sigma(i), \\ \phi^\sigma(i) &= \sum_n \alpha_n A_n^\sigma(i), \end{aligned} \tag{22}$$

where the sum over i runs over all $N/2$ sites of the sublattice U_σ only. The coefficients α_n can be evaluated.[16] They decrease to zero in space within a few lattice constants somewhat depending on the ratio t/J. Therefore the quasiparticles in local space can be considered as holes dressed with "clouds of spin defects" which have an extension of a few lattice sites and increase somewhat with increasing t/J. Note that without the transverse part of the exchange interaction of (1) and the influence of the so-called spiral paths, the wave function (22) would be localized; i.e., the one-hole excitations would be independent of $\mathbf{k}$. This is due to the fact that the hole is moving in this case in an Ising potential which roughly increases with the number of steps the hole jumps away from the original site i. The dispersion of the quasiparticles is mainly due to the influence of the transverse part of the Heisenberg interaction and only to a smaller part influenced by the spiral paths. This leads to a band $\epsilon_0(\mathbf{k})$ for the one-hole excitations with a width of order J.[16,17] For small doping, when the clouds do not strongly overlap, the quasiparticles anticommute to a good approximation. This becomes plausible from the fact that the anticommutation relations of two string operators, $A_n(i)$ and $A_{n'}(j)$, with $i \neq j$, are entirely determined by their annihilation operators which describe the hopping holes, provided the two strings do not cross. For this reason one may start for small doping from the approximate ground state (20). The quasiparticles fill up four "hole pockets" around the four degenerate minima of the band which are located at $(\pm\pi/2, \pm\pi/2)$. Deviations of the true ground state from the approximate ground state due to quasiparticle interactions will be neglected in the following.

As an example let us discuss somewhat in detail the evaluation of the self-energy $M_{22}(\mathbf{q},\omega)$. We first replace in (15) the projector $\mathcal{Q} = 1 - \mathcal{P}$ by 1. The effect of $\mathcal{Q}$ is to exclude processes which lead back to the original variables $N_x(\mathbf{q})$ and $S_y(\mathbf{q})$. Such processes will drop out in the following by the approximations used to evaluate M_{22}. Next note that the spin current operator splits,

$$j_{S^y}(\mathbf{q}) = j^J_{S^y}(\mathbf{q}) + j^t_{S^y}(\mathbf{q}), \tag{23}$$

corresponding to the two parts of the t-J Hamiltonian. The first part $j^J_{S^y}(\mathbf{q})$ is the same as in the pure Heisenberg antiferromagnet whereas the second one is only present for the doped system. It is given by

$$j^t_{S^y}(\mathbf{q}) = -(t/2q)\frac{1}{\sqrt{N}}\sum_{\langle i,j\rangle,\sigma}\sigma(e^{i\mathbf{q}\cdot\mathbf{R}_i} - e^{i\mathbf{q}\cdot\mathbf{R}_j})(\hat{c}^\dagger_{i,-\sigma}\hat{c}_{j,\sigma} + \hat{c}^\dagger_{j,\sigma}\hat{c}_{i,-\sigma}) \tag{24}$$

and describes the hopping of a hole to a neighboring site accompanied by a spin flip. We expect only the contributions to the self-energies of order t^2 from the hopping parts to be responsible for the renormalization of the spin-wave velocity and of the damping. Contributions from the Heisenberg spin current proportional to J^2 will be more or less the same as in the case of half-filling and will not be discussed any further. To apply $j^t_{S^y}(\mathbf{q})$ on the ground state $|\Psi_g\rangle$ we first replace the resolvent $1/(z - \mathcal{L})$ by $1/[z - (H - E_g)]$, where the definition of $\mathcal{L}$ was used and E_g is the ground state energy. Next $j^t_{S^y}(\mathbf{q})$ will be applied successively on all quasiparticles $\phi(\mathbf{k},\sigma)$ present in the Fermi state, i.e.,

