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Quantum spherical model with competing interactions

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ABSTRACT

We analyse the phase diagram of a quantum mean spherical model in terms of the temperature T , a quantum parameter g , and the ratio $p = -J_2/J_1$, where $J_1 > 0$ refers to ferromagnetic interactions between first-neighbour sites along the d directions of a hypercubic lattice, and $J_2 < 0$ is associated with competing antiferromagnetic interactions between second neighbours along $m \leq d$ directions. We regain a number of known results for the classical version of this model, including the topology of the critical line in the $g = 0$ space, with a Lifshitz point at $p = 1/4$, for $d > 2$, and closed-form expressions for the decay of the pair correlations in one dimension. In the $T = 0$ phase diagram, there is a critical border, $g_c = g_c(p)$ for $d \geq 2$, with a singularity at the Lifshitz point if $d < (m + 4)/2$. We also establish upper and lower critical dimensions, and analyse the quantum critical behavior in the neighborhood of $p = 1/4$.

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1. Introduction

The spherical model of magnetism has been used as an excellent laboratory to test ideas and concepts of phase transitions and critical phenomena [1–3]. There are several versions of the original model, including proposals of a quantum spherical model to correct some of the unphysical results at low temperatures [4–7]. The effects of frustration [8,9], random fields [10], and of disordered exchange interactions [11,12], have also been analysed in the context of quantum spherical models. With a view to describe the crossover between classical and quantum critical behaviour, Vojta [6] used a standard scheme of canonical quantization to analyse a quantum version of the ferromagnetic mean spherical model. We were then motivated to revisit this problem, with the addition of competing ferro and antiferromagnetic interactions, and the perspective to analyse a quantum Lifshitz point.

The mean spherical model, which has been originally proposed by Lewis and Wannier [2], is given by the partition function

$$Z_{cl} = \left[\prod_{\vec{T}} \int_{-\infty}^{+\infty} dS_{\vec{T}} \right] \exp \left[-\beta \mathcal{H} \{S_{\vec{T}}\} - \beta \mu \sum_{\vec{T}} S_{\vec{T}}^2 \right], \quad (1)$$

where $\beta = 1/(k_B T)$, T is the temperature and k_B is the Boltzmann constant, μ is a suitable chemical potential, \vec{T} is a lattice vector, and $\{S_{\vec{T}}\}$ is a set of continuous spin variables running over the N^d sites of a d -dimensional hypercubic lattice. The model Hamiltonian is written as

$$\mathcal{H} = - \sum_{(\vec{k}, \vec{T})} J_{\vec{k}, \vec{T}} S_{\vec{k}} S_{\vec{T}} - H \sum_{\vec{T}} S_{\vec{T}}, \quad (2)$$

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where (\vec{k}, \vec{l}) labels a pair of lattice sites, the exchange parameter $J_{\vec{k}, \vec{l}} = J(|\vec{k} - \vec{l}|)$ depends on the distance between sites \vec{k} and \vec{l} , and H is an external field. In this formulation, the chemical potential μ comes from the mean spherical condition,

$$\left\langle \sum_{\vec{l}} S_{\vec{l}}^2 \right\rangle = -\frac{1}{\beta} \frac{\partial}{\partial \mu} \ln Z_{cl} = N^d, \quad (3)$$

and it is well known that exact solutions for the thermodynamic functions can be obtained from the standard diagonalization of a quadratic form [3].

In a quantum version of this mean spherical model [4,6], the spin variable $S_{\vec{l}}$ becomes a position operator at lattice site \vec{l} , canonically conjugate to a momentum operator $P_{\vec{l}}$, with the commutation relations

$$[S_{\vec{l}}, S_{\vec{k}}] = 0, \quad [P_{\vec{l}}, P_{\vec{k}}] = 0, \quad [S_{\vec{l}}, P_{\vec{k}}] = i\delta_{\vec{l}, \vec{k}}, \quad (4)$$

where $\delta_{\vec{l}, \vec{k}}$ is a Kronecker delta and we assume that $\hbar = 1$. We then add a term of kinetic energy, depending on a quantum parameter g , and write the quantum quadratic form

$$\overline{\mathcal{H}} = \frac{1}{2}g \sum_{\vec{l}} P_{\vec{l}}^2 - \sum_{(\vec{k}, \vec{l})} J_{\vec{k}, \vec{l}} S_{\vec{k}} S_{\vec{l}} - H \sum_{\vec{l}} S_{\vec{l}} + \mu \sum_{\vec{l}} S_{\vec{l}}^2, \quad (5)$$

which can be diagonalised by a canonical method [6], leading to a solution of the problem for a general ferromagnetic pair interaction. At finite temperatures, the critical behaviour is essentially unchanged with respect to the classical spherical model. At zero temperature, depending on the parameter g , there is a quantum phase transition characterised by new (quantum) critical exponents. Also, the introduction of quantum fluctuations leads to a correction of the unphysical behaviour of the entropy at low temperatures.

