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Quantum phase transitions in the anisotropic three dimensional XY model

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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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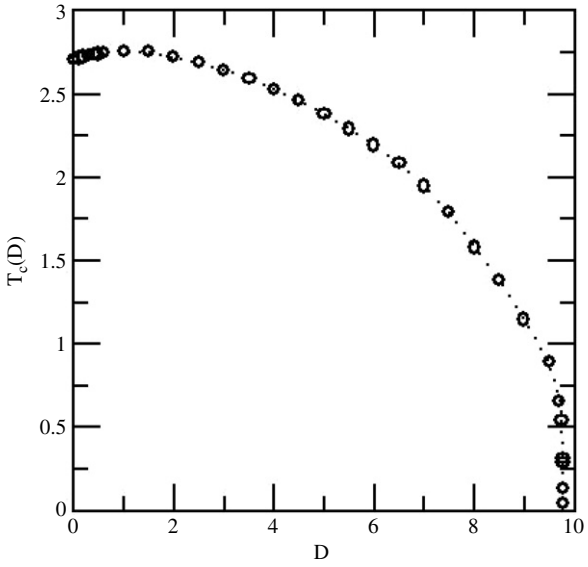

Fig. 1. The critical temperature T_c as a function of the anisotropy parameter D, for $D \leq D_c$. The dotted line is a guide for the eyes.

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:

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

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:

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

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

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

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.

2. Bond operator

A simple approach that can be used for a theoretical description of the large D phase is the method of bond operator, proposed by Sachdev [9] to study coupled dimer antiferromagnet with spin 1/2 and extended by Wang and Wang [8] to spin 1. This method has been widely applied, and in some cases provides an accurate quantitative description of numerical studies and experiments [8–13]. The method was employed previously at zero temperature and extended to finite temperature in Ref. [3]. In this formalism, three boson operators are introduced to denote the three eigenstates of S^z:

$$|1\rangle = u^+ |v\rangle\,, \qquad |0\rangle = t_z^+ |v\rangle\,, \qquad |-1\rangle = d^+ |v\rangle\,, \tag{8}$$

where $|v\rangle$ is some reference vacuum state which does not correspond to a physical state of the spin system. The physical states satisfy the constraint $u^+u + d^+d + t_z^+t_z = 1$. The spin operators are written as

$$S^+ = \sqrt{2}(t_z^+ d + u^+ t_z), \qquad S^- = \sqrt{2}(d^+ t_z + t_z^+ u), \qquad S^z = u^+u - d^+d. \tag{9}$$

In the large D phase we can assume that the t_z bosons are condensed and write: $\langle t_z^+\rangle = \langle t_z\rangle = t$. Using this approximation we get [8]:

$$\begin{aligned} H = {} & \frac{Jt^2}{2}\sum_{r,\delta}(d_r^+ d_{r+\delta} + u_{r+\delta}^+ u_r + u_r d_{r+\delta} + d_r^+ u_{r+\delta}^+ + H.c.) \\ & + \frac{J't^2}{2}\sum_{r,\delta}(d_r^+ d_{r+\delta} + u_{r+\delta}^+ u_r + u_r d_{r+\delta} + d_r^+ u_{r+\delta}^+ + H.c.) \\ & + D\sum_r (u_r^+ u_r - d_r^+ d_r)^2 - \mu\sum_r (u_r^+ u_r + d_r^+ d_r + t^2 - 1), \end{aligned} \tag{10}$$

where we have introduced a temperature dependent constraint parameter μ to enforce the condition of single occupancy. Since our starting point is the large D limit, a condition that the approximation is valid is that the quantum phase transition occurs at a relative large D. If the QPT occurs at a relative small D, the effect of the last term in the Hamiltonian (1) on the ground state energy is small and the present approximation is not valid. The present approach gives a very satisfactory description of the phase with $D \geq D_C$. As pointed out by Sachdev [14], an important feature of the bond operator approach is that the simplest mean field theory already yields ground states and excitations with the correct quantum numbers; so a strong fluctuation analysis is not needed to capture the proper physics of the problem.

Taking the Fourier transform and performing a Bogoliubov transformation defined by

$$u_k^+ = \tilde{u}_k \alpha_k - v_k \beta_k, \qquad d_{-k} = -v_k \alpha_k + \tilde{u}_k \beta_k, \tag{11}$$

where

$$\tilde{u}_k = \frac{1}{\sqrt{2\omega_k}}(\Lambda_k + \omega_k)^{1/2}, \qquad v_k = \frac{1}{\sqrt{2\omega_k}}(\Lambda_k - \omega_k)^{1/2}, \tag{12}$$

we obtain

$$H = \sum_k \omega_k(\alpha_k^+\alpha_k + \beta_k^+\beta_k) + \sum_k(\omega_k - \Lambda_k) + \mu N(1 - t^2), \tag{13}$$

with

$$\omega_k = \sqrt{\Lambda_k^2 - \Delta_k^2}, \quad \Lambda_k = -D + d + t^2 F_k,\ \Delta_k = t^2 F_k, \tag{14}$$

