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Local Properties of an Ising Model on a Cayley Tree

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The Ising model on a Cayley tree displays a peculiar (continuous order) phase transition with zero long-range order at all finite temperatures. When one studies expection values of spins far removed from the surface (which contains a finite fraction of the total number of spins in the thermodynamic limit), however, one obtains the so-called Bethe approximation. Here we study such a local description by setting up a simple recurrence relation for successive shell magnetizations far removed from the surface. In the ferromagnetic case the local magnetization is a fixed point of the iterative transformation, while in the antiferromagnetic case the fixed point bifurcates to a two-cycle of the transformation (for low temperatures and fields) giving rise to local sublattice magnetizations. In both cases, local thermodynamical properties are obtained by integration.

KEY WORDS: Ising model; Cayley tree; phase transition; iteration; fixed point; bifurcation; ferromagnetic; antiferromagnetic.

1. INTRODUCTION

A Cayley tree is a lattice (or graph) on which no closed paths can be generated. The simplest version with two shells and coordination number 3 is shown in Fig. 1.

The Ising model on such lattices has received much attention and it is often claimed and widely believed that the Bethe approximation becomes exact for the "infinite" Cayley tree. If, however, one treats the problem in the accepted statistical mechanical fashion, by first considering the finite lattice and then proceeding to the thermodynamic limit, one does not recover the Bethe approximation. Instead, one obtains a peculiar type of phase transition with a singular free energy[1,2] but with zero long-range

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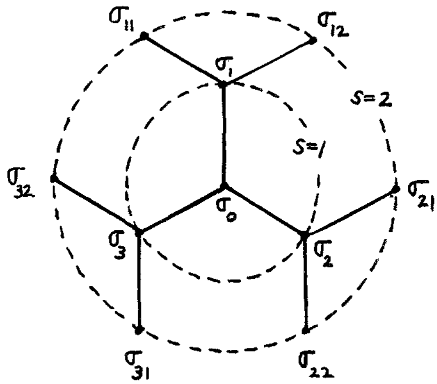

Fig. 1. Two shells of a Cayley tree with coordination number 3.

order at all finite temperatures.[3] This phenomenon may be attributed to the fact that in the thermodynamic limit a finite fraction of the sites on a Cayley tree lie on the surface. In order to avoid such peculiarities one must eliminate surface effects by considering local properties of sites, or groups of sites, in the interior of the lattice and far removed from its surface. This program was carried through by Runnels[4] for the hard repulsive lattice gas on a Cayley tree with coordination number 3. He showed that if "surface effects are eliminated" one obtains the quasichemical equation of state (the lattice gas version of the Bethe approximation) but only when the activity is strictly less than 4. He also foreshadowed future work on the nature of the transition when surface effects are not eliminated.

Our purpose here is to generalize the work of Runnels by considering, in spin language, the nearest-neighbor Ising model on a Cayley tree with coordination number z, for both ferromagnetic and antiferromagnetic interactions.

What we obtain in effect is an iterative scheme of the form

$$m_i = f(m_{i-1}), \qquad i = 1, 2, \ldots, N \tag{1.1}$$

for computing the magnetization per spin m_i in the ith shell from the surface of the lattice, in terms of m_{i-1}. In the ferromagnetic case the m_i's converge to the (stable) fixed point m^* of (1.1)

$$m^* = f(m^*) \tag{1.2}$$

which may be interpreted as a local magnetization per site. Alternatively, one can eliminate surface effects by defining the local magnetization to be

$$\lim_{n\to\infty} n^{-1} \sum_{i=1}^{n} m_i \tag{1.3}$$

which also equals m^* when the m_i converge to the fixed point. In any event the local magnetization so obtained corresponds to the Bethe approximation and by appropriate integration with respect to the magnetic field, as shown in Section 4, one obtains local thermodynamic quantities that also agree with the Bethe approximation.

The novel feature in the antiferromagnetic case is that when one makes the transition from ferromagnetic to antiferromagnetic coupling the fixed point of (1.1) bifurcates to a stable two cycle (m_+, m_-) given by

$$m_+ = f(m_-) \qquad \text{and} \qquad m_- = f(m_+) \tag{1.4}$$

for temperature and magnetic field below certain critical values. In this case m_+ and m_- have the obvious interpretations as sublattice magnetizations. The local magnetization (1.3), however, now becomes

$$\lim_{n\to\infty} n^{-1} \sum_{i=1}^{n} m_i = \frac{1}{2}(m_+ + m_-) \tag{1.5}$$

and all of these expressions agree with the appropriate antiferromagnetic Bethe approximation.[5]

In the following section we formulate the general Ising problem on a Cayley tree and derive the iteration scheme (1.1) for shell magnetizations. Local magnetizations are derived in Section 3 for both ferromagnetic and antiferromagnetic interactions, and in Section 4 these expressions are integrated to obtain corresponding local free energies. We conclude in Section 4 with a brief discussion of the "classical limit" $z \to \infty$.

