Quantum version of a spherical model: Crossover from quantum to classical critical behavior

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We investigate a quantum version of the spherical model which is obtained from the classical Berlin-Kac spherical model by a simple canonical quantization scheme. We find a complete solution of the model for short-range as well as for long-range interactions. At finite temperatures the critical behavior is the same as in the classical spherical model whereas at zero temperature we find a quantum phase transition characterized by new critical exponents. Based on a functional-integral representation of the partition function the free energy of the model is shown to be equivalent to that of the nonlinear σ model in the limit of infinite order-parameter dimensionality.

I. INTRODUCTION

The classical spherical model introduced by Berlin and Kac[1] is one of the simplest toy models in statistical physics showing nontrivial critical behavior. It appears to be universally applicable to studying a variety of critical phenomena. The classical spherical model can be solved exactly not only for nearest-neighbor interactions[1] but also for long-range power-law interactions,[2,3] random interactions,[4,5] systems in random magnetic fields,[6,7] and disordered electronic systems with localized states.[8] In addition it has been used as a test case for the finite-size scaling hypothesis.[9,10] Reviews on the classical spherical model were given by Joyce[3] and more recently by Khorunzhy *et al.*[11] for spherical models with disorder.

In recent years there has been a renewed interest in the theory of zero-temperature quantum phase transitions studied by Hertz[12] in 1976 in the context of itinerant ferromagnets. The newer investigations include metal-insulator transitions,[13] the superconductor-insulator transition,[14] as well as order-disorder transitions in quantum antiferromagnets[15] and spin glasses,[16] to name a few. Despite much effort we are far from having a complete picture of the behavior near quantum phase transitions. Thus it would be very useful to have a quantum version of the spherical model which can be used as universally as the classical spherical model.

Actually the idea of a quantum spherical model is not new; it dates back more than 20 years when Obermair[17] suggested a simple canonical quantization scheme for a dynamical spherical model. This was also used later to investigate a quantum spin glass.[18] However, these studies focused on the usual finite-temperature critical behavior and did not deal with the quantum phase transition at zero temperature. Similar models were also studied in the context of structural phase transitions.[19–21] Very recently a quantum version of the spherical model was suggested based on path-integral quantization.[22]

In this paper we consider a quantum version of the spherical model which is obtained by a canonical quantization scheme similar to that of Obermair. Like the classical model, the quantum model is exactly solvable, and we calculate the critical behavior at the finite-temperature classical fixed point as well as at the zero-temperature quantum fixed point. We also derive a functional-integral representation of our model. Based on this representation we investigate the relation to field-theoretic models and find that the free energy is identical to that of an $O(n)$ σ model in the limit $n\to\infty$.

II. CANONICAL QUANTIZATION OF THE SPHERICAL MODEL

We consider a classical spherical model[1] of $N=L^D$ (D is the spatial dimensionality) real variables S_i ranging from $-\infty$ to ∞ that interact via a pair potential U_{ij} which we assume to be translationally invariant [i.e., $U_{ij}=U(r_i-r_j)$] for simplicity. The Hamiltonian of the model is given by

$$H_{\rm cl}=\frac{1}{2}\sum_{i,j} U_{ij}S_iS_j+h\sum_i S_i\,, \tag{1}$$

where h is an external "magnetic" field. The values of the S_i are subject to the mean spherical constraint

$$\sum_i \langle S_i^2\rangle = N/4, \tag{2}$$

where $\langle\cdots\rangle$ denotes the thermodynamic average. In other studies of the spherical model this constraint is often imposed not on the averages but on the values of the variables themselves (strict spherical constraint). Usually both versions of the constraint yield the same results for the thermodynamic quantities[23] although different results have been reported for a spherical spin glass.[24] For a more detailed discussion of the relation between the mean spherical constraint and the strict spherical constraint see, e.g., Ref. 3. In the following we will see, however, that the mean spherical constraint (2) is easier to generalize to the quantum case than the strict constraint.

