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1975 J. Phys. A: Math. Gen. 8 905

(http://iopscience.iop.org/0305-4470/8/6/009)

J. Phys. A: Math. Gen., Vol. 8, No. 6, 1975. Printed in Great Britain.

Symmetry and the nature of the transition in the spin 1 Schrödinger exchange model

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Received 15 October 1974, in final form 23 December 1974

Abstract. The spin 1 Schrödinger exchange model is shown to have the same symmetry in fields as the three-component Potts model so that the zero-field quadrupolar ordering can be simply related to the dipolar ordering. The question of the nature of the transition is investigated using previously derived high-temperature series for the free energy as a function of an extensive variable. For $S = 1$, mean-field-like behaviour persists in our higher-order approximations on the face-centred cubic lattice, indicating a first-order transition in this model.

1. Introduction

The Schrödinger exchange model (SEM) of magnetism first considered by Allan and Betts (1967) and Joseph (1967) is a generalization of the spin $\frac{1}{2}$ Heisenberg model in the same sense that the Potts model (Alexander and Yuval 1974) is a generalization of the spin $\frac{1}{2}$ Ising model. The interaction between nearest-neighbour spins is via the Schrödinger exchange operator P_{ij} which permutes the states of spins on the ith and jth lattice sites and which reduces to the usual Heisenberg interaction for a spin $\frac{1}{2}$ system. The mean field approximation (MFA) for the spin S SEM yields exactly the same expression for the free energy as that of the q-component Potts model for $q = 2S+1$ (Kim 1974), and hence the SEM may be considered a quantum analogue of the Potts model.

For a spin 1 system with which the present study is primarily concerned, the operator P_{ij} is (Schrödinger 1941)

$$P_{ij} = (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) + (\boldsymbol{S}_i \cdot \boldsymbol{S}_j)^2 - 1. \tag{1}$$

Hence the spin 1 SEM is identical to the spin 1 Heisenberg model with an isotropic biquadratic interaction whose strength j is equal to that of the bilinear interaction J. Such a biquadratic perturbation interaction $-j(\boldsymbol{S}_i \cdot \boldsymbol{S}_j)^2$ is present in magnetic systems because of the superexchange mechanism (Anderson 1959), and the effect of this on the nature of the transition has been of some theoretical interest (Chen and Levy 1973 and references therein). For arbitrary values of j/J it is difficult to go much beyond the MFA, which can give misleading results just as for the Potts model (Baxter 1973). For $j/J = 1$, ie for the $S = 1$ SEM, Allan and Betts (1967) calculated the high-temperature susceptibility and free-energy series for the face-centred cubic lattice to the seventh

order in K, and later Chen and Joseph (1972) generalized this to the case of arbitrary spin and all lattices. From these works the values of the transition temperatures and the critical index γ are known approximately ($k_B T_c/J = 3{\cdot}1 \pm 0{\cdot}1$, $\gamma = 1{\cdot}2$–$1{\cdot}3$ for the FCC lattice for $S = 1$, for example), but the question of the nature of the transition still remains to be determined.

For a spin 1 system with isotropic interactions, only two order parameters, $m \equiv \langle S_{iz} \rangle$ and $x \equiv \langle S_{iz}^2 \rangle$, need be considered due to rotational invariance. Here, $\langle\ \rangle$ denotes a thermal average. The fields conjugate to the magnetic ordering m and the quadrupolar ordering x are the external magnetic field H and the single-ion anisotropy D respectively. Therefore, the complete Hamiltonian we shall consider takes the form

$$\mathscr{H} = -J \sum_{\langle ij \rangle} P_{ij} - H \sum_{i=1}^{N} S_{iz} + D \sum_{i=1}^{N} S_{iz}^2 \tag{2}$$

with $J > 0$, where the magnetic moment $g\mu_B$ is included in the factor H for notational convenience.

