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Phase transitions of the frustrated bilayer spin one XY model

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ABSTRACT

In this paper we use the SU(3) Schwinger boson representation, followed by a mean field decoupling, to study the disordered phases of the bilayer spin one quantum XY antiferromagnet on a square lattice with next near neighbor and a single ion anisotropy. The phase diagram at zero temperature is obtained. The ratio $\eta = J_\perp/J_1$ between the interlayer $J_\perp$ to the intralayer near neighbor J_1 exchange interactions exhibits a quantum phase transition at a critical ratio $\eta_c = 21.725$ that separates the small- η Nèel phase from the large η quantum disordered paramagnet. The effect of next near neighbor interactions is discussed. The Neel phase is studied using a self consistent harmonic approximation that takes into account topological effects.

1. Introduction

An important focus of condensed matter physics is the study of strongly-correlated systems. In these systems, quantum fluctuations give rise to many competing and exotic new phases. In this context, for over a decade, there has been considerable interest in the study of disordered magnetic phases mainly related with the subject of spin liquids. Quantum spin liquids (QSL) are systems of interacting spins that have a disordered ground state where their spin arrangements are constantly in flux, much like the molecules of an ordinary liquid. QSLs are of great interest in their own right, but they may also serve as platforms for "topological quantum computing". The search for a quantum spin liquid has focused mainly on spin ½ two dimensional quantum antiferromagnet [1]. The best studied example is the J_1–J_2 Heisenberg model. For small $\eta = J_2/J_1$ the ground state is Neel ordered. It has been found [2] that the system undergoes a second order quantum phase transition at a certain $\eta = \eta_{1c}$ from the Neel to a quantum disordered phase that is believed to be a spin-liquid state. For η larger than a critical value η_{2c}, one has a collinear ordered state, where the neighboring spins align ferromagnetically along one axis of the square lattice and antiferromagnetically along the other. As there is as yet no direct experimental confirmation of QSL alternative explanations have been proposed for some QSL candidates. For instance, Chen et al. [3] have argued that the observed phenomenology in a spin one triangular lattice can be understood in terms of a conventional picture arising as a crossover due to the proximity of a quantum critical point between spin spirals favored by the frustrated exchange and a quantum paramagnetic phase, favored by a single ion anisotropy, having in mind that single ion anisotropy should be common in $S > ½$ antiferromagnets.

Now let us consider another mechanism, besides frustration, that leads to disorder. When two planes of the two dimensional Heisenberg antiferromagnet on a square lattice are coupled together, forming a bilayer, the interplane coupling initially stabilizes but when it is made strong enough the long-range antiferromagnetic Néel order is destroyed. For spin ½, it is believed that the disordered phase is a spin liquid state. The model has being studied using SU(2) Schwinger boson formalism [4,5], quantum Monte Carlo simulations [6], series expansions [7], spin wave theory [8], modified spin wave theory [9], and the bond operator mean field method [10,11]. One reason for the interest in this model is that the normal-state magnetic properties of superconductors $YBa_2Cu_3O_{6+x}$, containing the weakly coupled CuO_2 planes, may be due to its lying close to a quantum phase transition in the bilayered antiferromagnetic model [4,11].

As the understanding of spin ½ models advanced, a next step was to investigate systems with spin one on frustrated lattices [12]. They present a middle ground between the quantum S = ½ system and the classical model. Several ground state phases that are realized in spin one systems are not found in $S = ½$ models. This includes the quantum paramagnetic nematic phase that appears in the presence of a single-ion anisotropy. In the simplest case, with axial symmetry, the spin quadrupole tensor has the same mathematical form as the orientational order parameter of nematic liquid crystals. There is a preferred axis in space without a preferred direction along this axis. The nematic order is characterized by a non-zero spin quadrupole tensor $Q_{ij} \equiv < S_i^\alpha S_j^\beta + S_j^\beta S_i^\alpha >$ which deviates from isotropy.

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Although the effect of frustration, bilayer coupling and single ion anisotropy [12] has been well studied in the Heisenberg model, less attention has been dedicated to the XY model.

