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Derivation of low temperature expansions for the Ising model with spin $S > \frac{1}{2}$

M F Sykes and D S Gaunt

Wheatstone Physics Laboratory, King's College, London, UK

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Abstract. The derivation of low temperature (high field) expansions for the Ising model with spin $S > \frac{1}{2}$ is described.

1. Introduction

This paper describes methods for the derivation of low temperature (high field) series for the Ising model with spin $S > \frac{1}{2}$. Such expansions were derived by Sykes (1956) but found difficult to interpret by the methods available at that time. The progress made in the last decade, both in the interpretation of low temperature series (Baker 1965, 1970, Guttmann 1969, Thompson *et al* 1969, Guttmann *et al* 1970) (see also the review by Gaunt and Guttmann (1973)), in cooperative phenomena and in methods for deriving them (Sykes *et al* 1965) has made it possible to re-examine this problem with profit (Fox and Gaunt 1970, 1972, Fox and Guttmann 1970, 1973, Fox 1972). The derivation of the raw data is of necessity a somewhat intricate matter and much of the process is best done by computer. We describe in outline how such expansions may be derived by direct enumeration; we also indicate briefly the necessary generalizations of the indirect method of partial generating functions. We assume throughout a general familiarity with the problem for spin $S = \frac{1}{2}$ which may be acquired from the reviews of Domb (1960) and Fisher (1963, 1965, 1967) and particularly the specialized papers of Sykes *et al* (1965, 1973a, b, c). The data derived by the methods described are published and analysed in the papers cited above.

2. The Ising model for general spin

The Ising model for general spin is defined by the Hamiltonian

$$\mathscr{H} = -\frac{J}{S^2}\sum_{ij} S_i^z S_j^z - \frac{mH}{S}\sum_i S_i^z \tag{2.1}$$

where S_i^z is the z component of the ith spin ($S_i^z = S, S-1, \ldots, -S$), m is the magnetic moment of each spin, H is the applied magnetic field in the z direction and J is the interaction energy defined precisely by (2.1). The first summation is taken over all interacting pairs of spins, and as we shall only consider the first neighbour model these pairs are equivalent to all edges of the lattice. The second summation is taken over all spins.

For the spin $\frac{1}{2}$ model the spins can be regarded as having two states: 'up' ($S^z = \frac{1}{2}$) and 'down' ($S^z = -\frac{1}{2}$). At absolute zero temperature all the spins point up, parallel to the applied magnetic field, to form an ordered state, the ground state. The energy of this ground state is, for a lattice of N sites and coordination number q,

$$-N(\tfrac{1}{2}qJ+mH). \tag{2.2}$$

As the temperature increases spins overturn and if two interacting spins change from parallel (either both up or both down) to antiparallel (one up and one down) the energy increases by $2J$, the so-called interspin interaction energy. The quantity $2m$ is a measure of the spin–field interaction energy and is the energy gained per unit field strength when a spin changes from parallel (up) to antiparallel (down) to the applied field.

In configurational terms the general spin model may be thought of as a replacement of the two spin states $S^z = \frac{1}{2}$ (up) and $S^z = -\frac{1}{2}$ (down) by $(2S+1)$ states with extremes of $S^z = S$ (fully up) and $S^z = -S$ (fully down). We shall call $S^z = S$ the zeroth (ground) state and number the $2S$ perturbed states 1 to $2S$. By virtue of the normalization (Sykes 1956, Domb and Sykes 1957, Fox 1972) in the Hamiltonian (2.1), the energy of the ground state is still given by (2.2). In addition, the interspin and spin–field interaction energies may be defined exactly as above, provided up and down are generalized to fully up and fully down and it is remembered that only interacting pairs of spins in these extreme states can properly be described as parallel or antiparallel.

3. Generalized linkage rule

For the spin $\frac{1}{2}$ model it is readily shown that if in the ground state s spins are perturbed, and there are r first neighbour bonds between them, the resultant energy gain is

$$2(qs-2r)J+2msH. \tag{3.1}$$

This result is conveniently called the linkage rule since it relates the energy of the perturbed state to the number of links between perturbed spins; it plays a fundamental role in the development of series expansions.