$$j^t_{S_y}(\mathbf{q})|\Psi_g\rangle = j^t_{S_y}(\mathbf{q})\prod_{\sigma\mathbf{k}\in\mathrm{FS}}\phi(\mathbf{k},\sigma)|\Psi_{\mathrm{AF}}\rangle = \sum_{\sigma\mathbf{k}\in\mathrm{FS}}\phi(\mathbf{k}_1,\uparrow)\ \cdots\ [j^t_{S_y}(\mathbf{q}),\phi(\mathbf{k},\sigma)]\ \cdots\ \phi(\mathbf{k}_N,\downarrow)|\Psi_{\mathrm{AF}}\rangle. \tag{25}$$

As approximation for $\phi(\mathbf{k},\sigma)$ we keep from the sum (22) over n only the dominant string $A^\sigma_n(i)$ of length $n=0$ with coefficient α_0. Contributions from higher strings are expected to change the final result only quantitatively. Since $A^\sigma_{n=0}(i) = \hat{c}_{i,\sigma}$ we immediately obtain for the commutator in (25)

$$[j^t_{S_y}(\mathbf{q}),\phi(\mathbf{k},\sigma)] \approx -\frac{\alpha_0}{\sqrt{N}}(t/2)\ g(\mathbf{k},\mathbf{q})\ \hat{c}_{\mathbf{k}+\mathbf{q},-\sigma}. \tag{26}$$

Here

$$g(\mathbf{k},\mathbf{q}) = (1/q)\sum_{j(\neq i)}[\cos(\mathbf{k}+\mathbf{q})\cdot(\mathbf{R}_i - \mathbf{R}_j) - \cos\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)], \tag{27}$$

where j is a nearest neighbor of i on the second sublattice. The effect of $j^t_{S_y}(\mathbf{q})$ is thus to create a hole with momentum $\mathbf{k}+\mathbf{q}$ and spin $-\sigma$ on the second sublattice. By use of (25) and (26) and by neglecting all interactions to the remaining quasiparticles in the ground state we arrive at the following result for $M^t_{22}(\mathbf{q},\omega)$:

$$M^t_{2,2}(\mathbf{q},\omega) = q^2\alpha_0^2\frac{t^2}{4N}\sum_{\sigma,\mathbf{k}\in\mathrm{FS}}{}' g(\mathbf{k},\mathbf{q})^2\{C_{-\sigma}[\mathbf{k}+\mathbf{q},\omega+\epsilon_0(\mathbf{k})] + C_{-\sigma}[\mathbf{k}-\mathbf{q},-\omega+\epsilon_0(\mathbf{k})]\}. \tag{28}$$

The quantities $C_\sigma(\mathbf{k},\omega)$ are one-hole correlation functions,

$$C_\sigma(\mathbf{k},\omega) = \left\langle \hat{c}^\dagger_{\mathbf{k},\sigma}\frac{1}{z-\mathcal{L}}\hat{c}_{\mathbf{k},\sigma}\right\rangle, \tag{29}$$

which enter since we have neglected all quasiparticle interactions so that quasiparticles in (20) with momenta and spins different from $\mathbf{k}$ and σ have dropped out. The two terms in (28) follow from the commutator metric. The prime above the sum over $\mathbf{k}$ indicates the influence of the Pauli principle. Only excited particles with $\mathbf{k}+\mathbf{q}$ (or $\mathbf{k}-\mathbf{q}$ in the second term) contribute which have energies above the Fermi level. Finally, the Liouville operator $\mathcal{L}$ was reintroduced in (28) again. In the one-hole correlation functions $\mathcal{L}$ acts on $\hat{c}_{\mathbf{k}+\mathbf{q},\sigma}$ (and on $\hat{c}_{\mathbf{k}-\mathbf{q},\sigma}$, respectively) and no longer acts on the two-particle operator j_{S^y} as in (15). This leads to the one-hole frequency shift $\epsilon_0(\mathbf{k})$ in (28). Equation (28) states that the spin-wave self-energy in a doped antiferromagnet is expressed by a sum over one-hole correlation functions. This coupling to the hole motion turns out to be responsible for the renormalization of the velocity and the damping of the spin waves. In the last step we have to evaluate $C_\sigma(\mathbf{k},\omega)$. This is done in first order Born approximation in close analogy to Ref. 18. As is well known, the one-hole spectral function Im $C_\sigma(\mathbf{k},\omega)$ obtained in this way exhibits a quasiparticle or coherent peak at low frequencies and an incoherent background structure at higher frequencies.

