Spin dynamics in a frustrated magnet with short-range order

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We analyze the stability of Néel and collinear orders for the frustrated J_1-J_2 model on a square lattice as a function of S and J_2/J_1 within the Schwinger-boson mean-field theory. For Néel order and *finite* S, the domain of stability extends beyond the classical boundary $J_2/J_1=\frac{1}{2}$, suggesting the possibility of stabilizing (with the help of quantum fluctuations) a state that is classically forbidden. We use the solution with short-range Néel order as an effective model for the magnetic properties of high-T_c Cu oxides. Predictions are made for the static susceptibility, the dynamical structure factor, and the nuclear relaxation rates (all observable experimentally) at all temperatures. We show that the spin waves are overdamped even at low T and that a gap opens in the spin-fluctuation spectrum. The susceptibility is nearly linear on a wide intermediate temperature range and obeys a Curie law at high temperature in agreement with $1/N$ fermionic expansion.

I. INTRODUCTION

From an experimental point of view, the magnetic properties of the normal state of high-T_c Cu oxides are now relatively well defined. First of all, it has been established using neutron scattering[1-3] that the antiferromagnetic (AF) long-range order (LRO) of the parent compounds is lost upon doping, but that AF short-range order (SRO) is still present in superconducting compounds. Second, NMR-NQR experiments performed on $YBa_2Cu_3O_{6+x}$ have shown that the static susceptibility, as measured by the Knight shift, has a nontrivial temperature dependence.[4,5] For $YBa_2Cu_3O_7$, it is temperature independent, like a regular Pauli susceptibility; but for intermediate dopings (e.g., $YBa_2Cu_3O_{6.63}$, $T_c=60$ K), the susceptibility decreases by a factor of 4 when T is lowered from room temperature to T_c, and the data extrapolate more or less to zero as T goes to zero. These data have been recently confirmed by experiments performed on $YBa_2Cu_4O_8$ ($T_c\simeq 60$ K), where the same T dependence as in $YBa_2Cu_3O_{6.63}$ has been observed.[6] In the case of $YBa_2Cu_4O_8$, one deals with a crystalline sample (the lower doping is a result of stoichiometry only) and this behavior can no longer be attributed to the effect of disorder.

A possible and simple way to account for these data is to assume that the strongly correlated fermions that are present in the CuO_2 planes have both itinerant and localized characters. As local moments, they have only SRO due to the frustration induced by the motion of the carriers. The static susceptibility then consists of two contributions: a T-independent term that arises from the Pauli mechanism for itinerant carriers, and a term that vanishes at $T=0$ and increases with T, and which comes from the local moments. If this picture is to make any sense, itinerant carriers should have a Pauli susceptibility that increases with doping, and the local moments should give a susceptibility that vanishes at $T=0$, increases with temperature, and saturates at higher temperature. The properties of the Pauli contribution are left for future investigation.[7] In this paper, we will concentrate on the properties of a specific model of local moments with SRO.

The first step is actually to find a model that exhibits AF SRO. In the case of high-T_c Cu oxides, the mechanism that triggers the loss of LRO is not known for sure, but it seems likely that the motion of the carriers induces strong quantum fluctuations that destroy the staggered magnetization. If the magnetic excitations can be separated into itinerant and localized ones, which is the basis of the picture we have in mind, this means that the carriers induce effective interactions between the local moments that will tend to destroy the staggered magnetization. This idea was first formulated by Inui *et al.*,[8] who proposed a Heisenberg Hamiltonian including coupling with more than just nearest neighbor (NN). At $T=0$, and if frustration effects are important enough, spin-wave fluctuations can destroy the staggered magnetization, which is equivalent to a loss of LRO. But this does not mean that the ground state retains SRO. In fact, the nature of the ground state of the Heisenberg model with AF nearest and next-nearest-neighbor (NNN) couplings has been recently studied by various authors,[9-13] and it seems likely that spin-Peierls order appears in the region of strong frustration ($J_2/J_1\simeq 0.5$).

Nevertheless, this does not imply that this model is un-

able to describe AF SRO. All we have to do is to force the system to have the right ground state by using an adequate mean-field theory. Given our goal, which is to describe the magnetic properties of high-T_c Cu oxides, this is a reasonable procedure because we *know* that there is antiferromagnetic SRO, but we do not know why. So, according to our picture of carriers modifying the interactions between local moments, there must be a contribution that stabilizes AF SRO against other possible ground states. As we do not understand what this contribution is, we include it by hand by using a mean-field theory that produces the required ground state.

Now, if some SRO persists, the most convenient method is the Schwinger-boson mean-field theory (SBMFT) developed by Arovas and Auerbach to study the finite-temperature properties of a two-dimensional (2D) Heisenberg antiferromagnet on a square lattice.[14,15] In fact, within the SBMFT, another way to destroy LRO at $T=0$ is to reduce the spin variable below a critical value $S_c \simeq 0.2$. The resulting model has already been studied,[16] and the T dependence of various quantities has been derived in the low-temperature limit. In the present paper, we wish to study a refined version of this model. There are several reasons for that. First of all, we would like to get rid of the unphysical hypothesis $S < S_c$ and to work with a model where $S=\frac{1}{2}$. Second, it is interesting to go to higher temperatures. But this is impossible within the nonfrustrated model because the high energy excitations yield a diverging $1/T_1$ due to density of state effects. Finally, frustrated Heisenberg Hamiltonians constitute an interesting problem per se for which a detailed analysis within a given mean-field approximation is a valuable piece of information.

