Random-field effect on the quantum ferromagnetic XY model

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The quantum version of the random-field spherical XY model on a d-dimensional hypercubic lattice is presented in the boson space, and solved exactly. We recover the Imry-Ma result concerning the lower critical dimension $d_c=4$, and calculate the critical exponents near the critical temperature. In particular, we obtain a general phase diagram of the model with arbitrary dimension d when $d>d_c$. The ferromagnetic ordering is reduced by quantum fluctuations, and destroyed completely by random-field fluctuations with sufficiently large values of the random-field variance σ. The entropy and the specific heat vanish as $T^{d/2}$ at low temperatures. Since the model is equivalent to a Bose system, we show a superfluid-Mott insulator transition at a critical chemical potential μ_c. [S0163-1829(98)00925-4]

In the last years, extensive attention has been lavished on the theory of disordered spin systems. One of the most fundamental questions is to know whether these random spin systems have an ordered phase. The most fruitful method to study disordered systems is the statistical field theory method,[1] which allows one to consider the infinite-range interaction case[2] where the saddle-point method provides the exact solution of the problem. While a large amount of work has been focused on the infinite-range model, which is expected to describe the transition in a short-range system of sufficiently high dimensions, the understanding of the real short-ranged disordered spin systems is still an incomplete and interesting problem. Thus it would be very useful to have a model which can be solved exactly, but which still retains the main features of the original short-range disordered spin model. Such a model is the spherical one which was first introduced by Berlin and Kac.[3] Since the classical spherical model in the spin representation can be solved exactly for nearest-neighbor interactions,[4,5] it has been successfully used to study a number of problems of phase transitions associated with order-disordered phenomena in random spin systems.[6] Lately, there has been renewed interest in the quantum version of disordered spin systems,[7–15] because of its relevance to the recently discovered high-T_c superconducting materials. Most theoretical work has been devoted to the study of the one-dimensional and infinite-range cases. These two limiting cases seem to capture some features induced by the quantum effects and randomness of the systems. However, very little is known about the phase transition behaviors of the quantum short-ranged spin systems, which are of experimental interest. The technical reason is that the quantum effects usually create a potentially difficult technical problem due to the requisite noncommutativity of spin operators in the Hamiltonian. On the other hand, 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,[16] granular superconductors and Josephson junctions,[17] and the superfluid-insulator transition and boson localization in disordered boson systems.[18,19] However, this quantum-disordered XY model is much more complicated, and few results are available.[20] Specifically, a phase diagram of the short-range quantum XY model in the presence of random fields has not been reported up to now. The construction of the quantum spherical model will provide a powerful method for studying these quantum phase transitions of disordered spin systems. In this paper, we report the exact result for the quantized spherical short-ranged XY model with a random field. Since the spin-$\frac{1}{2}$ XY model is equivalent to a hard-core boson model,[21,22] thinking of the spin problem in terms of the boson language, and vice versa, is a fruitful way to understand the physics of the XY model and related boson models. We will first introduce hard-core boson operators to map the quantum spin system into a boson system plus a local hard-core boson constraint, and construct a quantum spherical version of the model by relaxing the hard-core boson constraint in the boson space. Then it will be easy to use the coherent-state path integral to solve this equivalent boson model exactly. The phase diagram is obtained for arbitrary dimension, and the effects of quantum fluctuations and randomness on the phase transitions are examined. We find that the quantum fluctuations are to reduce somewhat the value of the magnetization, but do not destroy the ordered ferromagnetic phase. In contrast, the random fields have stronger fluctuations than quantum effects. The existence of the randomness leads to an increase of the lower dimension d_c by 2 from $d_c=2$ of the pure XY model. And for $d>d_c=4$, the model exhibits a transition from ferromagnetic to paramagnetic phases at a sufficiently large value of the random-field variance. Contrary to the classical spherical model in which the entropy gives a nonphysical low-temperature behavior, the entropy and specific heat in the present model are always positive at finite temperatures, and decay as $T^{d/2}$ at low temperatures. The model can also be used to describe the superfluid-Mott insulator transition of a Bose system. It is displayed that, at a critical chemical potential, there exists a phase transition between the disordered Mott insulator and the superfluid phases.

We consider a quantum XY model on a d-dimensional hypercubic lattice with N interacting spins. Its Hamiltonian is given by

$$\mathcal{H}=-\sum_{ij}^{N} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j-\sum_{i}^{N} \mathbf{h}_i\cdot\mathbf{S}_i, \quad (1)$$

where $\mathbf{S}_i=(S_i^x,S_i^y)$ is the quantum XY spin operator at site i, and J_{ij} are the strength of the exchange interactions between sites. $\mathbf{h}_i$ is the identically distributed random field at site i with the symmetric Gaussian probability distribution with zero mean and the variance σ^2.