In this work it is shown that the SEM has the same, exact symmetry in a three-dimensional field space as that of the Potts model. Consequently it is shown that the magnetic ordering and the quadrupolar ordering are simply related and that we have a situation in which either the transition is of first order or it is continuous but the transition point is a tricritical point when $H = D = 0$ (§ 2).

To investigate the question of the order of the transition for $H = D = 0$, the high-temperature series for the free energy on the face-centred cubic lattice previously reported (Kim and Joseph 1974*a*) are transformed from being a function of an intensive variable to that of an extensive variable so as to be able to consider the spontaneous ordering directly from the high-temperature series (§ 3). Analysis of the series is presented in § 4. We find that mean-field-like behaviour persists even with our higher-order approximation and that the general features of the ordering are much the same as for the $q = 3$ Potts model, even though the value of γ is appreciably different; $\gamma = 0{\cdot}9$–$1{\cdot}0$ for the Potts model (Kim and Joseph 1975).

2. Symmetry in fields

Since each spin state is completely equivalent as far as the two-spin interaction is concerned, we should expect a special symmetry in fields to exist similar to that in the Potts model (Kim and Joseph 1974b, Straley and Fisher 1973). We show in this section that this is indeed the case. Because the P_{ij} operator simply exchanges the states of two spins at the lattice sites i and j, it conserves the total number of spins in a state $S_z = M$ ($M = \pm 1, 0$). Therefore the Hamiltonian of equation (2) commutes with both ΣS_{iz} and ΣS_{iz}^2. Hence we can write the partition function Z_N as a sum of traces in each subspace where ΣS_{iz} is a constant and ΣS_{iz}^2 is a constant, that is:

$$Z_N = \mathrm{Tr}\, \mathrm{e}^{-\beta \mathscr{H}} = \sum_{l=0}^{N} \sum_{k=0}^{l} V(l-k, N-l, k) \exp[-lh_2 + (l-2k)h_1] \tag{3}$$

where $h_1 = \beta H$, $h_2 = \beta D$, $K = \beta J$, $\beta = 1/k_B T$ and

$$V(n_1, n_2, n_3) = \sum{}'' \left\langle M_1 M_2 \ldots M_N \middle| \exp\left(K \sum_{\langle ij \rangle} P_{ij} \right) \middle| M_1 M_2 \ldots M_N \right\rangle \tag{4}$$

is the trace of $\exp(K \Sigma_{\langle ij \rangle} P_{ij})$ in the subspace where

$$\sum_{i=1}^{N} M_i = n_1 - n_3 \quad \text{and} \quad \sum_{i=1}^{N} M_i^2 = n_1 + n_3 \qquad (n_1 + n_2 + n_3 = N),$$

that is, the sum over all configurations which have n_1 spins in the $M = 1$ state, n_2 spins in the $M = 0$ state and n_3 spins in the $M = -1$ state. Here $|M_1 M_2 \ldots M_N\rangle$ denotes a product state of eigenstates of S_{iz}. Now for each term in equation (3) we can change the states of n_1 spins of $M = 1$ to $M = 0$ and n_2 spins of $M = 0$ to $M = 1$, denoting the state obtained from $|M_1 \ldots M_N\rangle$ by this interchange as $|M'_1 \ldots M'_N\rangle$. The matrix element

$$\left\langle M'_1 \ldots M'_N \left| \exp\left(K \sum_{\langle ij \rangle} P_{ij} \right) \right| M'_1 \ldots M'_N \right\rangle$$

is the same as

$$\left\langle M_1 \ldots M_N \left| \exp\left(K \sum_{\langle ij \rangle} P_{ij} \right) \right| M_1 \ldots M_N \right\rangle$$

since any matrix element of P_{ij} is invariant under such an interchange. Consequently, after summing over all the $\binom{N}{n_1 n_2 n_3}$ configurations, we find the identity

$$V(n_1, n_2, n_3) = V(n_2, n_1, n_3). \tag{5}$$

Similarly we have $V(n_1, n_2, n_3) = V(n_3, n_2, n_1)$ etc. Hence we conclude that V is invariant under any permutation of its arguments.

