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The phase diagram and critical properties of the two-dimensional anisotropic XY model

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Abstract
In this paper we present a study of the phase diagram and critical properties of the square-lattice quantum XY model, with a single-ion anisotropy and spin $S = 1$, as a function of the anisotropy parameter D. For D less than a critical value D_C, which is the critical point for a quantum phase transition at $T = 0$, the model presents a Berezinskii–Kosterlitz–Thouless (BKT) transition. This region is adequately described by the self-consistent harmonic approximation. We show that, if we want to use a Schwinger boson theory in this region, we should include fluctuations around the mean-field approximation (which leads to a gauge field) to describe correctly the BKT transition. However both methods are inadequate to describe the large-D phase, and we show that this phase can be studied using the bond operator formalism which gives the correct behaviour for the correlation length as a function of the temperature in the critical point and above. Our results agree with scaling arguments.

1. Introduction

In the last decade considerable interest has been concentrated on quantum phase transitions (QPT). These transitions occur at zero temperature when a nonthermal parameter like pressure, chemical composition or magnetic field is varied [1, 2]. The effects of quantum criticality, different from the classical case, might be observed at high temperatures. This is, in many cases, the signature of a quantum critical point might extend to high temperatures. QPT are believed to provide keys to many new and exciting phenomena in condensed matter physics [3] and thus it is important to study the problem analytically. So far, only the simplest, and the most obvious cases have been studied in detail. One model where QPT can be well understood is the two-dimensional anisotropic quantum XY model described by the following Hamiltonian:

$$H = J \sum_{\langle n,m \rangle} (S_n^x S_m^x + S_n^y S_m^y) + D \sum_n (S_n^z)^2, \qquad (1)$$

where $\langle n, m\rangle$ represents the sum over nearest neighbours on the sites, n, of a regular lattice and $0 \leqslant D < \infty$. We consider the antiferromagnetic case given the present importance of this model. However, the Hamiltonian (1) is invariant under the transformation $J \to -J$, and a shift of the Brillouin zone $k \to k + \pi$. Due to the form of the single-ion anisotropy we should have $S > 1/2$ and so we take $S = 1$. For D less than a critical value D_C, the system has a thermal phase transition at a temperature T_{BKT}, the Berezinskii–Kosterlitz–Thouless temperature. This is another reason why this model is so interesting to study. This phase transition is associated with the emergence of a topological order, resulting from the pairing of vortices with opposite circulation. The BKT mechanism does not involve any spontaneous symmetry-breaking and emergence of a spatially uniform order parameter. The low-temperature phase is associated with a quasi-long-range order, at finite temperature, with the correlation of the order parameter decaying algebraically in space. Above the critical temperature the correlation decays exponentially. This picture is applicable to a wide variety of two-dimensional phenomena [4]. A recent experiment in a trapped atomic gas [5] not only confirms the BKT theory in a new system, but also reveals for the first time the role played by local topological defects or vortices.

For strong planar anisotropy in the Hamiltonian (1) we have the so called large-D phase. This phase consists of a unique ground state with total magnetization $S^z_{\text{total}} = 0$

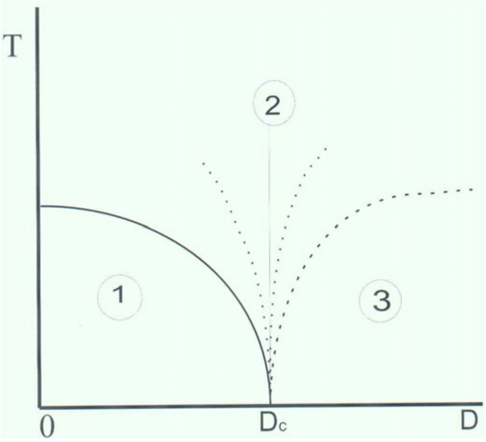

Figure 1. Phase diagram of the model described by the Hamiltonian (1) as a function of the anisotropy parameter D and temperature T. The solid line in region (1) describes the BKT transition. There is a quantum phase transition at $T = 0$, $D = D_C$. Region (2) is the critical region where $\xi \propto T^{-1}$. There is an energy gap above the ground state for $D > D_C$.

separated by a gap from the first excited states which lie in the sectors $S^z_{\text{total}} = \pm 1$. The elementary excitations are *excitons*, with $S = 1$ and an infinite lifetime at low energies. For small D the Hamiltonian (1) is in a gapless phase well described by the spin wave formalism. The increase of the anisotropy parameter D reduces the transition temperature and at D_C the phase vanishes. Thus, at D_C the system undergoes a QPT, at $T = 0$, from a gapless to a gapped phase.

