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Quantum phase transition in the anisotropic one-dimensional XY model with long-range interactions

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ABSTRACT

In this paper we study the one-dimensional XY model with single ion anisotropy and long-range interaction that decay as a power law. The model has a quantum phase transition, at zero temperature, at a critical value D_c of the anisotropy parameter D. For values of D below D_c we use a self-consistent harmonic approximation. We have found that the critical temperature increases with D for small values of this parameter. For values of D above D_c we use the bond operator technique and calculate the gap as a function of D, at zero temperature.

It is very convenient to study quantum phase transition (QPT) in low-dimensional systems because by changing the interactions in the system one changes the amount of quantum fluctuations [1]. One interesting model to study QPT is the anisotropic XY model. The ground state of this model is not trivial; it shares many properties with the antiferromagnetic Heisenberg model. The model with short-range interaction has been well studied [2]. Here we will be interested in interactions that decay as power law. The phase diagrams for the two models are different. In the first case, the singularity in the free energy is present only at T=0 at a quantum critical point D=D_c. In the latter case there is a line of $T>0$ phase transition that terminates at D_c.

Long range interactions can be studied either for experimental reasons like dipolar or Ruderman–Kitell–Kasuya–Yosida interactions or simply because of theoretical interest. As pointed out by Laflorence [3], a theoretical interest comes from the possibility to interpolate between discrete dimensions by turning continuously the exponent that governs the decay of interactions with the distance. Long range interactions tend to suppress quantum as well as thermal fluctuations, thus increasing the range of interaction having an effect that is somewhat similar to increasing the dimensionality of the system.

For the one-dimensional Heisenberg and XY model with ferromagnetic interactions decaying as r^p, it has been shown [4–6] that an ordinary transition, at finite temperature, to a ferromagnetically ordered phase exists when $1<p<2$. The condition $p>1$ is needed in order to avoid a ground state with an infinite energy per spin. Thermal fluctuations destroy the order for $p\geq 2$ at any finite temperature.

We will start with the Hamiltonian:

$$H=-\sum_{n,m}J_{nm}(S_n^xS_m^x+S_n^yS_m^y)+D\sum_n(S_n^z)^2 \tag{1}$$

with J_{nm}=$J|n-m|^{-p}$. Due to the form of the single ion anisotropy we will take S=1. The spectrum of Hamiltonian (1) changes drastically as D varies from very small to very large values. The 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 excitations in this phase is a gaped S=1 exciton with an infinite lifetime at zero temperature. For small D, Hamiltonian (1) is in a gapless phase described by the spin wave theory.

The characteristic energy scale Δ of fluctuations above the ground state vanishes as D approaches D_c. In the large D phase, Δ is the energy of the lowest excitation above the ground state, this is, the energy gap. In the small D phase, Δ is the scale at which there is a qualitative change in the nature of the frequency spectrum from its lowest frequency to its higher frequency behavior. Here, $\Delta\propto\rho$, where ρ is the stiffness (to be introduced later) [1].

The small D phase can be studied using the self-consistent harmonic approximation (SCHA). The details are given in Ref. [7]. Introducing the Villain's representation:

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

and following Ref. [7] we obtain

$$H_0=\sum_q[aS_q^zS_{-q}^z+b(q)\phi_q\phi_{-q}], \tag{3}$$

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where

$$a = J(0) + D, \quad b(q) = \rho[J(0) - J(q)], \tag{4}$$

$$J(q) = \sum_{n,m} J_{nm} e^{-iq(n-m)}, \tag{5}$$

and the stiffness ρ, which takes into account quantum and thermal fluctuations, is given by [7]

$$\rho = (1 - \langle (S_n^z)^2 \rangle) \exp\left[-\tfrac{1}{2}\langle (\phi_n - \phi_{n+1})^2 \rangle\right]. \tag{6}$$

From Eq. (3) we obtain

$$\langle (S_n^z)^2 \rangle = \frac{\tilde{S}}{2} \frac{1}{\pi} \int_0^{\pi} \mathrm{d}q \coth\left(\frac{\omega(q)}{2T}\right), \tag{7}$$

$$\langle \phi_q \phi_{-q} \rangle = \frac{1}{2\tilde{S}} \sqrt{\frac{q}{b(q)}} \coth\left(\frac{\omega(q)}{2T}\right) \tag{8}$$

with the dispersion relation

$$\omega(q) = 2\tilde{S}\sqrt{ab(q)}, \tag{9}$$

where $\tilde{S} = \sqrt{S(S+1)}$.