2. FORMULATION

For the general lattice with coordination number z, we start from a central spin σ_0 and label spins in successive shells $s = 1, 2, \ldots, N$ by $\sigma_{i_1, i_2, \ldots, i_s}$, $i_1 = 1, 2, \ldots, z$ and $i_k = 1, 2, \ldots, z-1$ for $k = 2, \ldots, s$. The special case $N = 2$ and $z = 3$ is shown in Fig. 1.

For arbitrary nearest neighbor couplings in a uniform magnetic field H, the interaction energy is given by

$$\begin{aligned} E\{\sigma\} = & -\sum_{i_1=1}^{z} J_{0,i_1}\sigma_0\sigma_{i_1} - \sum_{i_1=1}^{z}\sum_{i_2=1}^{z-1} J_{i_1,i_1 i_2}\sigma_{i_1}\sigma_{i_1 i_2} - \cdots \\ & - \sum_{i_1=1}^{z}\sum_{i_2=1}^{z-1}\cdots\sum_{i_s=1}^{z-1} J_{i_1 i_2 \ldots i_{s-1}, i_1 i_2 \ldots i_s}\sigma_{i_1 i_2 \ldots i_{s-1}}\sigma_{i_1 i_2 \ldots i_s} \\ & - \sum_{i_1=1}^{z}\sum_{i_2=1}^{z-1}\cdots\sum_{i_N=1}^{z-1} J_{i_1 i_2 \ldots i_{N-1}, i_1 i_2 \ldots i_N}\sigma_{i_1 i_2 \ldots i_{N-1}}\sigma_{i_1 i_2 \ldots i_N} \\ & - H\left(\sigma_0 + \sum_{i_1=1}^{z}\sigma_{i_1} + \cdots + \sum_{i_1=1}^{z}\sum_{i_2=1}^{z-1}\cdots\sum_{i_N=1}^{z-1}\sigma_{i_1 i_2 \ldots i_N}\right) \end{aligned} \tag{2.1}$$

Separating off the central spin and those in the first shell, we can write the partition function as

$$Z_N = \sum_{\{\sigma\}} \exp(-\beta E\{\sigma\})$$

$$\equiv \sum_{\sigma_0=\pm 1} \sum_{\{\sigma_{i_1}=\pm 1\}} \prod_{i_1=1}^{z} \exp\left(B\sigma_0 + K_{0,i_1}\sigma_0\sigma_{i_1}\right) Y^{i_1}(\sigma_{i_1}) \tag{2.2}$$

which reduces to

$$Z_N = \prod_{i=1}^{z} \left[Y^i(1) Y^i(-1) \right]^{1/2} \times \left[e^B \prod_{i=1}^{z} 2\cosh(K_{0i} + X_i) + e^{-B} \prod_{i=1}^{z} 2\cosh(K_{0i} - X_i) \right] \tag{2.3}$$

where

$$K_{0,i} = \beta J_{0,i}, \qquad B = \beta H \tag{2.4}$$

and X_i is defined by

$$e^{2X_i} = Y^i(1)/Y^i(-1) \tag{2.5}$$

If we now separate off the first shell in the reduced partition function $Y^i(\sigma)$ defined by (2.1) and (2.2) and repeat the above steps shell by shell we obtain the general expression for the partition function[5]

$$Z_N = \prod_{s=1}^{N} T_s \tag{2.6}$$

where

$$T_1 = e^B \prod_{i=1}^{z} 2\cosh(K_{0,i} + X_i) + e^{-B} \prod_{i=1}^{z} 2\cosh(K_{0,i} - X_i) \tag{2.7}$$

and ($s > 1$)

$$T_s = \prod_{i_1=1}^{z} \prod_{i_2=1}^{z-1} \cdots \prod_{i_s=1}^{z-1} \left\{ 2\cosh\left(K_{i_1 \ldots i_{s-1}, i_1 \ldots i_s} + X_{i_1 \ldots i_s}\right) \times 2\cosh\left(K_{i_1 \ldots i_{s-1}, i_1 \ldots i_s} - X_{i_1 \ldots i_s}\right)\right\}^{1/2} \tag{2.8}$$

with the $X_{i_1 \ldots i_s}$ defined recursively by

$$X_{i_1 \ldots i_s} = B + \sum_{i_{s+1}=1}^{z-1} \operatorname{ar\,tanh}\left[\left(\tanh K_{i_1 \ldots i_s, i_1 \ldots i_{s+1}}\right)\left(\tanh X_{i_1 \ldots i_{s+1}}\right)\right] \tag{2.9}$$

Having successively removed all shells we are left with the boundary condition,

$$Y^{i_1 \dots i_N}(\sigma) = e^{B\sigma} \qquad \text{or} \quad X_{i_1 \dots i_N} = B \tag{2.10}$$

