Cayley trees, the Ising problem, and the thermodynamic limit

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Proofs have been given that the Bethe-Peierls approximation solves exactly the Ising problem on a Cayley tree. For a tree with coordination number $\gamma > 2$, the approximation predicts, among other things, a phase transition in zero field at $T_c = 2J\{\ln[\gamma/(\gamma-2)]\}^{-1}$, with a discontinuity in the specific heat. On the other hand, the partition function in zero field can be calculated exactly and turns out to be analytic for all T. This paradox is analyzed and resolved. The transition occurring on a Cayley tree is found not to be of the type usually studied in thermodynamics.

In a well-known review article on cooperative phenomena,[1] Domb gave a proof that the Bethe-Peierls approximation solves exactly the Ising problem on a Cayley tree. This is a connected lattice in which each site has the same number γ of nearest neighbors, and in which there exist no closed loops. The Cayley tree has since then also received the name of "Bethe lattice." Figure 1 represents a portion of such a lattice for the case $\gamma - 1 \equiv K = 3$. Domb's proof is based on an expansion in Mayer diagrams given by Rushbrooke and Scoins,[2] and on the observation that the Bethe-Peierls approximation is obtained by summing all diagrams involving no closed configurations. More recently, Wheeler and Widom[3] proved a similar result for the lattice solution with an arbitrary number of components. Because of the mathematical similarity between the Ising problem and the lattice solution, their result was a confirmation and generalization of Domb's result. The above seemed to be a well-established result, frequently quoted in the literature. It was therefore a surprise for the present author to realize that the partition function in zero magnetic field can be calculated explicitly and is analytic for all T. The calculation can be done as follows: consider the usual Ising Hamiltonian

$$H = -J \sum_{(i,j)} \sigma_i \sigma_j \ , \quad J > 0 \tag{1}$$

where each σ_i takes the values ± 1, and the symbol (i,j) means that the summation is over all pairs of nearest neighbors. We consider a Cayley tree and choose an arbitrary site 0 which we call the origin; let the corresponding spin be σ_0. We associate with each bond α a variable $\theta_\alpha \equiv \sigma_r \sigma_s$, where r and s are the atoms at the end of that bond. It is clear that the $\{\theta_\alpha\}$ are all independent (since there are no closed loops), that each θ_α takes only the values ± 1, and that the set $\{\sigma_0, \{\theta_\alpha\}\}$ is a complete set of coordinates in the sense that to each configuration $\{\sigma_i\}$ there corresponds a unique $(\sigma_0, \{\theta_\alpha\})$ and vice versa. The partition function is:

$$Z(\beta) = \sum_{\text{all states}} e^{-\beta E} = \sum_{\sigma_0} \sum_{\theta_1} \cdots \sum_{\theta_{N_b}} e^{\beta J \sum \theta_\alpha} = \sum_{\sigma_0} \prod_{\alpha=1}^{N_b} (e^{\beta J} + e^{-\beta J}) = \sum_{\sigma_0} (2\cosh\beta J)^{N_b} = 2(2\cosh\beta J)^{N_b} \ , \tag{2}$$

where N_b is the total number of bonds on the tree. It is also easy to see that $N_b = N_s - 1$ (N_s = number of sites). In fact, for each site $i \neq 0$, there is a unique self-avoiding path leading from i to 0. If we associate with each site $i \neq 0$, the first bond along this path, we have a one to one correspondence between sites $i \neq 0$ and bonds; thus $N_s - 1 = N_b$. Therefore, in the thermodynamic limit $N_s \to \infty$ the free energy per atom is

$$f = \lim_{N_s \to \infty} \frac{F}{N_s} = -\lim_{N_s \to \infty} \frac{kT}{N_s} \ln Z = -kT \ln(e^{\beta J} + e^{-\beta J}) \ . \tag{3}$$

The specific heat per atom is $c = -Td^2 f/dT^2$ which is continuous for all T. The Bethe-Peierls approximation does not agree with the exact solution. The explanation of this paradox is that on a Cayley tree there is a huge number of surface atoms. The ratio of surface atoms to total number of atoms tends to $(K-1)/K$ and not to zero in the thermodynamic limit, and this makes some of the usual arguments illegal. In the diagrammatic approach there are three steps which become incorrect on a Cayley tree for this reason:

(i) The energy cannot be expressed in the usual way:

$$E = E_0 + 2J\gamma N_+ - 4JN_{++} \ , \tag{4}$$

where E_0 is the energy of the ferromagnetic ground state $\sigma_i = -1$ for all i, N_+ is the number of

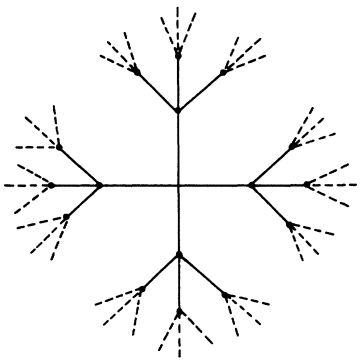

FIG. 1. Portion of a Cayley tree with $K=3$.

up spins, and N_{++} is the number of pairs of neighbors with both spins up. Equation (4) gives incorrect energies for up spins placed on the boundary, a possibility that can be neglected in a real lattice but not on a Cayley tree.

