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Group probabilities in the two-dimensional Ising model

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Abstract. Onsager's solution of the two-dimensional Ising model provides expressions for the spontaneous magnetisation and pair correlation functions. More detailed information, which provides insight into the clustering or ordering process, is obtained by expressing these correlation functions in terms of group probabilities. Each group consists of a central atom and its four nearest neighbours. Sum-rule equations for the twelve basic groups are solved to provide expressions for the group probabilities and the behaviour of the group probabilities as a function of temperature is discussed.

1. Introduction

The exact Onsager solution (McCoy and Wu 1973) of the two-dimensional Ising model provides explicit expressions for thermodynamic quantities and the pair correlation functions. A considerable effort has gone into the evaluation and visualisation of the groupings or clusters which occur in magnetic or alloy systems (Clapp 1971, Domb *et al* 1975, Domb and Stoll 1977). Although the pair correlation functions allow the short-range order parameters to be derived they do not directly give information relevant to larger particle groupings. The work of Verhagen and Harding (1979) showed that the magnetisation and correlation functions may be transformed into group probabilities, where a group is defined as an atom or spin with its four nearest neighbours. In the present work this idea is extended by developing sum rules for the group probabilities. The resultant sum-rule equation, which gives the magnetisation and correlation functions in terms of the group probabilities, is then inverted to give explicit expressions for the group probabilities.

As the pair correlation function averages the spin correlation over the 32 group configurations of the square lattice, it is not surprising that the group probabilities display temperature and critical point behaviour not apparent in the pair correlation results. As each type of group is clearly associated with the volume, surface, line element, or point defect of a cluster, the insight gained into the group behaviour is useful in envisaging the general cluster development of the system. The calculations also provide accurate reference data gainst which the accuracy and convergence of Monte-Carlo algorithms can be determined.

Although the Ising model applies equally well to magnetic, lattice-gas, or alloy studies, we have expressed the problem in terms of spin clustering in a ferromagnet. This allows the Ising model, and its solution in terms of the spin groups, to be seen in their simplest form and the results can be easily extended to the other areas if required.

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2. Ising model

The Hamiltonian of the spin-$\frac{1}{2}$ Ising model in a field H is

$$H_m = -\sum_{(ij)} J(\boldsymbol{r}_{ij}) s_i s_j - mH \sum_i s_i$$

where the spin variables s_i take the values ± 1 and the first sum runs over all pairs of spins. In the present work we shall assume that only nearest-neighbour (NN) interactions are significant such that $J(\boldsymbol{r}_{ij}) = J$ when $\boldsymbol{r}_{ij}$ is a NN vector and is zero otherwise. The magnetic moment per spin is denoted by m.

It is convenient to define the reduced spin-pair correlation function by

$$\Gamma(\boldsymbol{r}) = (\langle s_0 s_r \rangle - \langle s_0 \rangle^2)/(\langle s_0^2 \rangle - \langle s_0 \rangle^2) \tag{1}$$

where s_r is the spin at position $\boldsymbol{r}$, and the angular brackets denote the thermodynamic expectation value in an infinite system. For a two-dimensional square lattice

$$\langle s_{0,0} s_{0,N} \rangle = \pm \begin{vmatrix} a_0 & a_{-1} & a_{-2} & \dots & a_{-N+1} \\ a_1 & a_0 & a_{-1} & & a_{-N+2} \\ a_2 & a_1 & a_0 & \dots & a_{-N+3} \\ \vdots & & \vdots & & \vdots \\ a_{N-1} & a_{N-2} & a_{N-3} & \dots & a_0 \end{vmatrix} \tag{2}$$

where the sign is chosen to make $\langle s_{0,0} s_{0,N} \rangle$ positive, and

$$a_n = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\theta \, \mathrm{e}^{-\mathrm{i}n\theta} \phi(\theta) \tag{3}$$

with

$$\phi(\theta) = \left(\frac{(1-\alpha_1 \mathrm{e}^{\mathrm{i}\theta})(1-\alpha_2 \mathrm{e}^{-\mathrm{i}\theta})}{(1-\alpha_1 \mathrm{e}^{-\mathrm{i}\theta})(1-\alpha_2 \mathrm{e}^{\mathrm{i}\theta})} \right)^{1/2}. \tag{4}$$