Specializing now to the equal coupling case

$$K_{i_1 \dots i_s, i_1 \dots i_{s+1}} \equiv \beta J_{i_1 \dots i_s, i_1 \dots i_{s+1}} = K \tag{2.11}$$

and defining recursively

$$L_1 \equiv X_{i_1 i_2 \dots i_N} = B \tag{2.12}$$

$$L_{k+1} = B + (z-1)\,\mathrm{ar\,tanh}(\tanh K \tanh L_k), \qquad k = 1, 2, \dots, N-1 \tag{2.13}$$

we obtain from the above

$$Z_N = \prod_{k=1}^{N-1} \left[4\cosh(K + L_k)\cosh(K - L_k)\right]^{z(z-1)^{N-k}/2} \times \left\{ e^{B}\left[2\cosh(K + L_N)\right]^{z} + e^{-B}\left[2\cosh(K - L_N)\right]^{z} \right\} \tag{2.14}$$

The number of spins in shell s is clearly $z(z-1)^{s-1}$ so the total number of spins in the N shell lattice is

$$\nu(N) = 1 + \sum_{s=1}^{N} z(z-1)^{s-1} = \left[z(z-1)^{N} - 2\right]/(z-2) \tag{2.15}$$

It follows that in the thermodynamic limit the free energy per spin ψ is given by

$$\begin{aligned} -\beta\psi &= \lim_{N\to\infty} \nu(N)^{-1}\log Z_N \\ &= \left[(z-2)/2\right] \sum_{k=1}^{\infty} (z-1)^{-k} \log\left[4\cosh(K + L_k)\cosh(K - L_k)\right] \end{aligned} \tag{2.16}$$

A detailed analysis of this expression has been given by Müller-Hartmann and Zittartz.[1] Notice in particular, that when $B = 0$, all $L_k = 0$ from (2.13), and (2.16) reduces to the one-dimensional Ising model expression.[6] In fact, this follows easily from (2.2) by summing first over spins on the boundary, noting that for a boundary spin σ and its neighboring spin σ' in the $(N-1)$th shell,

$$\sum_{\sigma=\pm 1} e^{K\sigma'\sigma} = 2\cosh K \qquad \text{for} \quad \sigma' = 1 \quad \text{or} \quad -1 \tag{2.17}$$

Repeated application of (2.17) to spins in shells $N-1, N-2, \dots, 1$ gives the stated result.

Our aim here is to maintain the boundary condition $L_1 = B > 0$ and investigate the behavior of shells deep inside the lattice. In particular, the expectation value of the central spin is easily found by the above methods to be given in general[5] by

$$\langle \sigma_0 \rangle = Z_N^{-1} \sum_{\{\sigma\}} \sigma_0 e^{-\beta E\{\sigma\}}$$
$$= \tanh\left[B + \sum_{i=1}^{z} \operatorname{ar}\tanh(\tanh K_{0,i} \tanh X_i) \right] \tag{2.18}$$

where the X_i's are obtained recursively from (2.9) and (2.10).

In the equal coupling case we have

$$\langle \sigma_0 \rangle = \tanh\left[B + z \operatorname{ar}\tanh(\tanh K \tanh L_N) \right] \tag{2.19}$$

where L_N is obtained by iterating the recurrence (2.13).

As we will see in a moment, L_N iterates to a fixed point of (2.13) when $K > 0$ and (2.19) reduces to the Bethe approximation expression for the magnetization per spin.

In order, however, to utilize the more general expression (1.3) for local magnetization in terms of the shell magnetizations m_i, we follow Runnels[4] and begin with the bulk expression for the magnetization obtained from (2.16) as

$$m(\beta, B) = \frac{\partial}{\partial B}(-\beta\psi)$$
$$= \frac{(z-2)}{2} \sum_{k=1}^{\infty} (z-1)^{-k}$$
$$\times \left[\tanh(K + L_k) - \tanh(K - L_k) \right] \frac{\partial L_k}{\partial B} \tag{2.20}$$

where from (2.13)

$$\frac{\partial L_{k+1}}{\partial B} = 1 + \frac{z-1}{2} \left[\tanh(K + L_k) + \tanh(K - L_k) \right] \frac{\partial L_k}{\partial B} \tag{2.21}$$

Defining

$$r_k = \tfrac{1}{2} \left[\tanh(K + L_k) + \tanh(K - L_k) \right] \tag{2.22}$$

and

$$N_k = r_k \frac{\partial L_k}{\partial B} \tag{2.23}$$

we obtain from (2.21) the recurrence for N_k:

$$N_{k+1} = r_{k+1}\left[1 + (z-1) N_k \right] \tag{2.24}$$

yielding

$$N_k = r_k + (z-1)r_{k-1}r_k + (z-1)^2 r_{k-2}r_{k-1}r_k + \cdots$$
$$+ (z-1)^{k-1} r_1 r_2 \ldots r_k \tag{2.25}$$