Consequently, from equation (6) of Kim and Joseph (1974b) we have exactly the same symmetries in the two fields h_1, h_2 as for the Potts model, ie the free energy $f(K, h_1, h_2)$ obeys the relation

$$\beta f(h'_1, h'_2, K) = \beta f(h_1, h_2, K) - (h_1 + h_2) \tag{6}$$

where $2h'_1 = -h_1 + h_2$, $2h'_2 = -3h_1 - h_2$. When $h_1 = h_2 = 0$, which is the situation of interest to us, following Kim and Joseph (1974b) we see that the order parameters (m, x) in the ordered state can take on three sets of values, depending on the path along which we take the limits $h_1 \to 0$ and $h_2 \to 0$. Furthermore, they can be all expressed in terms of one unknown parameter, that is $(0, x_0)$, $(1 - \frac{3}{2}x_0, 1 - \frac{1}{2}x_0)$, $(-1 + \frac{3}{2}x_0, 1 - \frac{1}{2}x_0)$ for $0 \leqslant x_0 \leqslant \frac{2}{3}$.

Knowledge of the rigorous ground state (Kim and Joseph 1974c) together with phenomenological considerations enables us to identify the $(0, x_0)$ pair as the limit when $h_2 \to 0^+$ along the line $h_1 = 0$. Hence the quadrupolar ordering $x_0(T)$, which is $\frac{2}{3}$ in the high-temperature region and zero at $T = 0$, becomes the quantity of central interest to us. If $x_0(T)$ decreases continuously from the value $\frac{2}{3}$ as we lower the temperature through the transition temperature T_0, then we have a continuous transition and the point T_0 in zero field can be identified as a tricritical point in the three-dimensional field space because of the three-fold symmetry (Straley and Fisher 1973). The MFA predicts a discontinuity of $\frac{1}{3}$ in $x_0(T)$ at $T_0 = zJ/4k_B \ln 2$ (Nauciel-Bloch *et al* 1972).

3. Transformations of the high-temperature series

The free energy of the spin S SEM with arbitrary single-ion contributions has previously been calculated to seventh order in K (Kim and Joseph 1974a) in terms of the structure

functions $G_l \equiv g_l/g_1^l$. For the case under present consideration ($S = 1$) where the Hamiltonian is given by equation (2), the g_l functions become

$$g_l = 1 + 2\cosh(lh_1)\exp(-lh_2) \tag{7}$$

and the trace is to be taken with the product state of the eigenstates of S_{iz}. We shall now utilize these high-temperature series to investigate the quadrupolar ordering $x_0(T)$, as defined in § 2.

For this purpose it is necessary to transform the free energy $f(T, h_1, h_2)$ to the 'Gibbs' free energy $g(T, m, x)$ for $m = 0$. From now on we reserve the letter g to represent the free energy as a function of extensive variables. Since βf is a concave and even function in h_1, we note that

$$\begin{aligned}\beta g(T, 0, x) &= \sup_{h_1 h_2}(\beta f(T, h_1, h_2) - xh_2) \\ &= \sup_{h_2}(\beta f(T, 0, h_2) - xh_2).\end{aligned} \tag{8}$$

When $h_1 = 0$,

$$G_l = \frac{1 + 2\exp(-lh_2)}{[1 + 2\exp(-h_2)]^l}, \tag{9}$$

and if we define a quantity τ by

$$\tau \equiv \frac{2\exp(-h_2)}{1 + 2\exp(-h_2)}, \tag{10}$$

then each G_l becomes a polynomial of order l in τ. Hence the free energy can be expressed in the form

$$-\beta f(T, 0, h_2) = -\ln(1-\tau) + \sum_{n=1}^{\infty} \frac{K^n}{n!2^n} \sum_{k=0}^{2n} a_{n,k}\tau^k, \tag{11}$$

from which we get

$$\begin{aligned}x &= \partial(\beta f(T, 0, h_2))/\partial h_2 = \tau(1-\tau)\partial(-\beta f)/\partial\tau \\ &= \tau \sum_{n=0}^{\infty} \frac{K^n}{n!2^n} \sum_{k=0}^{2n} b_{n,k}\tau^k.\end{aligned} \tag{12}$$