where

$$F_k = 2(\cos k_x + \cos k_y + \alpha \cos k_z). \tag{15}$$

Here we have written $\alpha = J/J'$, and taken $J = 1$. In the mean-field approximation the Gibbs free energy is given by:

$$G = Ne_0 - \frac{2}{\beta}\sum_k \ln[1 + n(k)], \tag{16}$$

where $n(k) = 1/(e^{\beta\omega_k} - 1)$, and e_0 is the ground state energy per site:

$$e_0 = \frac{1}{N}\sum_k(\omega_k - \Lambda_k) + \mu(1 - t^2). \tag{17}$$

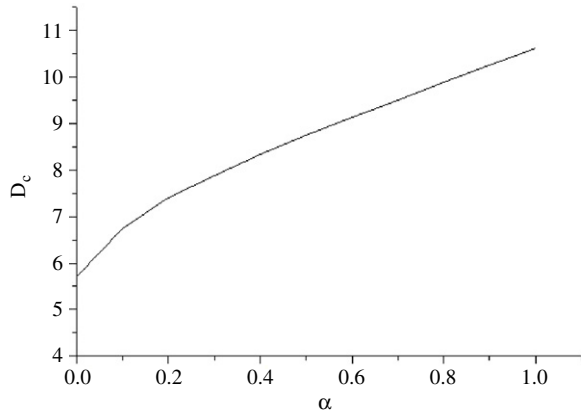

Fig. 2. The critical anisotropy parameter D_c as a function of $\alpha = J'/J$.

Minimizing G with respect to μ and t^2, we obtain the following self-consistent equations, which should be solved numerically:

$$\mu = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{F_k \mathrm{d}\vec{k}}{\sqrt{1+yF_k}} \coth\left(\frac{\beta\omega_k}{2}\right), \tag{18}$$

$$(2-t^2) = \frac{1}{2\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \mathrm{d}\vec{k}\left[\frac{1}{\sqrt{1+yF_k}} + \sqrt{1+yF_k}\right]\coth\left(\frac{\beta\omega_k}{2}\right), \tag{19}$$

where $y = 2t^2(-\mu + D)^{-1}$ and we can write $\omega_k = (-\mu + D)\sqrt{1+yF_k}$. At $D = D_C$ the gap vanishes, so

$$y_c = \frac{1}{2(2+\alpha)}. \tag{20}$$

For $D > D_C$ the gap is given by

$$m = (-\mu + D)\sqrt{1 - 2y(2+\alpha)}. \tag{21}$$

When $y \to y_c$, the energy gap goes to 0, indicating a transition from the large D phase to the Néel phase. An equation for the critical point where the gap goes to zero can be obtained:

$$D_C = 4(2+\alpha)(2 - I_1), \tag{22}$$

where

$$I_1 = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{\mathrm{d}\vec{k}}{\sqrt{1+y_cF_k}}. \tag{23}$$

In Fig. 2 we show $D_C(\alpha)$.

As D approaches D_C from above, at $T = 0$, the energy gap vanishes as

$$m = a(D - D_C)^\beta. \tag{24}$$

For $\alpha = 0$, we found $\beta = 1$, in agreement with Refs. [3,8], and for $\alpha = 1$, we obtained $\beta = 0.5$ in agreement with Ref. [8]. For $0 < \alpha < 1$, we got the result $\beta \approx 0.6$. In Fig. 3 we show the gap m, at $T = 0$, as a function of $\Delta = D - D_C$ for $\alpha = 0.5$. For $\Delta \to 0$ we have $m = 2.6\Delta^{0.6}$.

At the critical point, we have found that the gap increases linearly with the temperature, as expected from general scaling arguments. For $D > D_C$ we have a quantum paramagnetic ground state with no long range order. In Fig. 4 we show the gap as a function of temperature for $D = 20$ and $\alpha = 0.1, 0.5, 1.0$. We have found that the gap can be fitted to the following expression:

$$m^2 = c_0 + c_1 T^{3/2}\exp(-c_2/T), \tag{25}$$

where the parameters c_0, c_1 and c_2 depends on D and α. As we can see, a nonzero temperature induces an exponentially small density of thermally excited excitons.

In the limit $D \gg D_C$ we have $t^2 = 1$, $y = 2/D$, and the excitation spectrum, for $\alpha = 1$, takes the form

$$\omega_k = D + 2(\cos k_x + \cos k_y + \cos k_z), \tag{26}$$

in agreement with a calculation using standard perturbation theory.

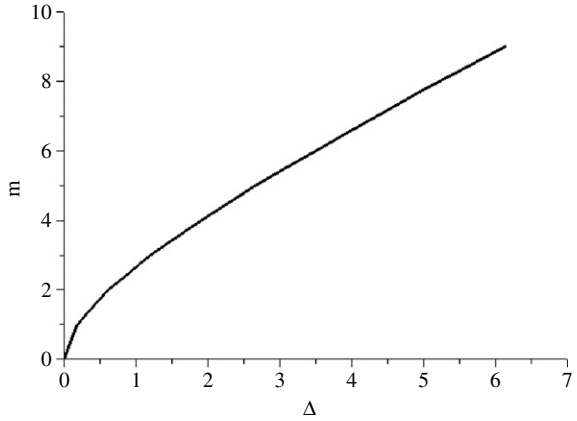

Fig. 3. The gap m, at $T = 0$, as a function of $\Delta = D - D_c$, for $\alpha = 0.5$.