(ii) It is assumed to derive Mayer's theorems that the weight of a graph having articulation points[4] is the product of the weights of the composing stars. That this is not true on a tree can easily be verified by computing explicitly the diagrams $(1-2)^2 \neq (1-2-3)$ (the numbers 1, 2, and 3 would be encircled in the usual notation[5,6]). It is crucial to take into account that particle 2 in the right-hand side may be on the surface.

(iii) The numbers of bonds and sites are related by $N_b = N_s - 1$ and not by $N_b = \frac{1}{2}N_s\gamma$ as would be the case for a lattice with a negligible fraction of surface atoms.

It seems that the errors introduced by (i) and (ii) cancel to some extent, and that it is (iii) which invalidates Domb's discussion. If, in his analysis, the correct relation $N_b \approx N_s$ is used, no phase transition results.

The proof given by Wheeler and Widom would go roughly as follows when specialized to the Ising problem:

(a) Choose one site as the origin 0, and let $i = 1, 2, \ldots, \gamma$ be its nearest neighbors. Let $P(\sigma_0, \sigma_i)$ be the joint probability for finding the values σ_0, σ_i, in thermal equilibrium. Let

$$P_c(\sigma_i/\sigma_0) \equiv P(\sigma_0, \sigma_i)[P(\sigma_0, +1) + P(\sigma_0, -1)]^{-1}$$

be the conditional probability that σ_i will occur if the central atom has spin σ_0.

(b) Because in a Cayley tree there are no closed loops, the probability $Q(\sigma_0, \xi)$ of finding a value σ_0 of the central spin and ξ spins up and $\xi - \gamma$ spins down among its nearest neighbors is exactly

$$Q(\sigma_0, \xi) = \binom{\gamma}{\xi} P_c(+1/\sigma_0)^{\xi} P_c(-1/\sigma_0)^{\gamma-\xi} \times [P(\sigma_0, +1) + P(\sigma_0, -1)] \,. \quad (5)$$

(c) For every ξ the ratio $Q(+1, \xi)/Q(-1, \xi)$ must be given by the corresponding Boltzmann factor:

$$Q(+1, \xi)/Q(-1, \xi) = e^{2J\beta(2\xi-\gamma)} \,, \quad \xi = 0, 1, 2, \ldots, \gamma \,. \quad (6)$$

(d) Because of the arbitrariness in the choice of the origin, we must have

$$P(+1, -1) = P(-1, +1) \,. \quad (7)$$

Among the four numbers $P(1,1)$, $P(1,-1)$, $P(-1,1)$, and $P(-1,-1)$, only three are independent because they must add up to unity. Equation (7) further reduced the number of independent quantities to two. Finally, there are two of the equations (6) which are independent ($\xi = 0$ and $\xi = 1$, for example) so that all probabilities can be determined. We will not give details of the algebra here[7]; suffice it to say that the resulting equations are exactly the Bethe-Peierls equations.

We can note again that this argument, based on the equivalence of all sites in thermal equilibrium, breaks down for atoms close to the surface. Since these constitute the majority of the atoms in the tree,[8] they will dominate the behavior of all thermodynamic functions. Thus, no contradiction exists between the Wheeler-Widom result and the analiticity of $f(\beta)$ [Eq. (3)]. The above discussion suggests, moreover, that even though no phase transition in the thermodynamic sense occurs at $T_c = J/\{k \ln [\gamma/(\gamma-2)]\}$, the magnetization *in the central region of the tree* will change suddenly from zero to its Bethe-Peierls value when the temperature is lowered below T_c.

