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Phase diagram in the quantum XY model with long-range interactions

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Abstract. We study the d-dimensional quantum XY model with ferromagnetic long-range interaction decaying as r^{-p} in terms of boson operators, by employing the coherent state path integral approach. We have obtained a finite critical temperature as a function of the dimension (d) for $d < p < 2d$. For $p > 2d$ the system becomes disordered at all temperatures. For the particular values $p = 3/2$ and $d = 1$ our theoretical calculations are comparable to those from Monte Carlo simulations.

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1 Introduction

In recent years, extensive attention has been applied to on the investigation of low-dimensional magnetism. It has been proved by Mermin and Wagner [1] that the one- and two-dimensional isotropic Heisenberg and XY models with short-range interaction do not present any spontaneous magnetization at any finite temperature ($T > 0$). The Mermin-Wagner theorem has been recently generalized by Bruno [2] to include long-range exchange interactions decreasing as $J_{ij} = \frac{J}{r_{ij}^p}$ (r_{ij} is the distance between sites) and it has been shown that for $p \geq 2d$ (d is the dimension of the lattice) the Heisenberg and XY models cannot be ferromagnetic, where the condition $p > d$ is needed in order to avoid a ground state with an infinite energy per spin. For the parameter $p \in (d, 2d)$ a ferromagnetic ordered phase exists [3]. In the case of the Ising model, where we have a discrete broken symmetry, the ordered phase survives for $p \in (d, 2d)$. For $p = 2$ the spontaneous magnetization of the one-dimensional Ising model is discontinuous at $T = T_c(p = 2)$ (the so-called Thouless effect) [5].

Long-range interactions are always of interest in different fields of physics because they can give rise to a variety of unusual macroscopic behavior, the best example in condensed matter being the dipole-dipole interaction ($p = 3$). It is well known that the long-range nature of interactions can drastically modify the critical behavior in low-dimensional classical and quantum systems. Using the Onsager reaction field theory on the one-dimensional Heisenberg and XY models, Pires has shown [7] that for $1 < p < 2$ the critical temperature T_c is finite ($T_c > 0$). For $p > 2$ these models are disordered at finite temperatures (i.e., $T_c = 0$). On the other hand, the borderline case $p = 2$ of the one-dimensional planar rotator system presents a transition to a phase with a slow decrease of correlation functions and an infinite susceptibility (Kosterlitz-Thouless-like transition-KTLT) [8]. This KTLT has been obtained in the framework of the harmonic approximation [8,9] and a self-consistent harmonic approximation [10]. In the region $p \in (0, d)$ the systems are nonextensive [11], where the best known examples are the gravitational N-body problem, black holes and superstrings, Lévy-like and correlated like anomalous diffusion, two-dimensional turbulence, granular matter, such as sandpiles, etc. These systems have been investigated in the context of mean field theory and generalized thermostatistics [11]. New methods have been proposed to study nonextensive spin systems in the framework of the generalized thermostatistics, such as renormalization group [12], the broad histogram Monte Carlo method [13] and the two-time Green's function technique [14]. However, all the above theoretical results are related to Boltzmann-Gibbs statistics ($p > d$).

Our work is organized as follows. In Section 2, we introduce the model and theoretical technique. The results of the phase diagram and discussions are presented in Section 3. We conclude in Section 4 with a summary of the results.

2 Model and formalism

In this paper we will study the d-dimensional quantum XY model with long-range ferromagnetic interaction described

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by the Hamiltonian

$$\mathcal{H} = -\sum_{n,m} J_{nm} \left(S_n^x S_m^x + S_n^y S_m^y \right) - H \sum_n S_n^x, \qquad (1)$$

with

$$J_{nm} = \frac{J}{|\overrightarrow{n} - \overrightarrow{m}|^p}, \qquad (2)$$

where S_l^α is the $\alpha(= x, y)$ component of the spin operator at site l and H the magnetic field. Notice that as $p \to \infty$ the model described by equation (1) approaches the nearest-neighbor model, which for $d = 1, 2$ has no order-disorder transition, but a transition to a low-temperature phase possessing infinite susceptibility and asymptotic power-law decay for the correlation function, the so-called Kosterlity-Thouless transition (KT) [15].

In the boson language, the spin operators in each lattice site are replaced by the boson creation a_i^+ and annihilation a_i operators (i.e., $S_j^+ = S_j^x + iS_j^y = \sqrt{2S}a_j^+$ and $S_j^- = S_j^x - iS_j^y = \sqrt{2S}a_j$) [16] with commutation relation $\left[a_i, a_j^+\right] = \delta_{ij}$. Therefore, the Hamiltonian (1) in the boson space can be rewritten as

$$\mathcal{H} = -2S \sum_{n,m} J_{nm} a_n^+ a_m + 2S\mu \sum_{n=1}^N a_n^+ a_n - \mu S^2 N - H\frac{\sqrt{2S}}{2} \sum_{n=1}^N (a_n^+ + a_n), \qquad (3)$$