Here we consider the case of the spin one XY model with near and next near neighbor exchange interactions and single ion anisotropy on the square-lattice bilayer, described by the Hamiltonian

$$H = \sum_{<ij>}\sum_{l=1}^{2} J_1^{(l)}(S_{i,l}^x S_{j,l}^x + S_{i,l}^y S_{j,l}^y) + J_2 \sum_{<<ij>>}\sum_{l=1}^{2}(S_{i,l}^x S_{j,l}^x + S_{i,l}^y S_{j,l}^y) + J_\perp \sum_i (S_{i,1}^x S_{i,2}^x + S_{i,1}^y S_{i,2}^y) + D\sum_i (S_i^z)^2, \quad (1)$$

where i denotes the ith unit cell containing two spin one (associated to the two layers, l = 1,2, that we call A and B) and $J_1^{(1)}$ and $J_1^{(2)}$ are the near neighbor intralayer exchanges on lattice A and B respectively, J_2 is the next near neighbor intralayer exchange in each layer and $J_\perp$ is the interlayer exchange interaction. We will be interested mainly in the case $J_1^{(1)} = J_1^{(2)} \equiv J_1$, but we will present the general expressions which could be of interest to some readers. $J_1^{(2)} = 0$ corresponds to a square lattice spin system with a local impurity spin attached to each lattice, i.e. a Kondo necklace model with XY exchange interaction [13].

This model for spin ½, $J_1^{(1)} = J_1^{(2)} \equiv J_1, J_2 = 0$ and $D = 0$ was studied by Stoudemire et al. [14], using quantum Monte Carlo simulations. They have found that the model exhibits a quantum phase transition at a critical coupling ratio $\eta_c = J_\perp/J_1 = 5.46$, between a low η-phase with long-range transverse antiferromagnetic order to a large η magnetic disordered phase.

For large values of the anisotropy parameter D in Hamiltonian (1) the system is in a magnetically disordered phase. The anisotropy term forces each spin to be predominantly in the nonmagnetic state $|S_n^z = 0\rangle$ and there is a finite gap to spin excitations. Decreasing D, the energy gap decreases and goes to zero at a critical D_C, where a quantum phase transition to a ordered phase (depending on the values of the parameters η and α, where $\alpha = J_2/J_1$) takes place [15,16]. In the classical model with $D = 0$, the interlayer coupling $J_\perp$ does not introduce frustration and then does not affect the classical ground state. In the quantum case, as mentioned before, the Néel order disappears above a critical value of $J_\perp$ giving rise to a non-magnetic phase.

The outline of the paper is as follows: In Sec. II we introduce the SU(3) Schwinger boson formalism in a mean field approximation. In Sec. III we present results of the calculations using this technique. In Sec. IV we calculate the Kosterlitz-Thouless transition temperature for $D = 0$ using a self consistent harmonic approximation, and finally in Sec. IV we present our conclusions.

2. SU(3) Schwinger boson formalism

Papanicolaou [17] has shown that the standard spin wave theory is not appropriate to treat spin one Hamiltonians which present magnetically disordered phase such as the Hamiltonian with easy plane single ion anisotropy. To overcome this problem, he proposed the SU(3) Schwinger boson theory, which is a generalization of the SU(2) representation. This formalism has also been called flavor wave theory in the literature.

In the SU(3) Schwinger boson representation the spin operators are replaced by three species of bosons via the relation [15,16]

$$S^x = -i(t_y^+ t_z - t_z^+ t_y), \quad S^y = -i(t_z^+ t_x - t_x^+ t_z), \quad S^z = -i(t_x^+ t_y - t_y^+ t_x), \quad (2)$$

with the constraint

$$t_x^+ t_x + t_y^+ t_y + t_z^+ t_z = 1. \quad (3)$$

To study magnetically disordered phases it is convenient to introduce another two bosonic operators u^+ and d^+ given by [15]

$$u^+ = -\frac{1}{\sqrt{2}}\left(t_x^+ + it_y^+\right), \quad d^+ = \frac{1}{\sqrt{2}}\left(t_x^+ - it_y^+\right). \quad (4)$$

we have

$$|1\rangle = u^+|v\rangle, \quad |0\rangle = t_z^+|v\rangle, \quad |-1\rangle = d^+|v\rangle, \quad (5)$$

where $|v\rangle$ is the vacuum state and $|n\rangle$ are eigenstates of S^z. The constraint (3) can then be written as $u^+u + d^+d + t_z^+t_z = 1$. The spin operators are now given by

$$S^+ = \sqrt{2}(t_z^+ d + u^+ t_z), \quad S^- = \sqrt{2}(d^+ t_z + t_z^+ u), \quad S^z = u^+u - d^+d. \quad (6)$$

