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Bond operator theory for the frustrated anisotropic Heisenberg antiferromagnet on a square lattice

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ABSTRACT

The quantum anisotropic antiferromagnetic Heisenberg model with single ion anisotropy, spin $S=1$ and up to the next-next-nearest neighbor coupling (the J_1–J_2–J_3 model) on a square lattice, is studied using the bond-operator formalism in a mean field approximation. The quantum phase transitions at zero temperature are obtained. The model features a complex $T=0$ phase diagram, whose ordering vector is subject to quantum corrections with respect to the classical limit. The phase diagram shows a quantum paramagnetic phase situated among Neél, spiral and collinear states.

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1. Introduction

Low-dimensional frustrated quantum antiferromagnets can display an intriguing interplay between order and disorder, and understanding such magnetically disordered states is important for the search of fractionalized excitations in two dimensions [1,2]. The search for spin liquid phases is one of the main interests in the study of magnetic systems with competing interactions and, in this context, the $S=\frac{1}{2}$, isotropic Heisenberg antiferromagnet on a square lattice with the nearest neighbors interactions J_1, next to nearest neighbors interactions J_2 and third neighbors interactions J_3 has been studied extensively by various analytical and numerical techniques [2–7].

Additional terms, as for instance single ion anisotropy, are possible when $S>\frac{1}{2}$ and can lead to new physical features, such as a quantum phase transition to a large D phase [8–11]. Studies of these models are not only of an academic interest since materials with $S=1$ and single ion anisotropy have been synthesized recently [12]. The system is more complex as there are now two mechanisms by which we can vary the quantum fluctuations. One mechanism is the introduction of anisotropy, another is by adding competing interactions to the bare model and varying the relative strengths of the competing exchange interactions, or the dimensionality and lattice type of the system. The combined effect of competing interactions J_1, J_2, and J_3 and single ion anisotropy may lead (or not lead) to frustrations, depending on their mutual values. The frustration enhances the importance of quantum effects because the classical order is suppressed. Motivated by these considerations, we will study the $S=1$, anisotropic, frustrated antiferromagnet on a square lattice, given by the Hamiltonian

$$H=\frac{J_1}{2}\sum_{r,\delta}(S_r^x S_{r+\delta}^x+S_r^y S_{r+\delta}^y+RS_r^z S_{r+\delta}^z)+\frac{J_2}{2}\sum_{r,d}(S_r^x S_{r+d}^x+S_r^y S_{r+d}^y+RS_r^z S_{r+d}^z)+\frac{J_3}{2}\sum_{r,\delta}(S_r^x S_{r+2\delta}^x+S_r^y S_{r+2\delta}^y+RS_r^z S_{r+2\delta}^z)+D\sum_r (S_r^z)^2, \quad (1)$$

where $\sum_{r,\delta}$ sums over the nearest neighbors, $\sum_{r,d}$ over the next-nearest neighbors, which are along the diagonals, and $\sum_{r,2\delta}$ over the next-next-nearest neighbors.

At infinite D, the ground state is a trivial product of states of $|S^z=0\rangle$ on all sites. In this state the average spin vanishes, $<S>=0$, and there is an excitation gap from the singlet to the doublets. On decreasing D, the energy gap decreases and goes to zero at a critical D_C, where a quantum phase transition takes place. For $D\leq D_C$ and positive, the system is in a gapless phase, which is ordered at $T=0$ in the non frustrated case. Previous study on this model with $J_3=0$ was performed in Ref. [8]. Here we will be concerned mainly with the effect of the J_3 term.

