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Nonclassical disordered phase in the strong quantum limit of frustrated antiferromagnets

H. A. Ceccatto, C. J. Gazza, and A. E. Trumper
Instituto de Física Rosario, Universidad Nacional de Rosario, Boulevard 27 de Febrero 210 Bis, 2000 Rosario, Argentina
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The rotationally invariant Schwinger-boson approach to quantum helimagnets is discussed. It is shown that in order to get quantitative agreement with exact results on finite lattices, parity-breaking pairing of bosons must be allowed. For the J_1-J_2-J_3 model on the special line $J_2 = 2J_3$, a quantum disordered phase is found, though notably only in the strong quantum limit $S = \frac{1}{2}$. The theory predicts the direct melting of biaxial helimagnetic order into an isotropic spin fluid, without the formation of an intermediate spin-nematic phase as recently suggested.

The insulating phase of copper oxide high-T_c compounds is well described by a two-dimensional spin-$\frac{1}{2}$ square lattice Heisenberg model,[1] displaying long-range antiferromagnetic order at zero temperature.[2] Upon doping this Néel order is rapidly suppressed due to the frustrating effects of hole movement, leaving a conducting state which has been suggested[3] to be different from a normal Fermi liquid. Unusual properties of this spin-liquid state might provide a mechanism for driving the system into a superconducting phase.

How the antiferromagnetic order is destabilized by doping, and the nature of the disordered state so generated, are central problems in the theoretical understanding of high-T_c superconductivity. One simple approach to these questions[4] consists in integrating out the holes for small doping, leaving an effective spin Hamiltonian with further-neighbor interactions:

$$H = J_1 \sum_{\mathbf{x},\mu} \mathbf{S_x} \cdot \mathbf{S_{x+\mu}} + J_2 \sum_{\mathbf{x},\mu'} \mathbf{S_x} \cdot \mathbf{S_{x+\mu'}} + J_3 \sum_{\mathbf{x},\mu''} \mathbf{S_x} \cdot \mathbf{S_{x+\mu''}}. \quad (1)$$

Here J_2 and J_3 measure the frustration strength between a given spin and its second and third neighbors, respectively, and the region of interest is $J_2 \sim 2J_3$. Since in this approximation the dynamical frustration produced by holes has been replaced by a static one, clearly (1) captures only gross features of the physics involved. On the other hand, Hamiltonian (1) is interesting *per se* as a model of a helimagnet, with the frustration known[5] to produce a spiral phase in some region of parameter space. In fact, classically, when $J_3 < \frac{1}{8}J_1$ the ground state of the system is in a Néel phase for $J_1 > 2J_2 + 4J_3$, while for $2J_2 > J_1 + 4J_3$ it goes to a collinear order which is ferromagnetic in one direction and antiferromagnetic in the other. These two phases are separated by a twisted spiral phase ordered at wave vector $\mathbf{Q} = (\pi, Q)$, with Q satisfying $\cos Q = \frac{2J_2 - J_1}{4J_3}$. For $J_3 > \frac{1}{8}J_1$, a new symmetric spiral phase ordered at wave vector $\mathbf{Q} = (Q, Q)$, with $\cos Q = \frac{-J_1}{2J_2 + 4J_3}$, appears. The two incommensurate phases are separated by the line $J_2 = 2J_3$, at which an infinite number of degenerate spiral states coexist.[6] The way strong fluctuations due to the quantum nature of spins alter this picture—particularly near the line $J_2 = 2J_3$—is an interesting question on its own, independently of the above mentioned connection with superconductivity.