The parameters are

$$\alpha_1 = \frac{z(1-|z|)}{1+|z|}$$

and

$$\alpha_2 = \frac{z^{-1}(1-|z|)}{1+|z|}$$

with $z = \tanh \beta J$ and $\beta = 1/kT$. The square root in (4) is defined such that $\phi(\pi) > 0$. The 'diagonal' spin correlation function $\langle s_{0,0} s_{N,N} \rangle$ may also be expressed as a Toeplitz determinant, similar to that given in (2)–(4). Expressions for the first and second NN correlation functions have been obtained by McCoy and Wu (1973). For $T > T_c$, where T_c is the critical temperature,

$$\langle s_{0,0} s_{0,1} \rangle = \coth 2\beta J [\tfrac{1}{2} + \pi^{-1} \cosh^2 2\beta J (2 \tanh^2 2\beta J - 1) K(k_>)]$$

and

$$\langle s_{0,0} s_{1,1} \rangle = (2/\pi k_>)[E(k_>) + (k_>^2 - 1) K(k_>)].$$

For $T < T_c$

$$\langle s_{0,0}s_{0,1}\rangle = \coth 2\beta J[\tfrac{1}{2} + \pi^{-1}(2 - \coth^2 2\beta J)K(k_<)]$$

and

$$\langle s_{0,0}s_{1,1}\rangle = (2/\pi)E(k_<)$$

where

$$k_> = \sinh^2 2\beta J = k_<^{-1}$$

and K and E are the complete elliptic integrals of the first and second kinds respectively (Cayley 1956, Erdélyi 1953). To obtain the third NN correlation function $\langle s_{0,0}s_{0,2}\rangle$ we need to evaluate the functions a_{-1} and a_1 in (2). For $T > T_c$

$$a_{-1} = \frac{2a}{\pi b}\left\{c\pi_1 + \frac{\alpha_1 a}{2\gamma}\left[\alpha_1^{-1}k_> K + (K - E) - \left(2\gamma - \nu\frac{d\gamma}{d\nu}\right)\pi_1\right]\right\}$$

and

$$a_1 = \frac{2a}{\pi b}\left\{-\alpha_1^{-1}bK + (\alpha_1^{-1}b + \alpha_2 a)\pi_1 + \frac{\alpha_2 a}{2\gamma}\left[\alpha_1^{-1}k_> K + (K - E) - \left(2\gamma - \nu\frac{d\gamma}{d\nu}\right)\pi_1\right]\right\}$$

where

$$\begin{aligned} &a = \alpha_1^{-1} - \alpha_1 \qquad && b = \alpha_2 - \alpha_1 \qquad && c = 1 - \alpha_1\alpha_2 \\ &\nu = \alpha_1 k_> \qquad && \gamma = \alpha_1\alpha_2(a/b)^2 \qquad && \nu(d\gamma/d\nu) = -ac/b \\ &K \equiv K(k_>) \qquad && E \equiv E(k_>) \qquad && \pi_1 \equiv \pi_1(\nu, k_>), \end{aligned}$$

π_1 being the complete elliptic integral of the third kind. For $T < T_c$, a_{-1} and a_1 were evaluated via the numerical integration of (3).

