Ordering in antiferromagnetic Potts models

1985 J. Phys. A: Math. Gen. 18 3375

(http://iopscience.iop.org/0305-4470/18/17/019)

J. Phys. A: Math. Gen. **18** (1985) 3375-3380. Printed in Great Britain

Ordering in antiferromagnetic Potts models†

B Hoppe and L L Hirst

Institut für Theoretische Physik, Universität Frankfurt, 6 Frankfurt am Main, West Germany

Received 1 April 1985

Abstract. Ordering in the antiferromagnetic Potts model on a simple cubic lattice with $q=3$ or 4 states per ion is investigated by Monte Carlo computer experiments. The results are analysed by forming the ion-pair correlation function, a technique permitting a more reliable identification of long-range order. In agreement with Banavar *et al*, we find a continuous phase transition to a two-sublattice ordered phase. The Monte Carlo results are used to test the mean-field approximation, which is found to yield qualitatively correct results for $q=3$ and 4, although exaggerating the ordering tendencies.

1. Introduction

The Potts model (Potts 1952, Wu 1982) is a semiclassical model in statistical mechanics which can be regarded as a generalisation of the Ising model. The Hamiltonian of the q-state Potts model can be written as

$$H=-J\sum_{(i,i')}\sum_{r}(|r\rangle\langle r|)_i(|r\rangle\langle r|)_{i'} \qquad r=1,2,\ldots,q \tag{1}$$

where $(|r\rangle\langle r|)_i$ is a projection operator for the state $|r\rangle$ at site i and the first summation is over all nearest-neighbour pairs. The antiferromagnetic case ($J<0$) has received less investigation than the ferromagnetic case ($J>0$), but the antiferromagnetic Potts model on a simple cubic (SC) lattice with $q=3$ or 4 states per ion was recently investigated by Banavar *et al* (1982) using Monte Carlo (MC) methods. These authors found indications for a continuous phase transition into a phase with long-range order in a two-sublattice scheme for both $q=3$ and $q=4$. Since the ionic polarisations obtained remain unsaturated in the low-temperature limit, it seems desirable to further check whether the non-zero values of the order parameter yielded by their MC calculations for a finite system might not result from short-range order only.

For this reason we have made new MC computations for the antiferromagnetic Potts model with 3 or 4 states per ion on the SC lattice. In addition to the usual plots of thermodynamic functions and a global order parameter, we have analysed our MC data by looking at ion-pair correlations as a function of interionic distance, which is found to provide an especially sensitive test for long-range order. We have also evaluated the simpler mean-field approximation and compared it to the MC results.

† Project of the Sonderforschungsbereich für Festkörperspektroskopie Darmstadt-Frankfurt, supported by the Deutsche Forschungsgemeinschaft.

0305-4470/85/173375+06$02.25

2. Monte Carlo results

We have applied standard Monte Carlo techniques as recently reviewed by Binder (1979). The system typically used was an $18\times18\times18$ lattice with periodic boundary conditions, with averaging performed over 800 MC steps per site. Results at low temperatures were obtained by cooling down from a high-temperature random configuration as discussed by Banavar *et al* (1982).

The pair correlation function $f(R)$ gives the probability of finding two ions i and i' at a distance R in the same state and is defined as

$$f(R)=\frac{1}{qN}\sum_{r}\sum_{i}\langle\langle(|r\rangle\langle r|)_i(|r\rangle\langle r|)_{i'}\rangle\rangle \tag{2}$$

where $\langle\langle\ \rangle\rangle$ denotes the thermodynamic average, r is summed over the q single-ion states, i is summed over the N sites of the lattice, and i' is fixed relative to i by $\boldsymbol{R}_{i'}-\boldsymbol{R}_i=\hat{\boldsymbol{u}}R$ where $\hat{\boldsymbol{u}}$ is a unit vector along one of the cube axes.

The correlation functions obtained for the three- and four-state models are shown in figures 1 and 2. At high temperatures we see short-range correlations which decay rapidly toward the value $1/q$ corresponding to uncorrelated ions as the separation R increases. At low temperatures the correlation function does not approach $1/q$ at large R but instead oscillates between different limiting values for even and odd R. This corresponds to ordering on the same scheme of two interpentrating FCC sublattices identified by Banavar *et al* (1982).