So, we have decided to study the Heisenberg Hamiltonian with nearest- and next-nearest-neighbor couplings (called J_1-J_2 model hereafter):

$$H = J_1 \sum_{\mathrm{NN}} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\mathrm{NNN}} \mathbf{S}_i \cdot \mathbf{S}_j \ . \tag{1}$$

The first thing to do is to determine for which value of J_2/J_1 the SBMFT predicts the disappearance of AF LRO and the existence of SRO for $S=\frac{1}{2}$. A linear spin-wave (LSW) calculation of Chandra and Doucot[17] suggests that this happens for big enough J_2/J_1. As we shall see below, this is also the case within SBMFT, but the loss of LRO occurs at a larger value of J_2/J_1 for $S=\frac{1}{2}$. In fact, the LSW phase diagram giving the domains of existence of LRO for various values of S and J_2/J_1 turns out to be significantly different from the one we got from the SBMFT, suggesting that corrections to the LSW calculation due to higher order effects might be qualitatively important. These results are presented in Sec. II.

The next step is to study the dynamic properties of this Hamiltonian for a given value of J_2/J_1 for which the SBMFT yields AF SRO. The qualitative results with respect to the previous analysis of such a model of SRO include a detailed description of the spin-spin correlation function $S(\mathbf{q},\omega)$ for different temperature regimes, and high T results for the susceptibility and the relaxation rate. This is the object of Sec. III.

II. PHASE DIAGRAM

Let us start our discussion by a short review of the properties of the classical J_1-J_2 model. For $J_2/J_1 < \frac{1}{2}$, the ground state is the Néel state [Fig. 1(a)]. For $J_2/J_1 > \frac{1}{2}$, J_2 dominates and the system separates into two sublattices, each of them having Néel order. For simple symmetry reasons, the classical energy is then independent of the angle θ between the two sublattices, and there is a continuous degeneracy between all these canted states [Fig. 1(c)]. Finally, for $J_2/J_1=\frac{1}{2}$, the ground-state manifold includes not only all the previous states, but also a class of helical states [Fig. 1(b)].

In the quantum case, these conclusions can be modified even at $T=0$ due to zero-point fluctuations. The main effect is a reduction of the order parameter that can lead in certain cases to a loss of LRO. This effect can be studied using linear spin-wave (LSW) theory.[18,19] In the case of the J_1-J_2 model, the phase diagram giving the critical value of the spin below which the LRO disappears as a function of J_2/J_1 has been determined with this method by Chandra and Doucot.[17] If the classical ground state is degenerate, another effect of quantum fluctuations can be to lift the degeneracy, as first proposed by Villain who called it "order from disorder."[20]

Now, for the purpose of the present paper, all we need is the region of existence of Néel LRO within the SBMFT. We start by noting that this method gives exactly the same reduction of the sublattice magnetization as the LSW calculation for $J_2=0$, i.e., for the usual AF case. Does it mean that the phase diagram will remain unchanged with respect to the LSW case? *A priori,* no. The argument is the following. In the LSW theory, quantum fluctuations cannot modify the shape of the spin-wave spectrum, whereas in the SBMFT, there is such a possibility. This was first pointed out by Chandra *et al.*,[12] who realized that Villain's "order from disorder" shows up as the opening of gaps in the excitation spectrum of twisted magnets. But if the spin-wave spectrum is modified, the reduction of the order parameter will also be modified, which can lead *a priori* to a different phase diagram. In fact, this has been recently observed by various authors[21,22] on the basis of an essentially equivalent method developed by Takahashi.[23] We nevertheless present the SBMFT analysis is some details because our

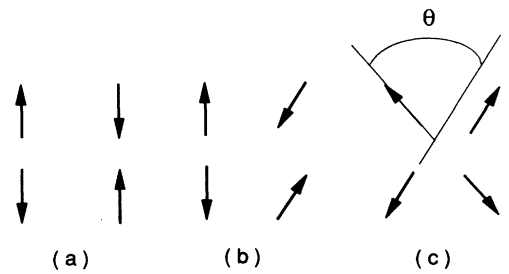

FIG. 1. Various possible orders in the classical case: (a) Néel state ($J_2/J_1 \leq \frac{1}{2}$); (b) helical states ($J_2/J_1=\frac{1}{2}$); (c) canted states ($J_2/J_1 \geq \frac{1}{2}$).

calculation yields significant improvements with respect to the previous results.

Let us now turn to a brief description of the method. For clarity, we will discuss only the collinear states in the present article.[24] In the large-S limit, this is quite natural, as we expect them to be stabilized against the other states by quantum fluctuations (order from disorder). In fact, it can be shown that within the SBMFT these states play no role in the interesting part of the phase diagram.[25]

The Schwinger-boson method starts from a faithful representation of spin operators

$$\mathbf{S}_i=\tfrac{1}{2}b_{i\sigma}^{\dagger}\boldsymbol{\sigma}_{\sigma\sigma'}b_{i\sigma'} , \tag{2a}$$

$$b_{i\sigma}^{\dagger}b_{i\sigma}=2S , \tag{2b}$$

where $b_{i\uparrow},b_{i\downarrow}$ are boson operators, and the second equation ensures that $\mathbf{S}_i^2=S(S+1)$. Then, to describe quantum fluctuations in a state with LRO, Chandra *et al.* pointed out that it is convenient, as in spin-wave theory, to work in a reference frame where spins are ferromagnetically aligned by performing a suitable local rotation. For details of the general method, the reader is referred to their original paper.[12] For collinear states, the method is very simple. After a rotation of π in spin space at the appropriate sites, the general Hamiltonian