If the 'up' spins of the system are referred to by the letter A and the 'down' spins by the letter B the fractional composition variables are

$$x_A = \tfrac{1}{2}(1 + \langle s_0\rangle) \qquad x_B = \tfrac{1}{2}(1 - \langle s_0\rangle). \tag{5}$$

As $\langle s_0\rangle$ is equal to the magnetisation $M(H)$ of the spin system it is given by the expression

$$\begin{aligned} \langle s_0\rangle = M(H) &= (1 - \sinh^{-4} 2\beta J)^{1/8} && \beta > 1/kT_c \\ &= 0 && \beta < 1/kT_c. \end{aligned} \tag{6}$$

A pair of spins separated by the vector $\boldsymbol{r}$ may be of AA, AB, BA or BB type and the fraction of such spin pairs occurring in the lattice is denoted by $x_{AA}(\boldsymbol{r})$, $x_{AB}(\boldsymbol{r}) = x_{BA}(\boldsymbol{r})$ and $x_{BB}(\boldsymbol{r})$ respectively. These spin-pair fractions may be expressed as a function of the composition variables x_A and x_B and the reduced spin correlation function $\Gamma(\boldsymbol{r})$:

$$\begin{aligned} x_{AA}(\boldsymbol{r}) &= x_A^2[1 + (x_B/x_A)\Gamma(\boldsymbol{r})] \\ x_{AB}(\boldsymbol{r}) &= x_A x_B(1 - \Gamma(\boldsymbol{r})) \\ x_{BB}(\boldsymbol{r}) &= x_B^2[1 + (x_A/x_B)\Gamma(\boldsymbol{r})]. \end{aligned} \tag{7}$$

3. Group relations

The 12 groups of the two-dimensional square lattice are shown in figure 1 and are referred to as A or B groups depending on the spin of the central site. The probability of forming a group having a positive central spin and n positive nearest-neighbour spins is

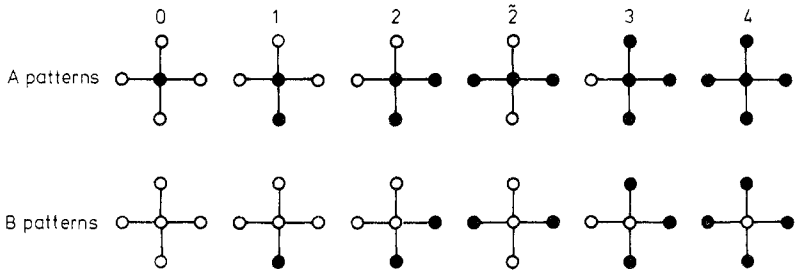

Figure 1. The 12 basic groups of the two-dimensional square lattice.

denoted as A_n and the corresponding probability of having a negative spin surrounded by n positive spins is B_n. It will also be useful to refer to each of the possible spin configurations by the index c, with the probability of forming such a configuration being denoted by P_c. Including the possible degeneracies of each of the spin groups there are 32 different configurations. Knowledge of the configuration probabilities P_c allows the calculation of the magnetisation and pair correlation functions, and conversely knowledge of these quantities determines the configurational probabilities for the square lattice via the application of the following three sum rules:

$$\sum_c P_c = 1 \tag{8}$$

$$\sum_c s_r^{(c)} P_c = \langle s_0 \rangle \tag{9}$$

$$\sum_c s_{r_0}^{(c)} s_{r-r_0}^{(c)} P_c = \langle s_0 s_r \rangle \tag{10}$$

where $s_r^{(c)}$ refers to the spin at position $\boldsymbol{r}$ relative to the central site in a group of configuration c. The sum rules (9) and (10) may also be expressed in terms of the spin and pair fractions x_A and $x_{AA}(\boldsymbol{r})$:

$$\tfrac{1}{2}\sum_c (s_r^{(c)} + 1) P_c = x_A$$

$$\tfrac{1}{4}\sum_c (s_{r_0}^{(c)} + 1)(s_{r-r_0}^{(c)} + 1) P_c = x_{AA}(\boldsymbol{r}).$$