It is crucial how to determine the correct small $\mathbf{q}$ and ω behavior. In (28) the limit $\mathbf{q} \to 0$ can be performed in $g(\mathbf{k},\mathbf{q})^2$. However, this is not allowed inside the bracket $[\cdots]$, as one would do in case the Kubo-Green relation could be applied. To make this transparent let us consider for a moment only the coherent part of $M^t_{22}(\mathbf{q},\omega)$,

$$M^t_{2,2}(\mathbf{q},\omega)|_{\text{coh}} = q^2 \alpha_0^4 \frac{t^2}{4N} \sum_{\sigma,\mathbf{k}\in\text{FS}} g(\mathbf{k},\hat{\mathbf{q}})^2 \left(\frac{\Theta[\epsilon_0(\mathbf{k}+\mathbf{q}) - \epsilon_F]}{z - [\epsilon_0(\mathbf{k}+\mathbf{q}) - \epsilon_0(\mathbf{k})]} + \frac{\Theta[\epsilon_0(\mathbf{k}-\mathbf{q}) - \epsilon_F]}{-z - [\epsilon_0(\mathbf{k}-\mathbf{q}) - \epsilon_0(\mathbf{k})]} \right). \tag{30}$$

This expression is obtained from the decomposition of $\hat{c}_{\mathbf{k}+\mathbf{q},-\sigma}$ and $\hat{c}_{\mathbf{k}-\mathbf{q},-\sigma}$ into one-hole eigenmodes where only the coherent excitations are taken into account. Except for the prefactor $g(\mathbf{k},\hat{\mathbf{q}})^2$ and a minus sign the sum over $\mathbf{k}$ in (30) is identical to the Lindhard function for the coherent excitations. Thus (30) describes the coupling to coherent quasiparticle-hole excitations. In order to see why the small ω and $\mathbf{q}$ dependence of (30) is crucial remember that a linear dispersion law $\omega_{\mathbf{q}} \sim q$ for the spin-wave excitations is expected. The dispersion law is determined by an explicit equation for $\omega_{\mathbf{q}}$ which follows from setting the denominator of (11) equal to zero. One can easily verify that apart from the prefactor q^2 Eq. (30) and also the full self-energy M^t_{22} of Eq. (28) are functions of ω/q for small $\mathbf{q}$. This is why a linear $\mathbf{q}$ dependence for the spin-wave excitations is obtained. Figure 1 shows our results for Re $M_{22}(\mathbf{q},\omega)$, and Im $M_{22}(\mathbf{q},\omega)/\omega$ at small wave vector $\mathbf{q}$, as obtained from (28) and from the Born approximation for $C_\sigma(\mathbf{k},\omega)$. The dip in Re M_{22} and the peak structure in Im M_{22}/ω for small frequencies is due to the coherent part of the one-hole motion. For larger frequencies both quantities are at first almost ω independent and show some ω structure due to the incoherent part of the hole motion for still higher frequencies. The negative values of Re M_{22} for small frequencies give rise to the expected decrease of the spin-wave velocity. Finally note again that the quantity M^t_{22} is only nonzero for the doped case, $\delta \neq 0$.

