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Quantum spherical XY model in a random field: coherent state path integral approach

Y.Q. Ma[1,2,a] and W. Figueiredo[2]

[1] Department of Physics, Nanjing University, Nanjing 210093, China
[2] Departamento de Fisica, Universidade Federal de Santa Catarina, 88040-900, Florianopolis, Santa Catarina, Brazil

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Abstract. By introducing boson operators, a quantum spherical XY model in the presence of a random field has been studied by the coherent state path integral approach. The phase diagram is obtained, and the effects of the random-field fluctuations Δ on the possibilities of the existence of a ferromagnetic phase are discussed. At the critical point, Δ_c, the order parameter M describing the ordered ferromagnetic phase disappears as $\propto (\Delta_c - \Delta)^{1/2}$. Since the model is equivalent to a Bose system, we also show that the phase transition at zero temperature between the superfluid and the disordered Mott insulator phases occurs at the chemical potential $\mu = J_0/2$, where J_0 is the strength of the exchange interaction. As the temperature T goes to zero, the asymptotic behavior of the entropy and the specific heat are $(J_0/2T)\exp(-J_0/2T)$ and $(J_0^2/4T^2)\exp(-J_0/2T)$, respectively.

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In the last years, a great deal of work has been devoted to the understanding of the phase transitions of the classical spin systems. In contrast, little attention has been paid to the study of the quantum spin systems. The reason is that quantum effects usually create a potentially difficult technical problem [1] due to the requisite non-commutativity of spin operators in the Hamiltonian. Lately, there has been renewed interest in the field of strongly interacting and disordered systems as in the random field and spin glass problems. One of the most fundamental questions is to know whether these random spin models have an ordered phase. The most fruitful method to study disordered systems is the statistical field theory method [2-5] which allows one to consider the infinite-range case [6-8] or mean-field models where the saddle point method provides the exact solution of the problem. On the other hand, it would be useful to have a model which can be solved exactly, but which retains the main features of the original model. Such a model is the spherical one which will provide a good starting point for studying these spin systems with quenched disorder. The spherical model in the spin representation was first introduced by Berlin and Kac [9], and has been sucessfully used later to study a number of problems of phase transitions associated with order-disordered phenomena in random spin systems [10-17]. A review of this subject was given by Joyce [18].

The disordered XY model was introduced as a simplified model for a variety of physical systems. Among them are vortex glass in type-II superconductors [19], granular superconductors and Josephson junctions [20], and the superfluid-insulator transition and boson localization in disordered boson systems [21-26]. As is well known, the XY model dates back to 1956 and it is now a standard model in statistical mechanics [27]. However, quantum version of the XY model with quenched disorder is much more complicated, and few results are available [28,29]. Specifically, phase diagram of the quantum XY model in the presence of random fields has not been reported up to now. The purpose of this letter is to formulate the coherent state path integral technique for the quantum spherical XY model in a random field and to report our findings from calculations of the phase diagram. Since the spin-$\frac{1}{2}$ XY model is equivalent to a hard-core boson model [30], thinking of the spin problem in terms of the boson language and *vice versa* is fruitful way to understand the physics of the XY model and related boson model. We start with transforming the spin operators to bosonic operators, and then construct a quantum spherical version of the model in the boson space. The phase diagram is obtained, and the effects of quantum fluctuations and randomness on the phase transition are examined. We find that the ferromagnetic ordering is reduced by quantum fluctuations and destroyed completely by random-field fluctuations with sufficiently large values of the random-field variance. The model can also be employed to describe the superfluid-Mott insulator transition of a Bose system. We display the existence of

[a] e-mail: myqiang@netra.nju.edu.cn

the transition between the superfluid and the Mott insulator phases at a critical chemical potential.