Although there are 32 P_c values, symmetry arguments reduce the number of different group probabilities to 12, there being 6 A groups and 6 B groups. It is, however, possible to relate the A_n and B_n probabilities. Consider two spin systems, identical except that in one system a particular site (having n NN positive spins) has positive spin (system A), while for the other system the same site has negative spin (system B). The ratio of the probabilities of occurrence of these two systems is given by

the ratio of their respective Boltzmann factors:

$$\frac{P(\text{system A})}{P(\text{system B})} = \frac{\exp[-(-J\,\Sigma_{NN}\,s_j - mH)/kT]}{\exp[-(J\,\Sigma_{NN}\,s_j + mH)/kT]}$$
$$= \exp[(2mH - 8J)/kT][\exp(4J/kT)]^n$$
$$= \kappa\lambda^n \tag{11}$$

where

$$\kappa = \exp[(2mH - 8J)/kT] \tag{12}$$

and

$$\lambda = \exp(4J/kT). \tag{13}$$

As (11) is true for all states of the system we obtain

$$A_n/B_n = \kappa\lambda^n. \tag{14}$$

Expressing the sum rules in terms of the group probabilities A_n and B_n and using the relationship (14) leads to the reduced form of the sum-rule equation:

$$\begin{bmatrix} 1 \\ x_A \\ x_A \\ x_{AA}(0,1) \\ x_{AA}(1,1) \\ x_{AA}(0,2) \end{bmatrix} = \begin{bmatrix} (\kappa+1) & 4(\kappa\lambda+1) & 4(\kappa\lambda^2+1) & 2(\kappa\lambda^2+1) & 4(\kappa\lambda^3+1) & (\kappa\lambda^4+1) \\ \kappa & 4\kappa\lambda & 4\kappa\lambda^2 & 2\kappa\lambda^2 & 4\kappa\lambda^3 & \kappa\lambda^4 \\ 0 & (\kappa\lambda+1) & 2(\kappa\lambda^2+1) & (\kappa\lambda^2+1) & 3(\kappa\lambda^3+1) & (\kappa\lambda^4+1) \\ 0 & \kappa\lambda & 2\kappa\lambda^2 & \kappa\lambda^2 & 3\kappa\lambda^3 & \kappa\lambda^4 \\ 0 & 0 & (\kappa\lambda^2+1) & 0 & 2(\kappa\lambda^3+1) & (\kappa\lambda^4+1) \\ 0 & 0 & 0 & (\kappa\lambda^2+1) & 2(\kappa\lambda^3+1) & (\kappa\lambda^4+1) \end{bmatrix} \begin{bmatrix} B_0 \\ B_1 \\ B_2 \\ B_{\frac{5}{2}} \\ B_3 \\ B_4 \end{bmatrix}, \tag{15}$$

i.e. $X = RB$ where X and B are the column matrices and R is the sum-rule matrix in (15).

The spin fraction x_A may be evaluated from (5) and (6), and the spin-pair fraction $x_{AA}(\boldsymbol{r})$ from (7) and (1). The reduced sum-rule equation may be solved numerically for the group probabilities B_n. Alternatively, provided the field H is zero, such that $\kappa = \lambda^{-2}$, (15) may be inverted to give

$$B = R^{-1}X \tag{16}$$

where the inverse of the sum-rule matrix

$$R^{-1} = \frac{1}{2(\lambda-1)^3}$$
$$\begin{bmatrix} 2\lambda^2(\lambda-3) & 4\lambda^2(\lambda+1) & -4\lambda^2(2\lambda-3) & -4\lambda^2(\lambda+1) & 4\lambda^2(\lambda-1) & 2\lambda^2(\lambda-1) \\ 3\lambda & -3\lambda(\lambda^2+1) & 2\lambda(\lambda^2-3) & 4\lambda(\lambda^2+1) & -2\lambda(\lambda^2-1) & -\lambda(\lambda^2-1) \\ -(\lambda+1) & (\lambda+1)(\lambda^2+1) & -2(\lambda^2-2\lambda-1) & -2(\lambda+1)(\lambda^2+1) & (\lambda-1)(\lambda+1)^2 & 2\lambda(\lambda-1) \\ -(\lambda+1) & (\lambda+1)(\lambda^2+1) & -2(\lambda^2-2\lambda-1) & -2(\lambda+1)(\lambda^2+1) & 4\lambda(\lambda-1) & (\lambda-1)(\lambda^2+1) \\ 1 & -(\lambda^2+1) & -4 & 4(\lambda^2+1) & -2(\lambda^2-1) & -(\lambda^2-1) \\ 0 & 0 & 4 & -4(\lambda+1) & 4(\lambda-1) & 2(\lambda-1) \end{bmatrix}$$