We report an analysis of this version of the quantum mean spherical model in the presence of competing interactions. We consider ferromagnetic interactions, $J_1 > 0$, between pairs of first-neighbour sites along the d directions of a hypercubic lattice, and antiferromagnetic interactions, $J_2 < 0$, between second-neighbour sites along $m \leq d$ directions. Classical versions of this model [13–16], as well as more elaborate mean spherical models with competing interactions [17], have been studied by several authors. For $m = 1$, we regain a spherical analogue of the Axial-Next-Nearest-neighbour Ising, or ANNNI, model [18,19], which is known to display a rich phase diagram, including a Lifshitz point, in terms of the temperature T and a parameter $p = -J_2/J_1$ that gauges the strength of the competing interactions. We then analyse the T - p - g phase diagram, for different values of m , in particular the $T = 0$ behaviour, and establish the critical dimensions and critical exponents associated with this quantum model system. In the classical case, $g = 0$, we confirm a number of results, including a singularity of the critical border at the Lifshitz point for $2 < d < (m + 6)/2$. In one dimension, we derive analytic expressions for the decay of pair correlations, and determine the region of modulated behaviour in the T - p phase diagram.

2. The quantum mean spherical model with competing interactions

This problem can be treated either by a conventional reduction to a system of coupled harmonic oscillators or by a judicious application of the method of path integrals [5,20,21]. Let us first use the representation in terms of harmonic oscillators. We then introduce bosonic operators a_l^\dagger and a_l to write

$$S_l \equiv \frac{1}{\sqrt{2}} \left(\frac{g}{2\mu} \right)^{1/4} (a_l + a_l^\dagger) \quad (6)$$

and

$$P_l \equiv -\frac{i}{\sqrt{2}} \left(\frac{2\mu}{g} \right)^{1/4} (a_l - a_l^\dagger), \quad (7)$$

where we have omitted the vector notation. We now assume periodic boundary conditions, and change to a Fourier representation,

$$a_l = \frac{1}{N^{d/2}} \sum_q a_q \exp(iql), \quad (8)$$

where a_q and a_q^\dagger are bosonic operators,

$$[a_q, a_{q'}] = 0, \quad [a_q^\dagger, a_{q'}^\dagger] = 0, \quad [a_q, a_{q'}^\dagger] = \delta_{q, q'}, \quad (9)$$

and the sum is over the d -dimensional vectors q belonging to the first Brillouin zone. We then write the quantum quadratic form (5) in the Fourier representation,

$$\begin{aligned} \bar{\mathcal{H}} = & (2g\mu)^{1/2} \sum_q \left[1 - \frac{\hat{J}(q)}{4\mu} \right] a_q^\dagger a_q - \frac{1}{2} (2g\mu)^{1/2} \sum_q \frac{\hat{J}(q)}{4\mu} (a_q a_{-q} + a_q^\dagger a_{-q}^\dagger) \\ & - H \left(\frac{N^d}{2} \right)^{1/2} \left(\frac{g}{2\mu} \right)^{1/4} (a_0 + a_0^\dagger) + \frac{N^d}{2} (2g\mu)^{1/2}, \end{aligned} \tag{10}$$

with

$$\hat{J}(\vec{q}) = \sum_{\vec{h}} J(|\vec{h}|) \exp(i\vec{q} \cdot \vec{h}), \tag{11}$$

where the sum runs over all lattice vectors. The final diagonalization of this quadratic form comes from the introduction of new bosonic operators, c_q and c_q^\dagger , according to a well-known Bogoliubov transformation. We then have

$$\bar{\mathcal{H}} = \sum_q w(q) \left(c_q^\dagger c_q + \frac{1}{2} \right) - \frac{N^d H^2}{4 \left[\mu - \frac{\hat{J}(0)}{2} \right]}, \tag{12}$$

where

$$[w(q)]^2 \equiv (2g\mu) \left[1 - \frac{\hat{J}(q)}{2\mu} \right], \tag{13}$$

which requires that the chemical potential μ should be larger than a certain limiting critical value μ_c ,

$$\mu > \mu_c = \max_{\vec{q}} \frac{1}{2} \hat{J}(\vec{q}) = \frac{1}{2} \hat{J}(\vec{q}_c). \tag{14}$$