2. Bond operator mean field theory

An adequate approach that has given a reasonable description of the low-temperature quantum critical properties of many

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different spin systems is the bond operator formalism [8–11,13–17]. The bond operator representation was proposed by Sachdev and Bhatt [18] to understand the properties of dimerized phases in quantum $S=\frac{1}{2}$ spin systems and was lately extended by Wang and Wang [8] to treat the antiferromagnet with spin $S=1$. Following Ref. [8] we introduce three boson operators to denote the three eigenstates of S^z:

$$|1\rangle = u^+|v\rangle, \quad |0\rangle = t_z^+|v\rangle, \quad |-1\rangle = d^+|v\rangle, \tag{2}$$

where $|v\rangle$ is the vacuum state. The spin operators are written as

$$S^+ = \sqrt{2}(t_z^+ d + u^+ t_z), \quad S^- = \sqrt{2}\,(d^+ t_z + t_z^+ u), \quad S^z = u^+ u - d^+ d \tag{3}$$

Substituting (3) in the Hamiltonian (1) and supposing that the t_z bosons are condensed, i.e. $<t_z> = <t_z^+> = t$,we obtain:

$$\begin{aligned} H = \frac{J_1}{2}\sum_{r,\delta}&[t^2(d_r^+ d_{r+\delta} + u_{r+\delta}^+ u_r + u_r d_{r+\delta} + d_r^+ u_{r+\delta}^+ + H.c.) \\ &+ R\,(u_r^+ u_r - d_r^+ d_r)\,(u_{r+\delta}^+ u_{r+\delta} - d_{r+\delta}^+ d_{r+\delta})\,] \\ &+ \text{similar terms for } J_2 \text{ and } J_3 \\ &+ D\sum_r (u_r^+ u_r + d_r^+ d_r) - \sum_r \mu_r (u_r^+ u_r + d_r^+ d_r + t^2 - 1) \end{aligned} \tag{4}$$

A temperature-dependent chemical potential μ_r is introduced to impose the local constraint $S_r^2 = S\,(S+1) = 2$. We solve the Hamiltonian (4) by a mean-field approach. We replace the local parameter μ_r by a single parameter μ, and make a mean-field decoupling for the remaining operator terms, i.e, $\langle d_r^+ u_{r+\delta}^+\rangle = \langle d_r u_{r+\delta}\rangle = p$, $\langle d_r^+ u_{r+2\delta}^+\rangle = \langle d_r u_{r+2\delta}\rangle = p_2, \langle d_r^+ u_{r+d}^+\rangle = \langle d_r u_{r+d}\rangle = \tilde{p}$.

After a Fourier transformation of operators u and d, we diagonalize the Hamiltonian with a Bogoliubov transformation, and obtain

$$H = \sum_k \omega_k(\alpha_k^+ \alpha_k + \beta_k^+ \beta_k) + \sum_k (\omega_k - \Lambda_k) + C, \tag{5}$$

where C is a constant and

$$\omega_k = \sqrt{\Lambda_k^2 - \Delta_k^2}, \tag{6}$$

$$\Lambda_k = -\mu + D + 2R(1+\eta+\alpha)(1-t^2) + 4t^2 g(k), \tag{7}$$

$$\Delta_k = 4t^2 g(k) - 4R(p\gamma_k + \eta\tilde{p}\tilde{\gamma}_k + \alpha p_2 \gamma_{2k}), \tag{8}$$

$$\gamma_k = (1/2)(\cos k_x + \cos k_y), \quad \tilde{\gamma}_k = \cos k_x \cos k_y, \tag{9}$$

$$\gamma_{2k} = (1/2)(\cos 2k_x + \cos 2k_y), \quad g(k) = \gamma_k + \eta\,\tilde{\gamma}_k + \alpha\,\gamma_{2k}, \tag{10}$$

Here $\eta = J_2/J_1$, $\alpha = J_3/J_1$, and we have set $J_1 = 1$. The parameters t^2, μ, p, and $\tilde{p}$,p_2 are obtained by numerically solving the following self-consistent equations:

$$t^2 = 2 - \frac{1}{N}\sum_k \frac{\Lambda_k}{\omega_k}\coth\left(\frac{\beta\omega_k}{2}\right), \quad \mu = \frac{4}{N}\sum_k \left(\frac{\Lambda_k - \Delta_k}{\omega_k}\right) g(k)\coth\left(\frac{\beta\omega_k}{2}\right) \tag{11}$$