The self-energy $M_{11}(\mathbf{q},\omega)$ is obtained in analogy to $M_{22}(\mathbf{q},\omega)$. Since $N_x(\mathbf{q})$ is not a constant of motion at $\mathbf{q} = \mathbf{0}$ the prefactor q^2 is absent. It turns out that the hopping part of M_{11} is very small. This is mainly due to the fact that the coefficient $\hat{g}(\mathbf{k},\mathbf{q})^2$, which corresponds to the coefficient $g(\mathbf{k},\mathbf{q})^2$ in (28), is very small for $\mathbf{k}$ values inside the hole pockets. This leads to a concentration dependence of $M^t_{11} \sim \delta^2$ so that this quantity is almost negligible. Finally, also the frequency terms L_{11} and L_{22} and the staggered magnetization $\langle N_z \rangle$ have to be evaluated by use of the ground state $|\Psi_g\rangle$, Eq. (20). One finds

$$L_{11}(\mathbf{q}) = 2J \left[1 - \left(\gamma_1 \frac{1}{N} \sum_{\sigma,\mathbf{k}\in\text{FS}} \tilde{f}(\mathbf{k}) + \gamma_2\delta + \frac{t}{J}\gamma_3\delta \right) \right],$$

$$L_{22}(\mathbf{q}) = (aq)^2 \frac{J}{4} \left[1 - \left(\gamma_1 \frac{1}{N} \sum_{\sigma,\mathbf{k}\in\text{FS}} f(\mathbf{k},\hat{\mathbf{q}}) + \gamma_2\delta + \frac{t}{J}\gamma_3\delta \right) \right], \tag{31}$$

$$\langle N_z \rangle = \frac{1}{2}(1 - \gamma_4\delta),$$

where a is the lattice constant and

$$\gamma_1 = \frac{1}{\sqrt{12}}\alpha_0\alpha_2 + \frac{1}{4}\sum_{n>0} \alpha_n\alpha_{n+2},$$
$$\gamma_2 = 2\alpha_0^2 + \sum_{n>0}(2n+3)\alpha_n^2,$$
$$\gamma_3 = 2\alpha_0\alpha_1 + \sqrt{3}\sum_{n>0}\alpha_n\alpha_{n+1}, \tag{32}$$
$$\gamma_4 = \sum_{n\leq 0}(2n+1)\alpha_n^2,$$

and

$$\tilde{f}(\mathbf{k}) = \sum_{\langle ii'\rangle(\neq j)} \cos\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_{i'}),$$
$$f(\mathbf{k},\mathbf{q}) = \frac{2}{a^2} \sum_{\langle ii'\rangle(\neq j)} (\hat{\mathbf{q}}\cdot(\mathbf{R}_i - \mathbf{R}_j)) \cos\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_{i'})^2. \tag{33}$$

Here the summations run over all nearest neighbors i, $i'(\neq i)$ of a fixed site j. The frequency terms contain contributions from $\mathcal{L}_t$ and $\mathcal{L}_J$ linear in δ which lead to a decrease with increasing δ. The staggered magnetization also decreases with δ and would formally become zero at a concentration of about 27% for $J/t = 0.3$ and at 17% for $J/t = 0.1$. Here we have taken string states $A_n(i)$

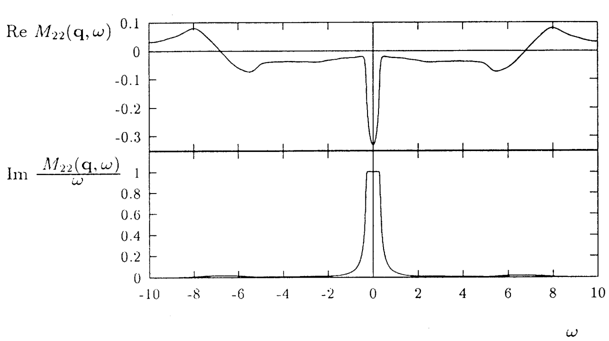

FIG. 1. Re $M_{22}(\mathbf{q},\omega)$ (in units of $q^2J/4$) and Im $M_{22}(\mathbf{q},\omega)/\omega$ (in units of $q^2/4$) as function of ω (in units of J) for $\mathbf{q} = (\pi/16, \pi/16)$, $J/t = 0.3$, and $\delta = 4\%$.

from the expansion (22) to very high order into account so that these values are rather accurate within our ground state wave function (20). As will be discussed below this result for $\langle N_z \rangle$ is expected to break down for hole concentrations δ close to the critical value δ_c at which the spin-wave excitations become soft. However, it should be rather reliable for small hole concentrations.