In this work we study the ground-state properties of Hamiltonian (1)—especially its incommensurate phases—with particular emphasis on the strong quantum limit $S = \frac{1}{2}$. First, we discuss the rotationally invariant Schwinger-boson approach to quantum helimagnets,[7] and a natural decoupling scheme for the effective (quartic) bosonic Hamiltonian. Secondly, we show that in order to get qualitative and quantitative agreement with exact results on finite lattices, parity-breaking pairing of bosons must be allowed, contrary to previous work in the literature.[8,9] We present evidence that a quantum disordered phase exists between the Néel and spiral phases, though notably only for physical spin $S = \frac{1}{2}$. On the other hand, it appears only for the third-neighbor coupling J_3 larger than a minimum finite value $J_{3\,\mathrm{min}} \simeq 0.038J_1$. Our approach predicts no intermediate spin-nematic phase between the biaxial quantum helimagnet and disordered isotropic spin fluid, contrary to a recent suggestion in the literature.[9] To our knowledge, this is the first thorough examination of the twelve-dimensional order-parameter space of (1) in the strong quantum limit. In addition, we assess the reliability of our approach by comparison with the few known exact (numerical) results on finite lattices.[6]

In order to obtain a rotationally invariant Hartree-Fock (HF) decomposition of H it is convenient to express the spin-operators in terms of the Schwinger representation:[10] $\mathbf{S_x} = \frac{1}{2}\mathbf{a}^\dagger_\mathbf{x} \cdot \boldsymbol{\sigma} \cdot \mathbf{a_x}$, where $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ are the Pauli matrices, and the bosonic spinors $\mathbf{a_x} = (a_{\mathbf{x}\uparrow}, a_{\mathbf{x}\downarrow})$ satisfy $\mathbf{a}^\dagger_\mathbf{x} \cdot \mathbf{a_x} = 2S$. Then, by means of the Fierz identity it is easy to show that $\mathbf{S_x} \cdot \mathbf{S_y} = \frac{1}{8} : \mathrm{Tr}(P\psi^\dagger_\mathbf{x}\psi_\mathbf{y}P\psi^\dagger_\mathbf{y}\psi_\mathbf{x}) :$, where

$$\psi_{\mathbf{x}} = \begin{pmatrix} a_{\mathbf{x}\uparrow} & -a^{\dagger}_{\mathbf{x}\downarrow} \\ a_{\mathbf{x}\downarrow} & a^{\dagger}_{\mathbf{x}\uparrow} \end{pmatrix} \quad , \quad P = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and, as usual, : : means normal order of the operators inside. The operator-valued matrix $\psi_{\mathbf{x}}$ transforms under rotations as $\psi_{\mathbf{x}} \rightarrow g\psi_{\mathbf{x}}$, with $g \in$SU(2), which naturally suggests the following invariant decomposition of (2):

$$(\mathbf{S_x} \cdot \mathbf{S_y})_{\rm HF} = \tfrac{1}{4}{\rm Tr}(W_{\mathbf{xy}}\psi^{\dagger}_{\mathbf{y}}\psi_{\mathbf{x}}) + \tfrac{1}{4}{\rm Tr}(\psi^{\dagger}_{\mathbf{x}}\psi_{\mathbf{y}}W_{\mathbf{yx}}) - \tfrac{1}{2}{\rm Tr}(W_{\mathbf{xy}}PW_{\mathbf{yx}}P). \quad (2)$$

The order-parameter matrix $W_{\mathbf{xy}}$ is given by

$$W_{\mathbf{xy}} \equiv \frac{1}{2}P\langle\psi^{\dagger}_{\mathbf{x}}\psi_{\mathbf{y}}\rangle P \equiv \begin{pmatrix} B^{*}_{\mathbf{xy}} & A^{*}_{\mathbf{xy}} \\ -A_{\mathbf{xy}} & B_{\mathbf{xy}} \end{pmatrix},$$

where $B^{*}_{\mathbf{xy}}=\frac{1}{2}\langle\sum_{\sigma} a^{\dagger}_{\mathbf{x}\sigma}a_{\mathbf{y}\sigma}\rangle$ and $A_{\mathbf{xy}}=\frac{1}{2}\langle\sum_{\sigma}\sigma a_{\mathbf{x}\sigma}a_{\mathbf{y}-\sigma}\rangle$. One can see that

$$\langle(\mathbf{S_x}\cdot\mathbf{S_y})_{\rm HF}\rangle = \tfrac{1}{2}{\rm Tr}(W_{\mathbf{xy}}PW^{*}_{\mathbf{xy}}P) = |B_{\mathbf{xy}}|^2 - |A_{\mathbf{xy}}|^2, \quad (3)$$

