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LETTER TO THE EDITOR

A Schwinger boson approach to Heisenberg antiferromagnets on a triangular lattice

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Abstract. The ground-state properties of generalized $S = \frac{1}{2}$ Heisenberg antiferromagnets on a triangular lattice are studied by means of the Schwinger boson approach. The generalizations considered include second-neighbour interactions and nearest-neighbour couplings breaking the rotational symmetry of the lattice. Unlike in previous work using the same representation of spin operators, good quantitative agreement with exact numerical results and with other approximate methods is obtained. The results point to the existence of magnetic long-range order, with a local magnetization $M = 0.275$ for the standard nearest-neighbour model.

The ground-state structure of the triangular-lattice Heisenberg *antiferromagnet* (TLHA) has been debatable for a long time [1]. Recently, the hunt for exotic spin-liquid states in connection with magnetic mechanisms of high-T_c superconductivity [2] has generated a new surge of interest on this problem. However, there is now a steadily growing conviction, with support from a variety of methods [3–5], that the model displays the conventional three-sublattice Néel order in its ground state, even in the strong quantum limit $S = \frac{1}{2}$.

We have recently shown [6] how to apply the Schwinger boson technique to general helimagnets, studying the J_1–J_2–J_3 model on the square lattice as an example. The beauty of this approach resides in its capability of describing different ground-state structures in an unified formalism, without biasing the calculation in an obvious way toward the existence or non-existence of magnetic long-range order. Moreover, by comparison with exact results on finite lattices the method proved itself to be quantitatively accurate beyond previous expectations.

In view of the above, and since classically the TLHA is a commensurate helimagnet, it seems worthwhile to reconsider this model by means of the Schwinger boson approach as developed in [6]. We stress here that this representation of spin operators has already been used in studies of the TLHA [7, 8], although without quantitative success for the reasons given in our previous work, and further discussed below. In contrast, here we will show, again by comparison with exact results on finite lattices, that the Schwinger boson approach is capable of producing remarkable good predictions for the energy, and also magnetization values in rough agreement with results obtained by other approximate methods [3, 4].

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Our interest will be focused on ground-state properties of generalized $S = \frac{1}{2}$ Heisenberg models,

$$H = \frac{1}{2}\sum_{xy}^{N} J_{xy} \boldsymbol{S}_x \cdot \boldsymbol{S}_y \tag{1}$$

with arbitrary couplings J_{xy} between sites x, y of a triangular lattice. The generalizations considered include second-neighbour interactions and nearest-neighbour couplings breaking the rotational symmetry of the lattice. The motivations for studying these models are discussed below. We replace spin operators in terms of the Schwinger representation by $\boldsymbol{S}_x = \frac{1}{2}\boldsymbol{a}_x{}^{\dagger}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{a}_x$, where the bosonic spinors $\boldsymbol{a}_x = (a_{x\uparrow}, a_{x\downarrow})$ must satisfy the local constraint $\boldsymbol{a}_x{}^{\dagger}\cdot\boldsymbol{a}_x = 2S$ in order to have a faithful spin S representation of the algebra. In this way Hamiltonian (1) becomes quartic in Bose operators, requiring some kind of approximation to be solved. We have shown in [6] that a natural, rotationally-invariant Hartree–Fock decomposition of (1) is given by:

$$(\boldsymbol{S}_x\cdot\boldsymbol{S}_y)_{\mathrm{HF}} = (B_{xy}\hat{B}^{\dagger}_{xy} - A_{xy}\hat{A}^{\dagger}_{xy} + \mathrm{HC}) - \langle(\boldsymbol{S}_x\cdot\boldsymbol{S}_y)_{\mathrm{HF}}\rangle \tag{2}$$

where the operators $\hat{A}^{\dagger}_{xy} = \frac{1}{2}\sum_{\sigma}\sigma a^{\dagger}_{x\sigma}a^{\dagger}_{y-\sigma}$ and $\hat{B}^{\dagger}_{xy} = \frac{1}{2}\sum_{\sigma}a^{\dagger}_{x\sigma}a_{y\sigma}$. The variational parameters A_{xy}, B_{xy} satisfy $A_{xy} = \langle\hat{A}_{xy}\rangle$ and $B_{xy} = \langle\hat{B}_{xy}\rangle$ to achieve full autoconsistency. Then, from the mean value

$$\langle(\boldsymbol{S}_x\cdot\boldsymbol{S}_y)_{\mathrm{HF}}\rangle = |B_{xy}|^2 - |A_{xy}|^2$$