$$H=\sum_{\langle i,j\rangle}J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j \tag{3}$$

can be written

$$H=\tfrac{1}{2}\sum_{\langle i,j\rangle_{\text{ferro}}}J_{ij}(D_{ij}^{\dagger}D_{ij}-2S^2) -\tfrac{1}{2}\sum_{\langle i,j\rangle_{\text{AF}}}J_{ij}(B_{ij}^{z\dagger}B_{ij}^{z}-2S^2) , \tag{4}$$

where $D_{ij}^{\dagger}=b_{i\sigma}^{\dagger}b_{j\sigma}$, $B_{ij}^{z\dagger}=b_{i\sigma}^{\dagger}b_{j-\sigma}^{\dagger}$, and $\langle ij\rangle_{\text{ferro}}$ ($\langle ij\rangle_{\text{AF}}$) means summation over pairs of parallel (antiparallel) spins. A mean-field decoupling is then performed with respect to the order parameters $\alpha_{ij}=\frac{1}{2}\langle D_{ij}^{\dagger}\rangle$ and $\gamma_{ij}=\frac{1}{2}\langle B_{ij}^{z\dagger}\rangle$, and the local constraint is replaced by a global one and is treated with a Lagrange multiplier λ. The resulting Hamiltonian is quadratic and can be diagonalized in Fourier space by a Bogolioubov transformation. The parameters α_{ij}, γ_{ij}, and λ are finally determined by minimizing the free energy.

Let us follow the details of the method in the cases of interest here. In the Néel case, we need two order parameters α and γ, while in the collinear case,[24] we need three of them: α, γ_1, and γ_2 (see Fig. 2). Then, introducing the quantities $h_{\mathbf{q}}$ and $\Delta_{\mathbf{q}}$ given by

$$h_{\mathbf{q}}=4J_2\cos q_x\cos q_y\alpha , \tag{5a}$$

$$\Delta_{\mathbf{q}}=2J_1(\cos q_x+\cos q_y)\gamma \tag{5b}$$

in the Néel case, and by

$$h_{\mathbf{q}}=2J_1\cos q_x\alpha , \tag{6a}$$

$$\Delta_{\mathbf{q}}=2J_1\cos q_y\gamma_1+4J_2\cos q_x\cos q_y\gamma_2 \tag{6b}$$

in the collinear case, the Fourier-transformed Hamiltonian reads

$$H=E_c+\sum_{\mathbf{q}}(h_{\mathbf{q}}+\lambda)(b_{\mathbf{q}\uparrow}^{\dagger}b_{\mathbf{q}\uparrow}+b_{\mathbf{q}\downarrow}b_{\mathbf{q}\downarrow}^{\dagger}) -\sum_{\mathbf{q}}\Delta_{\mathbf{q}}(b_{\mathbf{q}\uparrow}^{\dagger}b_{-\mathbf{q}\downarrow}^{\dagger}+b_{\mathbf{q}\uparrow}b_{-\mathbf{q}\downarrow}) \tag{7}$$

with

$$E_c=2J_1(S^2+2\gamma^2)-2J_2(S^2+2\alpha^2)-2\lambda(S+\tfrac{1}{2}) \tag{8}$$

in the Néel case, and

$$E_c=2J_1(\gamma_1^2-\alpha^2)+2J_2(S^2+2\gamma_2^2)-2\lambda(S+\tfrac{1}{2}) \tag{9}$$

in the collinear case.

The energy spectrum deduced from a Bogolioubov transformation of Eq. (7) reads

$$\omega_{\mathbf{q}}=[(h_{\mathbf{q}}+\lambda)^2-\Delta_{\mathbf{q}}^2]^{1/2} . \tag{10}$$

To study the ground-state properties, we need the self-consistent equations at $T=0$. To include the possibility of Bose condensation, we must introduce a quantity S^* and write them

$$\alpha=S^*+\sum_{\mathbf{q}}\frac{h_{\mathbf{q}}+\lambda}{2\omega_{\mathbf{q}}}\cos q_x\cos q_y , \tag{11a}$$

$$\gamma=S^*+\sum_{\mathbf{q}}\frac{\Delta_{\mathbf{q}}}{4\omega_{\mathbf{q}}}(\cos q_x+\cos q_y) , \tag{11b}$$

$$S+\tfrac{1}{2}=S^*+\sum_{\mathbf{q}}\frac{h_{\mathbf{q}}+\lambda}{2\omega_{\mathbf{q}}} \tag{11c}$$

for the Néel case, and

$$\alpha=S^*+\sum_{\mathbf{q}}\frac{h_{\mathbf{q}}+\lambda}{2\omega_{\mathbf{q}}}\cos q_x , \tag{12a}$$

$$\gamma_1=S^*+\sum_{\mathbf{q}}\frac{\Delta_{\mathbf{q}}}{2\omega_{\mathbf{q}}}\cos q_y , \tag{12b}$$

$$\gamma_2=S^*+\sum_{\mathbf{q}}\frac{\Delta_{\mathbf{q}}}{2\omega_{\mathbf{q}}}\cos q_x\cos q_y , \tag{12c}$$

$$S+\tfrac{1}{2}=S^*+\sum_{\mathbf{q}}\frac{h_{\mathbf{q}}+\lambda}{2\omega_{\mathbf{q}}} \tag{12d}$$

for the collinear case. The unknowns are $(\alpha_{ij},\gamma_{ij},\lambda)$ or $(\alpha_{ij},\gamma_{ij},S^*)$ depending on the parameters J_{ij} and S. If there is a solution in $(\alpha_{ij},\gamma_{ij},\lambda)$ for $S^*=0$, then the sys-

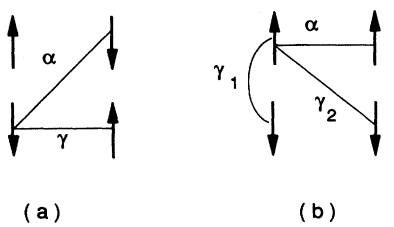

FIG. 2. Order parameters defined in the main text for (a) Néel order; (b) collinear order.

tem has no LRO. But if there is no such solution, there is Bose condensation;[26] the occupation of the lowest lying mode S^* is an unknown, and λ is fixed by the condition that the frequency of this mode vanishes. In the present context, this corresponds to LRO.