In analogy with a system of harmonic oscillators, we then write the partition function

$$Z_N(\beta, H, \mu) = \exp \left[\frac{\beta N^d H^2}{4 \left(\mu - \frac{\hat{J}(0)}{2} \right)} \right] \prod_q \left[2 \sinh \frac{1}{2} \beta w(q) \right]^{-1}, \tag{15}$$

and the free energy per site,

$$f(\beta, H, \mu) = - \frac{H^2}{4 \left[\mu - \frac{\hat{J}(0)}{2} \right]} + \frac{1}{\beta} \lim_{N \rightarrow \infty} \frac{1}{N^d} \sum_q \ln \left[2 \sinh \frac{1}{2} \beta w(q) \right], \tag{16}$$

with $\mu > \mu_c = \hat{J}(\vec{q}_c)/2$. The spherical constraint, given by Eq. (3), from which we determine the chemical potential μ , is written as

$$1 = \frac{H^2}{4 \left[\mu - \frac{\hat{J}(0)}{2} \right]^2} + \lim_{N \rightarrow \infty} \frac{1}{N^d} \sum_q \frac{g}{2w(q)} \coth \left[\frac{1}{2} \beta w(q) \right]. \tag{17}$$

In the classical limit, $g \rightarrow 0$, we regain most of the well-known results for the mean spherical model. The classical limit of this quantum free energy, however, includes an extra term of the form $\ln(\beta g)$, which corrects the classical behaviour at low temperatures. The particular limit $\hat{J}(q) \rightarrow 0$ corresponds to free quantum (spherical) rotors, with a finite energy gap, in contrast to the usual Heisenberg–Dirac spins.

These expressions also come from a straightforward application of the path integral formalism, which has been widely used to treat quantum statistical problems [5,20]. It is then interesting to write the Lagrangian associated with this problem,

$$\mathcal{L} = \frac{1}{2g} \sum_l \dot{S}_l^2 + \frac{1}{2} \sum_{k,l} J_{k,l} S_k S_l + H \sum_l S_l - \mu \sum_l S_l^2. \tag{18}$$

In the imaginary time formalism, with $t \rightarrow -i\tau$, the partition function is written as

$$\begin{aligned} Z = & \int \left(\prod_l \mathcal{D}S_l(\tau) \right) \exp \left\{ \int_0^\beta d\tau \left[- \frac{1}{2g} \sum_l \left(\frac{\partial S_l(\tau)}{\partial \tau} \right)^2 \right. \right. \\ & \left. \left. + \frac{1}{2} \sum_{l,l'} J_{l,l'} S_l(\tau) S_{l'}(\tau) + H \sum_l S_l(\tau) - \mu \sum_l S_l^2(\tau) \right] \right\}, \end{aligned} \tag{19}$$

where the first integral includes periodic conditions, $S_l(0) = S_l(\beta)$. We now introduce the Fourier transformation,

$$S_l(\tau) = \left(\frac{\beta}{N}\right)^{\frac{1}{2}} \sum_{q,w} \exp[i(ql + \tau w)] S_q(w), \quad (20)$$

where the vector q belongs to the first Brillouin zone, and $w \equiv w_n = (2n\pi)/\beta$, with integer n , is a Matsubara frequency. We then write the partition function

$$Z = \exp(\beta N \mu) \int \left(\prod_{n=-\infty}^{\infty} \prod_q dS_q(w_n) \right) \exp \left\{ (\beta N^d)^{\frac{1}{2}} \beta S_0(0) H + \sum_{q,n} \left[-\frac{\beta^2 w_n^2}{2g} + \frac{1}{2} \beta^2 \hat{J}(q) - \beta^2 \mu \right] S_q(w_n) S_{-q}(-w_n) \right\}, \quad (21)$$

where $\hat{J}(q)$ is given by Eq. (11), and we have omitted the vector notation. If we calculate the Gaussian integrals, and use the identity

$$\prod_{n=1}^{\infty} \left[1 + \left(\frac{w\beta}{n\pi} \right)^2 \right] = \frac{\sinh w\beta}{w\beta}, \quad (22)$$

it is straightforward to regain the partition function given by Eq. (15).