4. Group probabilities

The group probabilities B_n were calculated from (16) for the zero-field, $H = 0$, case. As no exact solutions for the magnetisation and spin correlation functions exist for

non-zero field this precluded calculation of the non-zero field group probabilities. The general solution of the nearest-neighbour, isotropic Ising model may be expressed in terms of the two parameters κ and λ, (12) and (13); however, for $H = 0$ $\kappa = \lambda^{-2}$ and the solution becomes a function of the single parameter λ. The Ising lattice is ferromagnetic when $\lambda > 1{\cdot}0$ $(J > 0)$ and antiferromagnetic when $\lambda < 1{\cdot}0$ $(J < 0)$. To describe the antiferromagnetic case the square lattice is subdivided into two equivalent sublattices 1 and 2 in such a way that all the nearest neighbours of a member of 1 belong to sublattice 2 and *vice versa*. The antiferromagnetic spin arrangement for a given $J < 0$ may then be obtained from the ferromagnetic arrangement corresponding to $|J|$ by reversing all spins on one of the sublattices. The resulting antiferromagnet has the same energy and thermal properties as the corresponding ferromagnet. For the antiferromagnet we define sublattice group probabilities $A(l)_n$ and $B(l)_n$ where the groups are centred on sublattices $l(l = 1, 2)$. If the antiferromagnet is formed by reversing the spins on sublattice 2 of a ferromagnet having group probabilities A_n and B_n, then on sublattice 1

$$A(1)_n = A_{4-n} \qquad B(1)_n = B_{4-n}$$

and on sublattice 2

$$A(2)_n = B_n \qquad B(2)_n = A_n.$$

The general behaviour of the ferromagnetic group probabilities in the range $1{\cdot}0 \leqslant \lambda \leqslant 6{\cdot}2$ is shown in figure 2. In a fully ordered antiferromagnetic spin system each spin is surrounded by unlike nearest neighbours while in a completely clustered

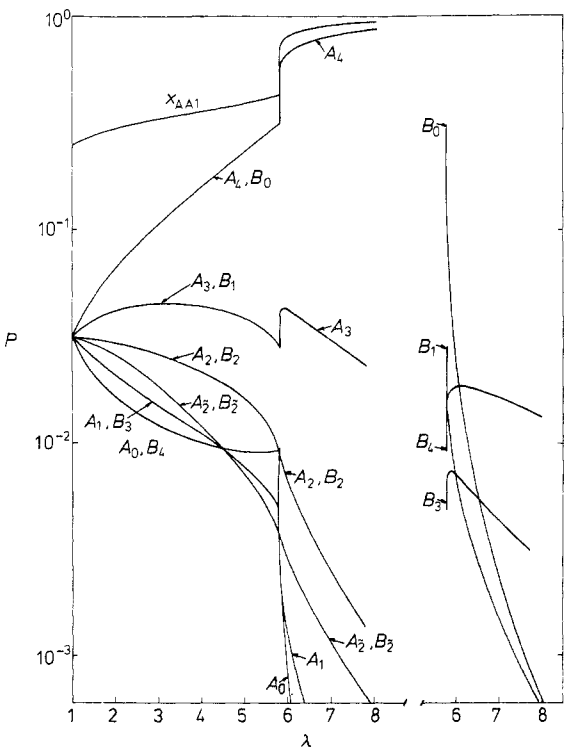

Figure 2. The group probabilities A_n, B_n, and the nearest-neighbour pair fraction x_{AA1} of the square lattice at zero magnetic field as a function of λ.

