Journal of Magnetism and Magnetic Materials 327 (2013) 1–6

Contents lists available at SciVerse ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Critical properties of the frustrated quasi-two dimensional XY-like antiferromagnet

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ARTICLE INFO

Article history:
Received 25 March 2012
Received in revised form
29 August 2012
Available online 27 September 2012

Keywords:
XY-model
Antiferromagnet
Frustration
Quantum phase transitions

ABSTRACT

We study, using a self-consistent harmonic approximation, the quasi-two-dimensional frustrated Heisenberg antiferromagnet with easy-plane single ion anisotropy. Besides the transition temperature from the high-temperature paramagnetic phase to the low-temperature ordered phase, we also obtain, at zero temperature, the critical single ion anisotropy parameter D_c that separates the low D region from the large D quantum paramagnetic phase. We have found disordered phases at zero temperature that could be possible candidates for spin liquids states.

1. Introduction

Frustrated quantum antiferromagnets on the square lattice have been the subject of intense research over the last decades, with particular interest in the spin $S=1/2$ case relevant for the cuprates, whereas interest in higher spin values increased with the discovery of the pnicitides [1]. As by now it is well known that the antiferromagnetic Heisenberg model on the square lattice has long-range order in the ground state even for $S=1/2$. It is also known that this long range order can be destroyed by frustration caused, for instance, by next nearest neighbor antiferromagnetic interactions [2–10].

On the other side, spin liquid is a hot topic in condensed matter physics since the discovery of high-T_C superconductivity. A spin liquid is a disordered state, but not all disordered states are a spin liquid [4]. So, a first step in the research of spin liquids is to look for disordered states. In this context, the antiferromagnetic Heisenberg model (AFHM) with competing interactions has been widely studied, but the same is not true for the XY model.

Several new magnetic materials characterized by competing interactions have been synthesized, but a detailed theoretical understanding of the ground state properties of simple models displaying both frustration and quantum fluctuations is still missing [11], and interpretations of the experimental results often relies on simple perturbative or semiclassical methods.

When $J_2/J_1 < 1/2$, where J_1 is the nearest-neighbor and J_2 the next-nearest neighbor interaction, the classical ground state has a Néel order. However when $J_2/J_1 > 1/2$, the ground state consists of two independent sublattices with antiferromagnetic order. The classical ground state energy does not depend on the relative orientations of both sublattices. However, quantum fluctuations lift this degeneracy and select a collinear order state, where the neighboring spins align ferromagnetically along one axis of the square lattice and antiferromagnetically along the other [3,4].

Additional terms, as for instance single ion anisotropy, are possible when $S > 1/2$ and can lead to new physical features, such as a quantum phase transition to a large D phase. Study 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 and get disordered phases. One mechanism is the anisotropy; the other is the competing interactions to the bare model where we can vary the relative strengths of the exchange interactions. 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. In real magnetic material, single-ion anisotropy plays a major role in determining the magnetic behavior of the system [12,13].

In this paper we will study a quasi-two-dimensional Heisenberg antiferromagnet with an easy-plane single ion anisotropy described by the following Hamiltonian:

$$H=\frac{J_1}{2}\sum_{r,a}(S_r^xS_{r+a}^x+S_r^yS_{r+a}^y+\lambda S_r^zS_{r+a}^z)+D\sum_r(S_r^z)^2 +\frac{J_2}{2}\sum_{r,d}(S_r^xS_{r+d}^x+S_r^yS_{r+d}^y+\lambda S_r^zS_{r+d}^z) +\frac{J_3}{2}\sum_{r,\delta}(S_r^xS_{r+\delta}^x+S_r^yS_{r+\delta}^y+\lambda S_r^zS_{r+\delta}^z). \quad (1)$$

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http://dx.doi.org/10.1016/j.jmmm.2012.09.006

Here J_1 is the nearest-neighbor, J_2 the next-nearest neighbor exchanges interactions, both in the XY-plane, and J_3 the inter-plane coupling. We take $S=1$, but our calculations can be applied for any $S>1/2$. The main physical motivation for our study is to find phases which do not carry a magnetic moment, and therefore are candidate for a spin liquid state.

The spectrum of the Hamiltonian (1) changes drastically as D varies from very small to very large values. A strong anisotropy favors a quantum paramagnetic ground state, which is separated from the ordered state by a quantum critical point. This phase consists of a unique ground state with total magnetization $S^z_{total}=0$, separated by a gap from the first excited states, which lie in the sectors $S^z_{total}=\pm 1$. The primary excitations is a gaped $S=1$ exciton with an infinite lifetime at low energies.

As it is well known, the isotropic 2D AFHM is ordered only at zero temperatures, while in the XY model a Kosterlitz–Thouless (KT) phase transition occurs when $J_3=0$, resulting from the unbinding of vortex–antivortex pairs. Therefore it is interesting to calculate the KT transition temperature T_{KT} for the XY model with competing interactions. For $J_3=0$ the critical behavior of the quantum XY model is of the KT-type, as in the classical case. Quantum fluctuations change the quantitative behavior of the model, but the qualitative picture of the classical system persists [14]. When $J_3>0$, we have the usual order-disorder phase transition.

For $J_3=0$, there is no spontaneous magnetization for $T>0$. However, for $T<T_{\mathrm{KT}}$ there is a quasi long-range order and the spin-spin correlation functions shows a power law decrease with distance (with an exponent proportional to T as $T\to 0$). A new property appearing below the phase-transition temperature is the stiffness ρ introduced by Berezinskii [15], by analogy with superfluid helium. At the KT temperature ρ drops to zero. Of course, for $J_3>0$, the magnetization is non null, but it is related to ρ, and thus goes to zero at the same point where ρ vanishes.