This general solution works for all forms of distance-dependent interactions, $J_{\vec{k},\vec{l}} = J(|\vec{k} - \vec{l}|)$. We now consider ferromagnetic interactions, $J_1 > 0$, between pairs of first-neighbour sites along the d directions of a hypercubic lattice, and antiferromagnetic interactions, $J_2 < 0$, between second-neighbour sites along $m \leq d$ directions. The Fourier transform of the exchange interactions is given by

$$\hat{J}(\vec{q}) = 2J_1 \sum_{j=1}^d \cos q_j + 2J_2 \sum_{j=1}^m \cos 2q_j, \quad (23)$$

where $\vec{q} = (q_1, q_2, \dots, q_d)$ is a wave vector in suitable (dimensionless) units. The maximum of $\hat{J}(\vec{q})$ depends on the ratio $p = -J_2/J_1$. If $p \leq 1/4$, the maximum is located at the critical value $\vec{q}_c = 0$, as in the simple ferromagnetic case. If $p > 1/4$, the maximum of $\hat{J}(\vec{q})$ is given by the critical vector

$$\vec{q}_c = (q_{c1}, q_{c2}, \dots, q_{cm}, 0, \dots, 0), \quad (24)$$

where

$$q_{c1} = q_{c2} = \dots = q_{cm} = \cos^{-1} \frac{1}{4p}. \quad (25)$$

The special case $p = 1/4$ corresponds to a Lifshitz point of degree m .

3. Phase diagrams and critical behaviour

In zero field, $H = 0$, the paramagnetic critical boundary in the T - p - g space comes from the spherical constraint, given by Eq. (17), supplemented by the critical limit of the chemical potential, $\mu = \mu_c$, given by Eq. (14). We then write

$$1 = \lim_{N \rightarrow \infty} \frac{1}{N^d} \sum_q \frac{g}{2w_c(q)} \coth \left[\frac{1}{2} \beta w_c(q) \right], \quad (26)$$

where

$$w_c(q) = g^{1/2} \left[\hat{J}(\vec{q}_c) - \hat{J}(\vec{q}) \right]^{1/2}. \quad (27)$$

In the classical limit, $g \rightarrow 0$, we have

$$1 = \lim_{N \rightarrow \infty} \frac{1}{N^d} \sum_q \frac{1}{\beta \left[\hat{J}(\vec{q}_c) - \hat{J}(\vec{q}) \right]}, \quad (28)$$

from which we obtain the critical temperature as function of p , for all values of d and m ,

$$\frac{k_B T_c}{2J_1} = \frac{1}{I(p, d, m)}, \quad (29)$$

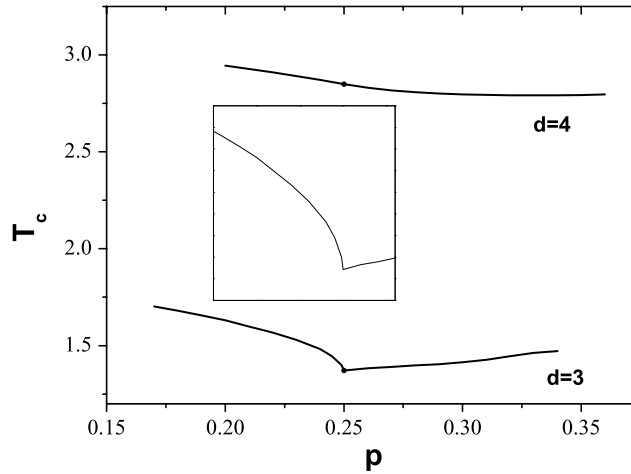


Fig. 1. Classical T - p phase diagrams, for dimensions $d = 3$ and $d = 4$, near a Lifshitz point ($p = 1/4$), with $m = 1$. The critical line separates ordered and disordered phases. Along the critical line, $\bar{q}_c = 0$ for $p \leq 1/4$, and $\bar{q}_c \neq 0$ for $p > 1/4$. The inset shows a magnification in order to emphasise the singular behavior of the paramagnetic border near the Lifshitz point in three-dimensions.

with

$$I(p, d, m) = \frac{1}{(2\pi)^d} \int d^d q \frac{1}{\sum_{j=1}^d (1 - \cos q_j) - p \sum_{j=1}^m (1 - \cos 2q_j)}, \tag{30}$$

for $p < 1/4$, and

$$I(p, d, m) = \frac{1}{(2\pi)^d} \int d^d q \frac{1}{\sum_{j=1}^d (1 - \cos q_j) - p \sum_{j=1}^m \left(\frac{1}{p} - \frac{1}{8p^2} - 1 - \cos 2q_j \right)}, \tag{31}$$

for $p > 1/4$.