To define a quantum version of the spherical model (1) we reinterpret the variables S_i as operators and define canonically conjugate "momentum" operators P_i so that the fol-

lowing commutation relations are obeyed (with $\hbar$ set equal to 1):

$$[S_i,S_j]=0, \quad [P_i,P_j]=0, \quad [S_i,P_j]=i\delta_{ij}. \tag{3}$$

The quantum spherical model is then obtained from (1) by adding a kinetic energy term. The choice of this term is by no means unique, and depending on the form of the kinetic energy the model shows different dynamical behavior. Here we choose the simplest possible kinetic energy, a sum over the squares of the ''momentum'' operators. Thus the Hamiltonian is given by

$$H=H_{\rm kin}+H_{\rm cl}=\frac{1}{2}\,g\sum_i P_i^2+\frac{1}{2}\sum_{i,j} U_{ij}S_iS_j + h\sum_i S_i+\mu\left(\sum_i S_i^2-\frac{N}{4}\right), \tag{4}$$

where the coupling constant g determines the importance of quantum fluctuations. Here $g\to 0$ corresponds to the classical limit. The mean spherical constraint (2) is taken care of by a Lagrange multiplier μ. It is easy to see that an implementation of the strict spherical constraint is more difficult in the quantum case, since here the S_i are not real variables but operators.

We want to emphasize that the commutation relations (3) together with the quadratic kinetic term in the Hamiltonian (4) do not describe quantum Heisenberg-Dirac spins but quantum rotors as will become clearer in Sec. V. The quantum rotors can be seen as a generalization of Ising spins in a transverse field.[16] The reader may also be aware of mappings between the low-temperature behavior of quantum Heisenberg antiferromagnets and models of quantum rotors.[15,25]

The quantum spherical model (4) is equivalent to a system of coupled harmonic oscillators. Therefore it can be solved very easily. A Fourier transformation of the Hamiltonian leads to

$$H=\sum_k\left[\frac{1}{2}\,gP(k)P(-k)+\frac{1}{2g}\,\omega^2(k)S(k)S(-k)\right] -\mu\,\frac{N}{4}-\frac{Nh^2}{4\mu}, \tag{5}$$

where $P(k)$ and $S(k)$ are the Fourier transforms of the operators and the frequencies $\omega(k)$ are given by

$$\omega^2(k)=2g\left(\mu+\frac{1}{2}\,U(k)\right). \tag{6}$$

Here $U(k)$ is the Fourier transform of the interaction matrix U_{ij} and we have fixed our energy scale by assuming that the Fourier component $U(0)$ to $k=0$ is equal to zero. In analogy to a system of harmonic oscillators we can immediately write down the partition function

$$Z=\prod_k\left(2\sinh\frac{1}{2}\,\beta\omega(k)\right)^{-1}\exp\left(\beta\mu\,\frac{N}{4}+\frac{\beta Nh^2}{4\mu}\right), \tag{7}$$

where β is the inverse temperature $\beta=1/k_BT$. Therefore the free energy per site reads

$$f=-\frac{1}{\beta N}\ln Z=-\frac{\mu}{4}-\frac{h^2}{4\mu}+\frac{1}{\beta N}\sum_k\ln\left(2\sinh\frac{1}{2}\,\beta\omega(k)\right). \tag{8}$$

The spherical constraint which determines μ is given by

$$0=\frac{\partial f}{\partial\mu}=-\frac{1}{4}+\frac{h^2}{4\mu^2}+\frac{1}{N}\sum_k\frac{g}{2\omega(k)}\coth\frac{1}{2}\,\beta\omega(k). \tag{9}$$

In the limit $g\to 0$ this equation approaches the corresponding classical result [note that the frequencies $\omega(k)$ also contain g], whereas the free energy (8) contains an extra term proportional to $\ln\beta g$ which is absent in the solution of the classical model (1). This is connected with the pathological thermodynamic behavior of the classical model at low temperatures, which is fixed by the extra term in the quantum case. Similar results were found in Refs. 18 and 22. It is also interesting to look at the limit of vanishing interactions $U(k)=0$ which corresponds to free spherical quantum ''rotors.'' In this case Eq. (9) yields a finite energy gap (finite μ) even for vanishing field h. In contrast, for free Heisenberg-Dirac spins the energy gap vanishes for vanishing field.