This result can now be inverted to give τ as a function of x. The series can be further manipulated to give

$$\begin{aligned}-h_2 &= \partial(\beta g(T, 0, x))/\partial x = \ln\left(\frac{\tau}{2(1-\tau)}\right) \\ &= \ln\left(\frac{x}{2(1-x)}\right) + \sum_{n \geqslant 1} \frac{K^n}{n!2^n} \sum_{k=0}^{2n-1} c_{n,k}x^k.\end{aligned} \tag{13}$$

Finally, equation (13) can be integrated to yield

$$\beta g(T, 0, x) = \beta g(T, 0, 0) + x\ln(x/2) + (1-x)\ln(1-x) + \sum_{n \geqslant 1} \frac{K^n}{n!2^n} \Psi_n(x) \tag{14}$$

where

$$\beta g(T, 0, 0) = \beta f(T, 0, +\infty) = -zK/2 \tag{15}$$

and

$$\Psi_n(x) = \sum_{k=1}^{2n} \frac{c_{n,k-1}}{k} x^k. \tag{16}$$

The known polynomials Ψ_n calculated in this way are tabulated in table 1 for the FCC lattice and $S = 1$. All calculations were carried out in integer arithmetic.

Table 1. Ψ_n polynomials of equation (14) for the FCC lattice.

$$\Psi_1 = 24x - 18x^2$$

$$\Psi_2 = -48x - 24x^2 + 108x^3 - 54x^4$$

$$\Psi_3 = -384x + 720x^2 - 1200x^3 + 2052x^4 - 1944x^5 + 648x^6$$

$$\Psi_4 = -1728x + 15552x^2 - 45648x^3 + 80352x^4 - 103464x^5 + 98496x^6 - 58320x^7 + 14580x^8$$

$$\Psi_5 = 46080x - 119808x^2 + 368640x^3 - 1607040x^4 + 4985280x^5 - 10468224x^6 + 14618880x^7 - 12577680x^8 + 5948640x^9 - 1189728x^{10}$$

$$\Psi_6 = 1674240x - 17150208x^2 + 77620608x^3 - 240371136x^4 + 520830432x^5 - 776297376x^6 + 772506720x^7 - 469612080x^8 + 126087840x^9 + 25544160x^{10} - 25194240x^{11} + 4199040x^{12}$$

$$\Psi_7 = 18063360x - 457883136x^2 + 2431005696x^3 - 7051500288x^4 + 9129383424x^5 + 11831732640x^6 - 82019044800x^7 + 200361916224x^8 - 316732187520x^9 + 354758110560x^{10} - 280211037120x^{11} + 148061299680x^{12} - 46823495040x^{13} + 6689070720x^{14}$$

4. Series analysis for the spin 1 face-centred cubic lattice

The spontaneous quadrupolar ordering $x_0(T)$ is obtained by the solution of

$$h_2 = -\partial(\beta g(T, 0, x))/\partial x = 0 \tag{17}$$

for the range $0 \leqslant x \leqslant \frac{2}{3}$. $x = \frac{2}{3}$ is a solution for all temperatures since $d\Psi_n/dx = 0$ at $x = \frac{2}{3}$ for all n. Note that if the series of equation (14) is cut off at first order in K, the result would be exactly the MFA expression for the free energy (Nauciel-Bloch *et al* 1972). Hence, if we define by g_N the series of equation (14) cut off at the Nth order in K, that is:

$$\beta g_N \equiv \beta g(T, 0, 0) + x \ln(x/2) + (1-x)\ln(1-x) + \sum_{n=1}^{N} \frac{K^n}{n!2^n} \Psi_n(x), \tag{18}$$

then g_N for $N \geqslant 2$ can be regarded as successive corrections to g_1, the MFA result.