that is, $A_{\mathbf{xy}}$ and $B_{\mathbf{xy}}$ measure, respectively, antiferromagnetic and ferromagnetic correlations between spins at sites **x** and **y**. In the following we will assume them to be real. Notice that (2) is also invariant under the (local) right transformation $\psi_{\mathbf{x}} \rightarrow \psi_{\mathbf{x}}\Lambda_{\mathbf{x}}$, with $\Lambda_{\mathbf{x}} = {\rm diag}(e^{i\varphi(\mathbf{x})}, e^{-i\varphi(\mathbf{x})})$. This gauge invariance is broken in (3), which means that strictly speaking $W_{\mathbf{xy}}$ must be zero (Elitzur's theorem[11]). The apparent contradiction of taking $W_{\mathbf{xy}} \neq 0$ in the calculations has been resolved in Ref. 12 in the context of lattice-gauge theories.

As stated above, our interest is mainly focused on spiral phases, i.e., stable magnetic structures with a uniform twist about some arbitrary axis **n**. For these structures, in the classical (large-S) limit, $A_{\mathbf{xy}} \sim S\sin\frac{\mathbf{Q}\cdot(\mathbf{y}-\mathbf{x})}{2}$ and $B_{\mathbf{xy}} \sim S\cos\frac{\mathbf{Q}\cdot(\mathbf{y}-\mathbf{x})}{2}$. Then, for finite systems the order parameters satisfy periodic or antiperiodic boundary conditions depending on whether $\frac{\mathbf{Q}}{2}$ is a normal mode of the lattice or not. Consequently, one must Fourier-transform Bose operators as $a_{\mathbf{x}\sigma} = \frac{1}{N}\sum_{\mathbf{k}} a_{\mathbf{k}\sigma}e^{i(\mathbf{k}-\sigma\frac{\mathbf{Q}}{2})\cdot\mathbf{x}}$, where $\sigma=\pm$, the **k**'s are the normal modes corresponding to periodic boundary conditions, and **Q** has to be found by minimizing the energy. In momentum space the Hartree-Fock Hamiltonian can be diagonalized by a standard Bogoliubov transformation, giving the quasiparticle dispersion relation $\omega_{\mathbf{q}} = \sqrt{[\gamma_B(\mathbf{q})-\lambda]^2-\gamma_A^2(\mathbf{q})}$ and ground-state energy $E_{\rm HF} = \frac{1}{2}\sum_{\mathbf{q}}\omega_{\mathbf{q}} + (S+\frac{1}{2})\lambda N$. We defined $\mathbf{q}=\mathbf{k}-\frac{\mathbf{Q}}{2}$,

$$\gamma_A(\mathbf{q}) = \frac{i}{2}\sum_{\mathbf{x}} J(\mathbf{x})A(\mathbf{x})e^{-i\mathbf{q}\cdot\mathbf{x}},$$

$$\gamma_B(\mathbf{q}) = \frac{1}{2}\sum_{\mathbf{x}} J(\mathbf{x})B(\mathbf{x})e^{-i\mathbf{q}\cdot\mathbf{x}}$$

and λ is the Lagrange multiplier that enforces (on average) the constraint condition on the number of bosons per site. Consistency equations require

$$A(\mathbf{x}) = \frac{1}{2N}\sum_{\mathbf{q}}\frac{\gamma_A(\mathbf{q})}{\omega_{\mathbf{q}}}\sin(\mathbf{q}\cdot\mathbf{x}) \ ,$$
$$B(\mathbf{x}) = \frac{1}{2N}\sum_{\mathbf{q}}\frac{\gamma_B(\mathbf{q})-\lambda}{\omega_{\mathbf{q}}}\cos(\mathbf{q}\cdot\mathbf{x}) \quad (4)$$

while the Lagrange multiplier forces

$$\frac{1}{2N}\sum_{\mathbf{q}}\frac{\gamma_B(\mathbf{q})-\lambda}{\omega_{\mathbf{q}}} = S+\frac{1}{2}. \quad (5)$$

