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.

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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 \( \tau_c \). As the critical point is approached the correlation time diverges as \( \tau_c \sim \xi^z \), where \( \xi \) 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:

\[
H = -J \sum_{(n,m)_1} (S^x_{n,m} S^x_{n+1,m} + S^y_{n,m} S^y_{n+1,m}) - J' \sum_{(n,m)_2} (S^x_{n,m} S^x_{n,m+1} + S^y_{n,m} S^y_{n,m+1}) + D \sum_n (S^z_n)^2,
\]

where \( (n, m)_1 \) denotes a pair of nearest-neighbor spins in the same plane, and \( (n, m)_2 \) 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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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:

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

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

\[
H = \sum_q \left[ \rho \tilde{S}(1 - \gamma_q)\phi_q \phi_{-q} + (1 + D/3)S_n^z S_{-n}^z \right],
\]

where \( \tilde{S} = \sqrt{S(S + 1)} \), \( \gamma_q = \frac{1}{2}(\cos q_x + \cos q_y + \cos q_z) \) and the stiffness \( \rho \), renormalized by thermal and quantum fluctuations, is given by

\[
\rho = (1 - \langle (S_n^z)^2 \rangle) \exp \left[ -\frac{1}{2}(\phi_n - \phi_{-n})^2 \right].
\]

From Eq. (2) we obtain:

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

\[
\langle (S_n^z)^2 \rangle = \frac{\tilde{S}}{2\pi^2} \int_0^\pi \int_0^\pi \int_0^{2\pi} d\tilde{\mu} \sqrt{\frac{\rho(1 - \gamma_q)}{1 + D/3}} \coth \left( \frac{\omega_q}{2T} \right),
\]

\[
\langle \phi_q \phi_{-q} \rangle = \frac{1}{2\pi} \sqrt{\frac{(1 - D/3)}{\rho(1 - \gamma_q)}} \coth \left( \frac{\omega_q}{2T} \right).
\]

The SCHA yields a critical Néel 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 $S^z$:

$$|1\rangle = u^+ |v\rangle, \quad |0\rangle = t^+_z |v\rangle, \quad |-1\rangle = d^+ |v\rangle,$$

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

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

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

$$H = \frac{Jt^2}{2} \sum_{i,j} (d^+_i d_{i+\delta} + u^+_i u_{i+\delta} + u_i d_{i+\delta} + d^+_i u^+_{i+\delta} + H.c.)$$

$$+ \frac{J't^2}{2} \sum_{i,j} (d^+_i d_{i+\delta} + u^+_i u_{i+\delta} + u_i d_{i+\delta} + d^+_i u^+_{i+\delta} + H.c.)$$

$$+ D \sum_r (u^+_r u_r - d^+_r d_r)^2 - \mu \sum_r (u^+_r u_r + d^+_r d_r + t^2 - 1),$$

where we have introduced a temperature dependent constraint parameter $\mu$ 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

$$u^+_k = \tilde{u}_k \alpha_k - v_k \beta_k, \quad d^+_{-k} = -v_k \alpha_k + \tilde{u}_k \beta_k,$$

where

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

we obtain

$$H = \sum_k \omega_k (\alpha^*_k \alpha_k + \beta^*_k \beta_k) + \sum_k (\omega_k - \Lambda_k) + \mu N (1 - t^2),$$

with

$$\omega_k = \sqrt{\Lambda^2_k - \Delta_k^2}, \quad \Lambda_k = -D + t^2 F_k, \quad \Delta_k = t^2 F_k,$$

where

$$F_k = 2(\cos k_x + \cos k_y + \alpha \cos k_z).$$

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

$$G = N e_0 - \frac{2}{\beta} \sum_k \ln[1 + n(k)],$$

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

$$e_0 = \frac{1}{N} \sum_k (\omega_k - \Lambda_k) + \mu (1 - t^2).$$
Minimizing $G$ with respect to $\mu$ and $t^2$, we obtain the following self-consistent equations, which should be solved numerically:

$$
\mu = \frac{1}{\pi^3} \int_0^{\pi} \int_0^{\pi} \int_0^{\pi} F_k \, dk \, \coth \left( \frac{\beta \omega_k}{2} \right) \cdot 
$$

$$
(2 - t^2) = \frac{1}{2\pi^3} \int_0^{\pi} \int_0^{\pi} \int_0^{\pi} dk \left[ \frac{1}{\sqrt{1 + yF_k}} + \sqrt{1 + yF_k} \right] \coth \left( \frac{\beta \omega_k}{2} \right). 
$$

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

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

For $D > D_c$ the gap is given by

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

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:

$$
D_c = 4(2 + \alpha)(2 - I_1),
$$

where

$$
I_1 = \frac{1}{\pi^3} \int_0^{\pi} \int_0^{\pi} \int_0^{\pi} \frac{dk}{\sqrt{1 + y_c F_k}}.
$$

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

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

$$
m = a(D - D_c)^\beta.
$$

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:

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

where the parameters $c_0$, $c_1$ and $c_2$ depends on $D$ and $\alpha$. 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

$$
\omega_k = D + 2(\cos k_x + \cos k_y + \cos k_z),
$$

in agreement with a calculation using standard perturbation theory.
3. External magnetic field

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

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

At a critical magnetic field $h_{c1} = \omega_k^{(1)}$, 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]:

$$S^+ = \sqrt{2} u t_c, \quad S^- = \sqrt{2} u t_c^+, \quad S^z = 1 - t_c^+ t_c,$$

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

$$H = \sum_k \omega_k b_k^\dagger b_k + E_g, \quad (29)$$
where $t^+_z = (1/\sqrt{N}) \sum_k e^{-i\vec{k}\cdot\vec{r}} h^+_k$, and

$$\omega_k = h - (D + \mu) + 4|\vec{u}|^2 \gamma_k, \quad \gamma_k = \frac{1}{2} (\cos k_x + \cos k_y).$$

(30)

$$\epsilon_0 = E_g/N = D\vec{u}^2 - h - \mu \vec{u}^2 + \mu,$$

(31)

where we have considered here the case $\alpha = 0$. Minimizing $G = \epsilon_0 - T \sum_k \ln(1 + n_k)$ we arrive at

$$1 - \vec{u}^2 = \sum_k n_k,$$

(32)

$$D - \mu = -4|\vec{u}|^2 \sum_k \gamma_k n_k.$$  

(33)

At $T = 0$ we have $\vec{u}^2 = 1, \mu = D$. The minimum of the spin-wave spectrum occurs at $Q = (\pi, \pi)$. The condition $\omega_0 \equiv 0$ defines the critical field

$$h_{c2} = (D + \mu) + 4|\vec{u}|^2,$$

(34)

which leads, for small $k$, to

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

(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 $\mu_n$ 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$_2$4SC(NH$_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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References