Let

$$\eta(q) = [J(0) - J(q)]. \tag{10}$$

From Eq. (5) we obtain

$$J(0) = J \sum_{p=1}^{\infty} \frac{1}{n^p} = J\varsigma(p), \tag{11}$$

where $\zeta(p)$ is the Riemann zeta function. The limiting form of $\eta(q)$ as $q \to 0$ is given by [8]

$$\eta(q) \propto q^{\min[(p-1),2]}, \tag{12}$$

and so the long-wavelength spin wave spectrum, for $p < 2$, takes the form $\omega_q \propto q^z$, where the dynamical critical exponent z is given by $z=(p-1)/2$. For $p \geq 3$ the spin wave spectrum is linear in q and the behavior is essentially the same as the spin wave calculations for nearest-neighbor interactions only.

The critical temperature T_c, for $p < 2$, is given as the temperature where ρ vanishes [7]. In Fig. 1 we show T_c as a function of the anisotropy parameter D, for $p=3/2$, and we have taken $J=1$. We can estimate the critical anisotropy parameter as $D_c=10.65$. An interesting result of our calculation is the increase of T_c with D, for small values of D. This feature was also found in the 3D model [9].

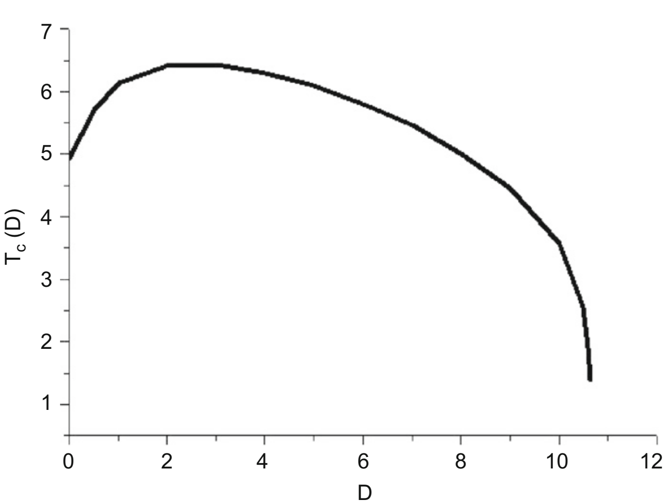

Fig. 1. The critical temperature T_c as a function of the anisotropy parameter D, for $D \leq D_c$ and $p=3/2$.

The in-plane magnetization M is given by

$$M = \exp\left[-\tfrac{1}{2}\langle (\phi_n)^2 \rangle\right]. \tag{13}$$

In Fig. 2, we show M as a function of D at zero temperature. As it is well known, the SCHA gives interesting information about the existence and location of critical points and reasonable values for critical temperatures, but one of its drawbacks is that it is not good for the evaluation of critical exponents. For instance, M drops discontinuously to zero at D_c.

An adequate method to treat the large D phase is the bond operator formalism, proposed by Wang and Wang [9] for $S=1$ and extended to finite temperatures by Pires and Gouvea [10]. The method has been used in two and three dimensions, but it can be extended to one dimension when we have long range order. In this formalism, three boson operators are introduced to denote the three eigenstates of S^z:

$$|1\rangle = u^+|v\rangle, \quad |0\rangle = t_z^+|v\rangle, \quad |-1\rangle = d^+|v\rangle, \tag{14}$$

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

$$S^+ = \sqrt{2}(t_z^+ d + u^+ t_z), \quad S^- = \sqrt{2}(d^+ t_z + t_z^+ u), \quad S^z = u^+ u - d^+ d, \tag{15}$$

with the constraint $u^+u+d^+d+t_z^+t_z=1$. In the large D phase we can assume that the t_z bosons are condensed and write $\langle t_z^+ \rangle = \langle t_z \rangle = t$. In this approximation we obtain:

$$H = \frac{t^2}{2} \sum_{n,m} J_{nm}(d_n^+ d_m + u_m^+ u_n + u_n d_m + d_n^+ u_m^+ + h.c.) + D\sum_n (u_n^+ u_n - d_n^+ d_n)^2 - \mu \sum_n (u_n^+ u_n + d_n^+ d_n + t^2 - 1), \tag{16}$$

where we have introduced a temperature dependent constraint parameter μ to enforce the condition of single occupancy.