It then follows from (2.20) that

$$m(\beta, B) = (z-2)\sum_{k=1}^{\infty}(z-1)^{-k}P_k \tag{2.26}$$

where

$$P_k = b_k N_k / r_k \tag{2.27}$$

and

$$b_k = \tfrac{1}{2}\left[\tanh(K + L_k) - \tanh(K - L_k)\right] \tag{2.28}$$

Using (2.25) and (2.27) and rearranging the terms in the sum (2.26) we have finally

$$m(\beta, B) = (z-2)\sum_{k=1}^{\infty}(z-1)^{-k}m_k \tag{2.29}$$

where

$$m_k = b_k + r_k b_{k+1} + r_k r_{k+1} b_{k+2} + r_k r_{k+1} r_{k+2} b_{k+3} + \cdots$$
$$= b_k + r_k m_{k+1} \tag{2.30}$$

Equation (2.29) can also be obtained from the expression for m in terms of a weighted sum of shell magnetizations. That is, for the finite lattice,

$$m_N(\beta, B) = \left[\nu(N)\right]^{-1}\sum_{s=1}^{N}\nu_s\langle\sigma\rangle_s \tag{2.31}$$

where

$$\nu_s = z(z-1)^{s-1} \tag{2.32}$$

is the number of spins in shell s from the central spin, $\langle\sigma\rangle_s$ symbolically denotes the average magnetization per site in shell s, and $\nu(N)$ is the total number of spins. Proceeding to the thermodynamic limit $N \to \infty$ one obtains (2.29) where m_k is now the average magnetization per site in shell k from the surface. What does not follow straightforwardly in this more direct approach is the recurrence (2.30) for shell magnetizations.

The "local magnetization" is now defined by

$$m^*(\beta, B) = \lim_{n\to\infty} n^{-1}\sum_{k=1}^{n} m_k \tag{2.33}$$

whenever the limit exists. From (2.30), this limit clearly depends on the limiting behavior of b_k and r_k, which in turn depend on the limiting behavior of L_k defined recursively by (2.13). We discuss this limiting behavior in the next section.

3. LOCAL MAGNETIZATION

In order to study the local magnetization we are led by the discussion in the previous section to consider the difference equation

$$x_{k+1} = f(x_k) \tag{3.1}$$

where

$$f(x) = \tanh\left[B + (z-1)\operatorname{ar\,tanh}(x \tanh K)\right] \tag{3.2}$$

and in terms of L_k defined previously in (2.12) and (2.13),

$$x_k = \tanh L_k \qquad \text{and} \qquad x_0 = 0 \tag{3.3}$$

The limiting behavior of the iterates x_k depends crucially on the sign of K as shown in Figs. 2 and 3. We consider the two cases separately and without loss of generality take $B \geqslant 0$.

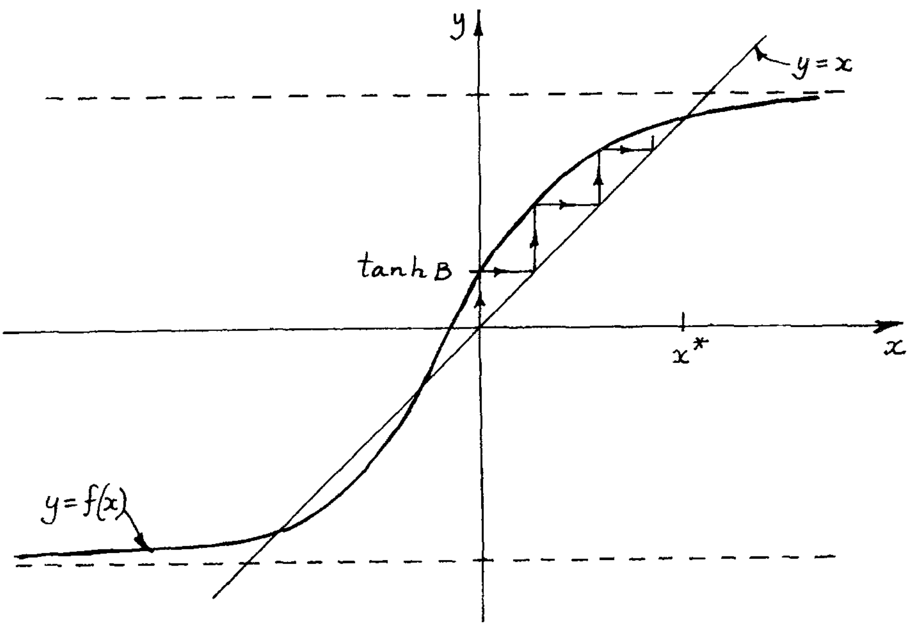

Fig. 2. Ferromagnetic state ($K > 0$): Iteration to a fixed point of (3.1). When $B = 0$, $f'(0) = (z-1)v$.