There is a long history associated with the calculations of similar lattice Green functions [3,22]. From the identity

$$\frac{1}{a^n} = \frac{1}{(n-1)!} \int_0^\infty dx x^{n-1} \exp(-ax), \tag{32}$$

where n is an integer, and $a > 0$, we write integral representations for $I(p, d, m)$, which are convenient to carry out an asymptotic analysis. For $d \leq 2$, the divergence of these integrals indicate that $T_c = 0$ for all values of m and $p \neq 1/4$. Also, we have $T_c > 0$ for $d > 2$, and for all values of m and $p \neq 1/4$. In particular, at the Lifshitz point, $T_c > 0$ for $d > (m + 4)/2$. We now consider the graphs of $T_c = T_c(p)$ versus the parameter p . It is easy to write an expression for dT_c/dp , for $p < 1/4$ and $p > 1/4$, and to show that there is common tangent at the Lifshitz point, $p = 1/4$. For example, for $d = 3$ and $m = 1$, we have

$$\left. \frac{\partial}{\partial p} \left(\frac{k_B T_c}{2J_1} \right) \right|_{p=1/4} = - \frac{1}{[I(\frac{1}{4}, 3, 1)]^2} \tilde{I},$$

with

$$\tilde{I} = \frac{1}{4(2\pi)^3} \int d^3 q \frac{1 - \cos 2q_1}{\left(\frac{11}{4} - \cos q_1 - \cos q_2 - \cos q_3 + \cos 2q_1 \right)^2}. \tag{33}$$

We then use the identity (32), with $n = 2$, to write an integral representation from which it is easy to show that the common tangent at the Lifshitz point, $p = 1/4$, is infinite for (i) $d < 2$, and (ii) $d > 2$, with $d < (m + 6)/2$, which includes the analogue of the ANNNI model ($d = 3$ and $m = 1$). In the numerically obtained graphs of Fig. 1, we sketch typical profiles of the critical line $T_c = T_c(p)$ for dimensions $d = 3$ and $d = 4$, and $m = 1$. Note the smooth behaviour of this paramagnetic border for $d = 4$ (and $m = 1$). The scale of this figure, however, is not enough to show the sharp singularity at the Lifshitz point for $d = 3$ (and $m = 1$), as pointed out in a sketch by Hornreich [23].

In the zero-temperature limit, $T \rightarrow 0$, Eq. (26) can be written as

$$1 = \frac{g^{1/2}}{2} \lim_{N \rightarrow \infty} \frac{1}{N^d} \sum_q \frac{1}{[\hat{J}(\vec{q}_c) - \hat{J}(\vec{q})]^{1/2}},$$

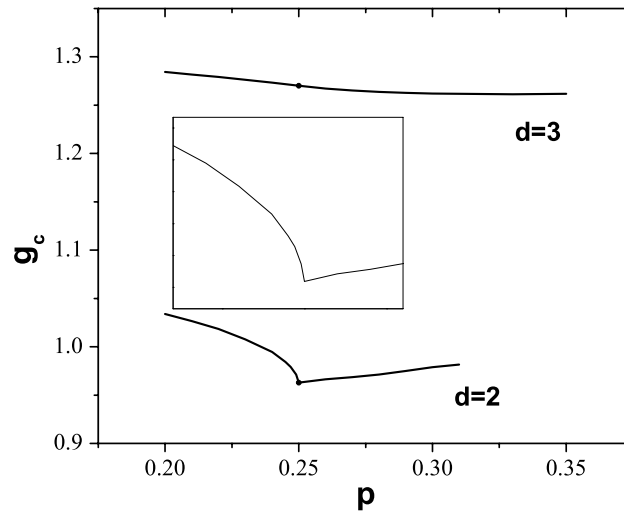


Fig. 2. Quantum phase diagram ($T = 0$) near a Lifshitz point with dimensions $d = 2$ and $d = 3$, and $m = 1$. Along the critical line, $g_c = g_c(p)$, we have $\vec{q}_c = 0$ for $p \leq 1/4$, and $\vec{q}_c \neq 0$ for $p > 1/4$. The inset shows a magnification of the border near $p = 1/4$ in two dimensions.

from which we obtain the critical quantum parameter, g_c , as a function of p , for all values of d and m ,

$$\frac{g_c}{2J_1} = \left[\frac{2}{I_Q(p, d, m)} \right]^2, \quad (34)$$

where

$$I_Q(p, d, m) = \frac{1}{(2\pi)^d} \int d^d q \frac{1}{\left[\sum_{j=1}^d (1 - \cos q_j) - p \sum_{j=1}^m (1 - \cos 2q_j) \right]^{1/2}}, \quad (35)$$

for $p < 1/4$, and

$$I_Q(p, d, m) = \frac{1}{(2\pi)^d} \int d^d q \frac{1}{\left[\sum_{j=1}^d (1 - \cos q_j) - p \sum_{j=1}^m \left(\frac{1}{p} - \frac{1}{8p^2} - 1 - \cos 2q_j \right) \right]^{1/2}}, \quad (36)$$

for $p > 1/4$. We now use an analytic continuation of the identity (32), for non integer values of n . From a similar analysis of convergence of these expressions, it is easy to show that there is a quantum phase transition ($g_c \neq 0$) for $d \geq 2$, independent of the value of m . In particular, there is a common derivative $\partial g_c / \partial p$ at the Lifshitz point, $p = 1/4$, with a singularity for $2 \leq d < (m + 4)/2$ (and a smooth behaviour for $d = 3$ and $m = 1$). In Fig. 2, we sketch typical profiles of this critical line in the $g - p$ plane for dimensions $d = 2$ and $d = 3$, and $m = 1$.

