Reaction-field calculation for the quantum Potts model

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Abstract. The reaction-field approximation is applied to the d -dimensional q -state quantum Potts model in an external transverse field. With the exception of $d \geq 3$, the tricritical value $q_c(d)$, below which the system has a second-order phase transition, decreases with increasing external field strength. From the ground state of the quantum d -dimensional model, an improved value of q_c is obtained for the classical model in $d + 1$ dimensions. A direct explanation is also obtained for the expected tricritical point in finite-thickness slabs of cubic ferromagnets (like DyAl_2) with a field in the (111) direction.

1. Introduction

In a previous paper (Dekeyser *et al* 1983) we have solved the general d -dimensional q -state Potts model on a hypercubic lattice in Onsager's reaction-field approximation. This approximation is an improvement on the molecular-field approximation (MFA), in the sense that it takes into account the direct influence on neighbouring sites of the particular state in which a given site may be found. More specifically, we focused our attention on the prediction for $q_c(d)$, giving the borderline between first- and second-order transitions. As is well known, a simple MFA gives the completely wrong prediction $q_c(d) = 2$ for this tricritical line. The result of our reaction-field approach was a remarkable qualitative improvement for $q_c(d)$.

In the present paper we apply the same method to the quantum mechanical case of the q -state Potts model in an external transverse field (Kogut and Sinclair 1981). The basic ideas of our derivation are equivalent to those of the calculation for the classical Potts system. The presence of the transverse field, however, complicates the necessary computational effort a great deal. Instead of reproducing these calculations in full detail, we will mainly stress the differences from the previous derivation due to the quantum mechanical nature of the Potts model in a transverse field. From the methodological point of view, this paper is a demonstration of how to apply the reaction-field idea to a quantum model.

After summarising the main formulae for the model and its MFA in § 2, the reaction-field approach is described in § 3. In § 4 we discuss a few applications of our calculation. First of all, from the ground-state result we may derive an improved prediction for $q_c(d + 1)$ for the classical zero-field model. Next we discuss the cubic ferromagnets such as DyAl_2 with a magnetic field in the (111) direction as a possible physical

realisation of the quantum three-state model. This allows us to explain the possible existence of tricritical points for slabs of finite thickness of these materials, not in terms of a dimensional crossover, but simply in terms of quantum effects.

2. Description of the model and MFA

When a transverse field is switched on, the q -state Potts model becomes a quantum model. A variable s_i is associated with each site i of a regular (hypercubic) lattice, where s_i may assume the integer values from 1 to q . Accordingly, we associate with each site a q -component column state vector s_i such that

$$(s_i)_j = \delta_{jk} \quad \text{when } s_i = k \ (k = 1, \dots, q).$$

The Hamiltonian of the model may be written as

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \mathbf{P}_i \cdot \mathbf{P}_j - h \sum_i B_i. \quad (1)$$

As usual, the first sum runs over nearest-neighbour pairs $\langle ij \rangle$. The q components P_i^k of the vector $\mathbf{P}_i$ are the projectors on the k th Potts state at site i :

$$(P_i^k)_{mn} = \delta_{mk} \delta_{nk}. \quad (2)$$

The first term of the Hamiltonian thus assigns an energy $-J$ to every set of neighbouring sites that are in the same Potts state. The transverse-field strength h is combined with the operators B_i where

$$(B_i)_{mn} = 1 - \delta_{mn}. \quad (3)$$

The transverse field thus tries to prevent condensation in any particular state.