Taking the Fourier transform, performing a Bogoliubov transformation and minimizing the free energy we obtain, following Refs. [9–11] where all the details of the calculation are presented, the following expression for the exciton energy:

$$\omega_q = (-\mu + D)\sqrt{1 + yf(q)}, \tag{17}$$

where

$$y = \frac{4t^2}{-\mu + D}, \quad t^2 = 2 - \frac{1}{2}(I_1 + I_2), \quad \mu = \frac{2}{y}(I_2 - I_1), \tag{18}$$

$$I_1 = \frac{1}{\pi}\int_0^{\pi} \frac{\mathrm{d}q}{\sqrt{1 + yf(q)}}, \quad I_2 = \frac{1}{\pi}\int_0^{\pi} \mathrm{d}q \sqrt{1 + yf(q)} \tag{19}$$

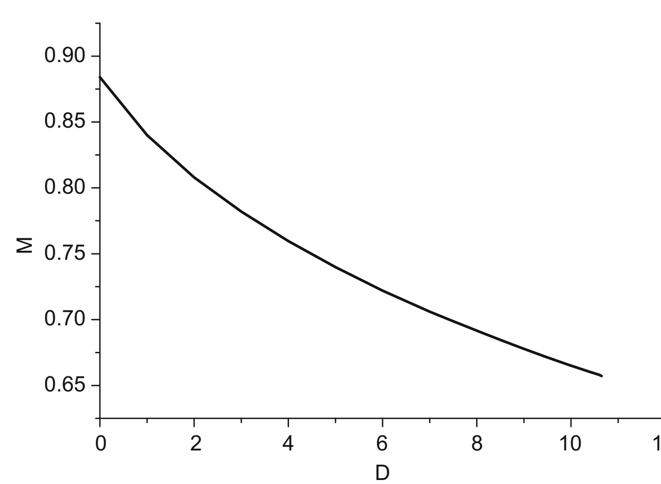

Fig. 2. The magnetization M as a function of D, for $D \leq D_c$.

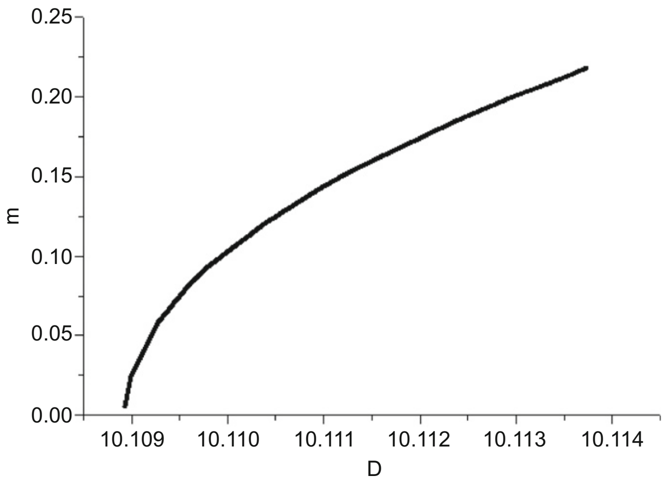

Fig. 3. The gap m, at T=0, as a function of D, for $D \geq D_c$, and p=3/2.

and

$$f(q) = \sum_{n=1}^{\infty} \frac{1}{n_p} \cos nq. \tag{20}$$

The energy gap, with J=1, is given by

$$m = (-\mu + D)\sqrt{1 - yf(0)}. \tag{21}$$

When $yf(0) \rightarrow 1$, the energy gap goes to 0, indicating a transition from the large D phase to the ordered phase. For p=3/2, we have obtained $D_c \approx 10.11$. This value is smaller than the one obtained using the SCHA. We believe this value is more reliable, since the bond operator technique is more suitable to treat the large D phase. In Fig. 3 we show the gap m as a function of the anisotropy parameter D. As D approaches D_c from above, the energy gap vanishes as $m \propto (D - D_c)^{\alpha}$, with $\alpha \approx 1.9$

In conclusion, we have studied the one-dimensional XY model with single ion anisotropy D and long range interaction decaying as a power law. In the small D phase we have used a self-consistent harmonic approximation and in the large D phase a bond operator technique. The phase diagram of the model for p=3/2 was obtained. Of course the SCHA is not very adequate, in one dimension, for short-range interaction. However, it is believed that it becomes asymptotically exact at large distance for long-range interaction. We remark that in the classical limit and D=0 the calculations using the SCHA are in good agreement with Monte Carlo simulations [12]. Since the quantum case at zero temperature and dimension d can be mapped to a classical model with dimension d+1 and finite temperature, the result should be even better for the quantum model. It is interesting to mention that in three dimensions, for the nearest-neighbor model, one has [9] $D_c \approx 10.48$, near the value obtained for the model studied in the present paper.

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