Spin-glass theory in the Bethe approximation: Insights and problems

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(Received 18 January 1982)

We set up and solve the Bethe approximation for a spin-glass with finite-range interactions. We obtain the finite-z analog of the Thouless-Anderson-Palmer equations and the free-energy functional at all T. In the configuration-averaged theory the entropy $\bar{S}(T)$ and all other properties are well behaved on a Cayley tree. For real lattices $\bar{S}(0)=0$, but the specific heat is negative near $T=0$ for all but small values of z.

In recent years much attention has focused on a model of a spin-glass with infinite-range interactions. The simplest mean-field theory of Sherrington and Kirkpatrick[1] (SK) contains one order parameter and leads to unphysical results. Thus far the only satisfactory approach appears to be one in which an infinite number of order parameters is introduced such as that of Thouless, Anderson, and Palmer[2] (TAP) and of Parisi[3] and others.[4] Intimately connected with the difficulties of the SK model is the fact that a spin-glass appears to have many metastable states leading to a highly complex free-energy surface. These metastable states are presumably the origin of the well known irreversibility and history dependent[5] effects in the spin-glasses.

The purpose of the present paper is to explore extensively the Bethe approximation to the finite-range random (Ising) model on real (loose packed) lattices, the exact solution of the model on a Cayley tree, and their mutual relationship. A study of the finite-range model will help form the basis for more elaborate configuration averaged theories (analogous to those of Parisi[3]), for treating localization effects[6] and for characterizing metastable states.

There have been several (incomplete) attempts[7–10] to study the Bethe approximation for a spin-glass. In the configuration-averaged theory, it was claimed[7,8] that the entropy $\bar{S}$ is ill behaved at $T=0$. We find this is not the case, in general. Only after performing a detailed analytic and numerical study did we find the "diseases" of this theory: For sufficiently large z the specific heat at low T is negative. Our other new contributions are to (1) demonstrate that the Cayley tree represents one (of a very small number of) model(s) which have a stable spin-glass phase. Imposing the boundary conditions discussed below serves to make the Cayley tree more like a real lattice. (2) To present an analog of the TAP equation for the free energy $F\{m_i\}$ and moments m_i at all T. (3) To show that a well-behaved entropy does not require a cavity in the effective field distribution.

We consider a Cayley tree of N atoms with random bonds in which the center site is labeled by 0 and a site on the nth generation by $\nu_n \equiv i_1, i_2, \ldots, i_n$ where the series gives the location of a site relative to the center. The free energy on a tree with K generations and coordination number z can be calculated recursively in terms of the effective fields $L_{\nu n}$, obtained by taking partial traces over all spins that are descendents of $\sigma_{\nu n}$. We define $H_{\nu n}$ as the site-dependent external fields and $J_{\nu n}$ as the random near-neighbor exchange coupling

$$F=-k_BT\left\{\ln\left[2\cosh\left(\beta H_0+\sum_{i_1=1}^{z}\tanh^{-1}(\tanh\beta J_{\nu_1}\tanh L_{\nu_1})\right)\right]\right.$$
$$\left.+\frac{1}{2}\sum_{n=1}^{K}\sum_{i_1=1}^{z}\sum_{i_2=1}^{z-1}\cdots\sum_{i_n=1}^{z-1}\ln[4\cosh(\beta J_{\nu n}+L_{\nu n})\cosh(\beta J_{\nu n}-L_{\nu n})]\right\} . \quad (1)$$

Here

$$L_{\nu n}=\beta H_{\nu n}+\sum_{i_{n+1}}^{z-1}\tanh^{-1}(\tanh\beta J_{\nu n+1}\tanh L_{\nu n+1}) , \quad (2)$$

where $i_1=1,\ldots,z$, $i_j=1,\ldots,z-1$ for $2\leq j\leq n$, for $n=1,\ldots,K-1$. The analog of Eq. (2) for $n=K$ is

$L_{\nu K}=\beta H_K$. The thermal averages of the spins $m_{\nu n}=\partial F/\partial H_{\nu n}$ are

$$m_0=\tanh\left(\beta H_0+\sum_{i_1=1}^{z}\tanh^{-1}(\tanh\beta J_{\nu_1}\tanh L_{\nu_1})\right) \tag{3}$$

and

$$m_{\nu n}=(m_{\nu n-1}\tanh\beta J_{\nu n}\operatorname{sech}^2 L_{\nu n}+\tanh L_{\nu n}\operatorname{sech}^2\beta J_{\nu n})(1-\tanh^2\beta J_{\nu n}\tanh^2 L_{\nu n})^{-1} \ . \tag{4}$$