Below a certain temperature and/or below a certain field strength we expect to find a condensation into, for example, the state $s = 1$, such that the thermal averages of the projectors are given by

$$p_1 = \langle P_i^1 \rangle = [1 + (q-1)m]/q \quad (4a)$$

$$p_n = \langle P_i^n \rangle = (1-m)/q \quad 2 \leq n \leq q. \quad (4b)$$

m is the order parameter. The MFA for this model is derived from the effective one-site Hamiltonian $\mathcal{H}_{\text{MFA}}$, which one obtains by replacing in (1) the projectors P_i^k on the z ($= 2d$ for hypercubic lattices) neighbours j of a particular site i by their expectation values (4):

$$\mathcal{H}_{\text{MFA}} = -Jz \left(p_1 P^1 + \sum_{n=2}^q p_n P^n \right) - hB. \quad (5)$$

Defining (with $\beta = 1/kT$)

$$-\beta \mathcal{H}_{\text{MFA}} = H \quad (6)$$

we thus obtain the matrix elements

$$H_{11} = \beta Jz p_1 \equiv \alpha \quad (7a)$$

$$H_{nn} = \beta Jz p_n \equiv \gamma \quad 2 \leq n \leq q \quad (7b)$$

$$H_{kl} = \beta h \equiv \eta \quad 1 \leq j \neq k \leq q. \quad (7c)$$

The relevant properties of the eigenvalues and eigenvectors of this matrix H are as follows.

(i) There are two eigenvectors e_+ and e_- with a non-zero first component. They belong to the eigenvalues λ_+ and λ_- respectively, with

$$\lambda_{\pm} = \alpha + u \pm w \quad (8)$$

where

$$u = \frac{1}{2}[\gamma - \alpha + (q - 2)\eta] \quad (9)$$

$$w = [u^2 + (q - 1)\eta^2]^{1/2}. \quad (10)$$

The (not yet normalised) eigenvectors have components

$$(e_{\pm})_1 = (q - 1)\eta \quad (11a)$$

$$(e_{\pm})_n = u \pm w \quad 2 \leq n \leq q. \quad (11b)$$

(ii) The third eigenvalue

$$\lambda_0 = \gamma - \eta \quad (12)$$

is $(q - 2)$ -fold degenerate. Its eigenspace is formed by all the vectors f with the properties

$$f_1 = 0 \quad \text{and} \quad \sum_{n=2}^q f_n = 0. \quad (13)$$

(iii) The unitary operator transforming from the standard Potts-state basis to the basis of eigenstates of H therefore has the following properties:

$$\begin{aligned} T_{11} &= (q - 1)\eta C_+ \\ T_{12} &= (q - 1)\eta C_- \\ T_{1n} &= 0 \quad 3 \leq n \leq q \\ \left. \begin{aligned} T_{n1} &= (u + w)C_+ \\ T_{n2} &= (u - w)C_- \end{aligned} \right\} \quad 2 \leq n \leq q \end{aligned} \quad (14)$$

where

$$C_{\pm} = [(q - 1)^2\eta^2 + (q - 1)(u \pm w)^2]^{-1/2}. \quad (15)$$

The matrix elements not defined by (14) depend on the particular choice made for the $(q - 2)$ -fold-degenerate eigenstates. We will not need a precise knowledge about these states, since we will use the unitarity of T , expressed by (T has real elements)

$$\sum_{n=3}^q T_{kn}T_{ln} = \delta_{kl} - T_{k1}T_{l1} - T_{k2}T_{l2}. \quad (16)$$

Let us come back now to the MFA. From (5) we obtain the self-consistency condition

$$\begin{aligned} p_1 &= Z^{-1} \text{Tr}(P^1 e^H) \\ &= Z^{-1}(T_{11}^2 e^{\lambda_+} + T_{12}^2 e^{\lambda_-}) \end{aligned} \quad (17)$$

where the single-site partition function is

$$Z = e^{\lambda^+} + e^{\lambda^-} + (q - 2) e^{\lambda_0}. \quad (18)$$

Equation (17) is the standard MFA equation of state for this model, giving in principle the order parameter m as a function of βJz , $\eta = \beta h$ and q . The right-hand side of (17) can indeed be written as a function of the difference

$$\alpha - \gamma = \beta Jzm. \quad (19)$$

By a series expansion, (17) then reduces to an equation

$$g(m) \equiv a_1 m + a_2 m^2 + \dots = 0. \quad (20)$$

This may be interpreted as the derivative of the free energy with respect to m . As is well known from the Landau theory, a second-order phase transition occurs when $a_1 = 0$ and $a_2 > 0$ (if only positive m are allowed, see Dekeyser *et al* 1983), while $a_2 < 0$ means that the system underwent a first-order transition. The tricritical point is then determined from $a_1 = 0 = a_2$. One easily verifies that for all values of h the approximation (17) suffers from the same fault as in the zero-field case: the transition is first order for all $q > 2$.