III. CRITICAL BEHAVIOR AT FINITE TEMPERATURES

In this section we will discuss the critical behavior of the quantum spherical model at a finite-temperature phase transition. As usual in the spherical model, the critical behavior is determined by the properties of Eq. (9) for the spherical constraint in the limit $\mu\to 0$. The system does not show a phase transition if the k sum on the right-hand side of (9) diverges for $N\to\infty$ and $\mu\to 0$. If it converges the system has a critical point at $h=0$ and $g=g_c$ with

$$0=-\frac{1}{4}+\frac{1}{N}\sum_k\frac{g_c}{2[g_cU(k)]^{1/2}}\coth\frac{1}{2}\,\beta[g_cU(k)]^{1/2}. \tag{10}$$

This integral converges for $D>x$, where x describes the asymptotic behavior of U_k: $U_k\sim|k|^x$ for $k\to 0$. Consequently, the lower critical dimension is given by x. (In the case of short-range interactions we have $x=2$.) In order to calculate the behavior of the system near this critical point we have to investigate (9) for small but finite μ. The main observation is that at any finite temperature (finite β) we can expand the coth terms in (9) and (10) in the long-wavelength limit $|k|\to 0$ and for small μ. From this it follows that the leading terms in (9) and (10) are the same as in the classical spherical model. After subtracting (10) from (9) and calculating the remaining k sums we find

$$-t_g\sim\left(\frac{h}{\mu}\right)^2+\begin{cases} C\mu^{(D-x)/x} & (D<2x)\\ C\mu\,\ln|\mu| & (D=2x)\\ C\mu & (D>2x),\end{cases} \tag{11}$$

where $t_g=(g-g_c)/g_c$ is the distance from the critical point and the prefactor C is a smooth function of g. If we define a ''magnetization'' $m=\partial f/\partial h=-h/2\mu$ [see Eq. (8)] we obtain the equation of state

TABLE I. Critical exponents for the quantum spherical model at the zero-temperature quantum fixed point and the finite-temperature classical fixed point as functions of dimensionality.

Exponent	Quantum fixed point ($D<D_u=3x/2$)	Classical fixed point ($D<D_u=2x$)	Both fixed points ($D>D_u$)
α	$(2D-3x)/(2D-x)$	$(D-2x)/(D-x)$	0
β	1/2	1/2	1/2
γ	$2x/(2D-x)$	$x/(D-x)$	1
δ	$(2D+3x)/(2D-x)$	$(D+x)/(D-x)$	3
ν	$2/(2D-x)$	$1/(D-x)$	$1/x$
η	$2-x$	$2-x$	$2-x$
z	$x/2$	$x/2$	$x/2$

$$-t_g \sim m^2 + \begin{cases} C(h/m)^{(D-x)/x} & (D<2x) \\ C(h/m)\lvert\ln(h/m)\rvert & (D=2x) \\ C(h/m) & (D>2x). \end{cases} \tag{12}$$

From this equation we can easily determine the critical exponents of the thermodynamic quantities and the upper critical dimension which is obviously given by $D_u=2x$. In order to find the critical exponent of the correlation length we notice that the only relevant length scale near the transition is determined by the long-wavelength behavior of $\omega(k)$ which is given by $\omega^2(k)\sim 2g(\mu+k^x)$, where we have omitted the prefactor in front of k^x. Consequently we get $\xi\sim\mu^{-1/x}$ and together with (11) this yields the critical exponent ν. The exponent η can be calculated from $\langle S_k S_{-k}\rangle \sim \omega_k^{-2}\sim k^{-x}$. The dynamical exponent z can be obtained from the divergence of the time scale at the phase transition, $\tau(k)\sim\omega(k)^{-1}\sim k^{-x/2}$. This yields $z=x/2$. The critical exponents at the finite-temperature fixed point are summarized in Table I. Except for the dynamical exponent which is not defined in the static classical model (1) all exponents at the finite-temperature critical point of the quantum model agree with those of the classical model. So at any finite temperature the asymptotic critical behavior is controlled by the classical fixed point as is expected from general renormalization-group arguments.[12]

IV. CRITICAL BEHAVIOR AT ZERO TEMPERATURE

We again investigate Eq. (9) for the mean spherical constraint, now for zero temperature. In this case the coth term in (9) is identical to 1 and the equation simplifies to

$$0=\frac{\partial f}{\partial \mu}=-\frac{1}{4}+\frac{h^2}{4\mu^2}+\frac{1}{N}\sum_k \frac{g}{2\omega(k)}. \tag{13}$$

The k integral converges for $D>x/2$ which is therefore the lower critical dimension. The critical coupling strength g_{c0} is given by

$$0=-\frac{1}{4}+\frac{1}{N}\sum_k \frac{g_{c0}}{2[g_{c0}U(k)]^{1/2}}. \tag{14}$$