For $i_1=1,\ldots,z$, $i_j=1,\ldots,z-1$ with $2\leq j\leq n$ for $n=1,\ldots,K$. Eliminating the $\{L_{\nu n}\}$ from Eqs. (3) and (4) yields

$$m_i=\tanh\left[\beta H_i+\sum_j\tanh^{-1}\left(\frac{1-g_{ij}^2-r_{ij}}{2(m_i-g_{ij}m_j)}\right)\right] \ , \tag{5}$$

where $g_{ij}\equiv\tanh\beta J_{ij}$ and

$$r_{ij}\equiv[(1-g_{ij}^2)^2-4g_{ij}(m_i-g_{ij}m_j)(m_j-g_{ij}m_i)]^{1/2} \ .$$

Here we have changed notation so that i, j denote sites in the lattice and J_{ij} the exchange interaction between them. The sum over j in Eq. (5) includes the z near neighbors in all generations except the Kth, in which case only one neighbor is involved. The free energy can be expressed in terms of the $\{m_i\}$ either by integrating Eq. (5) (which represents $\partial F/\partial m_i=0$) or by direct elimination of the $L_{\nu n}$ in (1). We obtain

$$\begin{aligned}F=k_BT&\sum_i\{[(1+m_i)/2]\ln[(1+m_i)/2]+[(1-m_i)/2]\ln[1-m_i)/2]\}\\&-k_BT\sum_{\langle ij\rangle}\left[m_i\tanh^{-1}\left(\frac{1-g_{ij}^2-r_{ij}}{2(m_i-g_{ij}m_j)}\right)+i\leftrightarrow j+\tfrac{1}{2}\ln\left(\frac{r_{ij}+1+g_{ij}^2-2g_{ij}m_im_j}{2(1-g_{ij}^2)}\right)\right]-\sum_i H_im_i \ .\end{aligned} \tag{6}$$

Equations (5) and (6) are exact on a Cayley tree. We may also apply them to a real lattice in which case they are equivalent to a Bethe approximation. As such they represent the analog of the Thouless, Anderson, and Palmer[2] equation for finite z. In particular, in the limit $z\rightarrow\infty$ the TAP results are recovered. It is important to note that unlike in the TAP theory, the ground-state solutions of (5) are not given by molecular-field theory.[10]

An exact expression for $\bar{F}$, the exchange averaged free energy as a function of the average distribution of fields $G_{ij}(h_{ij})$, is obtainable for a Cayley tree. We look for solutions to the self-consistent equation for $G_{ij}(h_{ij})$ of the form $G_{ij}(h_{ij})\equiv g(h_{ij})$ where h_{ij} is the effective field at site i due to its descendents from the jth branch down. This yields the following set of coupled equations:

$$g(h)=\int_{-\infty}^{\infty}dh'dJ\,g^{z-1}(h')P(J)\delta(h-\beta^{-1}\tanh^{-1}(\tanh\beta J\tanh\beta h')) \tag{7a}$$

and

$$g^m(h)=\int_{-\infty}^{\infty}\delta\left(h-H-\sum_{j=1}^m h_j\right)\prod_{j=1}^m[g(h_j)dh_j], \quad m=z \text{ or } z-1 \ . \tag{7b}$$

The free energy is given in terms of these effective fields as

$$\begin{aligned}\frac{B\bar{F}}{N}=(2b-1)\int_{-\infty}^{\infty}dh\ln(2\cosh\beta h)g^z(h)-\int_{-\infty}^{\infty}b\,dh_1dh_2dJ\,g^{z-1}(h_1)g^{z-1}(h_2)\\\times P(J)\ln[2\cosh(\beta h_1+\beta h_2)e^{\beta J}+2\cosh(\beta h_1-\beta h_2)e^{-\beta J}] \ ,\end{aligned} \tag{8}$$

where b is the number of bonds per site. For a Cayley tree ($b=1$) Eq. (8) is exact; for a regular lattice ($b=z/2$) this equation was previously derived[8] using the Bethe approximation. For a real lattice thermodynamic properties can be found by differentiating Eq. (8) with respect to the appropriate variable. In doing this it must be remembered that $g^z(h)$ and $g^{z-1}(h)$ depend implicitly on the external field and temperature. Use should also be made of the fact that $\bar{F}$ is stationary with respect to $g(h)$, subject to the constraint that $\int g(h)dh=1$. On the Cayley tree, it is essential that expressions for the thermodynamic variables be written in terms of the $G_{ij}(h_{ij})$ before making the ansatz that $G_{ij}(h_{ij})=g(h_{ij})$. The ansatz that $G_{ij}(h_{ij})$ is uniform implicitly imposes a temperature-dependent boundary condition; the surface spins are found to have a random external field distributed according to $g^{z-1}(h)$. The magnetization and Edwards-Anderson order parameter are given by

$$\begin{Bmatrix} q \\ m \end{Bmatrix} = \int_{-\infty}^{\infty} \begin{Bmatrix} \tanh^2\beta h \\ \tanh\beta h \end{Bmatrix} g^z(h)\,dh \quad . \tag{9}$$

The susceptibility is found to satisfy the Fischer relation: $\chi=\beta(1-q)$ for symmetric distribution functions $P(J)=P(-J)$. We find that $\bar{S}$ vanishes linearly with T in the form [for symmetric $P(J)$]:

$$\frac{\bar{S}}{k_B N} = (\pi^2/6)k_B T\left\{g^z(0) - 2b\int_{-\infty}^{\infty} dh\,[g^{z-1}(h)]^2 \int_{|h|}^{\infty} P(J)\right\} + O(T^2) \tag{10}$$

unless $P(J)$ is sufficiently singular to induce divergences in the field distribution functions.[11]