We will consider a spin-$\frac{1}{2}$ XY-model consisting of N interacting spins; the Hamiltonian of the model is given by

$$\mathrm{H} = -\sum_{ij} J_{ij}(\mathrm{S}_i^x \mathrm{S}_j^x + \mathrm{S}_i^y \mathrm{S}_j^y) - \sum_i h_i \mathrm{S}_i^x, \tag{1}$$

where S_i^α is the α component of a quantum XY-spin operator at site i, and the J_{ij} are the strength of the exchange interactions between sites, chosen to be $J_{ij} = \frac{1}{N} J_0$ for all pairs of spins. The scaling with N ensures a well-defined thermodynamic limit [3-5]. The random external field h_i is an independent random variable with zero mean and the variance Δ^2, *i.e.*,

$$\langle h_i \rangle_h = 0, \qquad \langle h_i h_j \rangle_h = \Delta^2 \delta_{ij}. \tag{2}$$

In the boson language, the spin operators are represented by the boson creation $\mathrm{a}^\dagger$ and annihilation a operators, and equation (1) can be rewritten as follows [30,27]:

$$\mathrm{H} = -\sum_{ij} J_{ij} \mathrm{a}_i^\dagger \mathrm{a}_j - \frac{1}{2} \sum_i h_i (\mathrm{a}_i^\dagger + \mathrm{a}_i), \tag{3}$$

with the local hard-core boson constraint $n_i = \mathrm{a}_i^\dagger \mathrm{a}_i = 0$ or 1. Since such a constraint defines boundaries in Hilbert space, it is extremely difficult to treat in a path-integral approach. To avoid the above difficulties, we impose the spherical constraint in the spin space $\sum_{i=1}^N [(\mathrm{S}_i^x)^2 + (\mathrm{S}_i^y)^2] = N$, which in the boson space, becomes a global hard-core boson one,

$$\sum_{i=1}^N \mathrm{a}_i^\dagger \mathrm{a}_i = \frac{1}{2} N. \tag{4}$$

The resulting path-integral theory is applicable to the present quantum XY model and related boson model under the relaxed constraint (4) which is enforced by introducing a Lagrange multiplier μ. The model Hamiltonian (3) with the constraint (4) is, in fact, a boson system with the boson hopping J_{ij} and the chemical potential μ in the strong on-site repulsion limit [21]; superfluidity in the boson model described by equation (3) corresponds to the magnetization in the XY plane. This model can also be applied to describe other physical systems such as the interaction properties between atoms and the electromagnetic field [31].

Once the Hamiltonian is written in terms of bosonic operators a_i the partition function, $Z = \mathrm{Tr}\ \mathrm{e}^{-\beta \mathrm{H}}$, can be expressed as the coherent state functional integral [32-34]

$$Z = \int \mathcal{D}(a, \bar{a}; \mu) \exp[-\frac{S(a, \bar{a}, \mu)}{\hbar}], \tag{5}$$

where the action $S(a, \bar{a}, \mu)$ is

$$S(a, \bar{a}, \mu) = \int_0^{\beta\hbar} \mathrm{d}t\, [\sum_i \bar{a}_i \frac{\partial}{\partial t} a_i - \frac{1}{N} \sum_{ij} J_0 \bar{a}_i a_j + \mu \sum_i \bar{a}_i a_i - \frac{1}{2} \sum_i h_i (\bar{a}_i + a_i) - \mu \frac{N}{2}], \tag{6}$$

where $a_i(t)$ is a c-number, $\bar{a}_i$ is its complex conjugate. In the following we will take the units $\hbar = 1$. Introducing a complex Hubbard-Stratonovich field,

$$M = \frac{1}{N} \sum_i \langle a_i \rangle, \tag{7}$$

the quadratic hopping terms may be decoupled by using the Hubbard-Stratonovich transformation, resulting in a single site problem:

$$Z = \int \mathcal{D}(a, \bar{a}; M, \bar{M}; \mu) \mathrm{e}^{-J} \tag{8}$$

where

$$\begin{aligned} J = \int_0^\beta \mathrm{d}t\, [&\sum_i \bar{a}_i \frac{\partial}{\partial t} a_i + \frac{1}{2} N J_0 M^2 - \frac{1}{2} J_0 \bar{M} \sum_i a_i \\ &- \frac{1}{2} J_0 M \sum_i \bar{a}_i + \mu \sum_i \bar{a}_i a_i \\ &- \frac{1}{2} \sum_i h_i (\bar{a}_i + a_i) - \mu \frac{N}{2}]. \end{aligned} \tag{9}$$