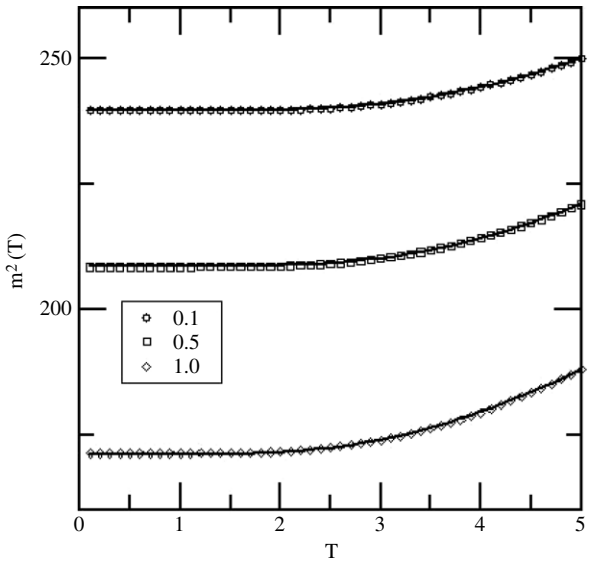

Fig. 4. The energy gap as a function of the temperature, for $D = 20$. The circles, squares and triangles are for $\alpha = 0.1$, 0.5 and 1.0 respectively. The lines were adjusted using Eq. (25).

3. External magnetic field

In the presence of an external magnetic field B applied along the z direction, we add a term $-h\sum S_r^z$, where $h = g\mu_B B$, to the Hamiltonian. The spin wave spectrum has now two branches given by:

$$\omega_k^{(1)} = \omega_k - h, \qquad \omega_k^{(2)} = \omega_k + h. \tag{27}$$

At a critical magnetic field $h_{c1} = \omega_0^{(1)}$ the energy gap vanishes and we have long-range order. When we increase the magnetic field, we assume the energy gap remains zero and part of the excitations condenses. For magnetic fields larger than a second critical field h_{c2} the spins are fully aligned with the field, below h_{c2} the system is in the antiferromagnetic phase. The magnetic ordering at h_{c2} can be identified as a Bose–Einstein condensation of the transverse components of the spins [15]. In this case we can express the bond operators as [15]:

$$S^+ = \sqrt{2}\bar{u}t_z, \qquad S^- = \sqrt{2}\bar{u}t_z^+, \qquad S^z = 1 - t_z^+ t_z, \tag{28}$$

where $u = u^+ = \bar{u}$. We find

$$H = \sum_k \omega_k b_k^+ b_k + E_g, \tag{29}$$

where $t_z^+ = (1/\sqrt{N})\sum_k e^{-i\vec{k}.\vec{r}} b_k^+$, and

$$\omega_k = h - (D+\mu) + 4J\bar{u}^2\gamma_k, \quad \gamma_k = \frac{1}{2}(\cos k_x + \cos k_y), \tag{30}$$

$$\varepsilon_0 = E_g/N = D\bar{u}^2 - h - \mu\bar{u}^2 + \mu, \tag{31}$$

where we have considered here the case $\alpha = 0$.

Minimizing $G = \varepsilon_0 - T\sum_k \ln(1+n_k)$ we arrive at

$$1 - \bar{u}^2 = \sum_k n_k, \tag{32}$$

$$D - \mu = -4J\sum_k \gamma_k n_k. \tag{33}$$

At $T = 0$ we have $\bar{u}^2 = 1$, $\mu = D$. The minimum of the spin-wave spectrum occurs at $Q = (\pi, \pi)$. The condition $\omega_Q \equiv 0$ defines the critical field

$$h_{c2} = (D+\mu) + 4J\bar{u}^2, \tag{34}$$

which leads, for small k, to

$$\omega_k = (h - h_{c2}) + J\bar{u}^2k^2, \tag{35}$$

showing that the QPT at h_{c2} has a dynamical critical exponent $z = 2$.

4. Conclusions

For the anisotropy parameter D above a critical D_C the system is in the quantum disordered regime with a spin gap. We have used the bond operator theory, in which the chemical potential is retained explicitly. Within a mean-field approximation, the operator t_z and the site-dependent chemical potential μ_n are replaced by uniform, global average values. These parameters are then determined self-consistently from a minimization of the Gibbs free energy. Among AFMs there is a family of materials where the single-ion anisotropy exceeds the exchange energy. These are the so-called Van Vleck, or singlet, antiferromagnets. These compounds show no magnetic ordering, in the absence of the external magnetic field, at any temperature down to $T = 0$ [16]. The compound $NiCl_24SC(NH_2)_2$ is a prototype of a three dimensional large-D model [17] with $D/J \approx 20$. Given the existence of materials with $D > J$, we hope that experimental data for the correlation length $\xi \propto m^{-1}$ will be available in the future so that we can verify our calculations.

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