IV. RESULTS AND DISCUSSION

After having determined all quantities from (11) we can now evaluate the dynamical spin susceptibility $\chi_{22}(\mathbf{q},\omega)$. In Figs. 2(a)–2(c) our final result for Im $\chi_{22}(\mathbf{q},\omega)/\omega$ as a function of ω is shown for $\mathbf{q} = (\pi/16, \pi/16)$ and $J/t = 0.3$ and for three different values of δ. In order to reproduce the experimental spin-wave linewidth for zero doping we have inserted a small finite value for Im M_{11}^J and for Im M_{22}^J. These self-energy contributions are also present for $\delta = 0$. As is clearly seen in Fig. 2 the spin-wave peaks shift towards smaller frequencies with increasing hole concentration δ. Moreover, the width of the peaks increases with doping. These features are in very good agreement with experiment. From the peak positions we have plotted in Fig. 3 the square of the spin-wave velocity v as a function of δ for two different values of J/t. To good approximation the points are located on straight lines, especially for $J/t = 0.1$. For $J/t = 0.3$ the δ dependence is at first slower and later steeper than linear. Therefore, a square root law approximately holds for the spin-wave velocity

$$v \simeq v_0 \sqrt{1 - \frac{\delta}{\delta_c}} \,, \tag{34}$$

where v_0 is the spin-wave velocity at $\delta = 0$ and δ_c is the critical hole concentration at which the spin-wave excitations cease to exist. This δ behavior is essentially a combined effect from the δ-dependent parts of L_{11} and L_{22} and from M_{22}. The critical concentration δ_c varies strongly with the ratio J/t. For $J/t = 0.3$ we find

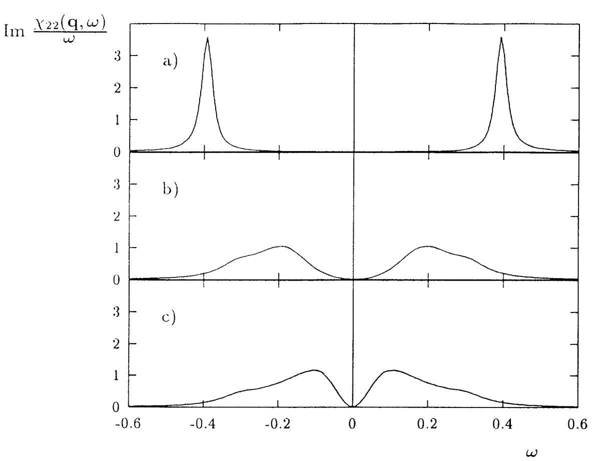

FIG. 2. Spectral function Im $\chi_{22}(\mathbf{q},\omega)/\omega$ (in units of $1/J^2$) as function of ω for $\mathbf{q} = (\pi/16, \pi/16)$, $J/t = 0.3$, and three different values of δ: (a) $\delta = 0\%$, (b) $\delta = 4\%$, (c) $\delta = 5\%$.

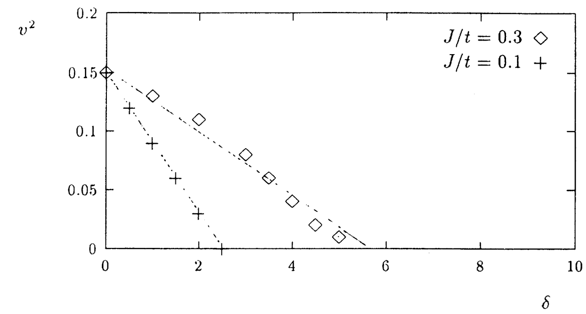

FIG. 3. Squared spin-wave velocity v^2 (in units of J^2a^2, where a is the lattice constant) as a function of hole concentration δ for two different values of J/t.