As the operators are now decoupled we can evaluate the trace of equation (8) as the trace over the boson operators on a single site raised to the power N and write

$$Z = \int \mathcal{D}(a, \bar{a}; M, \bar{M}; \mu) \mathrm{e}^{-\beta N f}. \tag{10}$$

In the thermodynamic limit, $N \to \infty$, the integral given by equation (8) with equation (9) can be performed by the method of the steepest descent, and the free energy f per site can be obtained after integration over the quadratic form in the bosonic variables inside the action J. Assuming that the Hubbard-Stratonovich field is replaced by a real and static parameter [33-35], the resulting free energy is easily obtained after averaging over any random external field distribution subject to the condition given by equation (2):

$$f = \frac{1}{2} J_0 M^2 - \mu - \frac{J_0^2 M^2}{4\mu} - \frac{\Delta^2}{4\mu} + T\, \ln(2\, \sinh \frac{\mu}{2T}), \tag{11}$$

where T is the temperature $T = \beta^{-1}$. In deriving equation (11) we have made use of the identity of the Gaussian integrals over pairs of complex conjugate variables

$$\int \prod_{i=1}^N \frac{\mathrm{d}\bar{a}_i\, \mathrm{d}a_i}{2\pi\, i} \exp(-\bar{a}_i M_{ij} a_j + \bar{\lambda}_i a_i + \lambda_i \bar{a}_i) = [\det M]^{-1} \exp(\bar{\lambda}_i M_{ij}^{-1} \lambda_j). \tag{12}$$

It is important to point out that in equation (11), the last term $T \ln(2\, \sinh \frac{\mu}{2T})$, which comes from the integral over the quantum harmonic oscillators, is different from the solution of the classical spherical model [18]. We will find that this term plays an important role in determining the phase transition behavior of the present quantum spherical XY model. The saddle-point equations, which can be found by minimizing the free energy f with respect to μ and M, yield

$$\frac{J_0^2}{4\mu^2}M^2 = 1 - \frac{1}{2}\coth\frac{\mu}{2T} - \frac{\Delta^2}{4\mu^2}, \tag{13}$$

$$\mu = \frac{1}{2}J_0. \tag{14}$$

The Hubbard-Stratonovich field M, which in fact, is the expectation value of the XY-plane spin component, corresponds to the order parameter describing the ferromagnetic ordering in the XY-model. The state with $M = 0$ is the paramagnetic one. Analogously, in the boson problem, $M = 0$ and $M \neq 0$ correspond to a Mott insulator phase and to a superfluid one, respectively.

It is important to consider some special cases at zero temperature. The first one is the case $\Delta = 0$, which is interesting in describing the superfluid-insulator transition of the pure Bose system. The corresponding Hamiltonian equation (3) with (4) simplifies to [36]

$$\mathrm{H} = -\sum_{ij} J_{ij}\mathrm{a}_i^\dagger \mathrm{a}_j + \mu\sum_i \mathrm{a}_i^\dagger \mathrm{a}_i. \tag{15}$$

In this case, the spherical constraint does not appear, and μ in equation (15) becomes the chemical potential fixing the average boson density $n = \mathrm{a}_i^\dagger \mathrm{a}_i$. The same steps as above lead to a free energy of the pure boson system given by

$$f = \frac{1}{2}J_0(1 - \frac{J_0}{2\mu})M^2. \tag{16}$$

This implies that for the chemical potential $\mu \leq \mu_c = J_0/2$ the ground stable state should be the superfluid phase, but when the converse is true, the only stable phase which remains is the disordered Mott insulator one.

The second case is $\Delta \neq 0$, and the corresponding saddle-point equations (13) and (14) reduce to

$$M = (\frac{1}{2} - \frac{\Delta^2}{J_0^2})^{1/2}. \tag{17}$$

It is straightforward to see from equation (17) that in the absence of random fields, $\Delta = 0$, the order parameter M of this XY model reduces from the classical value $M = 1$ to the present quantum result $M = \sqrt{2}/2$. This means that quantum fluctuations tend to weaken the ordered ferromagnetic behavior, but do not suppress completely the ferromagnetic ordering. On the other hand, as the strength of random field Δ approaches $\Delta_c = \frac{\sqrt{2}}{2}J_0$, the order parameter M disappears as $\propto (\Delta_c - \Delta)^{1/2}$, indicating that for $\Delta > \Delta_c$ the ground state becomes a paramagnetic one. In the present case, we find that the strength of random field at $T = 0$ plays a similar role as the temperature; the quantum effects are displayed only clearly by the reduction of the magnetization.