Let us pause at this point to discuss the differences between our calculations and those of recent works using the Schwinger-boson representation.[8–10] First, we have not referred spin operators to a twisted coordinate system with its z axis pointing at every site in the preferred direction of the local spin. This is only a matter of taste, but using a single (global) quantization axis helps in keeping the simplicity of the calculations. Secondly, we made no use of identities generated by means of the exact (operator) form of the constraint in order to simplify the Hamiltonian. We avoid their use since they are largely violated when the boson-number restriction is taken only on average. Actually this is the origin of the additional factor 2 obtained by Arovas and Auerbach[10] in the zero-point energies of the $S = \frac{1}{2}$ nearest-neighbor Heisenberg model. Since for the antiferromagnet $B=0, A\simeq 0.579$, according to (3) we found a ground-state energy $E_{\rm HF}/2N = -A^2 \simeq -0.335$. Instead, by using the identity : $\hat{B}^{\dagger}_{\mathbf{xy}}\hat{B}_{\mathbf{xy}}$: $+\hat{A}^{\dagger}_{\mathbf{xy}}\hat{A}_{\mathbf{xy}} \equiv S^2$, these authors obtained $E'_{\rm HF}/2N = S^2 - 2A^2 \simeq -0.420$. These values should be compared with the quantum Monte Carlo result[2] $E_{\rm MC}/2N \simeq -0.335$. Notice that, after removing the classical energy $-S^2$ from both results, what remains in the Arovas-Auerbach case is exactly *twice* our value for the zero-point energies.

The third difference, and the most important one, concerns our allowing of nonvanishing values for $\langle\mathbf{S}'_{\mathbf{x}}\wedge\mathbf{S}'_{\mathbf{y}}\rangle$ in the spiral phase, which is related to the parity-breaking pairing of bosons (here the prime means that spin operators are referred to the local quantization axis mentioned above). In Ref. 8, the condition $\langle\mathbf{S}'_{\mathbf{x}}\wedge\mathbf{S}'_{\mathbf{y}}\rangle = 0$ is explicitly introduced into the theory as a way of determining a privileged twisted reference system. This was interpreted as a simple gauge-fixing device, with the gauge invariance being associated to the independence of physics from the referential. Actually, this is a strong requirement which affects the results in a quantitative and even qualitative way. In order to show this we have evaluated (3) for a 20-site lattice with and without such a condition, and the results were compared with those of numerical studies of the same model.[6] As can be seen in Fig. 1, when the condition is used the energies of the spiral phases are much higher than the exact values. Moreover, it can be shown that they are never lower than those corresponding to the Néel and collinear phases. (For collinear magnets one has $\langle\mathbf{S}'_{\mathbf{x}}\wedge\mathbf{S}'_{\mathbf{y}}\rangle = 0$ automatically, so that, modulo the use of

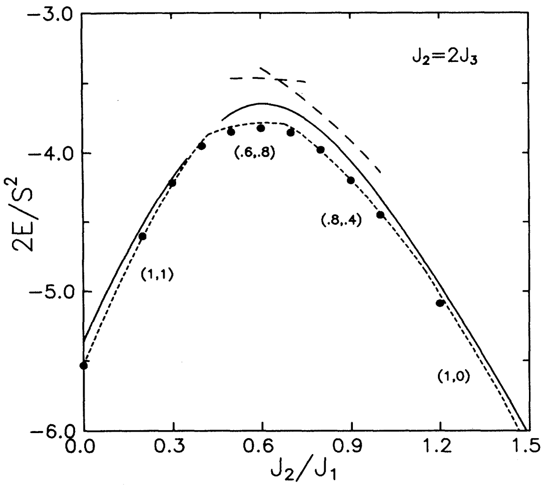

FIG. 1. Ground-state energy per bond for $S = \frac{1}{2}$. The small dashed line is our result for the 20-site lattice; the long dashed lines are the energies of the spiral phases when the gauge-fixing condition of Ref. 8 is used. Solid points are exact numerical values from Ref. 6. The labels (a,b) correspond to the $\frac{\mathbf{Q}}{\pi}$ wave vectors which minimize the energy. The solid line is our prediction for the infinite lattice.