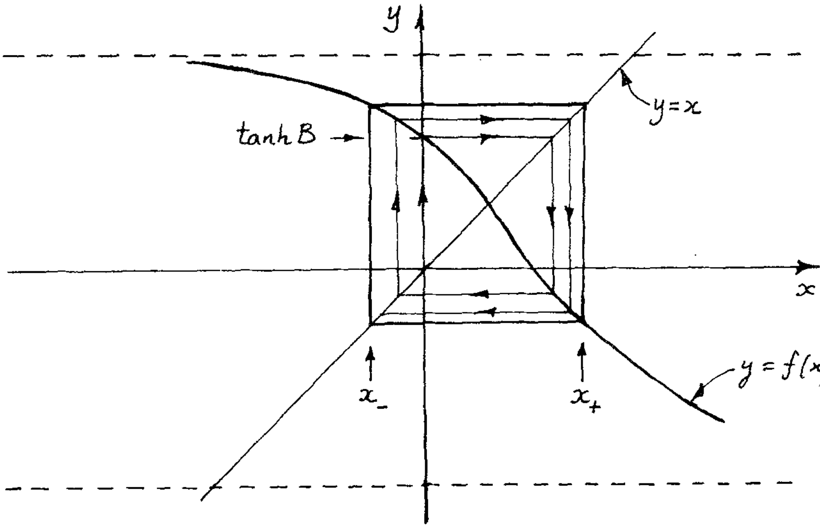

Fig. 3. Antiferromagnetic state ($K < 0$): Bifurcation to a two-cycle of (3.1).

(i) The Ferromagnetic Case $v = \tanh K > 0$

As shown in Fig. 2, the function $f(x)$ in this case is convex when $x \geqslant 0$ and monotone increasing. It then follows straightforwardly that we have monotonic convergence from $x = 0$ to the fixed point x^* as shown in Fig. 2.

From (3.1) and (3.2) we have

$$\tanh L^* \equiv x^* = \tanh\left[B + (z-1)\operatorname{ar}\tanh(x^* \tanh K)\right] > 0 \qquad (3.4)$$

and from (3.3), (2.22), and (2.28) as $k \to \infty$,

$$r_k \to r^* = \frac{1}{2}\left[\tanh(K + L^*) + \tanh(K - L^*)\right] = \frac{v(1 - x^{*2})}{1 - v^2 x^{*2}} \qquad (3.5)$$

and

$$b_k \to b^* = \frac{1}{2}\left[\tanh(K + L^*) - \tanh(K - L^*)\right] = \frac{x^*(1 - v^2)}{1 - v^2 x^{*2}} \qquad (3.6)$$

The local magnetization obtained from (2.30) and (2.33) is then given by

$$m_k \to m^* = \frac{b^*}{1 - r^*} = \frac{x^*(1 + v)}{1 + v x^{*2}} \qquad (3.7)$$

or using (3.4),

$$m^* = \tanh\left[B + z\operatorname{ar}\tanh(v x^*)\right] \qquad (3.8)$$

which is precisely the Bethe approximation expression for the magnetization. Notice also from (2.19) that this expression is also equal to the limiting value of $\langle \sigma_0 \rangle$ where σ_0 is the central spin. The critical temperature can also be seen by inspection from Fig. 2 to be given by

$$(z-1)\tanh K_c = 1 \tag{3.9}$$

since when $(z-1)\tanh K < 1$ $(K < K_c)$ $x^* \to 0$ as $B \to 0$, giving zero spontaneous magnetization, whereas when $K > K_c$, $\lim_{B\to 0} x^* > 0$, giving a nonzero spontaneous magnetization.

(ii) The Antiferromagnetic Case $v = \tanh K < 0$

In this case $f(x)$ is monotone decreasing from $+1$ (at $-\infty$) to -1 (at $+\infty$) and the possibility arises, as shown in Fig. 3, for $x_0 = 0$ to iterate to a 2-cycle (x_+, x_-) rather than to the fixed point x^*.

It would be amusing if this case also embodied the exotic bifurcations to 2^n-cycles and the transition to chaos,[7] but in view of the following elementary lemma (which is trivial to prove) this alas, cannot occur.

Lemma. Suppose that $x \geqslant y \Rightarrow f(x) \leqslant f(y)$ and

$$x_{k+1} = f(x_k), \qquad k = 0, 1, \ldots$$

Then

$$\text{(i) } x_2 \geqslant x_0 \Rightarrow x_{2k+2} \geqslant x_{2k} \quad \text{and} \quad x_{2k+1} \leqslant x_{2k-1}, \qquad k = 1, 2, \ldots$$
$$\text{(ii) } x_2 \leqslant x_0 \Rightarrow x_{2k+2} \leqslant x_{2k} \quad \text{and} \quad x_{2k+1} \geqslant x_{2k-1}, \qquad k = 1, 2, \ldots$$

Thus, when $f(x)$ is bounded (above and below) even and odd iterates form bounded monotonic sequences which converge either to the same limit (x^*) or to one or the other member of a 2-cycle.