3. The reaction-field approximation

In order to obtain the reaction-field approximation for this model, one has to replace the expectation values p_k in the effective single-site Hamiltonian (5) by the conditional expectation values p_k^c . These quantities give the thermal expectation value for finding site j in state k , under the condition that one of its z neighbours, s_i , is fixed in state k :

$$p_k^c = \langle P_j^k \rangle \Big|_{s_i=k}. \quad (21)$$

An exact calculation of these conditional expectation values would be equivalent to solving the model exactly. We will, however, limit ourselves to an approximate calculation, in which, starting from the MFA, the effect of fixing s_i in state k is taken into account in linear order in the quantities $(p_k^c - p_k)$. From a physical point of view this amounts to taking into account only the conditioning effects which propagate directly between nearest-neighbour sites; a higher-order calculation would also require us to take into account effects propagating through intermediate sites in the lattice.

The reaction-field calculation then runs parallel to the calculation of § 2, except for the fact that in (7) and subsequent equations we have to use

$$\begin{aligned} \alpha' &= \beta Jz p_1^c \\ \gamma' &= \beta Jz p_n^c \quad M2 \leq n \leq q \end{aligned} \quad (22)$$

instead of α and γ . The MFA Hamiltonian (5) is thus replaced by the reaction-field Hamiltonian

$$\mathcal{H}_R = -Jz \left(p_1^c P^1 + \sum_{n=2}^q p_n^c P^n \right) - hB. \quad (23)$$

The main problem resides in the calculation of the quantities α' and γ' , or rather of their difference $\alpha' - \gamma' = \beta Jz(p_1^c - p_n^c)$.

The calculation of p_1^c is rather simple, because this quantity can be obtained as the average of P^1 corresponding to the effective Hamiltonian (23), modified in such a way

that one of the neighbours is definitely fixed in state 1. Thus p_1^c can be obtained from equation (17), provided that α and γ are substituted for by

$$\begin{aligned}\alpha_1 &= \beta J(z-1)p_1^c + \beta J = \alpha' + \beta J(1-p_1^c) \\ \gamma_1 &= \beta J(z-1)p_n^c = \gamma' - \beta Jp_n^c.\end{aligned}\quad (24)$$

This would provide an explicit expression for p_1^c as a function of itself and the as yet unknown value of p_n^c . Since we will, in any case, resort to a linearisation in the $p_k^c - p_k$ in order to solve this equation and the analogous one for p_n^c , we will immediately use a first-order perturbation method for calculating the conditional probabilities. The conditional Hamiltonian for p_1^c is given by

$$\mathcal{H}_1^c = \mathcal{H}_R + V_1 \quad (25)$$

where

$$\begin{aligned}V_1 &= J(p_1^c - 1)P^1 + J \sum_{n=2}^q p_n^c P^n \\ &= Jp_n^c + J(p_1^c - 1 - p_n^c)P^1.\end{aligned}\quad (26)$$