A global order parameter corresponding to the above ordering scheme may be defined by

$$M(T)=\tfrac{1}{2}\sum_{r}|P_r(\mathrm{A})-P_r(\mathrm{B})| \tag{3}$$

where A and B label the two sublattices and P_r is the average population per ion of state r on the given sublattice. The dependence of this order parameter on temperature is shown in figures 3 and 4.

The MC data also yield curves (not shown) for the internal energy and specific heat as obtained from the energy fluctuations (Binder 1979). By integrating the internal energy over the inverse temperature (Binder 1981) we obtain the values for the zero-point entropy per ion listed in table 1, which for $q=3$ and $q=4$ are 34% and 51%, respectively, of the value $\ln q$ holding in the high-temperature limit. Also included in table 1 are MC values for the ordering temperature T_c and for the order parameter as extrapolated to $T=0$. Following prevailing practice, we take T_c as the turning point of $M(T)$, and the numerical uncertainty of this determination is also listed in table 1. The maximum of the specific heat defines values of T_c consistent with these, but with a considerably larger uncertainty. Table 1 and figures 1–4 pertain to calculations on crystals of L^3 ions where $L=18$ or 20 for $q=4$ or 3, and supplementary calculations with $L=10$ and 14 failed to yield any significant dependence of the results on crystal size.

3. The mean-field approximation

It is of interest briefly to compare the quasi-exact MC results obtained above to those yielded by the simpler MFA method.

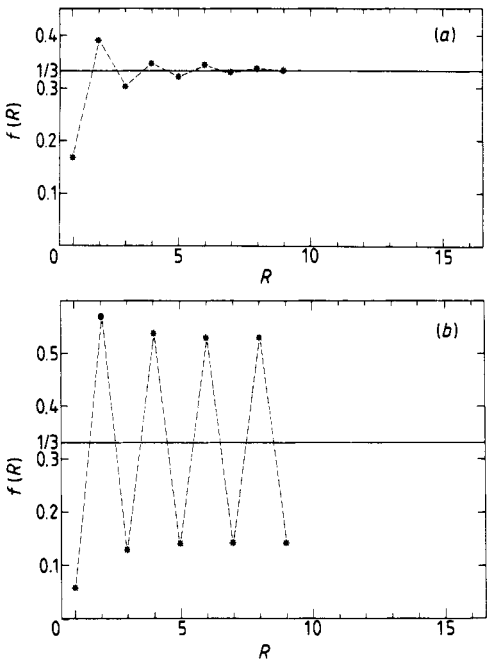

Figure 1. Monte Carlo results for the pair correlation function $f(R)$ in the three-state antiferromagnetic Potts model. (a) and (b) show high- and low-temperature curves, calculated for $T = 1.4\,|J|/k_B$ and $T = 0.98\,|J|/k_B$ respectively. For comparison the ordering temperature is $T_c = 1.28\,|J|/k_B$.

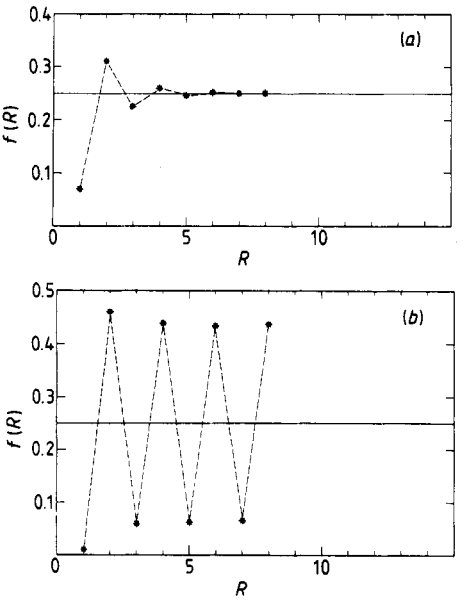

Figure 2. Monte Carlo results for the pair correlation function $f(R)$ in the four-state antiferromagnetic Potts model. (a) and (b) show high- and low-temperature curves, calculated for $T = 0.84\,|J|/k_B$ and $T = 0.35\,|J|/k_B$ respectively. For comparison the ordering temperature is $T_c = 0.68\,|J|/k_B$.