In the MFA there is a range of T for which multiple solutions of $dg_1/dx = 0$ exist and by choosing the one which gives the lowest energy g_1, a first-order transition results. To see the effect of the higher-order terms we can determine the $\partial g_N/\partial x = 0$ contours for $N = 2, 3, \ldots, 7$, successively. In practice it is easier to find T as a function of x, which we denote by $T_N(x)$. The first-order transition is manifested by the non-physical negative slope of $T_N(x)$ near $x = \frac{2}{3}$. For all $N \leqslant 7$ we find that a first-order transition exists. Table 2 shows the transition temperature T_0, defined as the temperature where the energy g_N for the solution $x = \frac{2}{3}$ becomes the same as that of the $x \neq \frac{2}{3}$ solution, and Δx is the discontinuity of $x_0(T)$ at T_0. Note that after an abrupt drop from $N = 2$

Table 2. T_0, Δx and T_c^* obtained from g_N for $N = 1$–7.

N	$k_B T_0/J$	Δx	$k_B T_c^*/J$
1	4·328	0·333	4·000
2	3·363	0·333	3·155
3	3·265	0·172	3·123
4	3·330	0·181	3·282
5	3·294	0·229	3·230
6	3·240	0·236	3·176
7	3·227	0·197	3·184

to $N = 3$, Δx remains nearly constant ($\Delta x \sim 0{\cdot}2$) and does not show any systematic decrease as N becomes larger. Also shown in table 2 is $T_c^* \equiv \lim_{x \to 2/3} T_N(x)$, the temperature at which the inverse of the zero-field, high-temperature susceptibility vanishes. In figure 1 we show the $T_N(x)$ curves for $N = 1, 2$ and 7. For $N = 3$–6 they are all roughly located between those for $N = 2$ and 7. Also shown is the corresponding discontinuity in the quadrupolar ordering at T_0. For the higher-order approximations the temperature range where multiple solutions exist is appreciably reduced. For an exact solution this range should be zero since g is rigorously convex in x.

The $T_N(x)$ curves just discussed are basically the zeroes of the $[0, N]$ Padé approximants (PA) to the $h_2(x, T)$ series of equation (17). For a better approximation to $T_\infty(x)$ it is necessary to construct PA to the logarithmic derivatives of the h_2 series to allow for a possible branch point behaviour (Baker *et al* 1970), that is

$$h_2 \sim A(T - T_\infty(x))^{-\gamma(x)}. \tag{19}$$

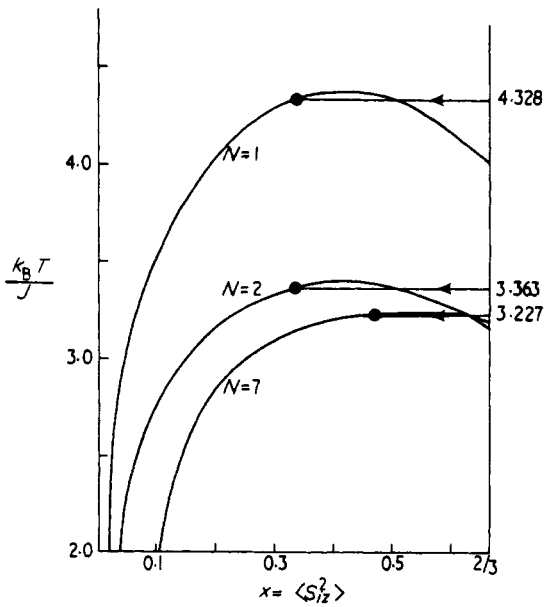

Figure 1. $T_N(x)$ curves and the discontinuities of the quadrupolar ordering obtained from g_N for $N = 1, 2$ and 7. $N = 1$ corresponds to the MFA. The transition is of first order (for all $N \leqslant 7$).