The critical behaviour in zero field, $H = 0$, comes from an asymptotic analysis of the spherical constraint in the neighbourhood of the transition. At finite temperatures, $T \neq 0$, in the limit $\mu \rightarrow \hat{J}(\mathbf{q})/2$, we have

$$\frac{1}{N^d} \sum_q \frac{g}{2w(q)} \coth \frac{1}{2} \beta w(q) = \frac{1}{12} g \beta + \frac{1}{N^d} \sum_q \frac{g}{\beta w^2(q)} + \mathcal{O}[w^2(q)]. \quad (37)$$

At zero temperature, $T = 0$, we have

$$\frac{1}{N^d} \sum_q \frac{g}{2w(q)} \coth \frac{1}{2} \beta w(q) = \frac{1}{N^d} \sum_q \frac{g}{2w(q)}. \quad (38)$$

We now expand $\hat{J}(q)$ as a Taylor series about $\vec{q} = \vec{q}_c$, in the classical and quantum cases. Although \vec{q}_c depends on the parameter p , the convergence of the sums in the right-hand side of Eqs. (37) and (38) does not depend on p , for $p \neq 1/4$. For finite temperatures, $T \neq 0$, the sum converges if $d > 2$ (which determines the lower critical dimension of the classical case), regardless of the value of m . At $T = 0$, the sum converges for $d > 1$, which leads to the lower critical dimension of the quantum case.

Let us consider some special situations.

3.1. Critical behaviour at finite temperatures and $p \neq 1/4$

In zero field, $H = 0$, at finite temperatures, $T \neq 0$, and for $p \neq 1/4$, we use Eq. (37) and perform a Taylor expansion about $T = T_c$ and $\mu = \mu_c$. We then have the asymptotic expression

$$0 \approx \frac{(T - T_c)}{2} \int d^d q \frac{1}{\mu_c - \frac{\hat{j}(q)}{2}} - (\mu - \mu_c) T_c \int d^d q \frac{1}{\left(\mu_c - \frac{\hat{j}(q)}{2}\right)^2}. \tag{39}$$

We now expand the integrands about $\vec{q} = \vec{q}_c$, and obtain

$$(\mu - \mu_c) \sim \begin{cases} \tau, & \text{for } d > 4 \\ \frac{\tau}{\ln \tau}, & \text{for } d = 4 \\ \tau^2, & \text{for } d = 3, \end{cases} \tag{40}$$

where $\tau = (T - T_c)/T_c$ gives the distance from the classical critical point. From these equations, supplemented by standard scaling considerations, it is possible to calculate the usual critical exponents associated with the classical spherical model. Although \vec{q}_c assumes different values for $p < 1/4$ and $p > 1/4$, the asymptotic behaviour is the same, regardless of the value of m .

3.2. Critical behaviour at $T = 0$ and $p \neq 1/4$

In analogy with the calculations for finite temperatures, we write

$$0 \approx (g - g_c) \int d^d q \frac{1}{\left(\mu_c - \frac{\hat{j}(q)}{2}\right)^{1/2}} - (\mu - \mu_c) g_c \int d^d q \frac{1}{\left(\mu_c - \frac{\hat{j}(q)}{2}\right)^{3/2}}. \tag{41}$$

From an expansion about $\vec{q} = \vec{q}_c$, we obtain the asymptotic behaviour

$$(\mu - \mu_c) \sim \begin{cases} \delta, & \text{for } d > 3 \\ \frac{\delta}{\ln \delta}, & \text{for } d = 3 \\ \delta^2, & \text{for } d = 2, \end{cases} \tag{42}$$

where $\delta = (g - g_c)/g_c$ gives the distance from the quantum critical point. As in the case of finite temperatures, Eq. (42) holds for $p \neq 1/4$ and any value of $m \leq d$. It is easy to use scaling arguments in order to obtain the (quantum) critical exponents for $p \neq 1/4$. With the necessary reinterpretations, and although critical dimensions are different, these values are in agreement with results of Vojta for the quantum ferromagnetic case [6].

3.3. Critical behaviour for $p = 1/4$

At the Lifshitz point, $p = 1/4$, the maximum of $\hat{J}(\vec{q})$ is still given by $\vec{q}_c = (0, 0, 0, \dots, 0)$, but the second derivative vanishes along the direction of competition. We then have to consider the quartic term in the expansion of $\hat{J}(\vec{q})$ about $\vec{q} = \vec{q}_c$.