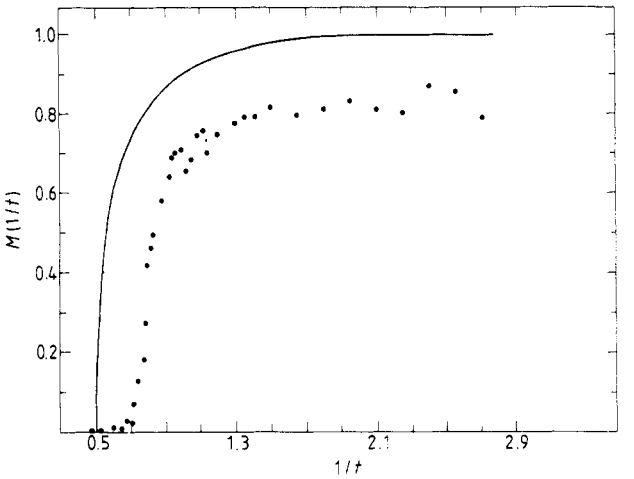

Figure 3. The order parameter M, as yielded by the mean-field approximation (full curve) and the Monte Carlo method (dots) for the three-state antiferromagnetic Potts model, plotted against the dimensionless inverse temperature $1/t = J/k_B T$.

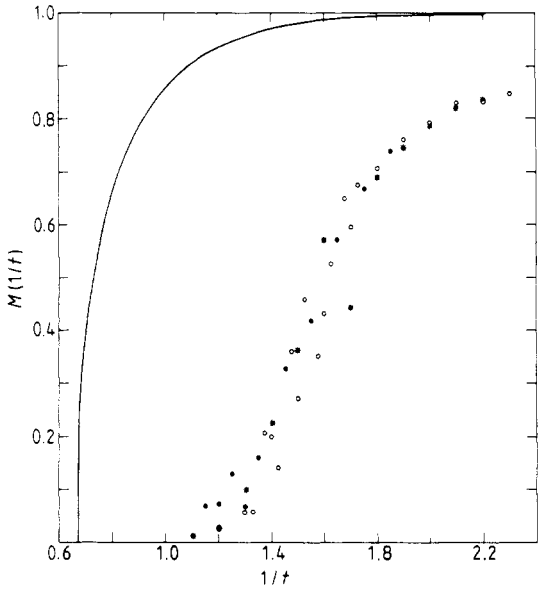

Figure 4. The order parameter M, as yielded by the mean-field approximation (full curve) and the Monte Carlo method (dots) for the four-state antiferromagnetic Potts model, plotted against the dimensionless inverse temperature $1/t = J/k_B T$.

The MFA solution, which is believed to be the absolutely stable one for the antiferromagnetic Potts model with q states per ion, has the following form. The SC chemical lattice is divided into interpenetrating FCC sublattices denoted A and B. The set of q single-ion states is divided into subsets C and C', where C contains any $\frac{1}{2}q$ states for q even or any $\frac{1}{2}(q-1)$ states for q odd, and where C' contains the remaining ones. Then occupation probabilities, depending on the sublattice and subset, are

Table 1. Values of the ordering temperature T_c, the order parameter in the low-temperature limit $M(0)$ and the zero-point entropy per ion $S(0)$ yielded by MFA and MC calculations for the antiferromagnetic Potts model with $q = 3$ or 4 states per ion.

	$q=3$		$q=4$	
	MC	MFA	MC	MFA
$k_B T_c/J$	1.28 ± 0.04	2	0.68 ± 0.06	$\frac{3}{2}$
$M(0)$	0.85	1	0.87	1
$S(0)$	0.376	0.347	0.708	0.693

assigned as indicated in table 2; for q even or odd the occupation probabilities contain one or two parameters, which are determined by minimising the free energy.

One arrives at MFA solutions of this form as follows (Hoppe and Hirst 1986). First one notes that the MFA problem on the SC lattice can be reduced to that on an elementary eight-ion cube with periodic boundary conditions. In the limits $T = 0^+$ and $T = T_c^-$ it is verified by series expansions that solutions of the indicated form are the absolutely stable ones. At intermediate temperatures local stability can be verified formally and absolute stability can hardly be doubted, although a formal proof has not been constructed. (Numerical verification of absolute stability by searching the whole parameter space is not feasible since even after reducing the problem to an eight-ion cube the general MFA trial state contains $8(q-1) = 16$ or 24 independent parameters.)