In general, for a given set of J_i and for small S, the system will have short-range order: $S^*=0$ and the spectrum has a gap. If the gap is finite for all values of S, the system cannot sustain LRO of the assumed symmetry. But if the gap vanishes for a certain range of spin values, there is Bose condensation, and LRO. In practice, one determines S_c as follows: (i) Assume that both S^* and the gap vanish (the second condition fixes λ); (ii) solve the self-consistent equations giving α_{ij} and γ_{ij}; (iii) deduce S from the last equation. The results for the Néel and collinear cases are given in Fig. 3, where we have plotted $1/S_c$ as a function of J_2/J_1. The main features agree with Xu and Ting.[22] For the collinear case, there is no qualitative difference with the LSW theory: $1/S_c$ vanishes at $J_2/J_1=\frac{1}{2}$, where the classical system undergoes a phase transition. For the Néel case, on the contrary, the phase boundary goes noticeably beyond $J_2/J_1=\frac{1}{2}$, which means that the spin liquid region found by Chandra and Doucot is considerably modified, and actually disappears for physical values of the spin.

Now, the large-S limit of this region of existence of Néel order is quite subtle. We have found that for $S\to\infty$ the boundary does *not* drop vertically to $J_2/J_1\sim 0.7$, as proposed by Xu and Ting,[22] but turns back to reach the classical limit $J_2/J_1=\frac{1}{2}$. We think that physically this is the only reasonable situation. In fact, when S goes to infinity, we have to connect one way or another to the classical result. In the classical case, the Néel state is unstable, which means that there are imaginary frequencies. So, increasing S should yield a vanishing spin-wave velocity before S becomes infinite. This actually cannot be observed in our calculation because quantum fluctuations will destroy the LRO before the spin-wave velocity vanishes. What we expect to observe is then a loss of LRO on increasing S. In other words, this region of Néel LRO has to be bounded from below. This is indeed what our numerical simulation has shown (see Fig. 3).

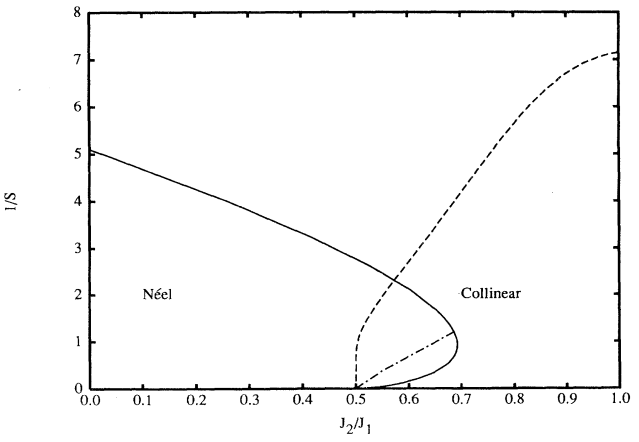

FIG. 3. Phase diagram obtained with the SBMFT. The solid line shows $1/S_c$ (Néel), the dashed line $1/S_c$ (collinear), and the dashed-dotted line the first-order transition boundary: Below the dashed-dotted line, the collinear state has a lower energy than the Néel state.

Another interesting question is raised by the coexistence of both types of order for $J_2/J_1\geq 0.5$. Within our approach, all we can do is to compare the ground-state energies of both states. They are given by

$$E_{\text{g.s.}}=E_{\text{zero}}+E_c\ , \tag{13}$$

where E_c is the constant part of the Hamiltonian [see Eqs. (7)–(9)] and $E_{\text{zero}}=\sum_{\mathbf{q}}\omega_{\mathbf{q}}$ is the zero-point energy. A straightforward calculation yields

$$E_{\text{g.s.}}(\text{Néel})=-2J_1(2\gamma^2-S^2)+2J_2(2\alpha^2-S^2)\ , \tag{14a}$$

$$E_{\text{g.s.}}(\text{collinear})=-2J_1(\gamma_1^2-\alpha^2)-2J_2(2\gamma_2^2-S^2)\ . \tag{14b}$$

These formulas can actually be obtained directly from Eq. (4). Let us note that these expressions are slightly different from those obtained by Xu and Ting[22] using Takahashi's method.[23] This is the essential difference between his variational approach and the large-N approach of the SBMFT. We have numerically computed these energies. It turns out that the collinear state is lower in energy in the region below the dashed-dotted line in Fig. 3. This means that there is a first order phase transition from the Néel state to the collinear state upon increasing S. However, we do not claim that we can make any statement as to what the real ground state is. Our Schwinger-boson approach is a mean-field theory, and its approximations are difficult to control. The nature of the ground state is actually still controversial (see Refs. 9–13 and 27). A likely candidate seems to be the spin-Peierls state first proposed in that case by Read and Sachdev,[11] a state beyond the reach of the present mean-field theory.