In order to prove this last statement, we still have to show that among the three solutions of the Bethe-Peierls equation[9] existing below T_c, the system will not choose the one corresponding to zero magnetization. To do this, we proceed as follows. We define first an "n-generation branch": take one atom and call it the "first-generation atom"; connect it to K other sites or atoms and call these the second generation, connect each second-generation atom to K other atoms and call these the third generation, etc. Stop the process when the nth generation has been added. The resulting graph, which is itself a Cayley tree, is an n-generation branch. We will study the Cayley tree obtained by attaching $\gamma = K+1$ n-generation branches to a central atom 0, and our aim will be to compute the magnetization of this central atom. To break the symmetry between the up and down directions, we use the well-known procedure of applying a magnetic field $B > 0$, and letting $B \to 0$ *after* the limit of an infinite system has been taken.

Let Λ_s be the partition function for an s-generation branch in a field B, and let σ be the spin of the first-generation atom. We can split

$$\Lambda_s = \sum_{\text{config.}} e^{-\beta E} = \Lambda_s^+ + \Lambda_s^- \tag{8}$$

where Λ_s^+ contains all terms in the sum Eq. (8) for which $\sigma = 1$, and Λ_s^- all terms for which $\sigma = -1$. Since an $(s+1)$-generation branch is obtained by attaching K s-generation branches to a new first-generation atom, we can immediately write down recurrence relations

$$\Lambda_{s+1}^+ = e^{\beta\mu B} \sum_{\xi=0}^{K} \binom{K}{\xi} (\Lambda_s^+)^{\xi} (\Lambda_s^-)^{K-\xi} e^{\beta J(2\xi - K)}$$

$$= e^{\beta\mu B} (\Lambda_s^+ e^{\beta J} + \Lambda_s^- e^{-\beta J})^K ,$$

$$\Lambda_{s+1}^- = e^{-\beta\mu B} (\Lambda_s^+ e^{-\beta J} + \Lambda_s^- e^{\beta J})^K , \tag{9}$$

which together with

$$\Lambda_1^+ = e^{\beta\mu B}, \quad \Lambda_1^- = e^{-\beta\mu B} \tag{10}$$

completely determine Λ_s^+ for all s. Similarly the partition function of the tree obtained by hanging $\gamma = K+1$ n-generation branches onto a central atom 0 is:

$$Z = Z^+ + Z^- , \tag{11}$$

$$Z^+ = e^{\beta\mu B} (\Lambda_n^+ e^{\beta J} + \Lambda_n^- e^{-\beta J})^{\gamma} , \tag{12}$$

$$Z^- = e^{-\beta\mu B} (\Lambda_n^+ e^{-\beta J} + \Lambda_n^- e^{\beta J})^{\gamma} .$$

Let $P_0(+1)$ and $P_0(-1)$ be the probabilities that σ_0 is $+1$ or -1, and define $z_s \equiv \Lambda_s^+ / \Lambda_s^-$. We have from elementary statistical mechanics and the use of (12)

$$\frac{P_0(+1)}{P_0(-1)} = \frac{Z^+}{Z^-} = e^{2\mu\beta B} \left(\frac{z_n e^{2\beta J} + 1}{e^{2\beta J} + z_n} \right)^{\gamma} \tag{13}$$

where z_n is determined by the equations

$$z_{s+1} = e^{2\beta\mu B} \left(\frac{z_s e^{2\beta J} + 1}{e^{2\beta J} + z_s} \right) \equiv g(z_s) ,$$

$$z_1 = e^{2\beta\mu B} . \tag{14}$$

The computation of the magnetization of the central atom, or more precisely of

$$\lim_{B \to 0} \lim_{n \to \infty} P_0(1)/P_0(-1)$$

can now be done as follows:

(i) With a fixed B and $z_1 = e^{2\beta\mu B}$, compute $z_2 = g(z_1)$; $z_3 = g(z_2)$; etc. Find the limit $z_\infty = z_\infty(B) = \lim_{s\to\infty} z_s(B)$. This amounts to taking the thermodynamic limit first.

(ii) Let $B \to 0$; define $z_\infty(0) = \lim_{B\to 0} z_\infty(B)$.

(iii) Compute $P_0(1)/P_0(-1)$ from (13) with z_n replaced by $z_\infty(0)$.

In Fig. 2, we sketch the shape of $g(z)$ for $T < T_c$ and a small field. The equation $z = g(z)$ has three roots which we indicate by $z_a(B)$, $z_b(B)$, and $z_c(B)$. We also indicate the position of z_1, namely, $z_b(B) < z_1 < z_c(B)$, and a geometric construction giving the successive iterations z_2, z_3, ... mentioned in (i) above. It is obvious from the figure that $z_\infty(B) = z_c(B)$, the biggest one of the three roots of $z = g(z)$. If $B \to 0$, $z_b(B) \to 1$ and the other two have well-defined limits $z_a(0)$, $z_c(0)$ which are different from 1 and are the inverse of each other. Thus, the magnetization of the central atom $m_0(B)$ has a nonvanishing value for $B \to 0$. If $T > T_c$, on the contrary, the equation $z = g(z)$ has only one root which tends to 1 for $B \to 0$, and

$$\lim_{B\to 0} \lim_{n\to\infty} m_0(B) = 0 .$$

This completes our calculation.