The temperature dependence of the order parameter $M(T)$ yielded by the MFA is compared to the MC results for $q = 3$ and 4 in figures 3 and 4. Here the low-temperature saturation at a value smaller than unity shown by the MC results is an indication of correlations which the MFA neglects.

Table 2. Occupation probabilities in stable MFA solutions for the antiferromagnetic Potts model with q states per ion. Here A and B label two interpenetrating FCC sublattices; C and C′ are substets of single-ion states and p and p' are variational parameters fixing the populations.

q	Sublattice	Subset	Probability
Even	A	C	$2p/q$
		C′	$2(1-p)/q$
	B	C	$2(1-p)/q$
		C′	$2p/q$
Odd	A	C	$2p/(q-1)$
		C′	$2(1-p)/(q+1)$
	B	C	$2(1-p')/(q-1)$
		C′	$2p'/(q+1)$

4. Discussion and conclusions

We have investigated the antiferromagnetic Potts model with $q = 3$ or 4 states per ion by means of Monte Carlo (MC) calculations and the mean-field approximation (MFA). In agreement with Banavar *et al* (1982), for both $q = 3$ and $q = 4$ we find a continuous

phase transition, leading to long-range order with two interpenetrating FCC sublattices. The ordering tendencies are less pronounced for $q = 4$ than for $q = 3$, as shown by the smoother increase of the MC order parameter against decreasing temperature (figures 3 and 4). This weaker ordering tendency in the $q = 4$ model may be related to the larger zero-point entropy, the MC value of which is 51% of that at $T = \infty$. Zero-point entropies as large as this are usually characteristic of models where long-range order is absent, the classical example being the Ising antiferromagnet on the two-dimensional triangular lattice (Wannier 1950), where the entropy at $T = 0$ is 49% of that at $T = \infty$.

Our MC computer experiments were analysed by evaluating not only the order parameter and thermodynamic functions but also the correlation function for ion pairs as a function of the separation, $f(R)$. At high temperatures $f(R)$ indicates only short-range order, decaying quickly with increasing R toward the value $1/q$ corresponding to uncorrelated pairs. At low temperatures $f(R)$ oscillates between different limiting values for R even or odd, providing clear evidence of long-range order in the above sublattice scheme. Our experience with this and related models (Hoppe and Hirst 1986) indicates that such an analysis of MC computations via the correlation function provides an indication of the existence of a phase transition in the infinite lattice which is substantially more direct and unambiguous than can be obtained by looking for incipient singularities in the thermodynamic functions, especially when the phase transition is continuous as in the present case. The present technique also compares favourably with analysis via a global order parameter because it separately exhibits the contributions from short-range order, which can give the order parameter a finite value in a finite sample even when genuine long-range ordering does not occur.

The simpler MFA method is also of interest despite its known tendency to exaggerate ordering effects. For the antiferromagnetic q-state Potts model, the MFA is found to imply long-range order for all q, whereas the 'satiation' effect (Hoppe *et al* 1983) implies that long-range order should disappear for sufficiently large q and the MC calculations of Banavar *et al* (1982) suggest that it is already absent at $q = 5$. Nevertheless, the MFA is found to work reasonably well for $q = 3$ and even for $q = 4$, as indicated by the comparison in table 1 of the MFA and MC results for the ordering temperature, the order parameter at $T = 0$ and the zero-point entropy per ion.

References

Banavar J R, Grest G S and Jasnow D 1982 *Phys. Rev.* B **25** 4639
Binder K 1981 *Z. Phys.* B **45** 61
Binder K (ed) 1979 *Monte Carlo Methods in Statistical Physics* (Berlin: Springer)
Hoppe B and Hirst L L 1986 to be published
Hoppe B, Liebmann R and Hirst L L 1983 *J. Phys. C: Solid State Phys.* **16** 1933
Potts R B 1952 *Proc. Camb. Phil. Soc.* **48** 106
Wannier G H 1950 *Phys. Rev.* **79** 357
Wu F Y 1982 *Rev. Mod. Phys.* **54** 235