From a physical point of view one would expect only sublattice magnetization to develop in such a simple antiferromagnetic model so the limitations of a 2-cycle are entirely reasonable in this case. For other systems with competing interactions it is possible, however, that more complicated and interesting bifurcation patterns will appear.[8]

In the present case, the transition or bifurcation to an antiferromagnetic state takes place when the fixed point x^* becomes unstable, which is easily seen by linearization of (3.1) to occur when

$$f'(x^*) < -1 \tag{3.10}$$

From (3.2) and the definition (3.4) of x^* this amounts to

$$(z-1)|v|(1 - x^{*2}) > 1 - v^2 x^{*2} \tag{3.11}$$

The first thing to notice is that since $|v| < 1$ and $x^{*2} < 1$, this condition can never be satisfied at high temperatures when $|K| < K_c$, with K_c defined by (3.9), for arbitrary $B \geqslant 0$. When $|K| > K_c$, however, the condition (3.11) is satisfied for $B < B_c$, where B_c, the so-called critical field, is obtained by "solving" (3.4), and (3.11) satisfied as an equality. Thus at $B = B_c$ we have from (3.11) that

$$(z-1)|v|(1-x^{*2}) = 1 - v^2x^{*2} \tag{3.12}$$

or

$$x^{*2} = \frac{|v|(z-1)-1}{|v|(z-1)-v^2} \tag{3.13}$$

B_c is then obtained from (3.4) by writing this equation in the form

$$\operatorname{ar\,tanh} x^* = B_c - (z-1)\operatorname{ar\,tanh}|v|x^* \tag{3.14}$$

yielding from (3.13) the result

$$B_c = \operatorname{ar\,tanh}\alpha + (z-1)\operatorname{ar\,tanh}|v|\alpha \tag{3.15}$$

where

$$\alpha = \left[\frac{|v|(z-1)-1}{|v|(z-1)-v^2}\right]^{1/2} \tag{3.16}$$

To summarize the situation for the antiferromagnetic case we have, firstly, a paramagnetic phase when the x_k in (3.1) iterate to the fixed point of f given by (3.4). This occurs when $|K| < K_c$ and $B \geqslant 0$ and when $|K| > K_c$ and $B > B_c$ where the critical field B_c is given by (3.15).

When $|K| > K_c$ and $0 \leqslant B \leqslant B_c$, the x_k in (3.1) iterate to a 2-cycle x_+, x_- given by

$$x_\pm = f(x_\mp) = \tanh\left[B + (z-1)\operatorname{ar\,tanh} vx_\mp\right] \tag{3.17}$$

It then follows from (2.22), (2.28), and (2.30) that the shell magnetizations m_k iterate to a 2-cycle, giving rise to sublattice magnetizations m_+ and m_- defined by

$$m_\pm = b_\pm + r_\pm m_\mp \tag{3.18}$$

where

$$b_\pm = \frac{x_\pm(1-v^2)}{1-v^2x_\pm^2}, \qquad r_\pm = \frac{v(1-x_\pm^2)}{1-v^2x_\pm^2} \tag{3.19}$$

Solving equations (3.18) for m_+ and m_- and using (3.19) one obtains after some tedious algebra the expressions

$$m_\pm = \frac{x_\pm + vx_\mp}{1+vx_+x_-} = \tanh(B + z\operatorname{ar\,tanh} vx_\mp) \tag{3.20}$$

with the $x_{\pm}$ given by (3.17). These expressions agree with those obtained previously for the antiferromagnetic Bethe lattice.[5]

In our terminology, the local magnetization when $|K| > K_c$ and $B \leqslant B_c$ is given by

$$m^*(\beta, B) = \lim_{n\to\infty} n^{-1} \sum_{k=1}^{n} m_k = \tfrac{1}{2}(m_+ + m_-)$$
$$= \tfrac{1}{2}\big[\tanh(B + z \operatorname{ar tanh} vx_+)$$
$$+ \tanh(B + z \operatorname{ar tanh} vx_-)\big] \tag{3.21}$$

In the following section we indicate how one can reconstruct a local free energy and derive local thermodynamic properties from the expressions given above for local magnetizations.