The phase diagram for the Hamiltonian (1) is expected to be as shown qualitatively in figure 1. In the continuum limit the Hamiltonian (1) is equivalent to the Hamiltonian describing the quantum rotor model and the phase diagram for this model was studied by Phillips [6], using the mean-field approximation. The solid line in figure 1 represents the line of critical points, determined by the BKT transition, that terminates at the critical point D_C. Below this line, the inverse correlation length, ξ^{-1}, vanishes. The mean-field theory, however, fails to give the BKT transition. The dashed line represents a crossover from the quantum critical region (where $\xi^{-1} \propto T$), to a region where quantum fluctuations dominate ($\xi^{-1} \gg T$). The aim of the present paper is to study the phase diagram of figure 1, using several methods.

The region $D \leqslant D_C$ has been well studied in the literature [8]. Starting with the Villain representation [7]:

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

using the semi-classical approach, taking the continuum limit of the Hamiltonian, and using a self-consistent harmonic approximation (SCHA) to take into account thermal and quantum fluctuations, the region $D \leqslant D_C$ in figure 1 was well described. The calculation is presented in [8]. The existence, nature, and the location of the transition was reasonably well established. The critical point was estimated as $D_C = 3.6$. An interesting fact is that the BKT transition can not be correctly obtained when we use only the harmonic Hamiltonian, since, as was said before, it is caused by topological excitations (unbinding of vortex–antivortex pairs) [9]. However, the behaviour of the spin correlation function is correctly given by the harmonic Hamiltonian using the expression:

$$\langle (S_0^x S_r^x + S_0^y S_r^y)\rangle \approx \langle [S(S+1) - (S_r^z)^2]\rangle \langle \cos(\varphi_0 - \varphi_r)\rangle$$
$$= \langle [S(S+1) - (S_r^z)^2]\rangle \exp\left[-\tfrac{1}{2}\langle(\varphi_0 - \varphi_r)^2\rangle\right]. \quad (3)$$

This happens because in (3) we have effectively bypassed the higher order perturbative theory.

In section 2 we present the Schwinger boson (SB) representation for Hamiltonian (1), and show how fluctuations around the mean-field approximation lead to a BKT transition. In section 3 we study the large-D phase and in section 4 we present our conclusions.

2. Schwinger boson representation

In this section we use the Schwinger boson representation, introduced by Arovas and Auerbach [10], to study the Hamiltonian (1). This formalism has been shown to be very successful in describing magnetism in various quantum systems. Qualitatively correct results are mostly obtained even in the mean-field approximation. As pointed out by Timm and Jensen [11] there are basically two reasons why the Schwinger boson mean-field theory (SBMFT) works well even in low dimensions: (i) since the bosonized spin degrees of freedom are integrated over in the functional integral, spin fluctuations are taken into account and (ii) the approach does not constitute an expansion around an ordered state, and thus works for both ordered and disordered ground states. Some papers where the SBMF was used to treat anisotropic models are listed below. The thermodynamic properties of the quantum XXZ model were studied by De Leone *et al* [12] in one dimension and by Fukumoto [13] in two dimensions. However, the model treated by these authors, where an exchange anisotropy is present, does not have a large-D phase. Cheng *et al* [14] studied the persistent spin current in an anisotropic spin ring (XXZ model) penetrated by a $SU(2)$ flux. Jiang *et al* [15] considered the effect of single-ion anisotropy on the Heisenberg antiferromagnetic chain and Xing *et al* [16] treated the field-induced transition in the antiferromagnetic chain with single-ion anisotropy in a transverse magnetic field. Here we treat, for the first time, the XY model with a single-ion anisotropy.

In the Schwinger boson representation [10, 17] the spin operators $\boldsymbol{S}_i$ are replaced by the bosons a_i and b_i at each site i as follows:

$$S_i^+ = a_i^+ b_i, \qquad S_i^- = a_i b_i^+, \qquad S_i^z = \tfrac{1}{2}(a_i^+ a_i - b_i^+ b_i), \quad (4)$$

with the constraint that only $2S$ bosons can occupy each site:

$$a_i^+ a_i + b_i^+ b_i = 2S. \quad (5)$$

We assume that the lattice is bipartite and that there is no frustration. On one sublattice we make the unitary transformation $a \to -b$, $b \to a$, i.e., $S^+ = -ab^+$, etc. Now we write (1) as:

$$H = -\frac{1}{2}\sum_{\langle i,j\rangle}(a_i^+ a_j b_i b_j^+ + a_i a_j^+ b_i^+ b_j) + \frac{D}{4}\sum_i (a_i^+ a_i - b_i^+ b_i)^2. \quad (6)$$