One of the advantages of the Schwinger boson theory is that it can be used in the ordered and disordered phases. In this section we will be interested in the disordered phase, where most of the spins are in the $S^z = 0$ state. In this case, the t_z bosons are condensate and we can take $< t_z >=< t_z^+ >= t$. Substituting (6) into the Hamiltonian (1), we obtain:

$$\begin{aligned} H = &\sum_l \sum_{r,\delta} \frac{J_1^{(l)}}{2}[t^2(d_r^+ d_{r+\delta} + u_{r+\delta}^+ u_r + u_r d_{r+\delta} + d_r^+ u_{r+\delta}^+ + H.c.) \\ &+ \sum_{r,a}\frac{J_2}{2}[t^2(d_r^+ d_{r+a} + u_{r+a}^+ u_r + u_r d_{r+a} + d_r^+ u_{r+a}^+ + H.c.) \\ &+ \frac{J_\perp}{2}\sum_{r,a}[t^2(d_r^+ d_{r+a} + u_{r+a}^+ u_r + u_r d_{r+a} + d_r^+ u_{r+a}^+ + H.c.) \\ &+ D\sum_r (u_r^+ u_r + d_r^+ d_r) - \sum_r \mu_r(u_r^+ u_r + d_r^+ d_r + t^2 - 1). \end{aligned} \quad (7)$$

A temperature-dependent chemical potential μ_r is introduced to impose the local constraint $S_r^2 = S(S+1) = 2$. In the mean-field approach, we replace the local parameter μ_r by a single parameter μ (which plays the role of a Lagrange parameter).

We Fourier transform the operators u and d independently on each layer A and B,

$$u_{r_n} = \sqrt{\frac{2}{N}}\sum_k e^{ik.r_n} u_k, \quad u_{r_m} = \sqrt{\frac{2}{N}}\sum_k e^{ik.r_m}\tilde{u}_k, \quad (8)$$

where $r_n \in A$, $r_m \in B$, with similar expressions for the d operator. The Fourier transformed Hamiltonian is:

$$\begin{aligned} H = &\sum_k f_k\Big\{[u_k^+ u_k + d_k^+ d_k + u_k u_k^+ + d_k d_k^+] + [u_k^+ u_k + d_k^+ d_k + u_k u_k^+ \\ &+ d_k d_k^+] + [u_k^+ d_{-k}^+ + d_k^+ u_{-k}^+ + u_k d_{-k} + d_k u_{-k}] + [u_k^+ d_{-k}^+ \\ &+ d_k^+ u_{-k}^+ + u_k d_{-k} + d_k u_{-k}]\Big\} + \sum_k g_k\Big\{[\tilde{u}_k^+\tilde{u}_k + \tilde{d}_k^+\tilde{d}_k + \tilde{u}_k\tilde{u}_k^+ \\ &+ \tilde{d}_k\tilde{d}_k^+] + [\tilde{u}_k^+\tilde{u}_k + \tilde{d}_k^+\tilde{d}_k + \tilde{u}_k\tilde{u}_k^+ + \tilde{d}_k\tilde{d}_k^+] + [\tilde{u}_k^+\tilde{d}_{-k}^+ + \tilde{d}_k^+\tilde{u}_{-k}^+ \\ &+ \tilde{u}_k\tilde{d}_{-k} + \tilde{d}_k\tilde{u}_{-k}] + [\tilde{u}_k^+\tilde{d}_{-k}^+ + \tilde{d}_k^+\tilde{u}_{-k}^+ + \tilde{u}_k\tilde{d}_{-k} + \tilde{d}_k\tilde{u}_{-k}]\Big\} \\ &+ h\sum_k\Big\{[u_k^+\tilde{u}_k + d_k^+\tilde{d}_k + u_k\tilde{u}_k^+ + d_k\tilde{d}_k^+] + [\tilde{u}_k^+ u_k + \tilde{d}_k^+ d_k \\ &+ \tilde{u}_k u_k^+ + \tilde{d}_k d_k^+] + [u_k^+\tilde{d}_{-k}^+ + d_k^+\tilde{u}_{-k}^+ + u_k\tilde{d}_{-k} + d_k\tilde{u}_{-k}] \\ &+ [\tilde{u}_k^+ d_{-k}^+ + \tilde{d}_k^+ u_{-k}^+ + \tilde{u}_k d_{-k} + \tilde{d}_k u_{-k}]\Big\}(D-\mu)\sum_k (u_k^+ u_k \\ &+ d_k^+ d_k + \tilde{u}_k^+\tilde{u}_k + \tilde{d}_k^+\tilde{d}_k), \end{aligned} \quad (9)$$

where

$$f_k = 4t^2(J_1^{(1)}\gamma_k + J_2\tilde{\gamma}_k) \quad , g_k = 4t^2(J_1^{(2)}\gamma_k + J_2\tilde{\gamma}_k),$$
$$h = t^2 J_\perp, \quad \gamma_k = 0.5(\cos k_x + \cos k_y), \quad \tilde{\gamma}_k = \cos k_x \cos k_y. \quad (10)$$