where N is the total number of sites, μ is a Lagrange multiplier to impose the spherical constraint in the spin space: $\sum\limits_{i=1}^N \left[(S_i^x)^2 + (S_i^y)^2 \right] = NS(S+1)$, which in terms of bosons becomes a mean hard-core boson constraint

$$\sum_{n=1}^N a_n^+ a_n = \frac{NS}{2}. \qquad (4)$$

The Hamiltonian (3) is an extended hard-core boson system with boson hopping J_{nm} and chemical potential μ, that has been studied in the context of a superfluid-Mott insulator transition [17]. Superfluidity in the boson model described in equation (3) corresponds to the magnetization in the XY plane. The condition (4) implies that the boson number $n_i = a_i^+ a_i$ could take on any value between 0 and ∞ (not just 0 or 1), subject only to the so-called mean hard-core boson constraint (4), like the original concept of the spherical model in the spin space [18].

Following the procedure used in reference [16] we obtain the Fourier transform of the Hamiltonian (3) with the constraint (4)

$$\mathcal{H} = \sum_k w_k a_k^+ a_k - \frac{H\sqrt{2S}}{2} \sum_k (a_k^+ + a_k) - \mu S^2 N, \qquad (5)$$

where a_k^+, a_k are the corresponding Fourier transforms of the boson operators and the dispersion relation is given by

$$w_k = 2S(\mu - J_k), \qquad (6)$$

with

$$J_k = \sum_{n,m} J_{nm} e^{i\overrightarrow{k}.(\overrightarrow{n} - \overrightarrow{m})}. \qquad (7)$$

The partition function $Z = \mathrm{Tr}e^{-\beta\mathcal{H}}$ is obtained using the coherent state functional integral representation in the Matsubara imaginary time formulation [19]. After integrating over the bosonic variables, the free energy per site, $f = -\frac{1}{\beta N} \ln Z$, is given by

$$f = \frac{1}{\beta N} \sum_k \ln \left(2 \sinh \frac{\beta w_k}{2} \right) - \frac{H^2}{4(\mu - J_o)} - \mu S(S+1), \qquad (8)$$

where $\beta = 1/k_B T$. The Lagrange multiplier μ is determined by minimizing the free energy, i.e., $\frac{\partial f}{\partial \mu} = 0$. The constraint (4) then becomes

$$\frac{S}{N} \sum_k \coth \frac{\beta w_k}{2} + \frac{H^2}{4(\mu - J_o)^2} = S(S+1), \qquad (9)$$

from which the parameter μ is determined.

The magnetization M defined by $M = -\frac{\partial f}{\partial H} = -\frac{H}{2(\mu - J_o)^2}$ is obtained from equation (8) and reads

$$M^2 = S(S+1) - \frac{S}{N} \sum_k \coth \frac{\beta w_k}{2}. \qquad (10)$$

The above equation shows a zero-temperature magnetization $M(T = 0) = S$, which is the expected result. The excitation energy spectrum $w_k = 2S(\mu - J_k)$ exhibits an energy gap $\Delta = 2S(\mu - J_o)$. Below a critical temperature T_c, long-range ferromagnetic order is achieved as a result of the Bose-Einstein condensation of the bosons. The second-order phase transition ($H = 0$) occurs when the energy gap Δ vanishes, and the Lagrange multiplier μ is given at $T = T_c$ by

$$\mu_c = J_o. \qquad (11)$$

The critical region ($T \simeq T_c$) is dominated by the long wavelength limit ($k \simeq 0$). Thus, substituting (11) in equation (10), expanding the $\coth x$, we obtain the critical temperature T_c

$$k_B T_c = \frac{S(S+1)}{I(p,d)}, \qquad (12)$$

with

$$I(p,d) = \frac{1}{N} \sum_k \frac{1}{J_o - J_k}. \qquad (13)$$

3 Results and discussion

In the thermodynamic limit $N \to \infty$, we can replace the summation in equation (13) by the integral $\int\limits_\Gamma \frac{d^d \overrightarrow{k}}{(2\pi)^d}$, where Γ denotes the first Brillouin zone. For small k (infrared behavior) and $d < p < 2d$ we have the behavior for $d = 1, 2$ [20]

$$w_k = J_o - J_k = A(p,d) k^{p-d}, \qquad (14)$$

with

$$A(p,d) = \frac{\pi^d d^{d-p}}{2\left[(p-1)!\right]^d \sin\left[\frac{\pi(p-d)}{2}\right]}. \qquad (15)$$

The critical temperature is finally given by

$$\frac{k_B T_c}{J} = \frac{S(S+1)(\frac{d}{2})!(2d-p)2^{d-1}}{\pi^{d/2-p} d^{p-d+1}\left[(p-1)!\right]^d \sin\left[\frac{\pi(p-d)}{2}\right]}. \qquad (16)$$

Using equation (16), the critical temperature near $p = 2d - \lambda$ ($\lambda \to 0^+$) can be estimated for $d = 1, 2$ as

$$\frac{k_B T_c(\lambda)}{J} \simeq S(S+1)B(d)\frac{\lambda}{\left[\sin(\frac{\pi d}{2}) - \lambda\cos(\frac{\pi d}{2})\right]}, \qquad (17)$$

where $B(d) = \frac{(\frac{d}{2})! 2^{d-1}\pi^{3d/2}}{d^{1+d}[(2d-1)!]^d}$.