In boson language, the spin operators in each lattice site are replaced by the boson creation $a^\dagger$ and annihilation a operators; Hamiltonian (1) can be rewritten as

$$\mathcal{H}=-\sum_{ij} J_{ij}a_i^\dagger a_j-\tfrac{1}{2}\sum_i (h_i^x-ih_i^y)a_i^\dagger-\tfrac{1}{2}\sum_i (h_i^x+ih_i^y)a_i, \quad (2)$$

by an exact mathematical transformation,[22] $S_i^x+iS_i^y=a_i^\dagger$ and $S_i^x-iS_i^y=a_i$. Here h_i^α is the αth component of the random external field $\mathbf{h}_i$ at site i. From the above exact mathematical transformation, one obtains the hard-core boson constraint condition $a_i^\dagger a_i=0$ and 1. Since such a model defines boundaries in Hilbert space with physical states $0\leqslant a_i^\dagger a_i\leqslant 2S$ (1 for spin-$\frac{1}{2}$), it is extremely difficult to handle in a function integral approach.[23] To avoid the above difficulties, we impose the spherical constraint in the spin space $(1/N)\Sigma_{i=1}^N\mathbf{S}^2=1$,[24,25] which, in boson language, becomes a mean hard-core bosonic constraint

$$\frac{1}{N}\sum_{i=1}^{N} a_i^\dagger a_i=\frac{1}{2}. \quad (3)$$

This means that the boson number $n_i=a_i^\dagger a_i$ is allowed to take on any value from 0 to ∞ (rather than just the values 0 and 1), subject only to the so-called mean hard-core boson constraint (3), like the original formulation of the spherical model in the spin space.[4] The advantage is that although one connects the physical states with $0\leqslant a^\dagger a\leqslant 1$ with unphysical states having $a^\dagger a>1$, which may lead to unphysical results, constraint (3) can effectively remove unphysical states in low dimensions, and the resulting path-integral theory is applicable to arbitrary spin-S case and related boson systems, corresponding to relaxing the hard-core boson condition $0\leqslant a^\dagger a\leqslant 2S$.[26] In particular, the technique presented here can be employed to study the soft-core boson Hubbard model with a finite on-site repulsion,[18] equivalent to the anisotropic $S=\frac{1}{2}$ Heisenberg model in which the expectation value of the boson number n is compared to $2S$, and the conventional spin-wave theory is no longer satisfying.[26] In the present case, the boson constraint appears as the natural way to eliminate the unphysical states, contrary to the modified spin-wave theory,[27] in which the Mermin-Wagner theorem[28] is enforced by hand (e.g., the total number of Holstein-Primakoff bosons per site is S on the average). Furthermore, in the spin space, the mean and strict spherical constraints lead to the same results for thermodynamics quantities.[4] However, for the present case we see that the relaxed mean boson constraint (3) can be easily extended to the quantum problems.[29]

Now a_i and $a_i^\dagger$ satisfy the standard boson commutation relations $[a_i,a_j^\dagger]=\delta_{ij}$. The price is that the constraint (3) is introduced into the Hamiltonian via a Lagrange multiplier μ which is determined by requiring that $(1/N)\Sigma_{i=1}^N a_i^\dagger a_i=\frac{1}{2}$. The parameter μ could be seen as an effective cutoff parameter of unphysical states in the boson space. Changing from the site representation to the momentum one, the Fourier transformation of Eq. (2) with constraint (3) is given by

$$\mathcal{H}=-\sum_{\mathbf{k}} J(\mathbf{k})a_{\mathbf{k}}^\dagger a_{\mathbf{k}}-\tfrac{1}{2}\sum_{\mathbf{k}} (h_{\mathbf{k}}^x-ih_{\mathbf{k}}^y)a_{\mathbf{k}}^\dagger -\tfrac{1}{2}\sum_{\mathbf{k}} (h_{-\mathbf{k}}^x+ih_{-\mathbf{k}}^y)a_{\mathbf{k}}+\mu\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}-\tfrac{1}{2}\mu N, \quad (4)$$