one can see that (the squared modulus of) A_{xy} and B_{xy} represent respectively the antiferromagnetic and ferromagnetic correlations between spins at sites x and y. In the following we will take these parameters to be real, which means that we are not considering flux phases. Since the formalism is completely invariant under rotations, by a judicious choice of A_{xy} and B_{xy} we can in principle describe any sort of (ordered or disordered) non-magnetic structure in the ground state of (1). The possibility of having magnetic long-range order is incorporated in the theory by allowing the Schwinger bosons to condense [7]. As stated above, in this way we have a unified formalism, capable of describing any possible ground state. Notice also that in this approach there is no need to partition the lattice into different sublattices nor to perform any rotation of spin operators to a local reference axis [8], as is customarily done in standard spin-wave theory. The advantages of using simultaneously the ferro and antiferro channels in decoupling (2) over previous approaches in the literature [7] have been discussed in [6], where it was shown that in this way one obtains very good qualitative and quantitative agreement with exact numerical results.

The Hartree–Fock Hamiltonian (1), (2) can be diagonalized by going to momentum space and performing a standard Bogoliubov transformation. If the system has incommensurate (spiral) magnetic order, for $S \to \infty$ the parameters $A_{xy} \sim S\sin(\boldsymbol{Q}/2)\cdot(\boldsymbol{y}-\boldsymbol{x})$ and $B_{xy} \sim S\cos(\boldsymbol{Q}/2)\cdot(\boldsymbol{y}-\boldsymbol{x})$, where $\boldsymbol{Q}$ is the spiral wave-vector. Then, in order to treat this case it is convenient to perform a Fourier transform on Bose operators as $a_{x\sigma} = (1/N)\sum_{q} a_{q\sigma}\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{x}}$, where $\boldsymbol{q} = \boldsymbol{k} - (\boldsymbol{Q}/2)$, $\boldsymbol{k}$ represents the normal modes corresponding to periodic boundary conditions, and $\boldsymbol{Q}$ has to be found by minimizing the energy. Carrying out this program one gets the quasiparticle dispersion relation $\omega_q = \sqrt{(\gamma_B(q) - \lambda)^2 - \gamma_A^2(q)}$ and ground-state energy $E_{\rm HF} = \frac{1}{2}\sum_q \omega_q + (S + \frac{1}{2})\lambda N$. We have defined

$$\gamma_A(q) = \frac{\mathrm{i}}{2}\sum_x J(x)A(x)\mathrm{e}^{-\mathrm{i}q\cdot x} \qquad \gamma_B(q) = \frac{1}{2}\sum_x J(x)B(x)\mathrm{e}^{-\mathrm{i}q\cdot x}$$

and λ is the Lagrange multiplier that enforces (on average) the constraint on the number of bosons *per site*:

$$\frac{1}{2N}\sum_q \frac{\gamma_B(q) - \lambda}{\omega_q} = S + \frac{1}{2}. \tag{3}$$

The consistency conditions are given by

$$A(x) = \frac{1}{2N}\sum_q \frac{\gamma_A(q)}{\omega_q}\sin(q\cdot x) \qquad B(x) = \frac{1}{2N}\sum_q \frac{\gamma_B(q) - \lambda}{\omega_q}\cos(q\cdot x). \tag{4}$$

The set of equations (3), (4) determine λ, A_{xy} and B_{xy}, and the longer the range of J_{xy} the larger is the number of parameters A_{xy}, B_{xy} to be determined. For finite systems these equations have to be solved for values of Q chosen from the normal modes of the lattice (because of the periodic boundary conditions), in order to find the one which minimizes the energy. For infinite lattices, and in the case where one has long-range magnetic order, equation (3) decouples from (4) and only determines the magnetization originated in the Bose condensation at the magnetic wavevector Q [9]. In such a case λ keeps to the value $\gamma_B(Q/2) + \gamma_A(Q/2)$, which produces the correct zero-mode (Goldstone) structure at $k = 0, Q$. Furthermore, to determine the (quasi)continuous variable Q one adds the equations $\partial E_{\rm HF}/\partial Q = 0$, which, by means of the chain rule for derivatives, can be shown to be equivalent to $\partial\lambda/\partial Q = 0$. In passing we note that since classically $\lambda \sim J(Q) = \sum_x J(x)\mathrm{e}^{-\mathrm{i}Q\cdot x}$, this last equation is the quantum equivalent of the classical condition which determines Q in the large-S spin-wave theory. For non-collinear magnets the non-zero value of the antisymmetric order parameter A_{xy} implies a parity-breaking pairing of bosons [6], whose consequences can be related to those connected to the inclusion of cubic (in Bose operators) terms in the Hamiltonian of the standard spin-wave approach to helimagnets [10].