ferromagnetic spin system each spin is surrounded by like nearest neighbours. In this sense it is convenient to describe the A_4 and B_0 groups as being fully clustered and the A_0 and B_4 groups as being fully ordered. The groups lying between these two extremes exhibit partial clustering or partial ordering, depending on their position in the group sequence of figure 1. At $\lambda = 1{\cdot}0$ (infinite temperature) the system is completely disordered and exhibits random mixing with all groups having the same probability of occurrence, $P_n = \frac{1}{32}$. At high temperature ($\lambda \simeq 1$) the effective mean field acting on each group is small; hence the groups appear to behave as independent units, and the group probabilities take the asymptotic high-temperature values

$$A_n = \tfrac{1}{32}\lambda^{\frac{1}{2}n-1} \qquad (\lambda \to 1{\cdot}0)$$

given by the Boltzmann factor. The group probabilities are therefore maximum for the fully clustered $A_4(B_0)$ group and range downwards through the sequence $A_3(B_1)$; $A_2, A_{\tilde{2}}(B_2, B_{\tilde{2}})$; $A_1(B_3)$ to the fully ordered $A_0(B_4)$ group.

The $A_4(B_0)$ probability increases monotonically to the critical point at $\lambda_c = 5{\cdot}828427$ and the partially clustered $A_3(B_1)$ probability exhibits a local maximum of $0{\cdot}044860$ at $\lambda = 3{\cdot}228$. At the opposite end of the clustering sequence the fully ordered $A_0(B_4)$ group initially decreases, as expected, but then exhibits a local minimum when $\mathrm{d}(\ln A_4)/\mathrm{d}(\ln \lambda) = 2$. This relation follows from (14) and the symmetry relation $B_n = A_{4-n}(\lambda \leqslant \lambda_c)$. The group probabilities at the critical point are given in table 1.

Table 1. Two-dimensional square lattice group probabilities at $\lambda_c = 5{\cdot}828427$.

$A_4(B_0)$	$A_3(B_1)$	$A_2(B_2)$	$A_{\tilde{2}}(B_{\tilde{2}})$	$A_1(B_3)$	$A_0(B_4)$
0·3161756	0·0281769	0·00882463	0·00358657	0·00483439	0·009307344

For $\lambda > \lambda_c$ the symmetry relation is no longer valid for all groups and in particular the (A_4, B_0), (A_3, B_1), (A_1, B_3) and (A_0, B_4) branches split into two separate arms at λ_c. The behaviour of the group probabilities in the vicinity of the critical point is shown in figures 3(*a*)–(*f*). Expressions for the separation between the A_n and B_{4-n} arms may be derived from the two sum rules (9), corresponding to $\boldsymbol{r}$ being taken as (i) the central site and (ii) one of the surrounding four 'boundary' sites, and (14):