In Eq. (10) the terms in large parentheses are evaluated at $T=0$. Note that in contrast to Eqs. (7) for the magnetic properties, the entropy, energy, etc., depend on the value of b and hence assume different values on a Bethe or real lattice. That $\bar{S}$ vanishes at $T=0$ should be contrasted with the SK ($z\to\infty$) result in which interchanging the order of taking limits yields $\lim_{T\to 0}\lim_{z\to\infty}\bar{S}(T)=(-1/2\pi)Nk_B$. Thus at $z=\infty$ the entropy is discontinuous at $T=0$. This $z=\infty$ "disease" manifests itself at finite z as a negative slope in $\bar{S}$ leading to a negative specific heat for large enough z and for real lattices only. This can be seen from Eq. (10) by noting that $\bar{S}$ will eventually become negative if b is large enough.

Equations (7) can be solved numerically by integrating out the δ function in Eq. (7a) and by Fourier transforming the convolution in Eq. (7b). We found that we could obtain numerical solutions for $P(0)=0$ at all $\bar{T}=T\sqrt{z}$ and for $P(0)\neq 0$ only at $T=0$. We considered two models (i) $P(J)=3^{3/2} J^2\exp(-3/2J^2/\bar{J}^2)/(\sqrt{2\pi}\bar{J}^3)$ and (ii) $P(J)=\exp(-\frac{1}{2}J^2/\bar{J}^2)/(\sqrt{2\pi}\bar{J})$. In the former case the specific heat C_h (on a real lattice) first becomes negative for $z\geq 4$, while in the latter $z\geq 5$ leads to negative C_h. For model (i), a numerical plot of $\bar{S}$ vs T in a real lattice (i) (solid lines) and for a Cayley tree (dot-dashed lines) for various z is shown in Fig. 1. The dashed line shows $z=200$ for a real lattice; the SK value is indicated on the figure. Our analytical and numerical results show that $d\bar{S}/d\bar{T}$ approaches $-\infty$ as $z\to\infty$. Note that the (exact) solution for the Cayley tree yields a well-behaved entropy. Since $\bar{S}$ is non-negative (for sufficiently small z on a real lattice) and Eqs. (7) can never admit a solution of the form $g^z(0)=0$, contrary to a suggestion in the literature,[7] a hole in $g^z(h)$ is not necessary in order for $\bar{S}$ to be positive.

We have found that the spin-glass phase on the Cayley tree has a lower free energy than that of the paramagnetic phase. This is not so for the real lattice. For the spin-glass phase in the limit $z\to\infty$, both the real lattice and the Cayley tree yield the SK ground-state energy. A complete study of all thermodynamic functions on a Cayley tree suggests that a well-behaved configuration-averaged theory can be obtained for this case. The reason that the configuration-averaged Bethe approximation leads to slightly unphysical results on a real lattice derives in part from a factorization assumption used in the derivation of Eqs. (7). Although this assumption is in the same spirit as the nonconfiguration-averaged

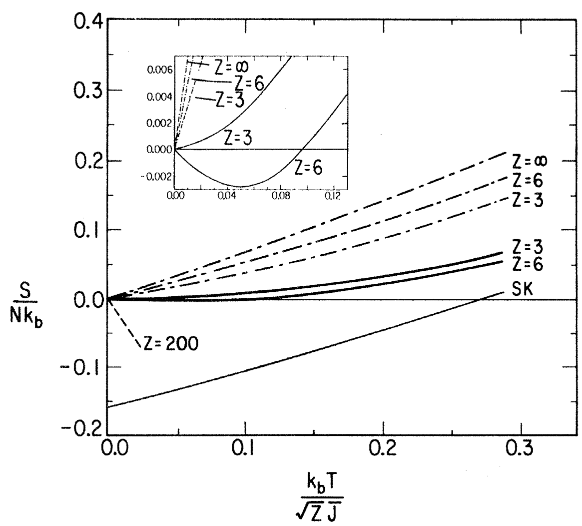

FIG. 1. Temperature dependence of the entropy S/Nk_B for the z values indicated for a Cayley tree (dot-dashed curves) and a real lattice (solid curves). The inset is an expanded scale plot of the very-low-temperature region.

Bethe approximation, it seems to violate the normalization conditions on the reduced density matrices. This problem does not occur in the Cayley tree, which is much less interconnected, so that the appropriate field distributions factor. In addition, limits on the validity[2] of the nonconfiguration-averaged theory on a real lattice will be discussed in a future publication.

ACKNOWLEDGMENTS

We acknowledge useful conversations with L. P. Kadanoff and G. F. Mazenko. This work was supported by the NSF DMR Grant No. 80-20609 and supported in part by the Materials Research Laboratory Program of the National Science Foundation at the University of Chicago under Grant No. 79-24007.

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