$$p = -\frac{1}{2N}\sum_k \frac{\Delta_k \gamma_k}{\omega_k}\coth\left(\frac{\beta\omega_k}{2}\right), \quad \tilde{p} = -\frac{1}{2N}\sum_k \frac{\Delta_k \tilde{\gamma}_k}{\omega_k}\coth\left(\frac{\beta\omega_k}{2}\right) \tag{12}$$

$$p_2 = -\frac{1}{2N}\sum_k \frac{\Delta_k \gamma_{2k}}{\omega_k}\coth\left(\frac{\beta\omega_k}{2}\right), \tag{13}$$

For a more detailed description of the formalism we refer the reader to Ref. [8]. For the XY model, $R=0$ and the terms with p do not contribute to Eq. (8). Therefore we have to solve only the self-consistent equations for t^2 and μ.

Once the self-consistent equations are solved, we can compute any kind of thermodynamical observable. The gap is obtained through the value of the minima of the dispersion relation (6) on the reciprocal lattice.

3. Results

In Fig. 1 we show the critical parameter D_C as a function of α, for $\eta=0$ and $R=0$. As we can see, the Neél order persists up to $\alpha_{1c}=0.226$ (quantum fluctuations stabilize the Neél order against spiral order). A different type of long range order arises at $\alpha_{2c}=0.387$, with ordering vector $\mathbf{Q}=(q,q)$ and q varying continuously. In Fig. 2 we show D_C as a function of α, for $\eta=1.0$ and $R=0$. The system shows columnar antiferromagnetic order for $\alpha<0.241$ and a spiral phase for $\alpha>0.545$. In the intermediate region the system is disordered. The behavior of $D_C(\eta)$ for $\alpha=0$, was presented in Ref.[13]. In Figs. 1 and 2 we have considered only the case $R=0$ since the self-consistent Eqs. (11)–(13) are more easily calculated in this limit. The behavior, however, is the same as the one for $R=1$.

For D larger than D_C the system is in a disordered phase with an energy gap. The gap vanishes at the critical point D_C, where a quantum phase transition from the large D phase to other phases occurs, with the minimum gap appearing at a wave vector Q, that depends on the parameters α and η.

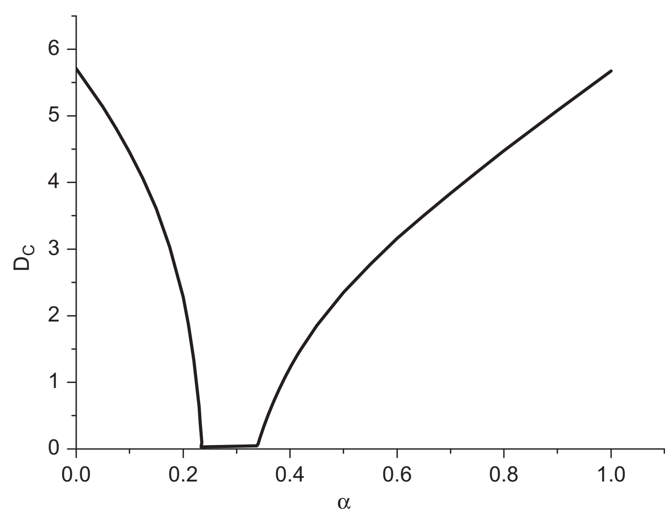

Fig. 1. Critical anisotropy parameter D_C as a function of α, for $\eta=0$ and $R=0$.

