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SU(N) Schwinger bosons and nematic phases in the bilinear–biquadratic $S=1$ triangular lattice antiferromagnet with third-nearest neighbor interactions

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ABSTRACT

I present in details the SU(N) Schwinger boson formalism, also known as flavor wave theory, that has been used several times in the literature. I use the method to study the ferroquadrupolar phase of a quantum biquadratic Heisenberg model with spin $S=1$ on the triangular lattice with third-nearest-neighbor interactions. Results for the phase diagram at zero temperature and the static and dynamical quadrupolar structure factors are presented. In principle, the results could be applied to $NiGa_2S_4$.

1. Introduction

Magnetic moments are expected to order for temperatures below a critical temperature. In most magnetic compounds these magnetic moments form a long-range ordered ferromagnetic or antiferromagnetic structure, depending on the nature and strength of the interactions of the spins. However, in some "frustrated" magnetic models, the low temperature phase has no long-range magnetic order. Instead, they develop some exotic states such as nematic order or spin liquid states [1].

As pointed out by Stoudenmire et al. [2], the triangular lattice antiferromagnet is of great interest because of its potential to exhibit exotic phases as a result of frustration and because it is the underlying lattice of many real materials.

The aim of this paper is to study the ferroquadrupolar phase of the biquadratic $S=1$ triangular lattice antiferromagnet with third-neighbor interactions, because, as Stoudenmire et al. [2] have shown, using Monte Carlo simulations, this model presents a ferroquadrupolar phase for certain values of the couplings. But before doing that I will present in full details the theoretical formalism adequate to treat nematic phases that has been used in the literature.

2. Schwinger boson formalism

One very useful analytical technique to study magnetic systems is the SU(2) Schwinger boson (SB) formalism [3]. In this representation two bosons operators a and b are introduced such that the spin components are written as

$$S^+ = a^+ b, \qquad S^- = b^+ a, \qquad S^z = \tfrac{1}{2}(a^+ a - b^+ b), \tag{1}$$

with the constraint

$$a^+ a + b^+ b = 2S. \tag{2}$$

The boson occupation $2S$ determines the representation of SU(2). The spin states are given by

$$|S, m\rangle = \frac{(a^+)^{S+m}(b^+)^{S-m}}{\sqrt{(S+m)!(S-m)!}}|v\rangle, \tag{3}$$

where $|S, m\rangle$ labels the S^2 and S^z eigenvalues and $|v\rangle$ is the Schwinger bosons vacuum. For $S=½$ we have

$$|+\rangle = a^+|v\rangle, \qquad |-\rangle = b^+|v\rangle. \tag{4}$$

If one has an ordered state one can condensate one of the bosons. For instance, if in Eq. (4) the ground state is the $|+\rangle$ state, one can condensate the a boson and take, using the constraint (2),

$$a, a^+ \to \sqrt{2S - b^+ b}. \tag{5}$$

This leads to the well known Holstein–Primakoff representation (HP), which single out the S^z direction, which defines their vacuum. The SB are useful to study the symmetric phases, while

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HP are convenient for the magnetically ordered broken symmetry phases.

We notice that in a truly disordered symmetric phase we have

$$<(S^z)^2> = <(S^x)^2> = <(S^y)^2> = \frac{S(S+1)}{3}. \tag{6}$$

To study the symmetric phase, for instance a two dimensional ferro or antiferromagnet at $T>0$, we define a bond operator [3]

$$F_{ij} \equiv a_i^+ a_j + b_i^+ b_j, \tag{7}$$

write the Hamiltonian in terms of F_{ij} and then decouple the four operator terms in a mean field approximation. However, if we take $T\to 0$, in order to satisfy a constraint equation, we must impose a macroscopic occupation at $\boldsymbol{k}=0$ (Bose condensation) and could obtain an ordered state at $T=0$ (as happens in the two dimensional Heisenberg model, for example). Thus the SB mean-field theory is more general than the HP approximation because the HP formalism starts from a prescribed ferro- or antiferro- order, while the SB has no bias on the order or disorder of the ground state in advance. The details are given in Ref. [3], and here I just want to note that the SB formalism describes magnetically disordered and ordered phase.

For spins $S>½$, several types of ordering, besides the well known dipolar ordering, such as nematic, octupolar or any higher multipolar ordering (where $<\boldsymbol{S}>=0$) are also possible. This is, multipolar ordering of the type $<S_{\alpha_1} S_{\alpha_2} \ldots S_{\alpha_n}>$ with $n=1$ (dipolar), $n=2$ (quadrupolar), $n=3$ (octupolar), etc., up to $n=2S$ can exist [4,5].

In these cases the ground state orderings do not have a classical counterpart at $T=0$ (states with $<\boldsymbol{S}_r>=0$ and finite higher multipolar orders are a purely quantum phenomenon [6]).