To compare with results of the one-dimensional planar rotator (classical XY model), we renormalize $\frac{k_B T_c}{J}$ as $t_c = \frac{k_B T_c}{JS(S+1)}$. For the particular case $p = 3/2$, the numerical value for the critical temperature found from (16) is $t_c = 2.22$ (same value obtained by numerical solution of the Eqs. (12) and (13)), which is in quite good accordance with $t_c = 2.16 \pm 0.01$ obtained by Monte Carlo simulation [9]. In particular, for $d = 1$ in equation (7) we have that t_c approaches to zero as

$$t_c(p) \simeq \frac{\pi^2}{2}(2-p). \qquad (18)$$

The above result is in agreement with that of the Green's function theory [21] in the one-dimensional Heisenberg model, except for an overall factor of 1/3.

On the other hand, by analyzing equation (17) for the two-dimensional XY model we observe a discontinuity in the critical temperature at $p = 2d = 4$ ($\lambda = 0$) that can be estimated to be

$$t_c^{2d}(p \to 4^-) \simeq \frac{\pi^3}{144}, \qquad (19)$$

while for $p > 4$ we have $t_c^{2d} = 0$. In the three-dimensional ($d = 3$) case we have the following behavior for w_k [20]

$$w_k \simeq \begin{cases} k^2, \ p > 5 \\ k^2 \ln(1/k), \ p = 5 \\ k^{p-3}, \ 3 < p < 5. \end{cases} \qquad (20)$$

Therefore, the integral in equation (13) is found to be convergent in the region of all $p > 3$ and we obtain $T_c > 0$, in accordance with Mermin-Wagner theorem [1]. The value of $t_c(p)$ decreases as p increases and diverges at $p = d = 3$.

In order to illustrate the critical behavior of the model (1), Figure 1 shows the dependence of the reduced transition temperature $t_c(p)$ as a function of p for the cases $d = 1$ (dashed line) and 2 (solid line). By performing the sum given by equation (13) numerically, we obtain the value of the critical temperature. We note that the critical temperature $t_c(p)$ increases as p decreases, and when p approaches $p = d$ we have a divergence in $t_c(p = d) \to \infty$. In two dimensions ($d = 2$) a discontinuity in $t_c(p)$ is obtained at $p = 4$ (see approximate value of this discontinuity in Eq. (19)) which vanishes just at that point, while in the one-dimensional ($d = 1$) case there is no discontinuity in $t_c(p)$ (see Eq. (18)).

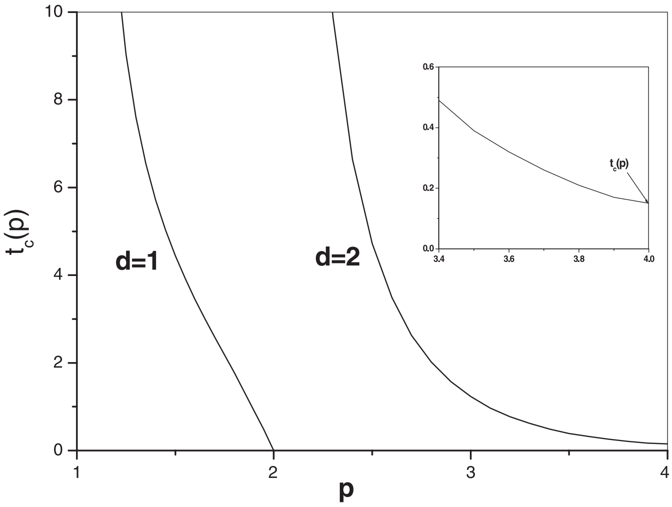

Fig. 1. The reduced critical temperature $t_c(p) \equiv \frac{k_B T_c(p)}{S(S+1)J}$ as a function of p for the quantum XY model with long-range interaction at low dimensions ($d = 1, 2$). Insert is the critical behavior of $t_c(p)$ versus p for $d = 2$ near of the discontinuity point at $p = 4$.

4 Conclusions

In summary, we have studied the d-dimensional XY model with long-range interaction in the boson space by using the coherent state path integral method [16,19]. The phase diagram of the model with arbitrary spin S and parameter p has been obtained. It is shown that the critical temperature T_c decreases with increasing p, and becomes infinite as $p \to d$. In the borderline case $p = 2d$ we have a transition to a phase with a slow decrease of correlation functions and an infinite susceptibility (Kosterlitz-Thouless-like transition-**KTLT**) [8]. Reasonable agreement with Monte Carlo simulations has been achieved for the case $p = 3/2$ in the one-dimensional planar rotator model.

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