For $T \neq 0$, the first and second integrals of Eq. (39) exist for $d > (m + 4)/2$ and for $d > (m + 8)/2$, respectively. We then have

$$(\mu - \mu_c) \sim \begin{cases} \tau, & d > (m + 8)/2, \\ \tau / \ln \tau, & d = (m + 8)/2, \\ \tau^{3/2}, & d = (m + 7)/2, \\ \tau^2, & d = (m + 6)/2, \\ \tau^{5/2}, & d = (m + 5)/2, \end{cases} \tag{43}$$

where $\tau = (T - T_c)/T_c$. From these asymptotic results, it is possible to obtain all the classical critical exponents.

At $T = 0$, the first integral in Eq. (41) exists for $d > (m + 2)/2$, and the second integral for $d > (m + 6)/2$. We then have

$$(\mu - \mu_c) \sim \begin{cases} \delta, & d > (m + 6)/2, \\ \delta / \ln \delta, & d = (m + 6)/2, \\ \delta^{3/2}, & d = (m + 5)/2, \\ \delta^2, & d = (m + 4)/2, \\ \delta^{5/2}, & d = (m + 3)/2, \end{cases} \tag{44}$$

where $\delta = (g - g_c)/g_c$. In conclusion, we have the same values for either classical or quantum exponents. As in the case of $p \neq 1/4$, the only difference is the critical dimension. According to an old conjecture about quantum critical behaviour, the quantum values of the critical exponents are given by the corresponding values of the classical version of the system in $d + z$ dimensions, where z is a dynamical critical exponent. For $m < d$ the dynamical critical exponent is $z = 1$ (anisotropic case); for $m = d$, it assumes the value $z = 2$ (isotropic case). It should be mentioned that Hamiltonian formulations of the mean spherical model have been considered by some authors [24].

3.4. Decay of pair correlations

Let us consider the system in a site-dependent field,

$$\mathcal{H} = - \sum_{(\vec{k}, \vec{\Gamma})} J_{\vec{k}, \vec{\Gamma}} S_{\vec{k}} S_{\vec{\Gamma}} - \sum_{\vec{\Gamma}} H_{\vec{\Gamma}} S_{\vec{\Gamma}}, \tag{45}$$

and write the partition function

$$Z_N(\beta, H, \mu) = \prod_q \exp \left[\frac{\beta N^d \widehat{H}(q) \widehat{H}(-q)}{4 \left(\mu - \frac{\widehat{j}(q)}{2} \right)} \right] \left[2 \sinh \frac{1}{2} \beta w(q) \right]^{-1}, \tag{46}$$

where $\widehat{H}(q)$ is the Fourier transform of $H_{\vec{\Gamma}}$, and we are omitting the vector notation. We then have

$$\langle S_q S_{-q} \rangle_N = \frac{4}{(\beta N^d)^2} \frac{\delta^2 \ln Z}{\delta \widehat{H}(q) \delta \widehat{H}(-q)} \Big|_{\widehat{H}(q)=\widehat{H}(-q)=0} = \frac{2g}{\beta N^d} \frac{1}{[w(q)]^2}, \tag{47}$$

from which we obtain the pair correlations in real space,

$$\langle S_r S_{r+h} \rangle_N = \frac{1}{\beta N^d} \sum_q \frac{\exp(iqh)}{2\mu - \widehat{j}(q)}. \tag{48}$$

As discussed by Pisani and collaborators [16], the analysis of $\langle S_r S_{r+h} \rangle$, for $d \geq 3$, below the critical temperature, leads to the introduction of a modulated order parameter, with characteristic oscillations for $p > 1/4$. A detailed analysis of the long-range correlations at Lifshitz point has been published by Frachebourg and Henkel [25]. There are also some investigations of the interplay between competing interactions and the decay of correlations [26].

We now show that these oscillations of the pair correlations in terms of distance are already present in the much simpler one-dimensional case. In the thermodynamic limit, Eq. (48) can be written as

$$\langle S_r S_{r+h} \rangle = \frac{1}{2\pi \beta} \int_{-\pi}^{\pi} dq \frac{\exp(iqh)}{[\mu - \cos q + p \cos 2q]}, \tag{49}$$

with the spherical condition

$$1 = \frac{1}{2\pi \beta} \int_{-\pi}^{\pi} dq \frac{1}{[\mu - \cos q + p \cos 2q]}, \tag{50}$$

where $p > 0$, μ and β are written in units of $J_1 > 0$, with the requirement that $\mu > \mu_c$. Therefore, $\mu > (1 - p)$ for $p < 1/4$, and $\mu > [1/(8p) + p]$ for $p > 1/4$. Eq. (49) can be rewritten as