We have also been able to prove that if the *average* magnetization is computed by the same means

$$m = \lim_{B\to 0} \lim_{N_s \to \infty} \frac{1}{N_s} \frac{\partial \ln Z(\beta, B)}{\partial B} , \tag{15}$$

the result is zero even below T_c. The proof is cumbersome and will not be given in detail; we only indicate briefly the essential steps. The main idea is again that the magnetization close to the surface goes continuously to zero with B, and that the thermodynamic functions are dominated by precisely these surface atoms.

For any given T, choose $n \gg e^{\beta J}$ and $B \ll J(K-1)/\mu K^{n+1}$. Consider an atom A n steps away from the surface. There are K^n paths leading from A to the surface, and these constitute an n-generation branch. The maximum magnetic energy of this n-generation branch is $E_{\max} \approx K^{n+1}\mu B/(K-1)$ obtained when all spins are aligned. Because of

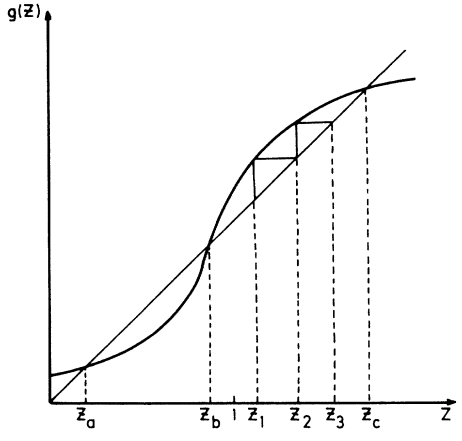

FIG. 2. Function $g(z)$ intersects the line at 45° at three points z_a, z_b, z_c when $T < T_c$. These points are roots at the equation $z = g(z)$. The point $z_1 = e^{2J\beta}$ is between z_b and z_c. The points $z_2 = g(z_1)$, $z_3 = g(z_2)$, etc., are indicated, and it is clear that $\lim_{s\to\infty} z_s = z_c$.

our condition on B, we have $E_{max} \ll J$; thus the magnetic part of the energy can be neglected in front of J in computing the configuration of this part of the tree.

Let us next look at one particular path from A to the surface. The mean number of spin flips along this path is $ne^{-\beta J} \gg 1$. This means that independently of what the spin at A was, the atoms close to the surface (say less than $\frac{1}{2}n$ steps away from the surface) have negligible magnetization.

Another remarkable fact is that both above and below T_c there coexist infinite clusters of up and down spins. T_c does not correspond to a percolation threshold in the usual sense. The proof of this statement will also be omitted since it is a straightforward application of the "birth-and-death" process considered for example in Feller's book.[10]

We conclude that the transition occurring at T_c in the central region of the tree is not of the type usually studied in thermodynamics. It does not show up as a singularity in the free energy; it is instead a process in which a large number of atoms cooperate to produce magnetization in a negligibly small portion of the system when $T < T_c$.

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[1]C. Domb, Adv. Phys. 9, 145 (1960).

[2]G. S. Rushbrooke and H. I. Scoins, Proc. Roy. Soc. A 230, 74 (1955).

[3]J. C. Wheeler and B. Widom, J. Chem. Phys. 52, 5334 (1970).

[4]For the nomenclature on graph theory as well as a proof of Mayer's theorems, see G. E. Uhlenbeck and G. W. Ford, *Studies in Statistical Mechanics* (North Holland, Amsterdam, 1962), Vol. 1, p. 121.

[5]K. Huang, *Statistical Mechanics* (Wiley, New York, 1963).

[6]S. A. Rice and P. Gray, *The Statistical Mechanics of Simple Liquids* (Interscience, New York, 1965).

[7]The proof sketched here is identical with Huang's (Ref. 5) provided his z, introduced phenomenologically, is identified with our $P_c(1/1)\exp(-2J)/P_c(-1/1)$.

[8]The number of atoms in the m outermost layers is a fraction $\approx 1 - K^{-m}$ of the total number N_s when $N_s \to \infty$.

[9]See Ref. 5 for details.

[10]W. Feller, *An Introduction to Probability Theory and its Applications* (Wiley, New York, 1961).