$\delta_c \approx 6\%$, whereas for $J/t = 0.1$ the critical concentration δ_c is $\approx 2.5\%$, i.e., closer to the experimental value of about 2% for Y-Ba-Cu-O (YBCO).[1] For very small hole concentrations the peak positions shift away at first very slowly from their value at $\delta = 0$ to smaller frequencies. This is the range where the decrease of the spin-wave velocity is mainly governed by the δ-dependent parts of L_{11} and L_{22} and where the spin-wave velocity is still larger than the Fermi velocity v_F of the quasiparticles. The decrease of v becomes faster when the spin-wave excitation moves inside the range of the coherent quasiparticle contributions, i.e., inside the dip region of Re $M_{22}(\mathbf{q},\omega)$ in Fig. 1. At the same time the spin-wave excitations become heavily damped. Therefore, for the doping concentrations $\delta = 4\%$ and 5% in Fig. 2, the line shift and the width of the spin waves are mainly governed by the ω dependence of the coherent part of $M_{22}^t(\mathbf{q},\omega)$. In this case the spin-wave velocity v is smaller than the Fermi velocity of the quasiparticles.

Let us finally compare our results with those given in the literature. Recently spin-wave excitations for the doped antiferromagnet have been investigated in the framework of the two-dimensional t-J model by a different theoretical method.[19–21] There, the starting point is a decomposition of the constrained electron operator $\hat{c}_{i,\sigma}$ into a Schwinger boson while keeping track of the spins, and into a slave fermion which generates a hole at site i. The requirement that a site should not be doubly occupied implies that the total number of fermions and bosons at each site should be $2S = 1$. However, this requirement is relaxed within this formalism by using a $1/S$ expansion.[18] This implies a number of approximations in the equations which govern the spin-wave excitations as compared to our exact relation (11). First, the δ-dependent contributions to L_{11} and L_{22}, which result from the hopping term, have been neglected. Second, the staggered magnetization $\langle N_z \rangle$ in Eq. (11) has been replaced by its value for $\delta = 0$. Furthermore, in Ref. 19 and also in Ref. 20, which is with respect to the spin excitation spectrum similar to Ref. 19, only hole concentrations δ are explicitly treated for which the spin-wave velocity is larger than the Fermi velocity of the holes. In that case the frequency ω in the self-energies can approximately be replaced by the bare spin-wave energy. The result was then extrapolated to the critical concentration δ_c. In contrast, the calculations in the present investigation are also explicitly performed in the δ regime, where the spin-wave velocity v has dropped below the Fermi velocity v_F and where the spin excitations lie within the electron-hole continuum. In that regime damping becomes important. Our theory provides for the doping dependence of the spin-wave damping—an important physical quantity for which measurements exist. In Ref. (21) also the case of $v < v_F$ has been considered, but the calculations were limited to the contributions from the coherent part. The additional condition $(t/J)\sqrt{\delta} \ll 1$ which appears in that work is probably related to the fact that the coupling of the two relevant variables (N_x and S_y) is neglected there. This gives rise to a single mode at $\omega_{\mathbf{q}}$ instead of two modes at $\omega_{\mathbf{q}}$ and $-\omega_{\mathbf{q}}$.