In table 3 we show the smallest positive real poles and their residues of PA to $d(\ln h_2(x, T))/dK$ for values of x ranging from $\frac{2}{3}$ to 0·05 for the three most significant PA: [3, 2], [4, 2] and [3, 3]. All of these poles first decrease (hence increase in T) slightly as x decreases and then eventually increase in the same manner as for the [0, 7] direct PA to h_2 shown in figure 1. Hence the mean-field-like 'bump', although small in magnitude, still persists in these approximants. Comparable results were observed in our analysis of the $q \geqslant 3$ Potts model (Kim and Joseph 1975). Similar type behaviour was also found for the [2, 4], [5, 1], [6, 0], [5, 0], [3, 1] and [4, 0] PA. However, for the [4, 1], [2, 3] and [2, 1] PA, there was a range of x near $\frac{2}{3}$ where a real pole did not even exist while the [2, 2], [3, 0] and [2, 0] PA showed an inverse type behaviour, ie monotonically increasing K as x decreases. However, since the latter three PA are lower-order approximants, this probably has no great significance.

Table 3. The smallest positive real poles (multiplied by 10^4) and their residue of the Padé Approximants to $d(\ln h_2(x, K))/dK$ for the three most significant approximants. §: no real pole exists.

	[3, 2]		[4, 2]		[3, 3]	
x	Pole	Residue	Pole	Residue	Pole	Residue
$\frac{2}{3}$	3201	1·16	3191	1·14	3191	1·14
0·65	3193	1·17	3184	1·16	3184	1·16
0·60	3175	1·20	3171	1·19	3171	1·19
0·55	3166	1·22	3166	1·22	3166	1·22
0·50	3165	1·23	3169	1·24	3169	1·24
0·45	3174	1·24	3183	1·25	3183	1·25
0·40	3196	1·24	3209	1·27	3209	1·26
0·35	3236	1·24	3253	1·28	3252	1·27
0·30	3303	1·25	3324	1·29	3323	1·29
0·25	3414	1·27	3439	1·31	3438	1·31
0·20	3600	1·30	3634	1·36	3632	1·36
0·15	3931	1·38	3993	1·48	3988	1·47
0·10	4642	1·57	4808	1·82	4779	1·76
0·05	7660	2·54	c.c.§	—	9557	5·42
0	∞		∞		∞	

5. Conclusion

We have shown that the spin 1 SEM, despite its quantum mechanical nature, possesses exactly the same symmetry in fields as the three-component Potts model. This result can easily be extended to arbitrary spin to show that the spin S SEM has the same symmetry as the $q(= 2S+1)$-component Potts model. Explicit quantitative considerations of these symmetry relations result in simple linear relations between the dipolar and the quadrupolar orderings in the $S = 1$ system. These two orderings, which might occur as separate phase transitions in other spin 1 systems (Blume and Hsieh 1969) are in fact two different aspects of a single quantity in the present case. That is, the phase transition (in zero fields) is characterized by just one order parameter for the SEM.

Successive corrections to the MFA for the order parameter $x_0(T)$ are found by Legendre-transforming the free-energy series. For all orders $N = 2$–7, we found a

discontinuous transition as in the $N = 1$ MFA. The discontinuity of $x_0(T)$ at the transition was in the range $0{\cdot}20 \pm 0{\cdot}04$ for all $N = 3$–7, whereas for $N = 1$ and 2 Δx is $\frac{1}{3}$. Also, the function $x_0(T)$ estimated from the appropriate PA showed that the non-physical, mean-field-like 'bump' did not disappear. We interpret these results as the manifestation of a discontinuous transition similar to the situation in the $q = 3$ Potts model.

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