4. LOCAL THERMODYNAMIC PROPERTIES

Consider first an arbitrary Ising model with spin–spin interaction energy $E_I\{\sigma\}$. In the presence of an external field $H = -B/\beta$, the partition function for M spins is given by

$$Z_M(\beta, B) = \sum_{\{\sigma\}} \exp(-\beta E_I\{\sigma\}) \exp\left(B \sum_{i=1}^{M} \mu_i\right) \tag{4.1}$$

The free energy per spin $\psi(\beta, B)$ is given in the thermodynamic limit by

$$-\beta\psi(\beta, B) = \lim_{M\to\infty} M^{-1} \log Z_M(\beta, B) \tag{4.2}$$

from which all thermodynamic properties can be derived. For example, the magnetization is given by

$$m(\beta, B) = \frac{\partial}{\partial B}\left[-\beta\psi(\beta, B)\right] \tag{4.3}$$

Suppose now that one were "given" a magnetization $m(\beta, B)$ and one wanted to reconstruct from it a corresponding free energy $\psi(\beta, B)$. Obviously one way of accomplishing this would be to integrate (4.3). Problems, however, appear with the range of integration, and for reasons which will become clear in a moment it is more convenient to start with auxiliary quantities $Q_M(\beta, B)$ and $\phi(\beta, B)$ defined, analogously to (4.1) and (4.2), by

$$Q_M(\beta, B) = \sum_{\{\sigma\}} \exp(-\beta E_I\{\sigma\}) \exp\left[B \sum_{i=1}^{M} (\mu_i - 1)\right] \tag{4.4}$$

and

$$-\beta\phi(\beta, B) = \lim_{M\to\infty} M^{-1} \log Q_M(\beta, B) \tag{4.5}$$

Evidently, we then have from (4.1), (4.2), and (4.3)

$$m(\beta, B) - 1 = \frac{\partial}{\partial B}(-\beta\phi) \tag{4.6}$$

$$\beta\phi(\beta, B) = \beta\psi(\beta, B) + B \tag{4.7}$$

and most importantly,

$$-\beta\phi(\beta, \infty) = -\lim_{B\to\infty} \beta\phi(\beta, B) = -\beta E_0 \tag{4.8}$$

where E_0 is the limiting value ($M \to \infty$) of $E\{\sigma\}/M$ when all spins σ_i are set equal to $+1$.

If we now integrate (4.6) from B to infinity we obtain from (4.7) and (4.8) the identity

$$\begin{aligned}\int_B^\infty \left[m(\beta, b) - 1\right] db &= \beta(\phi(\beta, B) - \phi(\beta, \infty)) \\ &= \beta\psi(\beta, B) + B - \beta E_0 \end{aligned} \tag{4.9}$$

Now if we are given a *local* magnetization $m^*(\beta, B)$ we simply use (4.9) to *define* a local free energy $\psi^*(\beta, B)$ by

$$\beta\psi^*(\beta, B) = \beta E_0 - B + \int_B^\infty \left[m^*(\beta, b) - 1\right] db \tag{4.10}$$

To illustrate this procedure for reconstructing local thermodynamic properties, consider the ferromagnetic case, and also the paramagnetic phase of the antiferromagnet, of the previous section for which the local magnetization is given by (3.8). For convenience we write

$$m^*(\beta, b) = \tanh(b + z \operatorname{ar}\tanh vx) \tag{4.11}$$

where $b \geqslant 0$ and $x = x(b)$ is the nonnegative solution of

$$x = \tanh\left[b + (z-1)\operatorname{ar}\tanh vx\right] \tag{4.12}$$

In the final expression we will use x^* to denote the solution of (4.12) when $b = B$. Also, since we have only nearest neighbor interactions, $\beta E_0 = -Kz/2$ in general for a regular lattice with coordination number z.

Consider now the integral

$$I = \int_B^\infty \left\{ \frac{\partial}{\partial b}\left[\log 2\cosh(b + z \operatorname{ar}\tanh vx)\right] - 1 \right\} db \tag{4.13}$$

Straightforward integration on the one hand (noting that $2\cosh\alpha \sim e^\alpha$ as $\alpha \to \infty$ and $x(b) \to 1$ as $b \to \infty$) gives

$$I = -\log 2\cosh(B + z \operatorname{ar}\tanh vx^*) + z \operatorname{ar}\tanh v + B \tag{4.14}$$

On the other hand, carrying out the differentiation with respect to b in

(4.13) gives

$$I = \int_B^\infty \left[\tanh(b + z \operatorname{ar}\tanh vx) - 1\right] db$$

$$+ \int_B^\infty \tanh(b + z \operatorname{ar}\tanh vx) \frac{zv}{1 - v^2x^2} \frac{\partial x}{\partial b} db$$

$$= \int_B^\infty \left[m^*(\beta, b) - 1\right] db + \int_B^\infty \frac{zx(1+v)v}{(1+vx^2)(1-v^2x^2)} \frac{\partial x}{\partial b} db$$

$$= \beta\psi^*(\beta, B) + \frac{Kz}{2} + B + \frac{z}{2} \int_B^\infty \frac{\partial}{\partial b} \left[\log(1 + vx^2) - \log(1 - v^2x^2)\right] db$$

$$= \beta\psi^*(\beta, B) + \frac{Kz}{2} + B + \frac{z}{2} \left[\log(1 - v^2x^{*2}) - \log(1 + vx^{*2}) - \log(1 - v)\right] \quad (4.15)$$

where in the second step we have used (4.11) and (3.7) and in the third step we have used (4.10).