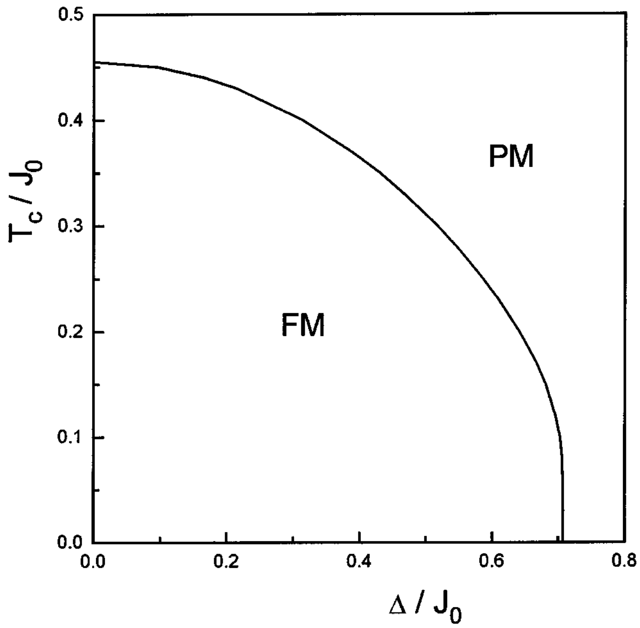

Fig. 1. Phase diagram for the quantum spherical XY model in a random field. Here T_c is the critical temperature and Δ is the intensity of the random field. T_c and Δ are scaled by J_0.

We now turn to the phase transition properties of the quantum spherical XY-model at a finite-temperature $T \neq 0$. From equations (13, 14) we will find that as one increases the temperature T, the order parameter M vanishes as $M \propto (T_c - T)^\beta$ with critical exponent $\beta = 1/2$. Figure 1 shows the dependence of the critical temperature T_c on the strength of random field Δ, *i.e.*, on the leftside of this curve the ferromagnetic phase is stable. The ferromagnetic transition temperature T_c decreases with an increase of the strength of the random field Δ, and vanishes for the critical value of the random-field variance $\Delta_c = \frac{\sqrt{2}}{2}J_0$. Finally, the present quantum bosonic theory gives the following asymptotic behavior for the entropy and the specific heat:

$$S(T)|_{T\to 0} \propto \frac{J_0}{2T}\exp(-\frac{J_0}{2T}), \tag{18}$$

$$C(T)|_{T\to 0} \propto \frac{J_0^2}{4T^2}\exp(-\frac{J_0}{2T}). \tag{19}$$

We see that in this model the entropy and the specific heat are always positive at finite temperatures and vanish as $T \to 0$. This result is in contrast to the classical spherical model [18] where the entropy approaches $-\infty$ and the specific heat keeps constant as $T \to 0$, respectively. This is a consequence of the logarithmic term present in equation (11), which is due to a pure quantum contribution.

In conclusion, we have investigated the static properties of the quantum spherical XY model in the presence of random fields. Replacing the spin operators by the boson ones in the bosonic representation, the model becomes equivalent to a boson one, and can be solved exactly by the use of the coherent state functional integral. This will provide a good starting point for further study of the coherent-state path integral approach of the quantum magnets and boson-Hubbard problems. We have obtained a set of saddle-point equations describing the phase transitions of the model considered. The model displayed a transition between the ferromagnetic and the disordered paramagnetic phases as a function of the strength of random fields. It was demonstrated that quantum fluctuations are to reduce somewhat the value of the magnetization, but do not destroy the ordered ferromagnetic phase. By contrast, the randnom fields make the ferromagnetic ordering unstable, and even the boundary of the ferromagnetic phase can be destroyed, which depends strongly on the variance Δ. We also showed a critical chemical potential $\mu_c = \frac{1}{2}J_0$ distinguishing the superfluid phase from the disordered Mott insulator phase in a pure boson system. We have seen that the entropy of this model exhibits the expected physical behavior when the temperature approaches zero.

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