We used the fact that for n and n' larger than one, we have

$$p_n^c = p_n^c. \quad (27)$$

and furthermore

$$\sum_{k=1}^q P^k = 1. \quad (28)$$

In the expression

$$p_1^c = \text{Tr}[P^1 \exp(-\beta \mathcal{H}_1^c)] [\text{Tr} \exp(-\beta \mathcal{H}_1^c)]^{-1} \quad (29)$$

we will now twice use the expansion

$$\exp(-\beta \mathcal{H}_1^c) = \exp(-\beta \mathcal{H}_R) \left(1 - \int_0^\beta d\mu \exp(\mu \mathcal{H}_R) V_1 \exp(-\mu \mathcal{H}_R) + \dots \right) \quad (30)$$

in order to obtain, up to first order in V_1 :

$$p_1^c = p_1(1 + \beta \langle V_1 \rangle) - \left\langle \int_0^\beta d\mu \exp(\mu \mathcal{H}_R) V_1 \exp(-\mu \mathcal{H}_R) P^1 \right\rangle. \quad (31)$$

The expectation values $\langle \dots \rangle$ in this expression are thermal expectation values with respect to the Hamiltonian $\mathcal{H}_R$. The first term in V_1 , being just a c -number, does not contribute to p_1^c .

A similar procedure may be followed for p_n^c . The conditional Hamiltonian, for example, for p_2^c is

$$\mathcal{H}_2^c = \mathcal{H}_R + V_2 \quad (32)$$

where

$$\begin{aligned}V_2 &= Jp_1^c P^1 + J(p_2^c - 1)P^2 + J \sum_{n=3}^q p_n^c P^n \\ &= Jp_n^c + J(p_1^c - p_n^c)P^1 - JP^2\end{aligned}\quad (33)$$

and a formula analogous to (31) yields p_2^c .

Combining the expression thus obtained, we finally obtain:

$$p_1^c - p_n^c = p_1 - p_n + \beta J(p_1 - p_n)[p_1(p_1 - p_n) - (p_1 + p_n) - (X_{11} - X_{1n})] + \beta J(X_{11} - X_{nn}) \quad (34)$$

where again $n > 1$, and

$$X_{ij} \equiv \frac{1}{\beta} \int_0^\beta d\mu \langle \exp(\mu \mathcal{H}_R) P^i \exp(-\mu \mathcal{H}_R) P^j \rangle. \quad (35)$$

We now have two relations between the order parameter m and $\alpha' - \gamma' = \beta Jz(p_1^c - p_n^c)$. Equation (17), adapted for the reaction-field Hamiltonian (23), yields a series expansion of m in powers of $\alpha' - \gamma'$. Analogous series expansions may be obtained for $X_{11} - X_{1n}$ and $X_{11} - X_{nn}$. Equation (34) thus establishes a second independent relation between m and $\alpha' - \gamma'$. Eliminating $\alpha' - \gamma'$ between (17) and (34) gives us a reaction-field equation of the form (20). The simultaneous vanishing of the coefficients a_1 and a_2 of the linear and quadratic terms of this series expansion determines the tricritical point.

In this way, we have determined numerically the line of tricritical points in the (q, d) -plane for several values of η . The results are illustrated in figure 1.

Figure 1. The line of tricritical points in the (q, d) -plane for: A, $\eta = 0$; B, $\eta = 1$; C, $\eta = \infty$ ($\eta = h/kT$).

4. Discussion

The results for $h = 0$ are obviously identical with the classical results obtained (with a single-site reaction-field approximation) in our previous paper (Dekeyser *et al* 1983). The other extreme situation, $\eta = \infty$, may be viewed as a ground-state calculation ($\beta = \infty$) for the Potts model in a transverse field. The ground-state phase transition in the transverse Ising model is a special example ($q = 2$), and is well known to be of second order. For general q , the simple MFA would predict that the transition in the ground

state of the transverse Potts model is first order as soon as $q > 2$, but our reaction-field result gives a much more realistic prediction for the borderline between first- and second-order transitions.