In a system with nematic order one has $<\boldsymbol{S}_r>=0$, but the order can manifest, for instance, as

$$<(S^z)^2> \neq \frac{S(S+1)}{3}. \tag{8}$$

As pointed out by Wang and Xu [7], in the SU(2) formalism there is no boson which condensation would lead to this order. This is, it is impossible to describe the spin nematic phase in this formulation as a boson condensate, because a nonzero condensate $<a>$ or $<b>$ necessarily produces a nonzero magnetic dipole moment. Besides that, Muniz et al. [4] have shown that for systems that have nematic order, the standard spin wave theory (SWT) is not adequate, even to describe the ordered phases. This problem was first considered by Papanicolaou [8], who considered the case of spin $S=1$. In this case, besides the three components of spin $S_r^\alpha(\alpha=x,y,z)$, one has the following operators (quadrupolar order parameters) that describe quadrupolar order:

$$Q = \begin{pmatrix} Q_r^{(0)} \\ Q_r^{(2)} \\ Q_r^{xy} \\ Q_r^{yz} \\ Q_r^{zx} \end{pmatrix} = \begin{pmatrix} (S_r^z)^2 - 2/3 \\ (S_r^x)^2 - (S_r^y)^2 \\ S_r^x S_r^y + S_r^y S_r^x \\ S_r^y S_r^z + S_r^z S_r^y \\ S_r^z S_r^x + S_r^x S_r^z \end{pmatrix}. \tag{9}$$

As it is well known, the three components of S_r^α (for any value of the spin S) obey the standard commutation rule and are therefore generators of the SU(2) representation. However if we want to take into account ordering described by the operators (9), we should enlarge the symmetry group. We have now 8 parameters (S_r^α,Q), which are generators of the SU(3) representation.

The same is true for higher values of spins. For $S=3/2$, one has octupolar order and thus to treat this order we should use a SU (4) representation [5].

The generators of SU(3) can be expressed in terms of three bosons operators (or fermions operators) a_n that obey the commutation relations [9,10]:

$$[a_n, a_m^+] = \delta_{nm}, [a_n, a_m] = 0, [a_n^+, a_m^+] = 0. \tag{10}$$

Defining the operator [9]

$$Q_\alpha = \frac{1}{2}\hat{a}^+ \lambda_\alpha \hat{a}, \quad \alpha = 1, 2, \ldots 8 \tag{11}$$

where $\hat{a} = (a_1^+, a_2^+, a_3^+)$ and λ_α are the Gell-Mann matrices that satisfy the commutation relations

$$[\lambda_\alpha, \lambda_\beta] = 2if_{\alpha\beta\gamma}\lambda_\gamma \tag{12}$$

where $f_{\alpha\beta\gamma}$ are the structure constants [9] we can show that

$$[Q_\alpha, Q_\beta] = if_{\alpha\beta\gamma}Q_\gamma, \tag{13}$$

this is, the operators Q_α obey the SU(3) Lie-algebra.

It has been shown that spin-1 models with single ion anisotropy [11–13], or biquadratic interactions [1,9,10] support $T=0$ nematic order, and models with spin-3/2 and cubic exchange term supports octupolar order [5]. Explicit magnetic anisotropy acts like a symmetry breaking field to the quadrupolar order parameter [2].

Papanicolaou [8] started by choosing the following basis

$$|x\rangle = i(|1\rangle - |-1\rangle)/\sqrt{2}, \qquad |y\rangle = (|1\rangle + |-1\rangle)/\sqrt{2}, \\ |z\rangle = -i|0\rangle, \tag{14}$$

where $|n\rangle$ are eigenstates of S^z. Next, one introduces a set of three boson operators t_α ($\alpha=x,y,z$) equivalent to the a's operators given in (10), defined by

$$t_x^+|v\rangle = |x\rangle, t_y^+|v\rangle = |y\rangle, t_z^+|v\rangle = |z\rangle, \tag{15}$$

where $|v\rangle$ is the vacuum state. We have the constraint

$$t_x^+ t_x + t_y^+ t_y + t_z^+ t_z = 1, \tag{16}$$

for single site occupancy on each site. In terms of the t operators we can write

$$S^\alpha = -i\varepsilon_{\alpha\beta\gamma} t_\beta^+ t_\gamma, \tag{17}$$

$$[S^\alpha, S^\beta] = i\varepsilon_{\alpha\beta\gamma} S^\gamma. \tag{18}$$

Writing the operators t's as a vector $\mathbf{t}=(t_x, t_y, t_z)^T$ we see that this representation has a U(1) gauge freedom $\mathbf{t}\to e^{i\theta}\mathbf{t}$ (and this explains the different notations used by different authors). In term of this operators Eq. (9) becomes

$$Q_n^{(0)} = \frac{1}{3}(t_{nx}^+ t_{nx} + t_{ny}^+ t_{ny} - 2t_{nz}^+ t_{nz}), \tag{19a}$$

$$Q_n^{(2)} = -(t_{nx}^+ t_{nx} - t_{ny}^+ t_{ny}), \tag{19b}$$

$$Q_n^{xy} = -(t_{nx}^+ t_{ny} + t_{ny}^+ t_{nx}), \tag{19c}$$

$$Q_n^{yz} = -(t_{ny}^+ t_{nz} + t_{nz}^+ t_{ny}), \tag{19d}$$

$$Q_n^{zx} = -(t_{nz}^+ t_{nx} + t_{nx}^+ t_{nz}). \tag{19e}$$

Finally we introduce another set of bosons operators

$$b_0^+ = \frac{1}{\sqrt{2}}(t_x^+ - it_y^+), \quad b_2^+ = -\frac{1}{\sqrt{2}}(t_x^+ + it_y^+), \quad b_1 = t_z, \tag{20}$$

and so