To obtain the appropriate generalization we start with the energy expressed as a sum over all the interactions. If two adjacent spins are in the xth and yth perturbed states respectively, the contribution of their interaction, taking the zeroth (ground) state as datum, is

$$-\frac{J}{S^2}(-Sx-Sy+xy). \tag{3.2}$$

The total energy from spin–spin interactions is therefore the sum over all edges

$$E = \frac{J}{S^2}\sum_{y\geqslant x}(Sx+Sy-xy)N_{x,y} \tag{3.3}$$

where $N_{x,y}$ is the number of edges joining spins in the xth and yth perturbed states. The key to the configurational method lies in regrouping this sum so as to eliminate the unperturbed spins from the summation. This is readily done through the relation

$$\sum_{y>0} qyN_y = \sum_{y>0} yN_{0,y} + \sum_{y\geqslant x>0}(x+y)N_{x,y} \tag{3.4}$$

where N_y is the number of spins in the yth perturbed state, which follows because from

every site there radiate q edges and each edge is shared with another site. From (3.3), on separating the terms for which $x = 0$,

$$\frac{S^2E}{J} = \sum_{y>0} SyN_{0,y} + \sum_{y\geq x>0} \{S(x+y)-xy\}N_{x,y} \tag{3.5}$$

and using (3.4)

$$\frac{S^2E}{J} = \sum_{y>0} qSyN_y - \sum_{y\geq x>0} xyN_{x,y} \tag{3.6}$$

which is the generalized form of the linkage rule for the interspin energy (Sykes 1956).

4. Low temperature enumerative problem

The low temperature (or high field) enumerative problem is a straightforward generalization of the spin $\frac{1}{2}$ problem. We suppose a perturbation with N_1 spins in the first perturbed state, N_2 in the second, and so on. Using the linkage rule (3.6) and including the contribution from the spin–field interaction the appropriate Boltzmann factor is

$$\exp\left\{-\frac{J}{S^2kT}\left(\sum_{y>0} qSyN_y - \sum_{y\geq x>0} xyN_{x,y}\right) - \frac{mH}{SkT}\sum_{y>0} yN_y\right\}. \tag{4.1}$$

If we choose variables

$$u = \exp\left(-\frac{J}{S^2kT}\right) \tag{4.2}$$

$$\mu = \exp\left(-\frac{mH}{kTS}\right) \tag{4.3}$$

the expansion for the free energy per spin can be written

$$F = -\tfrac{1}{2}qJ - mH - kT\ln\Lambda(\mu, u) \tag{4.4}$$

where

$$\ln\Lambda(\mu, u) = \sum_{n=1}^{\infty} L_n(u)\mu^n \tag{4.5}$$

and the coefficient of μ^n is a polynomial in u whose highest power is u^{nqs}. An exception occurs when q is odd (honeycomb lattice for example) and the spin is half-integer; u is then replaced by $z = u^{1/2}$.

The derivation of successive polynomials is now straightforward. The general case is cumbersome and as an illustration we particularize to $S = \frac{3}{2}$ on the triangular lattice. The first power of μ corresponds to one spin in the first perturbed state or

$$L_1 = u^9. \tag{4.6}$$

The second power of μ corresponds either to one spin in the second perturbed state (u^{18}) or two spins in the first; in the latter case the two perturbed spins may be separated ($-3\frac{1}{2}u^{18}$) or adjacent ($3u^{17}$) and

$$L_2 = 3u^{17} - 2\tfrac{1}{2}u^{18}. \tag{4.7}$$

The contributions to the third power of μ may be grouped:

$$N_1 = 3, N_2 = N_3 = 0 \qquad 2u^{24} + 9u^{25} - 30u^{26} + 19\tfrac{1}{3}u^{27} \tag{4.8}$$

$$N_1 = N_2 = 1, N_3 = 0 \qquad 6u^{25} \qquad -7u^{27} \tag{4.9}$$

$$N_1 = N_2 = 0, N_3 = 1 \qquad u^{27} \tag{4.10}$$

and

$$L_3 = 2u^{24} + 15u^{25} - 30u^{26} + 13\tfrac{1}{3}u^{27}. \tag{4.11}$$

To obtain the entries in (4.8) it suffices to notice that if all the spins are in the same perturbed state the coefficients required are numerically the same as those for the spin $\frac{1}{2}$ model; the contributions only differ in the powers of u. Thus for example the contribution to μ^6 if $N_2 = 3$ ($N_1 = N_3 = 0$) follows from (4.8) as

$$2u^{42} + 9u^{46} - 30u^{50} + 19\tfrac{1}{3}u^{54} \tag{4.12}$$

where successive powers now differ by 4 because each linkage must be reweighted in accordance with (3.6).

If all the perturbed states are not the same the underlying configuration must be reweighted to allow for any changes of symmetry. For example the leading term in (4.8) corresponds to a triangle of interacting spins. If all three change from the first to the second perturbed state the symmetry is unaffected; if only one changes it may be chosen in three ways and the contribution becomes $6u^{31}\mu^4$.

Proceeding systematically a useful number of terms can be derived if the underlying configurational information for the spin $\frac{1}{2}$ model is available. The first seven polynomials for $S = 1$ and $S = \frac{3}{2}$ on the triangular and face centred cubic lattices are given by Fox and Gaunt (1972). Polynomials for loose packed lattices may be derived similarly but it is usually better to exploit the sublattice division as outlined in the next section.