the above mentioned identities, our results and those of Ref. 8 do not differ.) In fact, introducing this condition is equivalent to ignoring terms with an odd number of operators in the standard (large-S) spin-wave approach to helimagnets, which produces gaps at $\mathbf{k} = \pm\mathbf{Q}$, therefore losing Goldstone modes.[13] Their recovery involves consideration of cubic spin-wave interactions that lead to spin-wave binding. On the contrary, our calculations keep the correct zero-mode structure, producing only gaps for the phason zero modes.[14] This can be seen from the fact that for $N \to \infty$ the chemical potential for bosons sticks to the value $\lambda = \gamma_B(\frac{\mathbf{Q}}{2}) + \gamma_A(\frac{\mathbf{Q}}{2})$, which leads to $\omega(\frac{\mathbf{Q}}{2}) = \omega(-\frac{\mathbf{Q}}{2}) = 0$. Since the Bogoliubov quasiparticles have dispersion relations $\epsilon_{\mathbf{k},\sigma} = \omega(\mathbf{k}-\sigma\frac{\mathbf{Q}}{2})$, we have gapless modes at $\mathbf{k} = \mathbf{0}, \pm\mathbf{Q}$. Notice that we pay a price for this: For $S \to \infty$ we do not recover the semiclassical magnon spectrum of a helimagnet.[15] We stress, however, that the excitations in the Schwinger-boson approach *are not* the conventional magnons. The Schwinger-boson Hamiltonian is quartic in Bose operators, so that magnon-magnon interactions are incorporated into the theory already at the saddle-point order. The excitations are built upon this interacting saddle-point background, which, as shown numerically below, seems to be a very good starting point for perturbative calculations in the strong quantum regime. Gaussian and higher-order fluctuations above the saddle point should become important for $S \to \infty$, restoring the agreement with semiclassical results. Finally, we would like to stress an additional feature of our approach: For $J_3 = 0$ the results obtained are exactly the same as predicted by Takahashi's modified spin-wave theory,[16] which is known to reproduce accurately exact results for the J_1-J_2 model.[17]

Numerical evaluation of Eqs. (4) and (5) involves finding the physical roots of 12 coupled nonlinear equations for the order parameters $A(\mathbf{x}), B(\mathbf{x})$, plus the additional constraint condition which determines λ. On a finite lattice this has to be performed for several choices of the mode $\mathbf{Q}$, in order to find the one which minimizes the energy. For the infinite lattice the constraint equation decouples and only determines the magnetization,[18] while one has to add an equation for the (quasicontinuous) variable Q. By means of the chain rule for derivatives it is easy to show that such an equation is $\partial\lambda/\partial Q = 0$. In the particular case $J_2 = 2J_3$, $S = \frac{1}{2}$, we have at our disposal numerical results[6] on finite lattices to compare with. Figure 1 shows a remarkable agreement between our prediction for the ground-state energy of a 20-site lattice and the corresponding exact values. In the same figure we have plotted the result for the infinite lattice, for which quantum fluctuations select the (π, Q) phase as the stable one. Notice also the missing segment for $0.38 \lesssim \frac{J_2}{J_1} \lesssim 0.47$. In this region of parameter space no solution of the proposed spiral form was found, which is better understood by looking at Fig. 2. There we plot $M(\mathbf{Q})$, the effective length of the rotating vector in the spiral phase [for $\mathbf{Q} = (\pi,\pi)$ it corresponds to the staggered magnetization in the Néel phase]. These values can be obtained by straightforward generalization of the calculations in Ref. 18, and are related to the long distance behavior of the spin-spin correlation function by $\lim_{|\mathbf{x}-\mathbf{y}|\to\infty}\langle \mathbf{S_x}\cdot\mathbf{S_y}\rangle \approx M^2(\mathbf{Q})\cos\mathbf{Q}\cdot(\mathbf{x}-\mathbf{y})$. As can be seen, for $S = \frac{1}{2}$ both Néel and spiral orders are melted by quantum fluctuations, leaving a window in the above mentioned region where no obvious structure is present. Our theory predicts a simple disordered phase with a gap, though other more interesting possibilities have been suggested in the literature (in the connection with superconductivity this phase should correspond to the sought spin-liquid phase). It is clear, however, that this approach predicts no intermediate spin-nematic phases as proposed in Ref. 9. Our ground-state wave function is