Following [12] we introduce the bond variables

$$A_{ij} = a_i^+ a_j + b_i^+ b_j, \qquad B_{ij} = a_i b_j + b_i a_j, \quad (7)$$

and rewrite the Hamiltonian (6) as

$$H = -\tfrac{1}{4}\sum_{\langle ij\rangle}(A_{ij}^+ A_{ij} + B_{ij}^+ B_{ij}) + \frac{D}{2}\sum_i (a_i^+ a_i a_i^+ a_i + b_i^+ b_i b_i^+ b_i) + \sum_i \lambda_i (a_i^+ a_i + b_i^+ b_i - 2S), \quad (8)$$

where the constraint on the number of bosons is enforced by the Lagrangian multiplier λ_i. In writing (8) we have neglected constant terms. Using a path integral representation, we perform a Hubbard–Stratonovich transformation [10] using the bond variables A_{ij} and B_{ij}, and the on-site coupling $P = \langle a_i^+ a_i\rangle = \langle b_i^+ b_i\rangle$. We chose A_{ij}, B_{ij}, and λ_i to be static and assume the spatially uniform values A, B and λ respectively. In the mean-field approximation, following the steps presented in [12] we obtain the saddle point equations:

$$\left(S + \frac{1}{2}\right) = \frac{1}{2N}\sum_k \frac{R_k}{\omega_k}\coth\left(\frac{\beta\omega_k}{2}\right), \quad (9)$$

$$A = \frac{1}{4N}\sum_k \gamma_k\left[1 - \frac{R_k}{\omega_k}\coth\left(\frac{\beta\omega_k}{2}\right)\right], \quad (10)$$

$$B = \frac{1}{4N}\sum_k \frac{\gamma_k T_k}{\omega_k}\coth\left(\frac{\beta\omega_k}{2}\right), \quad (11)$$

$$P = \frac{D}{8N}\sum_k \frac{R_k}{\omega_k}\coth\left(\frac{\beta\omega_k}{2}\right), \quad (12)$$

where

$$R_k = \gamma_k A z + \lambda - 2P, \qquad T_k = \gamma_k B z, \qquad \gamma_k = \frac{1}{z}\sum_\delta e^{i\vec{k}\cdot\vec{\delta}}, \quad (13)$$

and

$$\omega_k = \sqrt{R_k^2 - T_k^2}. \quad (14)$$

Here z is the coordination number and $\vec{\delta}$ indexes the nearest neighbours. From equations (9) and (11) we obtain

$$P = \frac{D}{4}\left(S + \frac{1}{2}\right). \quad (15)$$

Following [13] we assume that part of the magnons are condensed at $k = \pi$. To take into account the Bose condensation we replace the point $k = \pi$ with a parameter m_x and write equation (9) at $T = 0$ as:

$$\left(S + \frac{1}{2}\right) = m_x + \frac{1}{2}\left(I_0 + \frac{I_1}{2}\right), \quad (16)$$

where

$$I_n = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \frac{\gamma_k^n\, d\vec{k}}{\sqrt{1+\gamma_k}}. \quad (17)$$

We find, for $S = 1$, $m_x = 0.94$. This parameter m_x has a meaning of a long-range order parameter and the long-range order lies in the xy-plane.

Defining $\tilde{\lambda} = \lambda - 2P = \lambda - 3D/4$, where we have taken $S = 1$, we find that our results are similar to the ones for the isotropic XY model with a renormalized $\tilde{\lambda}$ parameter. Since, for this model [13], $A \approx B$, we will take $A = B$ and write the magnon frequency as

$$\omega_k = \tilde{\lambda}\sqrt{1 + \eta\gamma_k}, \quad (18)$$

where $\eta = 2Az/\tilde{\lambda}$. Numerical calculations give $\eta = 1$, $\tilde{\lambda} = 4$. Thus the SBMFT gives results similar to the ones obtained using the linearized spin wave theory. The correlation length ξ calculated using the SBMFT is finite for $T > 0$, even in the case $D = 0$, and therefore the theory cannot predict the BKT transition, and neither the critical point D_C.

