Physica A 388 (2009) 3779–3784

Contents lists available at ScienceDirect

Physica A

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

Quantum phase transitions in the anisotropic three dimensional XY model

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ARTICLE INFO

Article history:
Received 6 April 2009
Available online 6 June 2009

PACS:
75.10.jm
75.40.-s

Keywords:
XY model
Quantum phase transitions

ABSTRACT

In this paper we study the quantum phase transition in a three-dimensional XY model with single-ion anisotropy D and spin $S = 1$. The low D phase is studied using the self consistent harmonic approximation, and the large D phase using the bond operator formalism. We calculate the critical value of the anisotropy parameter where a transition occurs from the large-D phase to the Néel phase. We present the behavior of the energy gap, in the large-D phase, as a function of the temperature. In the large D region, a longitudinal magnetic field induces a phase transition from the singlet to the antiferromagnetic state, and then from the AFM one to the paramagnetic state.

1. Introduction

As is well known classical phase transitions are driven only by thermal fluctuations. On the other side, in a quantum system there are fluctuations driven by the uncertainty principle, even in the ground state, that can drive phase transitions at $T = 0$, the so called quantum phase transitions (QPT) [1]. These transitions take place by changing not the temperature, but some parameter in the Hamiltonian of the system. A zero temperature phase transition is a nonanalyticity in the ground state of an (infinite) system as a function of some parameter such as pressure or applied magnetic field. The quantum critical point (QCP) can be viewed, in some cases, as the endpoint of a line of finite-temperature transitions. At the QCP quantum fluctuations exist on all length scales and therefore can be observed at finite temperature. The typical time scale for a decay of the fluctuations is the correlation time τ_c. As the critical point is approached the correlation time diverges as $\tau_c \propto \xi^z$, where ξ is the correlation length and z is the dynamical critical exponent. The physics of the QPT is in general quite complex. One model where it can be well studied is the XY model with an easy-plane single ion anisotropy, described by the Hamiltonian:

$$H = -J \sum_{\langle n,m\rangle_1} (S_n^x S_m^x + S_n^y S_m^y) - J' \sum_{\langle n,m\rangle_2} (S_n^x S_m^x + S_n^y S_m^y) + D \sum_n (S_n^z)^2, \tag{1}$$

where $\langle n, m\rangle_1$ denotes a pair of nearest-neighbor spins in the same plane, and $\langle n, m\rangle_2$ in adjacent planes. Due to the form of the single ion anisotropy, we will take $S = 1$. The spectrum of the Hamiltonian (1) changes drastically as D varies from very small to very large values. The so called large D phase, $D > D_C$, consists of a unique ground state with total magnetization $S^z_{\text{total}} = 0$ separated by a gap from the first excited states, which lie in the sectors $S^z_{\text{total}} = \pm 1$. The primary excitation in this phase is a gapped $S = 1$ exciton with an infinite lifetime at zero temperature. At $T > 0$, thermally excited quasi-particles will collide with each other, and this leads to a finite lifetime. For small D, the Hamiltonian (1) is in a gapless phase described by the spin-wave theory. This model in one and two dimensions has been well studied in the literature [2,3]. For $J' = 0$, the critical behavior of the XY model in the low D region is of the Kosterlitz–Thouless type, resulting from the unbinding

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0378-4371/$ – see front matter
doi:10.1016/j.physa.2009.06.009

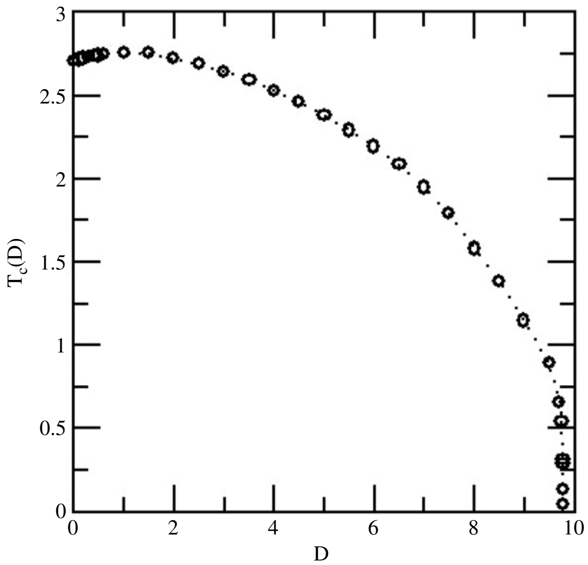

Fig. 1. The critical temperature T_c as a function of the anisotropy parameter D, for $D \le D_c$. The dotted line is a guide for the eyes.

of vortex–antivortex pairs. In this paper we consider the case with a non-null inter-plane coupling. The case $D = 0$, in the classical limit, was studied in Ref. [4]. Although we will be mainly interested in the large D phase, we will present the whole phase diagram.

Starting from the large D phase, one way to cause the onset of magnetic order is by increasing the exchange interaction. The application of pressure is expected to have just this effect [5].

The small D phase can be studied using the self-consistent harmonic approximation (SCHA). This approximation has been extensively studied in the literature [6,7] and here we present only the essentials. Starting with the Villain representation:

$$S_n^+ = e^{i\phi_n}\sqrt{(S+1/2)^2 - (S_n^z+1/2)^2},$$
$$S_n^- = \sqrt{(S+1/2)^2 - (S_n^z+1/2)^2}\, e^{-i\phi_n}, \tag{2}$$

and following, for instance, Ref. [7] we can write the Hamiltonian (1) for $J = J' = 1$, as

$$H = 3\sum_q [\rho\tilde{S}(1-\gamma_q)\phi_q\phi_{-q} + (1 + D/3)S_q^z S_{-q}^z], \tag{3}$$

where $\tilde{S} = \sqrt{S(S+1)}$, $\gamma_q = \frac{1}{3}(\cos q_x + \cos q_y + \cos q_z)$ and the stiffness ρ, renormalized by thermal and quantum fluctuations, is given by

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

From Eq. (2) we obtain:

$$\omega_q = 6\tilde{S}\sqrt{\rho(1-\gamma_q)(1+D/3)}, \tag{5}$$

$$\langle (S_r^z)^2\rangle = \frac{\tilde{S}}{2}\frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi d\vec{q}\sqrt{\frac{\rho(1-\gamma_q)}{1+D/3}}\coth\left(\frac{\omega_q}{2T}\right), \tag{6}$$

$$\langle \phi_q\phi_{-q}\rangle = \frac{1}{2\tilde{S}}\sqrt{\frac{(1-D/3)}{\rho(1-\gamma_q)}}\coth\left(\frac{\omega_q}{2T}\right). \tag{7}$$

The SCHA yields a critical Nèel line in three dimensions and in Fig. 1 we show $T_C(D)$ for $\alpha = 1$. We can estimate D_C as about 9.77 compared with the result $D_C = 10.6$ obtained using the bond operator method described in the next section. An interesting result of our calculation is the slight increase of T_C with D, for small D. A more pronounced effect was found by Wang and Wang [8], but we believe that the SCHA is more adequate to treat the model in the low D phase than the bond operator technique. It would be interesting to have numerical calculations data to check both predictions.

Both the energy gap m and the Néel order parameter vanish continuously as D_C is approached from either side.