What is then the physical meaning, if any, of the region of stability of the Néel order? We interpret this as a stability against long-wavelength fluctuations of the order parameter. But for the same value of J_2/J_1, the corresponding classical state is unstable and cannot serve as a starting point in a $1/S$ expansion. The existence of a quantum state with LRO that cannot be obtained by a perturbation of the corresponding classical state is not new in the context of spin systems. Studying the boundary between ferromagnetism and helimagnetism in a hexagonal model, Harris and Rastelli[28] have found that quantum fluctuations can stabilize a helical state which is forbidden classically, yielding what they have called a quantum helix. The SBMFT allows one to describe this effect because in this method, the quantum fluctuations modify the coupling constants, i.e., the dynamics of the order parameter. Further work along these lines is in progress.[29]

Finally, we should mention that this phase diagram is not complete. The noncollinear classical ground states define LRO that can be sustained outside the regions where the collinear ones can. Nevertheless, this corre-

sponds to $S \leq 0.42$ and is physically not very interesting. For all physical values of the spin, we have preliminary results that indicate that these states are never stabilized against one of the collinear states considered in this paper.[25]

III. SPIN DYNAMICS

Let us now turn to the study of the spin dynamics. We first note that the frequencies $\omega_{\mathbf{k}}$ correspond to the spectrum of the mean-field Hamiltonian and should be considered as elementary excitations. On the other hand the collective modes are directly obtained from the dynamical spin correlation function defined by $S(\mathbf{q},\omega) = \int dt\, e^{i\omega t}\langle \mathbf{S}_{\mathbf{q}}(t)\cdot\mathbf{S}_{-\mathbf{q}}(0)\rangle$, $\omega > 0$. It can be written $S(\mathbf{q},\omega)=S_1(\mathbf{q},\omega)+S_2(\mathbf{q},\omega)$, where $S_1(\mathbf{q},\omega)$ and $S_2(\mathbf{q},\omega)$ have a different physical origin and are given by

$$S_1(\mathbf{q},\omega)= \sum_{\mathbf{k}} (u_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}}-v_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}})^2 n_{\mathbf{k}}(1+n_{\mathbf{k}+\mathbf{q}}) \times \delta(\omega_{\mathbf{k}}-\omega_{\mathbf{k}+\mathbf{q}}+\omega)\,, \tag{15}$$

$$S_2(\mathbf{q},\omega)= \sum_{\mathbf{k}} (u_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}}-v_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}})^2 (1+n_{\mathbf{k}}) \times (1+n_{\mathbf{k}+\mathbf{q}})\delta(\omega_{\mathbf{k}}+\omega_{\mathbf{k}+\mathbf{q}}-\omega)\,, \tag{16}$$

$n_{\mathbf{k}}=1/(e^{\beta\omega_{\mathbf{k}}}-1)$ is the bosonic thermal factor, β the inverse temperature, and $u_{\mathbf{k}}=[(\lambda+h_{\mathbf{k}}+\omega_{\mathbf{k}})/2\omega_{\mathbf{k}}]^{1/2}$ and $v_{\mathbf{k}}=\mathrm{sgn}(\Delta_{\mathbf{k}})[(\lambda+h_{\mathbf{k}}-\omega_{\mathbf{k}})/2\omega_{\mathbf{k}}]^{1/2}$ are the coefficients of the Bogolioubov transformation that diagonalizes the mean-field Hamiltonian. The physical processes responsible for the first term are the simultaneous emission and absorption of two elementary excitations. This term vanishes identically at $T=0$ because thermally activated excitations are no longer available. On the other hand, the second term corresponds to the emission of two elementary excitations. This process is allowed even at zero temperature.

In the following we shall investigate the behavior of $S(\mathbf{q},\omega)$ in the disordered phase. We have chosen a value of $J_2=0.65$ ($J_1=1$), while the spin is set to $S=\frac{1}{2}$. This corresponds to a point in the phase diagram close to the boundary of the region of AF LRO. Let us emphasize again here that we do not consider J_2 as a real physical quantity but rather as a parameter we adjust to get the generic form of the dynamical correlation function for SRO antiferromagnets. So, we disregard the collinear phase which is predicted by the theory and we assume that we have instead a disordered Néel state.

Before we turn to the study of the disordered state let us summarize some of the main results relative to the pure Heisenberg model ($J_2=0$).[14] At $T=0$, $S(\mathbf{q},\omega)$ was shown to diverge on a surface in the 3D ω-$\mathbf{q}$ space given by $\omega=\omega_{\mathbf{q}}$ in complete agreement with large-S spin-wave theories. At finite temperature a gap develops [$\Delta(T)\sim T\exp(-C/T)<T$] leading to an exponential decay of the static spin-spin correlations. Near $\mathbf{q}_0=(\pi/a,\pi/a)$ (on the scale of the correlation length) the spin waves become overdamped, while sufficiently far away from $\mathbf{q}_0$ they recover a large lifetime. In other words, the spin waves are still defined in real space on the scale of the correlation length (exponentially large at low temperature). Our motivation to study here the disordered phase is threefold. (i) First, we are stimulated by the excellent agreement found for $S(\mathbf{q},\omega)$ between the SBMFT and exact diagonalizations on small clusters.[30] (ii) Second, we expect a behavior of $S(\mathbf{q},\omega)$ qualitatively different from the pure Heisenberg model. Indeed, the gap formation has a different origin in each case. For $J_2=0$, the disordering of the spins (at long distance) is due to thermal fluctuations and the gap is always exponentially small compared to T while in the case of interest here the disordering is due to frustration and at low temperature the gap becomes larger than T. (iii) Third, a disordered spin state is realized in the new high-T_c superconductors upon doping the Néel state. In the superconducting phase correlation lengths as short as 1 or 2 lattice spacings are typically observed. Moreover, the quantity $S(\mathbf{q},\omega)$ is directly accessible by inelastic neutron scattering (at least for $\mathbf{q}\sim\mathbf{q}_0$) and therefore a direct comparison with experiment is in principle possible.