Now we try to understand the limitations of the SBMFT. In a path integral formalism, as discussed by Tsvelik [18], we can write

$$a = \sqrt{2S}\exp[i(\psi + \varphi)/2]\cos(\theta/2), \qquad b = \sqrt{2S}\exp[i(\psi - \varphi)/2]\sin(\theta/2). \quad (19)$$

Tsvelik has shown that using the above representation, the Heisenberg antiferromagnetic model maps into the nonlinear sigma model with the topological term. The transformation (19) is equivalent, in the semi-classical limit, and in a path integral formulation, to the Villain representation (in the classical limit). Considering this result, the question is: why the SBMFT has failed? We try to answer this question. One way to improve the mean-field calculation is to include the fluctuations around the mean-field result. So, in the following, we will consider the effects of these fluctuations.

The action for the Hamiltonian (8) is given by [10, 12]:

$$S = \int_0^\beta d\tau\Big\{\frac{1}{2}\sum_i [a_i^+(\tau)\partial_\tau a_i(\tau) - \partial_\tau a_i^+(\tau)a_i(\tau) + b_i^+(\tau)\partial_\tau b_i(\tau) - \partial_\tau b_i^+(\tau)b_i(\tau)] + \sum_{\langle i,j\rangle}[4(A_{ij}^+ A_{ij} + B_{ij}^+ B_{ij}) + (A_{ij}^+ A_{ij} + A_{ij}^+ A_{ij} + B_{ij}^+ B_{ij} + B_{ij}^+ B_{ij})] + \sum_i \lambda_i (a_i^+ a_i + b_i^+ b_i - 2S)\Big\}, \quad (20)$$

where τ is the imaginary time and we have here, for simplicity, considered the isotropic XY model.

When we ignore the fluctuations of A, B and λ the excitations around the zeroth-order mean-field state are free bosons. This leads to the SBMFT discussed above [10]. In the following we will consider the effects of fluctuations in A, B and λ which describe the collective excitations above the mean-field ground state. Here, we will only consider the phase fluctuations a_{ij} around the mean-field solution as follows:

$$A_{ij} = \tilde{A}e^{-ia_{ij}}, \qquad B_{ij} = \tilde{B}e^{-ia_{ij}}. \quad (21)$$

Taking the above expressions into equation (20) it is easy to see that the action is invariant under the gauge transformation:

$$a_{ij} \to a_{ij} + (\theta_i - \theta_j), \qquad a_i \to a_i e^{i\theta_i}, \qquad b_i \to b_i e^{i\theta_i}. \tag{22}$$

Let us review briefly the concept of local gauge invariance in quantum electrodynamics. A change of gauge in a charged field ψ, coupled to the electromagnetic field, means a change of phase given by $\tilde{\psi} = \exp(i\alpha)\psi$. To preserve invariance one notices that in electrodynamics it is necessary to counteract the variation of α with the position $\mathbf{r}$, by introducing the electromagnetic field A_μ which changes under a gauge transformation as

$$\tilde{A}_\mu = A_\mu + \frac{1}{e}\partial_\mu\alpha, \tag{23}$$

where e is a constant, taken as the electron charge. The details can be found in any book of quantum field theory. The situation in equations (21) and (22) is somewhat similar to Abelian electrodynamics [19] and we can identify the field a_μ with a vector potential. Notice that here we have a lattice gauge field where $(\theta_i - \theta_j)$ replaces $\partial_\mu\theta$. The 'charged particles' of this two-dimensional gauge field can be associated with the 'vortices' of the XY model which interact through a logarithmic potential. As was shown by Minnhagen [20], a two-dimensional gas of Coulomb particles interacting through a logarithmic potential has a BKT transition. Thus we have shown that when we consider the fluctuations around the mean-field ground state the SB theory leads to the correct picture.

3. Large-D phase

Up to now we have shown that, for $D < D_C$, the SCHA gives reliable results for the phase diagram, and that we should include fluctuations in the SBMFT to get the correct results in this region. However, both methods fail for $D > D_C$, and at the critical point, $D = D_C$, for $T > 0$. Of course we could map the 2D quantum model into the 3D classical model [21], but this procedure gives information only at $T = 0$. The large-D phase is best studied using the bond operator formalism proposed by Wang and Wang [22] for $S = 1$, where three boson operators were introduced to denote the three eigenstates of S^z:

$$|1\rangle = u^+|v\rangle, \qquad |0\rangle = t_z^+|v\rangle, \qquad |-1\rangle = d^+|v\rangle, \tag{24}$$