where $a_{\mathbf{k}}$, $a_{\mathbf{k}}^\dagger$, and $h_{\mathbf{k}}$ are the Fourier transforms of the operators and the random field, respectively. The interactions $J(\mathbf{k})$ are given by $J(\mathbf{k})=2J\Sigma_{\alpha=1}^d\cos k_\alpha$, where J is the strength of the nearest-neighbor interactions. The model Hamiltonian (4) realizes the reformulation of the initial boson Hamiltonian (2) in terms of the standard bosons, and can be solved exactly. This will provide a good starting point for further study of statistical mechanics of the quantum magnets and related boson models. Since the XY model differs from the Heisenberg model by the absence of the term $JS_i^zS_j^z$ which leads to nonquadratic terms in the boson Hamiltonian, Eq. (4) is a quadratic form in the boson creation and annihilation operators $a_{\mathbf{k}}^\dagger$ and $a_{\mathbf{k}}$. Actually, the model Hamiltonian (4) is an extended hard-core boson system with the boson hopping J_{ij}, and the chemical potential μ in the strong onsite repulsion limit.[18] On the other hand, Eq. (4) can also be employed to describe other physical systems such as the interaction properties between atoms and the electromagnetic field.[30]

Once the Hamiltonian is written in terms of bosonic operators, we can express the partition function $Z=\mathrm{Tr}\,e^{-\beta\mathcal{H}}$ using the coherent state functional integral[23,26] in the Matsubara 'imaginary time' formulation. The advantage is that in the coherent-state path-integral representation, the boson operator will become a c number, and the trace in the partition function can be performed explicitly. Upon integrating out the bosons and then averaging over the Gaussian random fields in the partition function, the resulting free energy per site, $f=-(1/\beta N)\ln Z$, is given by

$$f=-\frac{1}{\beta N}\sum_{\mathbf{k}} \ln\{1-\exp[-\beta(\mu-J(\mathbf{k}))]\}^{-1} -\frac{1}{N}\sum_{\mathbf{k}} \frac{\sigma^2}{4[\mu-J(\mathbf{k})]}-\frac{1}{2}\mu, \quad (5)$$

where the summation is performed over the first Brillouin zone of the reciprocal lattice. The first term in Eq. (5), which comes from the integral over the quantum harmonic oscillators, is different from the solution of the classical spherical model.[4,5] It is easy to find that this quantum term also appears in other quantum-mechanical problems,[23,26,12–14,31] and plays a crucial role in determining the phase transition behavior of the quantum systems. The Lagrange multiplier μ is determined by minimizing the free energy with respect to it, $\partial f/\partial\mu=0$:

$$\frac{1}{N}\sum_{\mathbf{k}} n_{\mathbf{k}}+\frac{1}{N}\sum_{\mathbf{k}} \frac{\sigma^2}{4[\mu-J(\mathbf{k})]^2}-\frac{1}{2}=0, \quad (6)$$

with $n_{\mathbf{k}}=1/(\exp[\beta(\mu-J(\mathbf{k})]-1)$. The energy spectrum is given by $E_{\mathbf{k}}=\mu-J(\mathbf{k})$, and exhibits an energy gap $\Delta E=\mu-J(\mathbf{k}=0)$. There exists a second-order phase transition where μ sticks at $J(\mathbf{k}=0)=2Jd$. Actually, at this point $\mu=2Jd$, the boson condensation of the $\mathbf{k}=0$ mode occurs. This state will accumulate more and more bosons with the decrease of temperature T, so that at $T=0$ the ground state is achieved by populating the $\mathbf{k}=0$ mode only. Thus long-range ferromagnetic order is achieved as a result of the Bose-Einstein condensation of the bosons. Converting a sum into an integral in Eq. (6) must be accomplished by adding a Bose-Einstein condensate term corresponding to the case $\mu=2Jd$ and $\mathbf{k}=0$ in the thermodynamic limit. The resultant equation of state is obtained by calculating the spin-spin correlation function $M^2=\langle S_0^x\cdot S_{\mathbf{R}}^x\rangle|_{\mathbf{R}\to\infty}$. We have

$$M^2=\frac{1}{2}-\int\frac{d^dk}{(2\pi)^d}\frac{1}{\exp\{\beta[\mu-J(\mathbf{k})]\}-1}-\int\frac{d^dk}{(2\pi)^d}\frac{\sigma^2}{4[\mu-J(\mathbf{k})]^2}. \tag{7}$$