The summation in $S(\mathbf{q},\omega)$ was performed on finite lattices of typical sizes 400×400 or 600×600. Although the spectrum $\omega_{\mathbf{k}}$ is periodic of period $\mathbf{q}_0$, the dynamical spin correlation function is defined in the full Brillouin zone as expected since there is no LRO, hence no doubling of the unit cell.[31] Indeed, this can be seen directly from formulas (15) and (16) remembering that $v_{\mathbf{k}}$ changes sign when $\mathbf{k}$ crosses the $\cos k_x+\cos k_y=0$ pseudo-Fermi surface. Three-dimensional plots of $S(\mathbf{q},\omega)$ are shown in Figs. 4–6 for various temperatures and $\mathbf{q}\propto\mathbf{q}_0$. We show here the fluctuations in the vicinity of the AF wave vector where most of the spectral weight is concentrated at low temperature (around $\mathbf{q}\sim\mathbf{0}$ the spectral function is at least one order of magnitude smaller). Besides, we consider the low frequency regime ($\omega\sim0-20$ meV) because it is experimentally the most relevant. At $T=0$, as shown in Fig. 4, only S_2 gives a nonzero contribution. There is rigorously no weight for $\omega<2\omega_{\mathbf{q}_0}(T=0)$ and a sharp edge appears in $S(\mathbf{q},\omega)$ when $\omega\geq2\omega_{(\mathbf{q}-\mathbf{q}_0)/2}$. Since

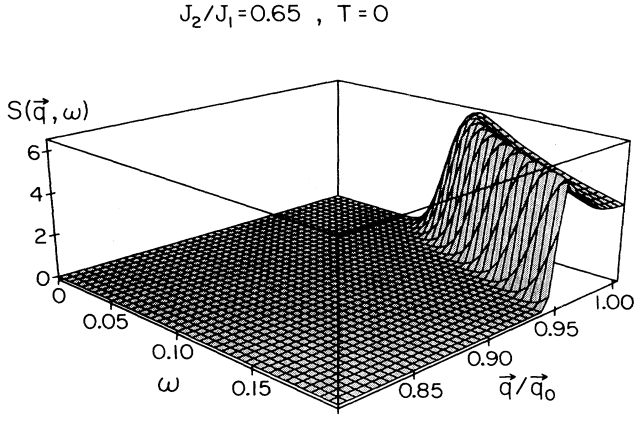

FIG. 4. Dynamical structure factor $S(\mathbf{q},\omega)$ vs ω and $\mathbf{q}\propto\mathbf{q}_0$ at temperature $T=0$ ($J_1=1$). The calculation was performed on a 400×400 lattice.

the spectrum $\omega_{\mathbf{k}}$ has a gap there is a minimum energy to create a pair of excitations. The edge is reminiscent of the spin-wave modes but the dispersion $\omega=\omega_{(\mathbf{q}-\mathbf{q}_0)/2}$ is quadratic near $\mathbf{q}=\mathbf{q}_0$ due to the gap and the maximum is not very pronounced. With increasing temperature (Figs. 5 and 6) the gap in the spectrum increases so that the contribution due to S_2 appears at larger frequency and the edge first rounds off because of the finite temperature and then becomes sharper again because of the reduction of the bandwidth. The integrated intensity of S_2, however, is reduced by T. Simultaneously, at low energy spectral weight grows with increasing temperature due to the S_1 component. Since thermal excitations are primarily created around $\mathbf{q}\sim\mathbf{q}_0$ the dynamical structure factor diverges at $\mathbf{q}_0$ and $\omega=0$, i.e., $S_1(\mathbf{q}_0,\omega)\propto\delta(\omega)$ at any finite T. From Fig. 5, it is clear that the spin-wave edge is split into two broad maxima. However, this structure might disappear if fluctuations are treated in a more elaborate way, for instance in the random-phase approximation (RPA).

Let us now briefly discuss the case $\mathbf{q}\sim 0$. From Eqs. (15) and (16) it is easy to realize that the behavior of the structure factor around $q=0$ or $\mathbf{q}=\mathbf{q}_0$ is very similar since $\omega_{\mathbf{k}+\mathbf{q}_0}=\omega_{\mathbf{k}}$. The only difference comes from the squares appearing as prefactors. S_1 is enhanced near $\mathbf{q}_0$ by the factor $[(\lambda+h_{\mathbf{k}})/\omega_{\mathbf{k}}]^2\geq 1$. On the other hand, in S_2 the prefactor vanishes at exactly $\mathbf{q}=0$ and $S_2(\mathbf{0},\omega)=0$ at all temperatures. At $T=0$, $S(\mathbf{0},\omega)=0$ for any frequency. We conclude then that the integrated spectral weight in the vicinity of $\mathbf{q}=\mathbf{0}$ is in general negligible compared to the one in the region around $\mathbf{q}_0$, at least at low temperature. We would also like to note that because of the gap our results do not give the hydrodynamic behavior at long wavelength speculated by several authors.[32,33] However, the possible existence of a diffusive behavior and of a pseudogap near $\mathbf{q}=\mathbf{0}$ is not expected to change the various physical properties studied here which are essentially dominated by the $\mathbf{q}_0$ fluctuations.