$$A_n - B_{4-n} = 2L_n\langle s_0\rangle \tag{17}$$

where

$$L_4 = \frac{\lambda^2(\lambda-3)}{2(\lambda-1)^3} \tag{18}$$

$$L_3 = \frac{\lambda}{2(\lambda-1)^3} \tag{19}$$

$$L_1 = \frac{-1}{2(\lambda-1)^3} \tag{20}$$

$$L_0 = \frac{-(\lambda-3)}{2(\lambda-1)^3}. \tag{21}$$

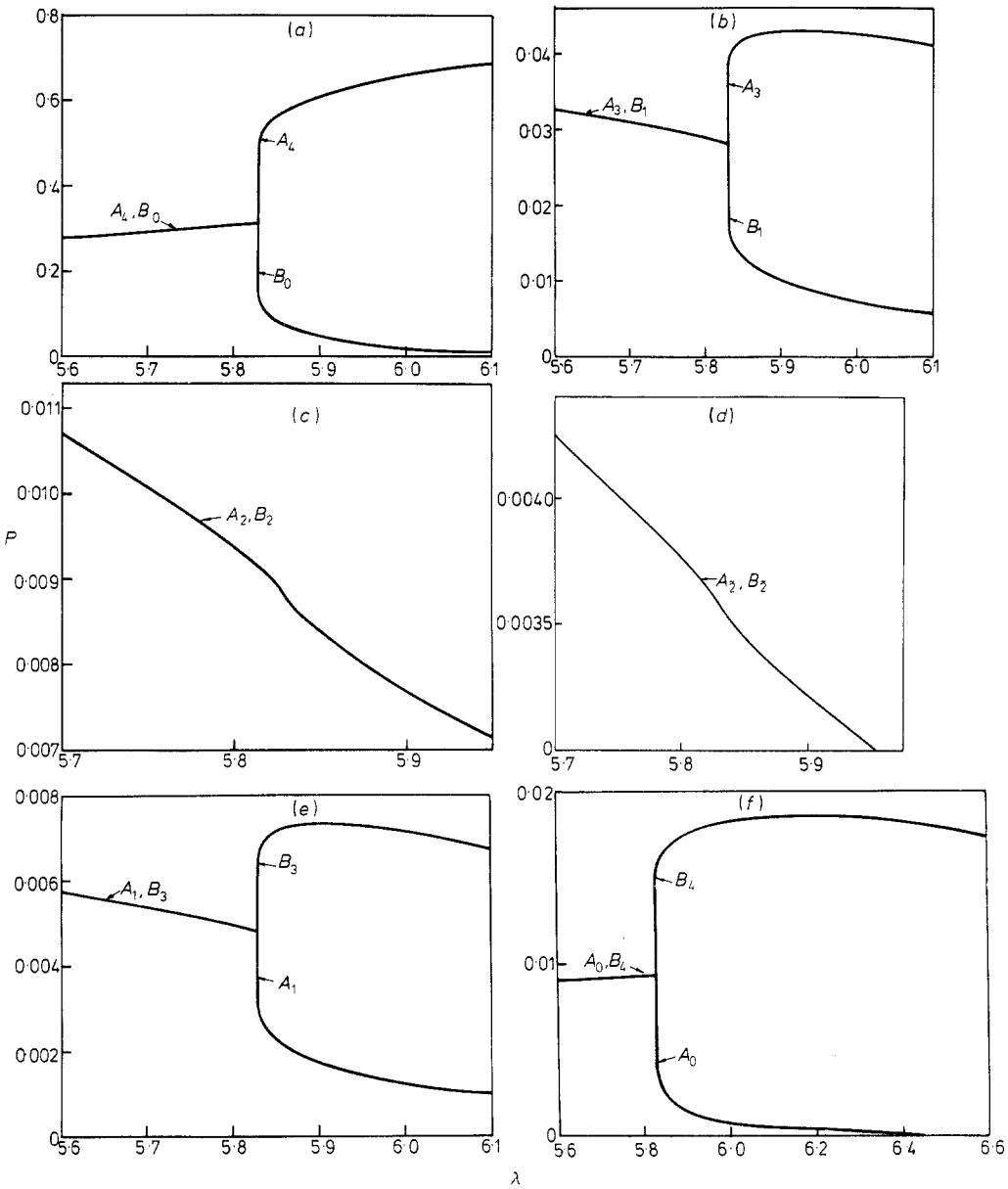

Figure 3. Group probabilities near $\lambda_c(H=0)$: (*a*) A_4, B_0; (*b*) A_3, B_1; (*c*) A_2, B_2; (*d*) $A_{\tilde{2}}, B_{\tilde{2}}$; (*e*) A_1, B_3; (*f*) A_0, B_4.