The critical temperature T_c below which the ordered ferromagnetic phase appears is determined by solving Eq. (7) for the spherical constraint in the limit $\mu=2Jd$. Expanding the exp term in Eq. (7), we obtain, in the limit $M\to 0$,

$$1-\frac{\sigma^2}{4J^2}g_1-\frac{T_c}{J}g_2=0, \tag{8}$$

with

$$g_1=\int\frac{d^dk}{(2\pi)^d}\frac{1}{2[d-\gamma(\mathbf{k})]^2},\quad g_2=\int\frac{d^dk}{(2\pi)^d}\frac{1}{d-\gamma(\mathbf{k})}, \tag{9}$$

where $\gamma(\mathbf{k})=\Sigma_{\alpha=1}^d\cos k_\alpha$. The values of the functions g_1 and g_2 depend only on the dimension d. Equation (8), with Eq. (9), exhibits an order-disordered phase transition, provided that the integrals in Eq. (9) converge. It is straightforward to see from Eq. (9) that the functions g_1 and g_2 converge for $d>4$ and $d>2$, respectively. Thus we conclude that the random-field fluctuations destroy the ordered ferromagnetic phase for $2<d\leqslant 4$, and the lower critical dimension for the present XY model is $d_c=4$, which is in agreement with the Imry-Ma result.[32] Since the random-field term in Eq. (7) contains the stronger singularity for $k\to 0$ than the second term on the right-hand side of Eq. (7), which corresponds to the quantum fluctuations, the leading contribution to the critical behaviors stems from the random-field term. The critical behavior near the critical temperature T_c is determined by the solution of state equation (7) for small but finite ΔE. Expanding the exp term in Eq. (7) in $k\to 0$ and for small ΔE, we have

$$|T-T_c|\sim M^2+C\sigma^2\begin{cases}(\Delta E)^{(d-4)/2} & (d<6)\\ \Delta E\ \ln\Delta E & (d=6)\\ \Delta E & (d>6).\end{cases} \tag{10}$$

Obviously the upper critical dimension is $d_u=6$. From Eqs. (10) we can determine the critical exponents of the thermodynamic quantities of the quantum XY model in the presence of random fields; this yields $\beta=1/2$, $\delta=d/(d-4)$, $\nu=1/(d-4)$, and $\gamma=2/(d-4)$ for $4<d<6$. Above $d_u=6$ we recover the mean-field results $\beta=1/2$, $\delta=3$, $\nu=1/2$, and $\gamma=1$.

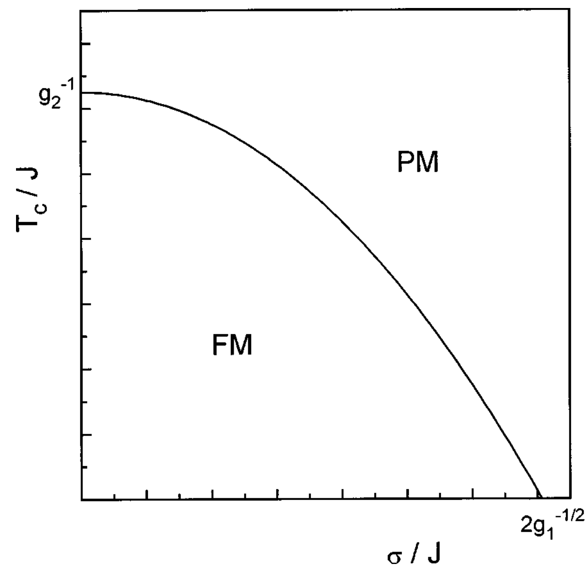

FIG. 1. Phase diagram in the plane T_c/J vs σ/J of the quantum spherical XY model in a random field for $d>4$. FM denotes the ferromagnetic phase, and PM the paramagnetic phase. The critical temperature T_c^t and the random-field strength σ are scaled by J.

In the following, we first consider the properties of the phase transition at zero temperature $T=0$. Equation (7) reduces to

$$M^2=\frac{1}{2}-\int\frac{d^dk}{(2\pi)^d}\frac{\sigma^2}{4[\mu-J(\mathbf{k})]^2}. \tag{11}$$

In the absence of random fields, $\sigma=0$, Eq. (11) shows that the magnetization $M=\sqrt{2}/2$, which differs from the classical result $M=1$, exhibits a quantum reduction effect. This means that quantum fluctuations tend to weaken the ordered ferromagnetic behavior, but do not completely suppress the onset of ferromagnetic order. On the other hand, as the strength of the random field σ reaches a critical strength of disorder, $\sigma_c=2J/g_1^{1/2}$, the magnetization M disappears as $\propto(\sigma_c-\sigma)^{1/2}$, showing a zero-temperature transition. For $\sigma>\sigma_c$ the ground stable state becomes a paramagnetic one. In the present study, we see that the random-field-induced fluctuations are stronger than quantum fluctuations, and thus the critical behavior close to phase transition is dominated by the random-field fluctuations; the quantum effects are displayed only clearly by the reduction of the magnetization.