5. Method of partial generating functions

For the spin $\frac{1}{2}$ model on a loose packed lattice the method of partial generating functions (Sykes *et al* 1965, 1973a, b, c) can be used with advantage. This exploits the fact that such lattices divide into two equivalent sublattices A and B so that no spin is connected to any other spin on the same sublattice. By providing the exact solution when the number of perturbed spins on one sublattice (by convention B) is restricted to some value λ the first $(2\lambda + 1)$ low temperature (or high field) polynomials are obtained. The method is described in detail in the papers cited. It requires a knowledge of the powerful technique of generating functions (described for example by Feller (1950) and Fisher (1962)).

We outline the modifications when $S > \frac{1}{2}$ by taking as an example the simple quadratic lattice of $2N$ sites with $\lambda = 2$; the arguments are quite general. When $S = \frac{1}{2}$ exploitation of the linkage rule (3.1) requires essentially a knowledge of the number of first neighbour bonds between perturbed spins. The two spins on the B sublattice cast 'shadows' on the A sublattice; these shadows can affect either 8, 7 or 6 spins as illustrated schematically in the figure. Any site on the A sublattice which is perturbed will yield

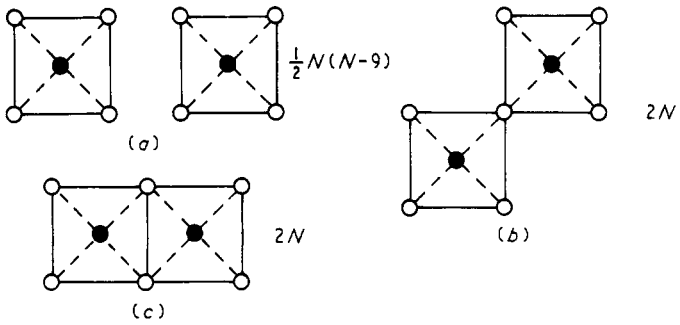

Figure 1. Simple quadratic lattice: the three types of shadow pattern cast on A spins by two B spins. ○ A spin, ● B spin, – – – possible bonds between perturbed spins.

one bond for each shadow in which it lies. Denoting perturbed A spins by x and perturbed B spins by y the appropriate generating function is

$$\tfrac{1}{2}N(N-9)y^2(1+bx)^8(1+x)^{-8}+2Ny^2(1+bx)^6(1+b^2x)(1+x)^{-7}$$
$$+2Ny^2(1+bx)^4(1+b^2x)^2(1+x)^{-6} \tag{5.1}$$

where the power of b in the expanded function corresponds to the number of bonds between perturbed spins in the resultant configuration.

To apply the technique when $S = 1$ we introduce x and X to denote perturbed spins on the A sublattice in the first and second state respectively, and y and Y on the B sublattice. In accordance with the linkage rule (3.6) (where x and y should not be confused with the notation of this section) bonds between x and y are to yield b, x and Y or X and y are to yield b^2, and X and Y are to yield b^4. In all the shadow patterns illustrated in the figure there are three ways of distributing two perturbed states on the B sublattice. The required generating function is now

$$\begin{aligned}
&\tfrac{1}{2}N(N-9)y^2(1+bx+b^2X)^8(1+x+X)^{-8}\\
&\quad+N(N-9)yY(1+bx+b^2X)^4(1+b^2x+b^4X)^4(1+x+X)^{-8}\\
&\quad+\tfrac{1}{2}N(N-9)Y^2(1+b^2x+b^4X)^8(1+x+X)^{-8}\\
&\quad+2Ny^2(1+bx+b^2X)^6(1+b^2x+b^4X)(1+x+X)^{-7}\\
&\quad+4NyY(1+bx+b^2X)^3(1+b^2x+b^4X)^3(1+b^3x+b^6X)(1+x+X)^{-7}\\
&\quad+2NY^2(1+b^2x+b^4X)^6(1+b^4x+b^8X)(1+x+X)^{-7}\\
&\quad+2Ny^2(1+bx+b^2X)^4(1+b^2x+b^4X)^2(1+x+X)^{-6}\\
&\quad+4NyY(1+bx+b^2X)^2(1+b^2x+b^4X)^2(1+b^3x+b^6X)^2(1+x+X)^{-6}\\
&\quad+2NY^2(1+b^2x+b^4X)^4(1+b^4x+b^8X)^2(1+x+X)^{-6}.
\end{aligned} \tag{5.2}$$

The generalization is conceptually simple and the derivation of a useful number of partial generating functions straightforward although tedious. The modification to $S > 1$ is obvious but the expressions become progressively heavier. The main practical problem lies in the performance of the manipulations required to obtain the high field polynomials explicitly; nevertheless the method has proved more productive than direct enumeration. The technique has been developed by Fox (1972) and the first ten

polynomials for the spin 1 model on the simple quadratic, simple cubic and body centred cubic lattices and the first twelve polynomials on the honeycomb and diamond lattices are given by Fox and Gaunt (1972).

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