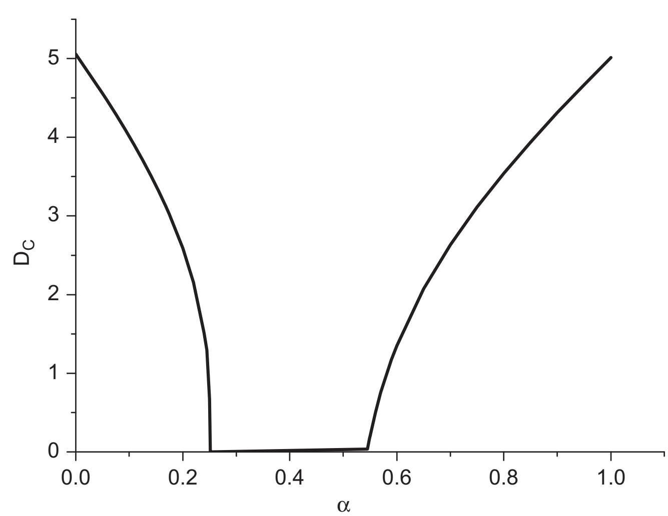

Fig. 2. Critical anisotropy parameter D_C as a function of α, for $\eta=1$ and $R=0$.

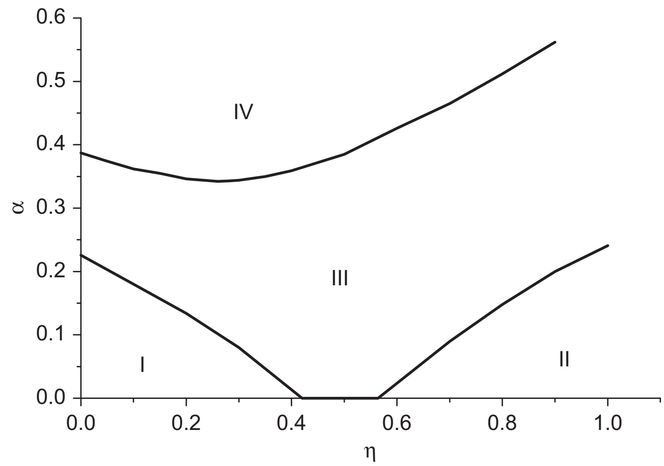

Fig. 3. Phase diagram at $T=0$ for $R=1$. Phase I is characterized by Néel order. Phase II is a collinear antiferromagnetic phase. In phase III the spins are disordered. Phase IV is spirally ordered.

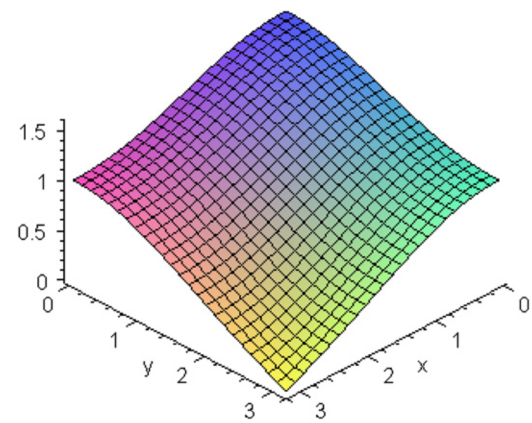

Fig. 5. Dispersion relation, $\omega_q/(-\mu+D)$, for $\alpha=\eta=0.1$.

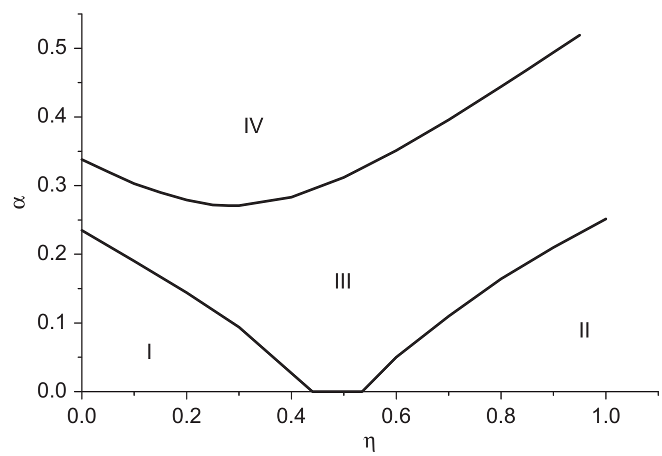

Fig. 4. Phase diagram at $T=0$ for $R=0$. The phases are the same as in Fig. 3.