With increasing T the bandwidth is reduced and above some critical temperature (~ 0.87 at $J_2=0.65$) the spectrum becomes dispersionless, $\omega_{\mathbf{k}}=\lambda(T)=T\ln(1+1/S)$. The structure factor is then $\mathbf{q}$ independent and fulfills $\sum_{\mathbf{q}}S(\mathbf{q},\omega)=S(S+1)\delta(\omega)$ (S_2 vanishes at the transition). We believe that this second-order transition is an artifact of the mean-field approach, but that it signals the crossover of behaviors between correlated spins at low T and free spins at high T. In the real system this crossover is expected to be smooth with T. It is also interesting to note that the fermionic $1/N$ expansion gives a very similar result.[34,35]

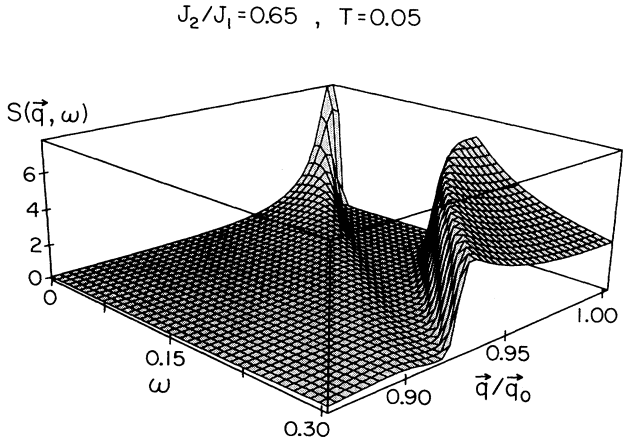

FIG. 5. Dynamical structure factor $S(\mathbf{q},\omega)$ vs ω and $\mathbf{q}\propto\mathbf{q}_0$ at temperature $T=0.05$ ($J_1=1$). The calculation was performed on a 600×600 lattice.

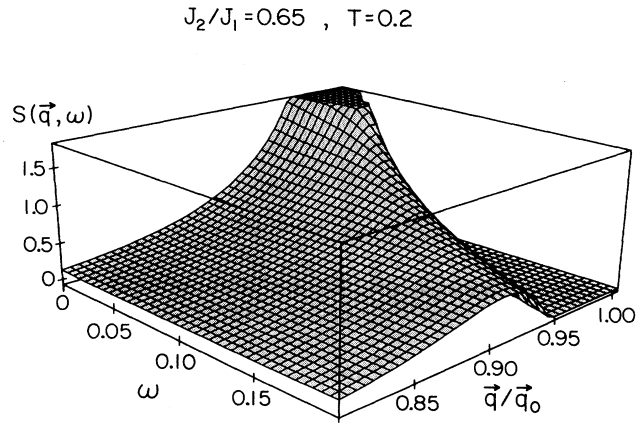

FIG. 6. Dynamical structure factor $S(\mathbf{q},\omega)$ vs ω and $\mathbf{q}\propto\mathbf{q}_0$ at temperature $T=0.2$ ($J_1=1$). The calculation was performed on a 400×400 lattice.

Since the total magnetization commutes with the Hamiltonian the uniform static susceptibility $\chi=\int_0^\beta d\tau\langle\mathbf{S}_{\mathbf{q}=0}(\tau)\cdot\mathbf{S}_{\mathbf{q}=0}(0)\rangle$ reduces to β times the equal-time correlation function:

$$\chi=\frac{\beta}{2\pi}\int d\omega\, S(\mathbf{q}=0,\omega)=\sum_{\mathbf{k}} n_{\mathbf{k}}(1+n_{\mathbf{k}})\,. \tag{17}$$

χ is shown in Fig. 7 versus T. We can distinguish three temperature ranges. First, at low temperature the gap in the spectrum produces an exponential behavior. Second, for intermediate temperature χ is nearly linear. Third, when T is increased further the short-range correlations are suppressed by thermal fluctuations and the susceptibility obeys a Curie law $\chi\propto S(S+1)/T$. This is again in very good agreement with the fermionic mean-field approach.[35]

Finally we investigate the nuclear relaxation rates given by

$$\frac{1}{T_1}=\sum_{\mathbf{q}} F_{\mathbf{q}}S(\mathbf{q},\omega_N)\,, \tag{18}$$

where ω_N is the Larmor nuclear frequency ($\omega_N\ll J_1$) and $F_{\mathbf{q}}$ is a form factor accounting for possible nonlocal couplings between the nucleus and the electronic spins. We consider the three form factors 1, $1+\cos q_x+\cos q_y$, and $1+\cos q_x+\cos q_y+\cos q_x\cos q_y$ corresponding to the Cu, O, and Y nuclei, respectively.[36,37] Since the spectral

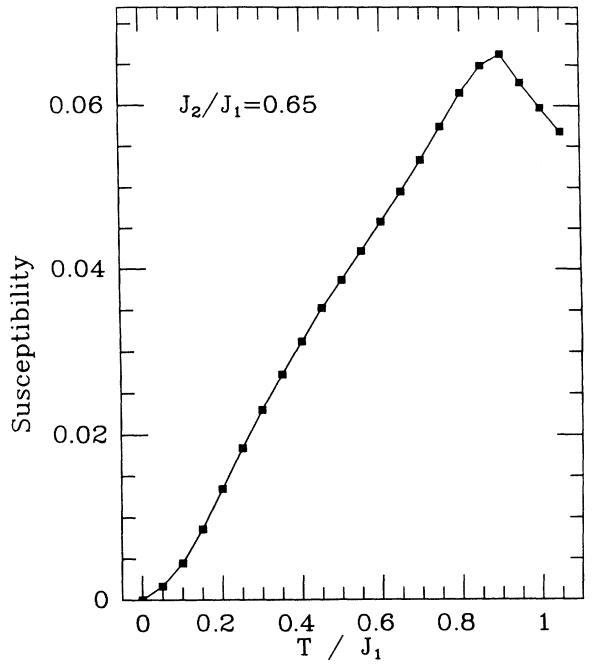

FIG. 7. Static susceptibility vs temperature (calculated on a 200×200 lattice).