$$\langle S_r, S_{r+h} \rangle = \frac{1}{\pi \beta i p} \oint_C dw \frac{w^{h+1}}{w^4 - \frac{1}{p} w^3 + \frac{2\mu}{p} w^2 - \frac{1}{p} w + 1}, \tag{51}$$

where the contour C is the unit circle and we assuming that $h > 0$. The fourth-order polynomial in the denominator is easily factorised, with two roots, w_1 and w_2 , inside the unit circle. After some straightforward algebra, we have

$$\langle S_r S_{r+h} \rangle = \frac{\cos[h\theta_1 + (\theta_1 - \alpha)]}{\cos(\theta_1 - \alpha)} \exp[h \ln |w_1|], \tag{52}$$

where α is a real phase depending on p and μ , and

$$w_1 = |w_1| \exp(i\theta_1) = \frac{1}{4p} (1 - A - 2B), \tag{53}$$

with

$$A = \sqrt{8p^2 - 8p\mu + 1}; \quad B = \sqrt{\frac{1}{2} - 2p(p - \mu) - \frac{1}{2}A}, \tag{54}$$

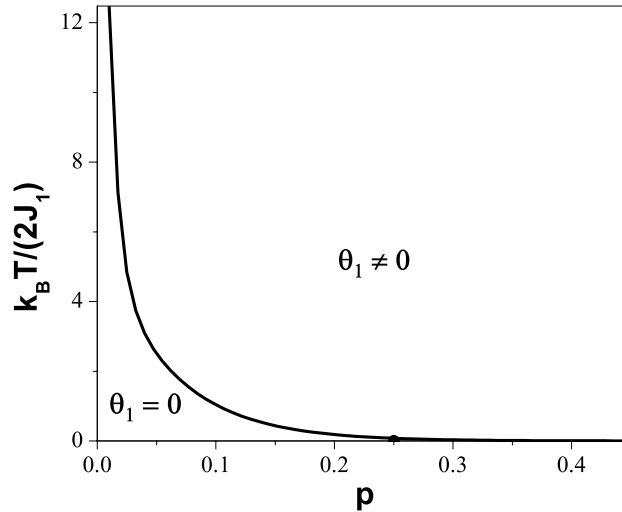


Fig. 3. Regions of the T - p plane of the one-dimensional model with simple exponential decay ($\theta_1 = 0$) and oscillatory exponential decay ($\theta_1 \neq 0$) of the pair correlations.

so that $|w_1| < 1$, which leads to the well-known exponential decay. The spherical condition (50) can be used to parametrically eliminate the chemical potential μ , and write the correlations in terms of T and p . In particular, oscillations are suppressed by $\theta_1 = 0$, which is equivalent to

$$\frac{k_B T}{2J_1} = \frac{1}{8p} - 2p, \quad (55)$$

with the asymptotic value $T = 0$ for $p = 1/4$. In Fig. 3, we draw this border, and indicate the region with oscillating correlations ($\theta_1 \neq 0$) in the T - p plane. From Eq. (52), we can write expressions for a modulation length, $L_D = 2\pi/\theta_1$, and the correlation length, $\xi = -1/\ln|w_1|$, in terms of temperature and the competition parameter p , which is a useful information to investigate the growth of modulated domains [26]. A similar behaviour has been found by Stephenson [27] in a calculation for the ANNNI chain.

4. Conclusions

We report an analysis of the phase diagram of a quantum mean spherical model in terms of temperature T , a quantum parameter g , and the ratio $p = -J_2/J_1$, where $J_1 > 0$ is a ferromagnetic interaction between first-neighbour sites along the d directions of a hypercubic lattice, and $J_2 < 0$ is associated with competing antiferromagnetic interactions between second neighbours along $m \leq d$ directions. We regain a number of results for the classical version of this model, including the topology of the critical line in the $g = 0$ space, with a singular behaviour at the Lifshitz point, $p = 1/4$, for $2 < d < (m+6)/2$, which includes the case of the usual analogue of the Axial-Next-Nearest-neighbour Ising, or ANNNI, model. We consider in particular the $T = 0$ phase diagram, which displays a quantum Lifshitz point, at $p = 1/4$. In the $g - p$ phase diagram, there is a critical border, $g_c = g_c(p)$ for $d \geq 2$, with a singularity at the Lifshitz point if $d < (m + 4)/2$. We establish upper and lower critical dimensions and analyse the critical behaviour in the neighbourhood of the Lifshitz point. In one dimension, we derive analytic expressions for the decay of pair correlations, and determine the region of modulated behaviour in the T - p phase diagrams.

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