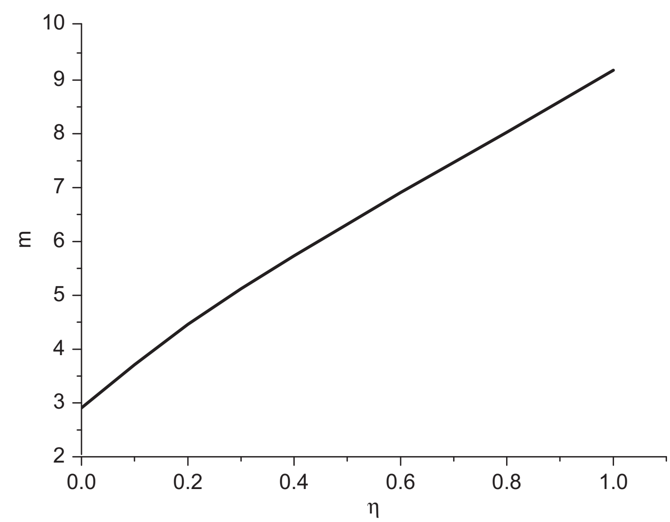

Fig. 6. Gap versus η, for $D=8$, $R=1$ and $\alpha=0$, at temperature 0.1.

The phase diagrams of the J_1–J_2–J_3 model are shown in Figs. 3 and 4, for $R=1$ and $R=0$, respectively, and are composed of four different phases:

(I) An antiferromagnetic Neél phase with $\mathbf{Q}=(\pi,\pi)$, just as in the unfrustrated square lattice.
(II) A columnar antiferromagnetic phase showing antiferromagnetic order in one direction of the lattice and ferromagnetic order in the other one. Here $\mathbf{Q}=(0,\pi)$ or $(\pi,0)$.
(III) A disordered phase. The combined effect of quantum fluctuations and competing interactions was strong enough to destroy the long-range order.
(IV) A spiral phase with ordering vector $\mathbf{Q}=(q,q)$, and q varying continuously.

Increasing D in the phases (in the α–η plane) where long range order occurs, we reach a disordered state. We have, thus, two mechanisms that may lead to disorder: the single ion anisotropy, whose strength is measured by D, and the competing interactions J_1, J_2 and J_3.

When the dispersion relation shows a zero mode, Bose condensation indicates an ordered phase. For illustration purpose, in Fig. 5 we show the dispersion relation at coupling values $\alpha=\eta=0.1$, well inside the Neél phase.

In the classical case (and with $D=0$, $\eta=0$) there is a conventional Neél order for $\alpha \le 0.25$ and a state with long range incommensurate antiferromagnetic order for $\alpha > 0.25$. However, for the quantum $S=\frac{1}{2}$ model, a modified spin-wave theory [2] shows that the Neél order persists up to $\alpha_{1c}=0.39$, and the long range spiral order arises at $\alpha_{2c}=0.52$. In the model studied here (for $R=1$), $\alpha_{1c}=0.226$ and $\alpha_{2c}=0.387$. The J_1–J_2 model with first and second-neighbor couplings has only collinear, commensurate spin correlations, and this makes both the classical and quantum theories quite different from that of the J_1–J_3 model.

Since the competing interactions increase the magnitude of quantum fluctuations, it is interesting to examine how the gap varies with these interactions at a fixed temperature. In Fig. 6 we plot the gap at (π,π) versus the coupling η, at $D=8$, $R=1$, $T=0.1$ and $\alpha=0$. The curve is almost a straight line. For $D=8$, $R=1$, $T=0.1$ and $\eta=0$, the gap increases linearly with α and could be fitted by $m=2.92+0.87\alpha$.

An interesting result of our theory is the existence of a gap in the nonmagnetic region $\alpha_{1c} < \alpha < \alpha_{2c}$, even for $D=0$. The gap, however, vanishes at α_{1c} and α_{2c}. In Fig. 7 we show the gap as a function of D, for $\alpha=0.3$ and $\eta=0$. As we can see, $m=0.46$ at $D=0$.