In order to calculate the critical exponents we proceed analogously to Sec. III by subtracting (14) from (13). After calculation of the k sum we obtain

$$-t_g \sim \left(\frac{h}{\mu}\right)^2 + \begin{cases} C\mu^{(2D-x)/2x} & (D<3x/2) \\ C\mu\ \ln\lvert\mu\rvert & (D=3x/2) \\ C\mu & (D>3x/2). \end{cases} \tag{15}$$

The equation of state is given by

$$-t_g \sim m^2 + \begin{cases} C(h/m)^{(2D-x)/2x} & (D<3x/2) \\ C(h/m)\lvert\ln(h/m)\rvert & (D=3x/2) \\ C(h/m) & (D>3x/2). \end{cases} \tag{16}$$

Obviously the upper critical dimension is $3x/2$. All the critical exponents can be easily calculated from (15) and (16). They are summarized in Table I. As at the classical fixed point the dynamical exponent z is given by $x/2$. A comparison with the results of Sec. III shows that the critical exponents at the quantum critical point of the D-dimensional model are equal to those of a $(D+z)$-dimensional model at the finite-temperature critical point, as is expected from general renormalization-group arguments.[12] Thus all scaling relations are obeyed if one substitutes D by $D+z$.

In order to investigate the crossover from quantum to classical critical behavior arising at small but finite temperatures we first calculate the shift of the critical coupling due to a small but finite temperature. To this end we subtract Eq. (14) from Eq. (10). After calculation of the k sum we find for all dimensionalities $D>x$

$$g_c - g_{c0} \sim T^{(2D-x)/x}. \tag{17}$$

Here g_c is the critical coupling at finite temperature T and g_{c0} is the critical coupling at zero temperature. Therefore the shift exponent is given by $\phi=(2D-x)/x$. To derive the crossover scaling form of the equation of state,

$$m=t_g^{\beta} f(h/t_g^{\beta\delta}, T/t_g^{\phi}), \tag{18}$$

we subtract (14) from (9). Here t_g measures the distance from the critical coupling at zero temperature. This yields

$$0=\frac{h^2}{4\mu^2}+\frac{1}{N}\sum_k \frac{g}{2\{2g[\mu+U(k)/2]\}^{1/2}} \times\left(\coth\frac{1}{2}\beta\{2g[\mu+U(k)/2]\}^{1/2}-1\right) +\frac{1}{N}\sum_k\left(\frac{g}{2\{2g[\mu+U(k)/2]\}^{1/2}}-\frac{g}{2[gU(k)]^{1/2}}\right) +\frac{1}{N}\sum_k\frac{\sqrt{g}-\sqrt{g_{c0}}}{2[U(k)]^{1/2}}, \tag{19}$$

where we have added two terms that are actually zero. Calculating the arising integrals requires some patience. Below the upper critical dimension $D_u=3x/2$ we eventually find

$$0=m^2+\left(\frac{h}{m}\right)^{1/\gamma}F\left(\frac{h}{mT^2}\right)+\left(\frac{h}{m}\right)^{1/\gamma}+t_g, \tag{20}$$

where we have omitted all prefactors and kept only the leading terms close to the zero-temperature fixed point. The function F stems from the first of the k sums in (19). Equation (20) can be easily transformed into a scaling form equivalent to (18):

$$T=t_g^{x/(2D-x)}\Upsilon\left(\frac{t_g}{m^2},\frac{h}{m^{(2D+3x)/(2D-x)}}\right), \tag{21}$$

from which we extract the crossover exponent to be $\phi=x/(2D-x)$. The crossover exponent is equal to the inverse of the shift exponent and given by $\phi=z\nu$, as is expected from the analogy between the quantum-to-classical crossover scaling in this model and finite-size scaling.

In dimensions above the upper critical dimension D_u crossover scaling breaks down. The equation of state cannot be written in a form analogous to (18). This behavior corresponds to the breakdown of finite-size scaling in the spherical model above D_u (see, e.g., Ref. 10). It can be explained in terms of a dangerous irrelevant variable in the renormalization group.[26] We note that in agreement with the breakdown of the crossover scaling the shift of the critical coupling g_c for $D>D_u$ is not given by the naive scaling form $(g_c-g_{c0})\sim T^{1/z\nu}$ but is much weaker [see Eq. (17)].