Finally, note that the softening of the spin waves is accompanied by a magnetic phase transition when δ approaches δ_c. This is easily seen by looking at the zero frequency limit (19) of $\chi_{11}(\mathbf{q},\omega)$, i.e., $\chi_{11}^{is} = \langle N_z\rangle^2/[L_{22}(\mathbf{q}) + M_{22}(\mathbf{q},\omega \to 0)]$. The denominator in this expression is the same factor as the one which enters the denominator of (11) and which is responsible for the disappearance of the spin-wave velocity at δ_c. Therefore, χ_{11}^{is} diverges at δ_c and the system undergoes at δ_c a phase transition from an antiferromagnetic ground state to a new ground state which is probably nonmagnetic. We expect that the phase transition is also accompanied by a softening of the order parameter $\langle N_z\rangle$ which should vanish at δ_c as well. However, the staggered magnetization $\langle N_z\rangle$, as evaluated from the ground state wave function (20), depends only weakly on the hole concentration δ. As mentioned above, for $J/t = 0.1$, $\langle N_z\rangle$ formally vanishes at $\delta \approx 17\%$ whereas the spin-wave velocity already goes to zero at $\approx 2.5\%$. This means the staggered magnetization $\langle N_z\rangle$, evaluated from (20), is still finite when δ reaches δ_c. The reason is that critical fluctuations, which become important close to δ_c, have been neglected in the nondegenerate ground state (20). The low-energetic spin-wave excitations, which are almost degenerate with (20) when δ approaches δ_c, should enter the evaluation of $\langle N_z\rangle$. We expect $\langle N_z\rangle$ to go to zero at δ_c if one takes quasiparticle interactions into account by which low-energetic spin-wave excitations should be mixed to the ground state (20). Therefore, the present calculation, based on (20), is limited to δ values smaller than δ_c, though the overall qualitative picture should remain correct also when δ reaches δ_c.

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[1] J. Rossat-Mignod *et al.*, Physica B **169**, 58 (1991).
[2] G. Aeppli *et al.*, Phys. Rev. Lett. **62**, 2052 (1989).
[3] R. J. Birgeneau and G. Shirane, in *Physical Properties of High Temperature Superconductors I*, edited by D. M. Ginsberg (World Scientific, Singapore, 1989).
[4] E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991).
[5] P. W. Anderson, Science **235**, 1196 (1987).
[6] F. C. Zhang and T. M. Rice, Phys. Rev. **37**, 3759 (1988).
[7] H. Mori, Prog. Theor. Phys. **34**, 423 (1965).
[8] D. Forster, in *Hydrodynamic Fluctuations, Broken Symmetry, and Correlation Functions*, Frontiers in Physics (Benjamin, New York, 1975).
[9] E. Fick and G. Sauermann, in *The Quantum Statistics of Dynamic Processes*, edited by Peter Fulde, Springer Series in Solid-State Sciences Vol. 86 (Springer, Berlin, 1990).
[10] S. Chakravarty, Phys. Rev. Lett. **66**, 481 (1991).
[11] P. Chandra, P. Coleman, and A. I. Larkin, J. Phys. Condens. Matter **2**, 7933 (1990).
[12] P. Kopietz and G. Castilla, Phys. Rev. B **43**, 11 100 (1991); see also P. Kopietz (unpublished).
[13] J. Gan, N. Andrei, and P. Coleman, J. Phys. Condens. Matter **3**, 3537 (1991).
[14] L. N. Bulaevskii *et al.*, Zh. Eksp. Teor. Fiz. **54**, 1562 (1968) [Sov. Phys. JETP **27**, 836 (1968)].
[15] B. I. Shraiman and E. D. Siggia, Phys. Rev. Lett. **60**, 740 (1988).
[16] R. Eder and K. W. Becker, Z. Phys. **78**, 219 (1990).
[17] K. W. Becker, R. Eder, and H. Won, Phys. Rev. B **45**, 4864 (1992).
[18] C. L. Kane, P. Lee, and N. Read, Phys. Rev. B **39**, 6880 (1989).
[19] J. Igarashi and P. Fulde, Phys. Rev. B **45**, 12 357 (1992).
[20] G. Khaliullin and P. Horsch, Phys. Rev. B **47**, 463 (1993); G. Khaliullin, Pis'ma Zh. Eksp. Teor. Fiz. **52**, 912 (1990) [JETP Lett. **52**, 289 (1990)].
[21] I. R. Pimentel and R. Orbach, Phys. Rev. B **46**, 2920 (1992).