2. Self-consistent Harmonic approximation

Simple approaches which yield an analytical description are very useful for practical purposes. For an XY-like model such as Hamiltonian Eq. (1), a very convenient theory is the self consistent harmonic approximation (SCHA), which replaces the Hamiltonian by an effective one with temperature-dependent renormalized parameters [14,16,17]. Although it is a semiclassical theory it has the advantage of being the only spin wave theory which gives the KT-transition. We write the spins components in the Hamiltonian (1) in terms of the Villain representation [18]

$$S_r^+ = e^{i\varphi_r}\sqrt{(S+1/2)^2-(S_r^z+1/2)^2},\; S_r^- = \sqrt{(S+1/2)^2-(S_r^z+1/2)^2}\,e^{-i\varphi_r}. \tag{2}$$

where φ is the operator corresponding to the azimuthal angle of the spin around the z axis. Taking Eq. (2) into Eq. (1), writing $\varphi=\phi+\pi$ for the near-neighbor term (antiferromagnetic order), and expanding the cosine term we obtain:

$$H_1=\frac{J_1}{2}\sum_{r,a}\left[\rho_1\tilde{S}^2(\phi_r^2-\phi_r\phi_{r+a})+\lambda S_r^zS_{r+a}^z\right]+D\sum_r (S_r^z)^2 \tag{3}$$

where $\tilde{S}^2=S(S+1)$, and the stiffness $\rho_1$for the near-neighbor spins is given by [14]

$$\rho_1=\left\langle\left[1-\left(\frac{S_r^z}{\tilde{S}}\right)^2\right]\right\rangle\langle\cos(\phi_r-\phi_{r+a})\rangle. \tag{4}$$

Here we are supposing that $|\phi_{r+a}-\phi_r|<<1$.This is true for $T<T_{\mathrm{KT}}$, but not for $T>T_{\mathrm{KT}}$ where the dissociation of vortices disorder the system. Therefore our calculation is valid only at low temperatures, i. e. $T<J$ [15].

Taking the Fourier transform we get

$$H_1=2J_1\sum_q[\rho_1\tilde{S}^2(1-\gamma_q)\phi_q\phi_{-q}+(1+d+\lambda\gamma_q)S_q^zS_{-q}^z] \tag{5}$$

where

$$\gamma_q=\tfrac{1}{2}(\cos q_x+\cos q_y),\quad \text{and}\quad d=D/2J_1.$$

A procedure similar can be used for the other terms. We remark that for the next-near-neighbor, in the Néel phase, the spins are in the same direction and we take $\varphi=\phi$. Doing all the calculations we arrive at the final result for the Néel phase

$$H=\sum_q[\tilde{S}^2a(q)\phi_q\phi_{-q}+b(q)S_q^zS_{-q}^z] \tag{6}$$

with

$$a(q)=2J_1\left[\rho_1(1-\gamma_q)-\eta\rho_2(1-\xi_q)+\frac{\alpha\rho_3}{2}(1-\cos q_z)\right] \tag{7}$$

$$b(q)=2J_1\left[1+d-\eta+\frac{\alpha}{2}+\lambda(\gamma_q+\eta\xi_q+\frac{\alpha}{2}\cos q_z)\right] \tag{8}$$

The stiffness constants, renormalized by quantum fluctuations, are given by

$$\rho_i=\left\langle\left[1-\left(\frac{S_r^z}{\tilde{S}}\right)^2\right]\right\rangle\exp\left[-\sum_q g_i(q)<\phi_q\phi_{-q}>\right] \tag{9}$$

where

$$g_1=(1-\gamma_q),\; g_2=(1-\xi_q),\; g_3=(1-\cos q_z). \tag{10}$$

$$\xi_q=\cos q_x\cos q_y,\quad \eta=J_1/J_2,\quad \text{and}\quad \alpha=J_3/J_1. \tag{11}$$

By introducing the canonical transformation

$$\phi_q=\left(\frac{b(q)}{a(q)}\right)^{1/4}(a_q^++a_{-q}),\; S_q^z=i\left(\frac{a(q)}{b(q)}\right)^{1/4}(a_q^+-a_{-q}) \tag{12}$$

where a_q^+ and a_q are the boson-creation and annihilation operators, respectively, we can write Eq. (6) as

$$H=\sum_q\omega_q(a_q^+a_q+1/2) \tag{13}$$

where

$$\omega_q=2\tilde{S}\sqrt{a(q)b(q)}. \tag{14}$$

Using Eq. (12), the static correlations can be calculated, and the result is

$$\left\langle(S_r^z)^2\right\rangle=\frac{\tilde{S}}{2\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi d^3q\sqrt{\frac{a(q)}{b(q)}}\cot h\left(\frac{\beta\omega_q}{2}\right) \tag{15}$$

$$\left\langle\phi_q\phi_{-q}\right\rangle=\frac{1}{2\tilde{S}}\sqrt{\frac{b(q)}{a(q)}}\cot h\left(\frac{\beta\omega_q}{2}\right). \tag{16}$$

In the collinear phase, Eqs. (7) and (8) are substituted by

$$a(q)=J_1\rho_1(\cos q_y-\cos q_x)+2J_2\rho_2(1-\cos q_x\cos q_y)+J_3\rho_3(1-\cos q_z). \tag{17}$$

$$b(q)=J_1\lambda(\cos q_x+\cos q_y)+D+2J_2(1+\lambda\cos q_x\cos q_y)+J_3(1+\lambda\cos q_z). \tag{18}$$

The other equations remain the same. The critical temperature T_C and the critical anisotropy parameter D_C can be evaluated where the stiffness drops to zero. We remark, once more, that for $\alpha=0$, T_C is the Kosterlitz–Thouless transition temperature T_{KT}.