We turn to the phase transition of the system at a finite temperature $T\neq 0$. From Eqs. (7)–(9) we see that at the phase transition, the magnetization M behaves $M\propto(T_c-T)^{1/2}$. In Fig. 1, we present the $T-\sigma$ phase diagram of the model for $d>d_c$, i.e., on the left of this curve the ferromagnetic phase occurs. The ferromagnetic phase transition temperature T_c as a function of σ decreases continuously from its maximum value $T_c=J/g_2$, as σ grows, and vanishes for the critical value of the random-field variance $\sigma_c=2J/g_1^{1/2}$. In addition, from Eq. (5) we obtained that the entropy and the specific heat behave as $\propto T^{d/2}$ at low temperature T, contrary to the classical spherical model,[4,5] where the entropy appraches $-\infty$ and the specific heat keeps constant as $T \to 0$, respectively. This is a direct consequence of the logarithmic term present in Eq. (5), which is due to a pure quantum contribution.

Finally, since the present XY model is equivalent to a boson system, we would like to shed some light on the properties of the superfluid-Mott insulator transition of the pure Bose system. The Hamiltonian can now be written as

$$\mathcal{H}=-\sum_{ij} J_{ij}a_i^\dagger a_j-\tfrac{1}{2}\sum_i (H^x-iH^y)a_i^\dagger -\tfrac{1}{2}\sum_i (H^x+iH^y)a_i+\mu\sum_i a_i^\dagger a_i . \tag{12}$$

Here H_i^α is the αth component of the external magnetic field $\mathbf{H}_i$. In the present case, the spherical constraint does not appear, and μ in Eq. (12) becomes the chemical potential determining the average boson density $n=a_i^\dagger a_i$. The corresponding free energy of the pure boson system becomes

$$f=\frac{1}{\beta N}\sum_{\mathbf{k}} \ln 2\sinh\frac{1}{2}\beta[\mu-J(\mathbf{k})] -\frac{H^2}{4[\mu-J(\mathbf{k}=0)]}-\frac{1}{2}\mu. \tag{13}$$

The superfluid order parameter M is equal to $M=-\partial f/\partial H =H/2[\mu-J(\mathbf{k}=0)]$. Equation (13) gives an energy gap $\Delta E=\mu-2Jd=H/2M$, which vanishes in the ordered superfluid phase $(M\neq 0)$ at zero field, i.e., $\mu=2Jd+0(H)$ for the ordered superfluid phase. In the disordered Mott insulator phase, there exists a finite energy gap $\mu-\mu_c$ for $\mu>\mu_c =2Jd$. The system undergoes a second-order phase transition, from a disordered Mott insulator to an ordered superfluid phase at a critical chemical potential $\mu=\mu_c$, in agreement with the result of Pazmandi and Domanski.[33]

In conclusion, we have studied the phase transition and the critical properties of the quantum short-range XY model with random fields in the exactly soluble spherical limit. We have obtained a general expression describing the phase transition of the model with arbitrary dimension d for $d>4$. It was shown that the main effect of quantum fluctuations is a reduction of the ferromagnetic ordering. On the other hand, the random-field-induced fluctuations destroy the ferromagnetic phase for $2<d\leqslant 4$, and, when $d>4$, randomness makes the ferromagnetic ordering unstable, and even the boundary of the ferromagnetic phase can be destroyed, which depends strongly on the variance σ. At the critical point σ_c, the magnetization M disappears as $\propto(\sigma_c-\sigma)^{1/2}$. We calculated the critical exponents near the phase transition, and showed that the random-field fluctuations rather than the quantum fluctuations dominate the critical behavior. We have seen that the entropy of this model displays the expected physical behavior when the temperature $T\to 0$. The present model also demonstrated the existence of the transition from the superfluid into the Mott insulator phases, as the chemical potential μ approaches a critical value μ_c. The Mott insulator phase has a finite energy gap $\mu-\mu_c$, but for the superfluid phase the energy gap vanishes for vanishing field. Replacing the quantum spin operators by the boson ones in the bosonic representation, the present quantum bosonic theory can be applied to make contact with a set of the quantum XY models with other types of disorders, and the related disordered Bose ones. In particular, generalizations to the quantum XY models with random-bond interactions and the inclusion of anisotropy will be straightforward.

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