We have numerically solved equations (3) and (4) for J_{xy} coupling a site with its first (J_1) and second (J_2) neighbours. Classically [11], the second-neighbour interaction allows one to move the magnetic wave-vector from $Q = (\frac{4\pi}{3}, 0)$ for $0 \leqslant J_2 < \frac{1}{8}J_1$ (corresponding to the three-sublattice Néel order, or commensurate spiral order), to $Q = (0, \frac{2\pi}{\sqrt{3}})$ for $\frac{1}{8}J_1 < J_2 \leqslant J_1$ (which produces a collinear spin arrangement, antiferromagnetic along two sides of a triangle and ferromagnetic along the third one). For larger values of J_2 the system becomes an incommensurate helimagnet, with Q moving continuously from $Q = (0, \frac{2\pi}{\sqrt{3}})$ to $Q = (0, \frac{4\pi}{3\sqrt{3}})$.

In figure 1 we plot our result for the energy *per bond* of a 12-site lattice as a function of the ratio J_2/J_1 for spin $S = \frac{1}{2}$. One can see that for this finite lattice there is a remarkable agreement with exact numerical results taken from [11]. In the same figure we show the corresponding result for the infinite lattice. In particular for the nearest-neighbour model we obtained $E = -0.1899$, a value which should be compared with $E_{sc} = -0.183 \pm 0.003$, coming from numerical diagonalization of small clusters [12], $E_{var} \leqslant -0.179$, obtained by variational methods [3], and $E_{sw} = -0.180$ and -0.182, predicted by different versions [4,5] of the spin-wave theory. In contrast to the findings for the square lattice with further-neighbour interactions [6], there seems to be no non-classical (non-magnetic) phase in any region of coupling space. In figure 2 we plot the local magnetization $M(Q)$ corresponding to the different phases, as obtained from the long-distance behaviour of correlation functions: $\lim_{|x-y|\to\infty}\langle S_x S_y\rangle \approx M^2(Q)\cos Q\cdot(x-y)$. (Actually $M(Q)$ can be obtained from (3) by straightforward generalization of the considerations in [9].) For $J_2 = 0$ we obtained $M = 0.275$, a value strongly reduced from its classical maximum by the quantum fluctuations, although not as low as predicted by standard spin-wave calculations [4] ($M_{sw} = 0.239$). For the sake of comparison, the variational result for the energy in [3] was obtained with a sublattice magnetization $M_{var} = 0.34$. The value we obtained is not too far from the corresponding result for the square lattice $M = 0.303$, despite the lack of frustration in this last case. We believe that the inherent frustration of the triangular lattice is somehow compensated by its large coordination number, which helps in sustaining magnetic order.

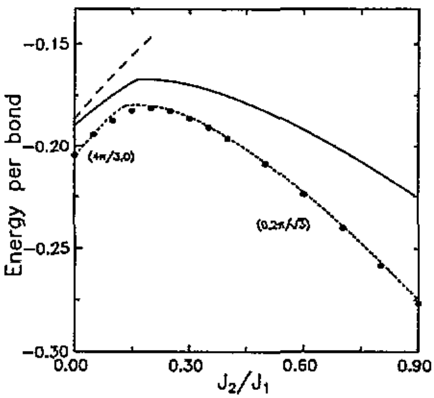

Figure 1. Energy *per bond* for the TLHA with first-(J_1) and second-(J_2) neighbour interactions. ···· is our prediction for a 12-site lattice. Points are exact numerical results from [11]. – – – is the corresponding result for the energy in the Néel phase as obtained from the theory developed in [8]. —— is our prediction for the infinite lattice.

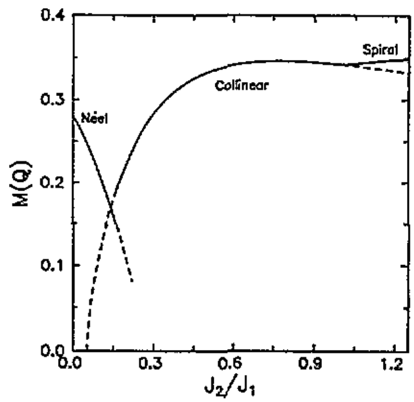

Figure 2. Local magnetization in the different phases. The full curves indicate the effective stability regions of each phase. There is a first-order transition from Néel to collinear order at $J_2/J_1 \simeq 0.16$, and a continuous transition from this collinear order to an incommensurate spiral phase at $J_2/J_1 \simeq 0.95$.