If the four boundary spins of a group are in an $n=2$ configuration the probability of the central spin being 'up' (A) or 'down' (B) is equal. Therefore $A_2 = B_2$ and $A_{\tilde{2}} = B_{\tilde{2}}$ and the symmetry splitting for $n=2$ does not occur.

Equations (17)–(21) give the high-temperature symmetry relation $A_n = B_{4-n}$ for $\lambda < \lambda_c$ and show that the sharp splitting which develops at λ_c is due to the rapid development of spontaneous magnetisation $\langle s_0 \rangle$. Inspection of figure 3 shows that the mean of A_n and B_{4-n} for $\lambda \geqslant \lambda_c$ is a smooth continuation of the high-temperature

$A_n(B_{4-n})$ curve. The A_n and B_{4-n} group probabilities differ from this mean value by $\pm L_n\langle s_0\rangle$. In particular, in the region of the critical point

$$A_n \simeq A_n(\lambda_c) + L_n\langle s_0\rangle. \tag{22}$$

In a ferromagnetic system like spins tend to group together to form clusters of A or B spins. The boundary surface between clusters is defined by the existence of AB spin pairs and the total surface 'area' is equal to the number of AB spin pairs in the system. The total cluster surface area per lattice site is

$$\begin{aligned}\langle S\rangle_{\text{site}} &= 4(A_3 + 2A_2 + A_{\tilde{2}} + 3A_1 + A_0) \\ &= 4(B_1 + 2B_2 + B_{\tilde{2}} + 3B_3 + B_4).\end{aligned} \tag{23}$$

Inserting (22) into (23) we find that in the close vicinity of the critical point $S(\lambda) \simeq S(\lambda_c)$, that is there is no change in total cluster surface area during the initial rapid development of spontaneous magnetisation. This is an interesting result in view of the large change in cluster volumes due to spin reversal at λ_c. In figure 4 $\langle S\rangle_{\text{site}}$ is plotted as a function of λ. The total surface area is a relatively slowly varying monotonic function of λ with a point of inflection at λ_c.

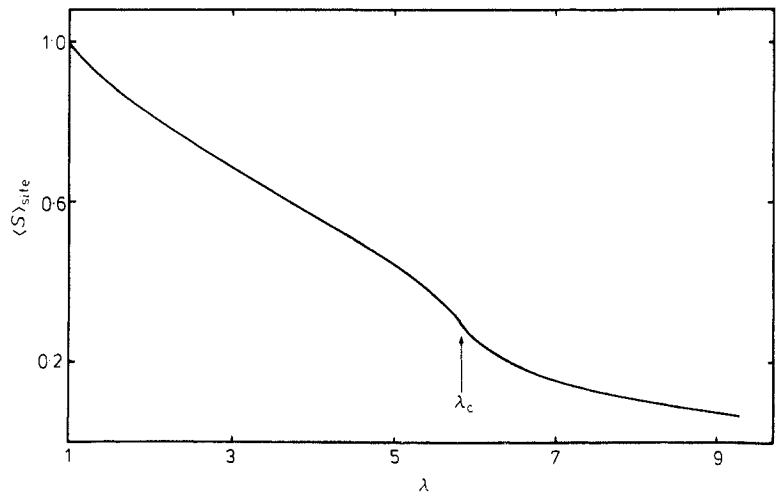

Figure 4. The total surface area of the square lattice at zero magnetic field, per lattice site, as a function of λ.

5. Conclusion

The determination and knowledge of group probabilities provides detailed knowledge of the local configurations in an Ising lattice. Changes in cluster size and topology, for instance, are reflected in the relative magnitudes of the group probabilities and offer an alternative way of characterising clusters. Information on the total cluster surface can also be obtained from the group probabilities. As the group terminology is closer to that employed in Monte-Carlo simulation than the pair correlation or spontaneous magnetisation functions they provide an excellent reference against which the accuracy of simulation studies can be determined.

Acknowledgments

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