function has no weight at low energy $1/T_1$ vanishes at $T=0$ as shown in Figs. 8(a) and 8(b). At low temperature the behavior is exponential as noted earlier.[25] For O and Y sites, the form factors are responsible for the suppression of the $\mathbf{q}_0$ fluctuations leading to a drastic decrease of the relaxation rates compared to the Cu one [Fig. 8(a)]. However, this is effective only at low temperature, $T<0.1$ (assuming $J_1\sim1500$ K, this means $T<150$ K). At higher temperature, when the spectrum becomes dispersionless, all the relaxation rates become nearly identical [Fig. 8(b)]. The only processes contributing to the relaxation of the nuclear spins are the simultaneous emission and absorption of two excitations of same energy above the gap. However, at the second order transition the bandwidth drops to zero while the density of states becomes infinite at $\omega=\lambda$. Therefore $1/T_1$ diverges at the transition as the spins become free. The same artifact occurs for fermionic mean-field theory.[35] In real systems, this density of state effect is expected to be smoother so that $1/T_1$ may saturate eventually at large temperature as seen experimentally.

IV. CONCLUDING REMARKS

Searching for a model to describe part of the magnetic fluctuations in high-T_c superconductors, we have studied the J_1-J_2 frustrated Heisenberg model by the Schwinger-boson mean-field theory. The $(1/S,J_2/J_1)$ phase diagram exhibits significant differences with that obtained by an LSW analysis. The most surprising feature is that, in the quantum case, long-range Néel order can be stabilized for $J_2/J_1>0.5$, i.e., in a region where it is classically forbidden. When this is not the case (e.g., $J_2/J_1=0.65$ for $S=\frac{1}{2}$), the system has short-range Néel order, in agreement with neutron-scattering data obtained on

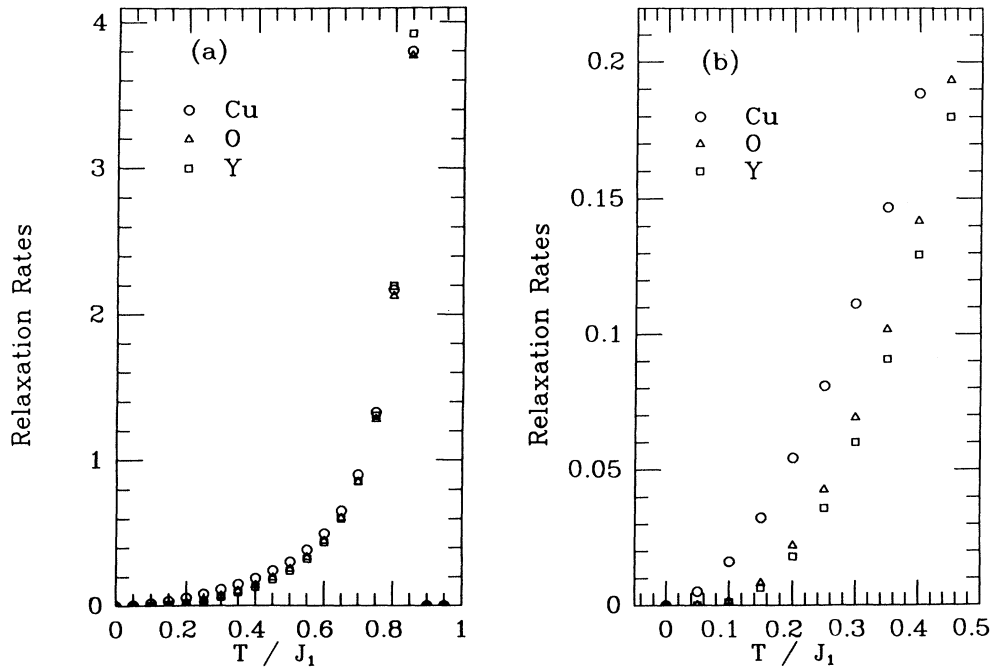

FIG. 8. Nuclear relaxation rates vs temperature (calculated on a 160×160 lattice). The full temperature range and the low-temperature region are shown in (a) and (b), respectively. Due to a very small but finite nuclear frequency ω_N $1/T_1$ vanishes above some critical temperature ~0.87.

high-T_c Cu oxides. A detailed analysis of the spin dynamics shows a number of interesting features of this model. At low temperature, the results are qualitatively similar to those obtained for the J_1 model with $S < S_c \sim 0.2$. In particular, a gap opens in the spin-wave spectrum, leading to a drastic increase of the spin-wave lifetime at short wavelength and to an exponential behavior of the static susceptibility and the Cu relaxation rate. At higher but still low temperature, one gets a linear behavior for the susceptibility and for the various relaxation rates. This is the most promising result insofar as high-T_c Cu oxides are concerned. Finally, at higher temperature, there is a phase transition to free spins, in qualitative agreement with large SU(N) theories. At the transition, $1/T_1$ diverges, while beyond this point, the susceptibility recovers the usual Curie behavior.

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