In order to compare more closely with the situation for the square lattice, we have also considered the nearest-neighbour model with the coupling along one side of a basic triangle (J_1') different from the value on the other two sides. In this way the triangular lattice can be considered a distorted square lattice with second-neighbour interaction along one of its diagonals, a model which classically displays a continuous deformation from Néel order ($Q = (\pi, \frac{\pi}{\sqrt{3}})$) for $J_1' = 0$, to commensurate spiral order ($Q = (\frac{4}{3}\pi, 0)$) for $J_1' = J_1$. The results obtained are plotted in figure 3. As can be seen, switching on the frustrating interaction J_1' decreases the two-sublattice magnetization of the distorted square lattice. When J_1' reaches a value near 0.6, the system prefers to start rotating the local magnetization instead of reducing it further, going continuously into a spiral phase. At $J_1' = J_1$ the wavevector $\boldsymbol{Q}$ accomodates perfectly to the triangular lattice, and the system displays the three-sublattice Néel order with sublattice magnetizations pointing at 120° to each other (commensurate spiral). Since the square lattice is believed to be Néel ordered [13], the smooth behaviour between the extreme values of J_1' supports our conviction about the existence of magnetic long-range order in the TLHA.

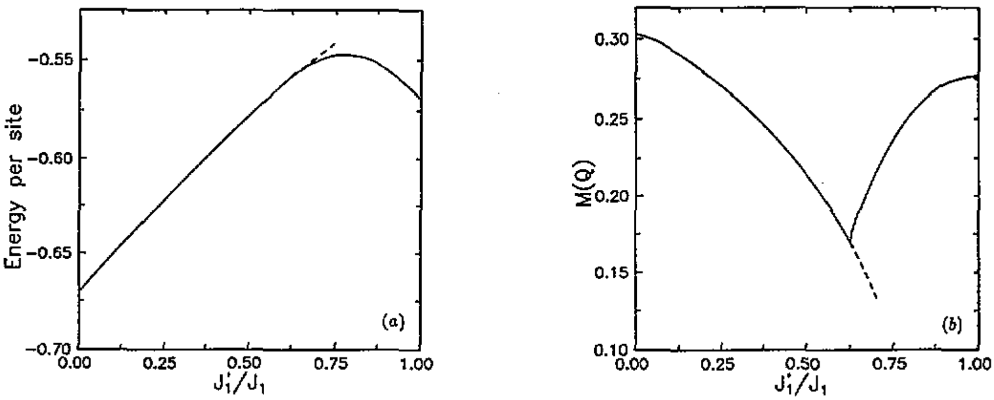

Figure 3. (*a*) Energy *per site*, and (*b*) local magnetization, for the nearest-neighbour TLHA with couplings breaking the rotational symmetry of the lattice. For $J_1' = 0$ the system reduces to a Heisenberg model on a distorted square lattice, while for $J_1' = J_1$ one regains the symmetry of the triangular lattice. The broken curves represent the behaviour of energy and magnetization when the spiral wavevector is locked at $\boldsymbol{Q} = (\pi, \frac{\pi}{\sqrt{3}})$, corresponding to the distorted square lattice.

A few final comments in connection with related works in the literature on the TLHA. Yoshioka and Miyazaki [7] have recently considered the nearest-neighbour TLHA using a similar Schwinger boson approach. Leaving aside minor details, the main difference between their work and ours comes from their introduction in the Hamiltonian of a term which vanishes because of the exact (operator) form of the constraint. In this way they simplify the Hamiltonian, which becomes a function only of the RVB-like parameter A_{xy}. However, since the restriction on the number of bosons *per site* is imposed on average, this term gives an incorrect, sizeable contribution to the ground-state energy. Ritchey and Coleman [8] have also applied the Schwinger boson approach to the TLHA. They introduce into the theory the arbitrary condition $\langle S_x' \wedge S_y' \rangle = 0$, as a way of determining a privileged twisted reference frame (the prime on spin operators means that they are referred to the local quantization axis). This condition is satisfied automatically by collinear magnets. However, in the spiral phase the vector product between spin operators must be allowed to be different from zero in order to have quantitative agreement with exact results (see figure 1).

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