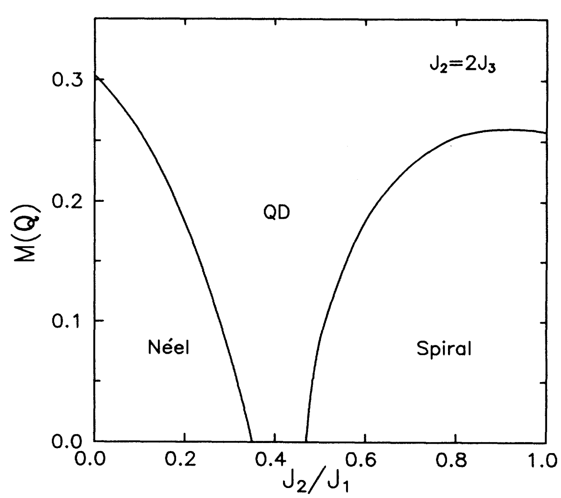

FIG. 2. Staggered magnetization per site in the Néel phase and effective length of the rotating vector in the spiral phase for $S = \frac{1}{2}$.

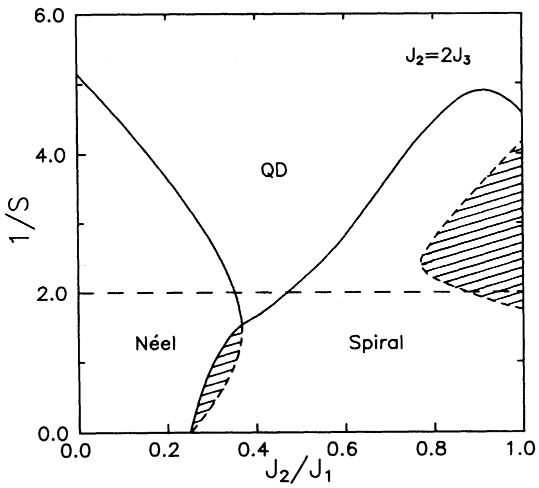

FIG. 3. Phase diagram showing lines of stability (solid) and metastability (dashed) for the different phases. Hatched areas are metastability regions for antiferromagnetic and collinear orders.

an isotropic singlet, with long-range magnetic order appearing as a Bose condensation phenomenon. When the local moment vanishes, the condensate disappears and no long-range tensor order can be sustained.

In Fig. 3 we show the stability regions of the Néel and spiral phases for general spin S. Hatched areas are metastability regions for Néel and collinear orders (for $J_2 = 2J_3 < \infty$ the collinear order is neither classically nor quantum stable). For physical spins $S \geq 1$ the spiral phase goes continuously to an antiferromagnetic order, but, quite remarkably, for $S = \frac{1}{2}$ there is a window between both phases where the ground state is disordered, in accordance with Figs. 1 and 2. We stress here that this result questions the reliability of semiclassical expansions based on the large-S limit,[8,19] which predict a narrow disordered phase for finite but arbitrarily large S. However, the inclusion of random-phase-approximation fluctuations might modify this part of the phase diagram, bringing it in line with spin-wave and nonlinear σ-model results. The observed window shrinks by reducing J_3, and finally closes at $J_{3\,\mathrm{min}} \simeq 0.038J_1$. For $J_3 = 0$ there is a large overlap of the (meta)stability regions of Néel and collinear orders, with a first-order transition between them, and no disordered phase even for $S = \frac{1}{2}$.[16] However the small value of $J_{3\,\mathrm{min}}$ lends some support to the suggestion that dynamical generation of J_3 could produce a disordered phase for the J_1-J_2 model.[20]

In closing, we mention that other physical quantities like the spin-spin correlation functions and structure factor have also been considered. For the structure factor we found again very good agreement with exact values on the 20-site lattice. These results, as well as a study of the geometry-frustrated triangular lattice, will be presented elsewhere.

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