where $|v\rangle$ is the vacuum state. Although a mean-field approximation is also used here the method predicts correctly a quantum phase transition. In the low D region the bond operator method gives results equivalent to the linearized spin wave theory. As pointed out by Lu *et al* [23] the starting point in the bond operator formalism is the large-D limit. Thus we can see why the method seems more appropriated to describe the strong coupling regime. For the Hamiltonian (1) the self-consistent equations presented in [22] become

$$\mu = \frac{z}{\pi^2}\int_0^\pi\int_0^\pi \frac{\gamma_k\, d\vec{k}}{\sqrt{1+y\gamma_k}}\coth\left(\frac{\beta\omega_k}{2}\right), \tag{25}$$

$$2(2-t^2) = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi d\vec{k}\left[\frac{1}{\sqrt{1+y\gamma_k}} + \sqrt{1+y\gamma_k}\right] \times \coth\left(\frac{\beta\omega_k}{2}\right), \tag{26}$$

$$\omega_k = (-\mu + D)\sqrt{1+y\gamma_k}, \tag{27}$$

where $y = 2zt^2(-\mu + D)^{-1}$. The value of D_C, where the energy gap goes to zero, obtained using the bond operator method is $D_C = 5.72$. This value is larger than previous estimates. We believe that this value is more reliable, since the method used here is more suitable to treat the large-D phase.

Here we concentrate only in new results presented below and refer the reader to [22] for more details. At low temperatures the integrals in the above equations can be evaluated analytically using the procedure presented by Takahashi [24]. Using

$$\omega(x) = \frac{2}{N}\sum_k \delta(x - \gamma_k), \tag{28}$$

we find

$$\int \frac{d\vec{k}}{(2\pi)^2}\frac{1}{\sqrt{1-y\gamma_k}}\coth\left(\frac{\beta\omega_k}{2}\right) = I_0 + \frac{T\omega(1)}{\tilde{D}}\ln\left[\frac{T^2}{\tilde{D}^2(1-y)}\right], \tag{29}$$

$$\int \frac{d\vec{k}}{(2\pi)^2}\frac{\gamma_k}{\sqrt{1-y\gamma_k}}\coth\left(\frac{\beta\omega_k}{2}\right) = I_1 - 12\omega(1)\zeta(3)\left(\frac{T}{\tilde{D}}\right)^3, \tag{30}$$

where $\tilde{D} = -\mu + D$ and $\zeta(x)$ is the zeta function. Using the above expressions and a little algebra we find for the gap at $D = D_C$

$$\Delta = \omega_{k=\pi} \propto T. \tag{31}$$

So, the inverse correlation length scales linearly with temperature, in agreement with the analysis of scaling dimensions at a quantum critical point [1]. Directly above D_C, the dynamics are controlled by thermal fluctuations. This regime is referred to as *quantum critical*. In this regime, quasi-particle excitations are not well defined. For $D > D_C$, the correlation length reach a finite value as $T \to 0$, leading to a quantum paramagnetic ground state with no long-range order. As D approaches D_C from above, the energy gap vanishes as $\Delta \propto (D - D_C)$, also in agreement with scaling arguments [1].

We have also solved equations (25) and (26) numerically, and obtained

$$\Delta = 1.22(D - D_C), \tag{32}$$

at $T = 0$, and

$$\Delta = \Delta_0 + c_1 T^{1/2}\exp(-c_2/T), \tag{33}$$

for $D > D_C$. Here c_1 and c_2 are constants which depend on D. The ground state, as expected, has a gap, and nonzero T induces an exponentially small density of thermally excited excitons. Equation (33) has the same form as the one presented by Sachdev [1] for the Ising chain in a transverse field in the quantum paramagnetic side. This confirms the universal behaviour of the model studied here.

4. Conclusions

For D less than a critical value D_C (which is the critical point for a quantum phase transition at $T = 0$) the model described by the Hamiltonian (1) presents a Berezinskii–Kosterlitz–Thouless (BKT) transition. This region is adequately described by the self-consistent harmonic approximation. We have shown that, if one wants to use a Schwinger boson theory to study this region, one should include fluctuations around the mean-field approximation (which leads to a gauge field) to describe correctly the BKT transition. Finally, we have shown also that the large-D phase can be best studied using the bond operator formalism, which is more suited to this phase and gives the correct behaviour for the correlation function as a function of the temperature in the critical point and above. We have a crossover from the quantum–critical region where $\Delta \propto T$, to the disordered regime where quantum fluctuations dominate. Thus, to explain the phase diagram of the model, for all positives values of D, we have to use different methods.

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