We have found that the behavior of the gap with temperature, in any region, has the behavior expected from scaling theories [19]. In order to illustrate, in Fig. 8 we show the gap as a function

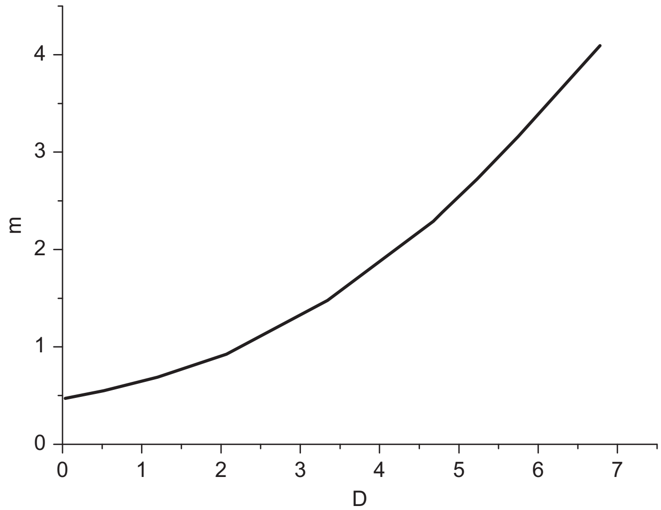

Fig. 7. Gap in the paramagnetic phase as a function of the anisotropy parameter D, for $\eta=0$ and $\alpha=0.3$.

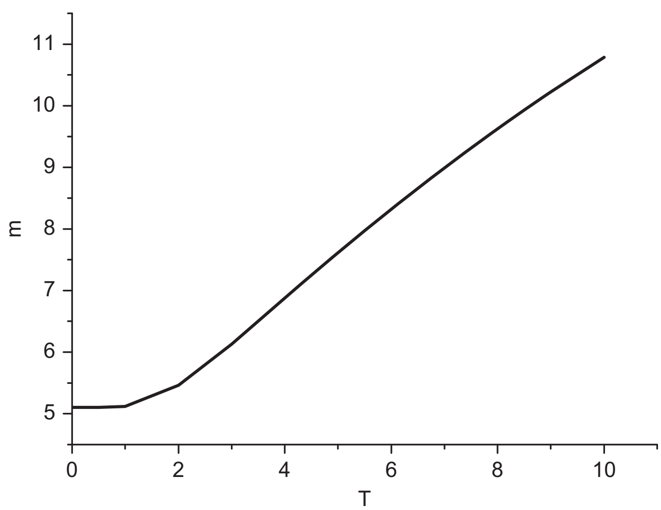

Fig. 8. Gap as a function of temperature for $D=8$, $R=1$, $\alpha=0$ and $\eta=0.3$.

of temperature for $D=8$, $R=1$, $\alpha=0$ and $\eta=0.3$. The curve can be fitted to the following expression:

$$m = m_0 + c_1 T^{1/2} \exp(-c_2/T), \tag{14}$$

where c_1 and c_2 are constants which depend on D, α and η.

4. Conclusions

In this paper we have used the bond operator technique to study the low temperature critical properties of the anisotropic, frustrated $S=1$ Heisenberg antiferromagnet on a square lattice. A very dramatic effect of quantum fluctuations seems to be the disappearance of an ordered state in phase III in the classical phase diagram, characterized by magnetic order at a pitch vector [2] $\mathbf{Q}=(q,\pi)$ with continuously varying q.

Isaev et al. [20] have shown that for the isotropic $S=\frac{1}{2}$ Heisenberg antiferromagnet with $J_3=0$, the intermediate quantum paramagnetic phase, $\eta_{1c}<\eta<\eta_{2c}$, is a (singlet) *plaquette* crystal, and the ground and first excited states are separated by a finite gap. It should be interesting to calculate the ground state in this interval in our model and see the effect of the single ion anisotropy in this ground state.

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