V. FUNCTIONAL-INTEGRAL REPRESENTATION OF THE PARTITION FUNCTION

To shed some further light on the properties of the model and its relations to other models for quantum phase transitions we derive a functional-integral representation of the partition function by a method analogous to the Feynman functional integral[27] for the propagator. We start with the Trotter formula[28]

$$Z=\mathrm{Tr}e^{-\beta(H_{\mathrm{kin}}+H_{\mathrm{cl}})}=\mathrm{Tr}\lim_{n\to\infty}(e^{-\beta H_{\mathrm{kin}}/n}e^{-\beta H_{\mathrm{cl}}/n})^n. \tag{22}$$

Inserting appropriate sets of eigenstates of the operators S_i and P_i between the exponentials allows us to perform the trace. In the limit $n\to\infty$ the partition function may now be written as the functional integral

$$Z=\int D[S_i(\tau)]\exp\left\{-\int_0^\beta d\tau\left[\frac{1}{2g}\sum_i\left(\frac{\partial S_i}{\partial\tau}\right)^2+H_{\mathrm{cl}}[S_i(\tau)]\right]\right\}. \tag{23}$$

Here $D[S_i(\tau)]$ is, up to a normalization constant, the product of the dS_i for all sites i and all infinite imaginary time steps. In this form the partition function is similar to that of a model very recently suggested by Nieuwenhuizen.[22] The kinetic energy of his model, however, contains a first derivative with respect to imaginary time τ, whereas our model contains a second derivative (after partial integration). As a consequence, his model can be defined only for complex S_i or by considering the system and its dual at the same time. However, its behavior is closer to the behavior of quantum Heisenberg-Dirac spins. In particular, there is no energy gap for vanishing interactions and vanishing field. Consequently, although both models are similar, the differences in the kinetic energy result in different dynamical behavior. In particular, the models belong to different universality classes at the zero-temperature quantum critical point.

The critical properties of our model are determined only by the long-wavelength behavior of the interaction $U(k)$; thus we can omit all but the leading term of $U(k)$ without changing the critical behavior. After a Fourier transformation the partition function then reads

$$Z=\int D[S(k,\omega)] \times\exp\left\{-\beta\sum_\omega\sum_k\left(\frac{\omega^2}{2g}+ck^x\right)S(k,\omega)S(-k,-\omega)\right\}, \tag{24}$$

where c is a model-dependent constant. In the case of short-range interactions ($x=2$) this partition function can be seen as the spherical version of the usual field-theoretic nonlinear σ model.[29] As follows from the arguments given by Stanley[31] for the classical models its free energy is identical to the large-n limit of the $O(n)$ nonlinear σ model[30] which describes quantum rotors instead of Heisenberg-Dirac spins. (One major difference between rotors and spins is that the different components of an n-component rotor commute with each other whereas the components of Heisenberg-Dirac spin operators do not commute.)

VI. CONCLUSIONS

In this paper we have investigated the critical properties of a quantum version of the spherical model. We have obtained a quantum description by reinterpreting the spherical ''spins'' as operators and defining conjugate ''momentum'' operators via the canonical commutation relations. The Hamiltonian of the quantum model is given by the sum of a quadratic kinetic energy term and the classical spherical Hamiltonian. Therefore our model describes quantum ''rotors'' rather than Heisenberg-Dirac spins. Such rotors can be seen as generalization of Ising spins in a transverse field. They arise, e.g., in effective models for the low-temperature behavior of quantum Heisenberg antiferromagnets.[15,25]

Writing the partition function as a functional integral shows that the free energy of our model with short-range interactions is identical to that of the large-n limit of the field-theoretic $O(n)$ σ model. Obviously there are many possible choices for the kinetic term (one being that of Ref. 22) different from ours. In general they lead to different universality classes at the quantum critical point whereas the classical finite-temperature critical behavior is determined only by the form of the classical spherical Hamiltonian. It is therefore not influenced by the choice of the kinetic energy.

For our choice of the kinetic energy the critical properties of the D-dimensional model at the quantum critical point are identical to those of a $(D+z)$-dimensional model at the finite-temperature critical point. The dynamical exponent z is given by $x/2$ where the exponent x describes the behavior of the interaction $U(k)$ in the limit of small k. We consider this model as a starting point for the investigation of more complicated problems which arise, for instance, by adding quenched disorder to the model, which breaks the symmetry between spatial and temporal directions.

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