Comparing (4.14) and (4.15) and noting that

$$\frac{zK}{2} = \frac{z}{2} \operatorname{ar}\tanh v = \frac{z}{4} \log \frac{1+v}{1-v} \quad (4.16)$$

we find, on rearrangement, the expression for the local free energy

$$\beta\psi^*(\beta, B) = -\log 2\cosh(B + z \operatorname{ar}\tanh vx^*) + \frac{z}{2}\left[\tfrac{1}{2}\log(1 - v^2) - \log(1 - v^2x^{*2}) + \log(1 + vx^{*2})\right] \quad (4.17)$$

which agrees with the form for the free energy obtained in the Bethe approximation.[9]

Recall that this expression is appropriate for $K \geqslant 0$ and $B \geqslant 0$ and also for $K < 0$ provided $|K| \leqslant K_c$ and $B \geqslant 0$ or $|K| > K_c$ and $B \geqslant B_c$. In the truly antiferromagnetic phase $|K| > K_c$ and $B < B_c$ we rewrite (4.10) as

$$\beta\psi^*(\beta, B) = \int_B^{B_c} \left[m^*(\beta, b) - 1\right] db + B_c - B + \psi^*(\beta, B_c) \quad (4.18)$$

where $\psi^*(\beta, B_c)$ is given by (4.17) with B replaced by B_c, Eq. (3.15), and $m^*(\beta, b)$ in the integrand is given by (3.21).

To evaluate the integral in (4.18) one proceeds exactly as above but now in place of (4.13) one considers the integral

$$I' = \int_B^{B_c} \left(\frac{1}{2} \frac{\partial}{\partial b} \left\{\log 2\cosh\left[b + z \operatorname{ar}\tanh vx_+(b)\right] + \log 2\cosh\left[b + z \operatorname{ar}\tanh vx_-(b)\right]\right\} - 1\right) db \quad (4.19)$$

By following the steps above leading from (4.13) to (4.17) one obtains the expression

$$\begin{aligned}\beta\psi^*(\beta, B) = & -\tfrac{1}{2}\big[\log 2\cosh(B + z\,\mathrm{ar}\tanh vx_+) \\ & + \log 2\cosh(B + z\,\mathrm{ar}\tanh vx_-)\big] \\ & + (z/2)\Big\{\tfrac{1}{2}\log(1 - v^2) \\ & - \tfrac{1}{2}\big[\log(1 - v^2x_+^2) + \log(1 - v^2x_-^2)\big] \\ & + \log(1 + vx_+x_-)\Big\}\end{aligned} \tag{4.20}$$

where x_+ and x_- are solutions of (4.17). This expression is valid for $K < 0$, $|K| > K_c$, and $B < B_c$. (It should perhaps be noted that when $B = B_c$, $x_+ = x_- = x^*$.)

As a final note we obtain the corresponding classical expressions by taking the limit $z \to \infty$ after first normalizing the coupling constant by replacing J by J/z or equivalently for large z, by replacing $v = \tanh K$ by K/z.

In this limit, (4.17) and (4.18) become, respectively,

$$\beta\psi^*(\beta, B) = -\log 2\cosh(B + Kx^*) + Kx^{*2}/2 \tag{4.21}$$

and

$$\beta\psi^*(\beta, B) = -\tfrac{1}{2}\log\big[4\cosh(B + Kx_+)\cosh(B + Kx_-)\big] + Kx_+x_-/2 \tag{4.22}$$

where from (3.4) and (3.17) ($B > 0$)

$$x^* = \tanh(B + Kx^*) > 0 \tag{4.23}$$

and

$$x_\pm = \tanh(B + Kx_\mp) \tag{4.24}$$

Moreover, from (3.8) and (3.20), x^* is in fact the magnetization and $x_\pm$ the sublattice magnetizations.

Recall that (4.21) and (4.23) are appropriate for the ferromagnet ($K > 0$) and for the paramagnetic phase ($|K| \leqslant K_c$ and $B \geqslant 0$ or $|K| > K_c$ and $B \geqslant B_c$) of the antiferromagnet ($K < 0$) and (4.22) and (4.24) describe the antiferromagnetic phase ($K < 0$, $|K| > K_c$ and $B < B_c$).

Also, the critical values K_c and B_c, from (3.9) and (3.15), are given in the limit $z \to \infty$ by ($|K| > K_c$)

$$K_c = 1 \quad \text{and} \quad B_c = \mathrm{ar}\tanh\left(1 - \frac{1}{|K|}\right)^{1/2} + \left(1 - \frac{1}{|K|}\right)^{1/2} \tag{4.25}$$

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