On the other hand, it is known (Kogut 1979) that the ground state of a d -dimensional quantum system with transverse field is equivalent to the finite-temperature D -dimensional classical system without a field, with $D = d + 1$. Since this equivalence is based on a transfer matrix treatment of the extra dimension, our $\eta = \infty$ results may also be interpreted as an improvement on the reaction-field calculation for the classical Potts model without a field. The reaction-field is then effectively working between infinite one-dimensional chains of lattice sites, and this must be expected to be a better approximation than the single-site reaction-field. From this point of view, we understand why the general trend (for $d \leq 3$) of our result is a shift of $q_c(d)$ towards lower values when η increases from zero to infinity: it is the result of shifting the $q_c(d)$ curve to the left. Ideally we would expect $q_c(d, \eta = 0) = q_c(d - 1, \eta = \infty)$. The observed shift in dimensionality is, however, smaller than unity. This may be understood from the fact that our classical single-site reaction-field calculation underestimated the tricritical dimensionality corresponding to a certain value of q (see Dekeyser *et al* 1983). Any improvement on this approximation is thus expected to shift the curve towards higher values of d . The approximation obtained here for $\eta = \infty$ is then the superposition of (i) the above mentioned shift of the $q_c(d)$ curve from d to $d - 1$, and (ii) a shift to the right due to the implicit exact transfer matrix treatment of one dimension. We also believe that the crossing of the curves for $d \geq 3$ is caused by the growing importance of effect (ii). In this way we now obtain from our $\eta = \infty$ calculation the following approximations for the classical Potts model: $q_c(4) \approx 2.219$, $q_c(3) \approx 2.764$ and $q_c(2) \approx 3.428$ (exact value: 4.0). Our value for $q_c(3)$ is in good agreement with the estimate obtained by Kogut and Sinclair (1982) on the basis of a $1/q$ -expansion.

Even if the quantitative results are not very accurate, there is an interesting qualitative prediction in our calculation. For a certain range of q - and d -values we have shown that, by increasing the strength of a transverse field, it is possible to change the nature of the phase transition from second order to first order. As a numerical example, a two-dimensional Potts system with $q = 2.9$ in zero field is predicted to have a second-order phase transition in our approach, whereas it has a first-order transition in strong fields. The tricritical point would be found at $h/J \approx 0.816$ and $\beta J \approx 0.98$. Taking into account the estimated deviation of our results from the true values in zero field, it may be expected that in reality such a phenomenon will also occur for $d = 2$, $q = 3$.

In this sense our calculation gives a direct description of the tricritical point that is expected to be found in a finite slab of a cubic ferromagnet such as DyAl_2 by increasing the magnetic field along the (111) direction (Shnidman and Domany 1981). Such a system is supposed to be a realisation of the $d = 2$, $q = 3$ model with the three Potts states corresponding to magnetised states along the three easy axes (100), (010) and (001), with a second-order phase transition (Mukamel *et al* 1976, Barbara *et al* 1978). The effect of the (111) field, apart from creating the easy axes that correspond to the three Potts states, is to add to the Hamiltonian a transverse-field term as described by our formula (3). Indeed, the Larmor precession induced on a magnetic moment by an external field corresponds in our discretised three-state Potts model to the transition probabilities caused by the second term of Hamiltonian (1). Our calculation then suggests that the phase transition for such a $d = 2$ model is indeed of second order up to a particular field strength, above which a first-order transition should be seen (see figure 2).

Figure 2. Qualitative phase diagram expected for the two-dimensional three-state quantum Potts model. The full and broken curves represent second- and first-order transitions respectively.

The previously mentioned authors are of course correct when claiming that an increasing transverse field corresponds to an increase of the effective dimensionality. We have already mentioned the fact that the system behaves like a $(d + 1)$ -dimensional system when η becomes infinite. Finite values of η then correspond to a finite number of d -dimensional layers, forming a slab of finite thickness in the $(d + 1)$ -dimensional space (Hertz 1976). In this sense, our calculation provides a very simple approach to the expected tricritical point for a thin slab of the three-state Potts model (Andelman and Berker 1981, Shnidman and Domany 1981). Since increasing the transverse-field strength corresponds effectively to a growing slab thickness, this is a special case of dimensional crossover, due to quantum effects.

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