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Entropy of a random-bond Ising chain

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We study the one-dimensional Ising model in a magnetic field with each nearest neighbor J_i assigned at random. For $J_i = \pm J_0$ with equal probability, Nernst's law is violated, just as Kirkpatrick has found; however, when some uncertainty is introduced into the value of J_0 the entropy vanishes linearly with the temperature, much as in the mathematical two-level model for glasses of Anderson *et al.*

The low-temperature properties of spin-glasses are not very well known. Recently, there has been a fair amount of interest in the possible violation of the third law of thermodynamics[1,2] in these systems. Kirkpatrick[3] has recently found that a model in two and three dimensions with a Hamiltonian given by

$$H = -\sum_{(i,j)} J_{ij}\sigma_i\sigma_j \quad , \tag{1}$$

with $\sigma_i = \pm 1$ and J_{ij} being $\pm J_0$ randomly for nearest neighbors and zero otherwise, has a nonvanishing entropy in the $T \rightarrow 0$ limit. The question arises as to what happens if each J_{ij} is not restricted to be $\pm J_0$ exactly but is governed by a continuous probability distribution.

Here we present results on a model that is (a) simple enough so that a few exact results (in addition to numerical results) can be obtained, and (b) we believe it answers, at least partially, the question just posed.

The model we study is the one-dimensional random-bond Ising model[4,5] described by the Hamiltonian

$$H = -\sum_{i=1}^{N} J_i\sigma_i\sigma_{i+1} - H\sum_{i=1}^{N}\sigma_i \quad , \tag{2}$$

where the value of each J_i is fixed (quenched) independently and at random. Each J_i is set equal to $\pm J_0 \pm \delta J$ with equal probability and δJ is any number satisfying $|\delta J| \leq \frac{1}{2}\Delta J$, where ΔJ is a given quantity (i.e., the value of each J_i is independently assigned by a probability distribution which is given by two square hats centered about $+J_0$ and $-J_0$, each having a width ΔJ). Note that $\sum_{i=1}^{N} J_i = 0$ is only satisfied in the average. Previous results[5] on this model for $J = \pm J_0$ ($\Delta J \equiv 0$) show a low-temperature discontinuity of the magnetization (M) versus the applied field (H) which already suggested a violation of the third law of thermodynamics at the points of discontinuity.

We find that, if each $J_i = \pm J_0$ ($\Delta J \equiv 0$), then for a wide range of values of H, the entropy (S) does not vanish in the $T \rightarrow 0$ limit (and furthermore, S depends on H in that limit). This result is the one-dimensional version of Kirkpatrick's two- and three-dimensional results for $H = 0$. On the other hand, for $\Delta J \neq 0$ and $\Delta J << J_0$, then S takes the same values as for $\Delta J = 0$ if $kT \gtrsim \Delta J$, but $S = F(H)T$ for $kT << \Delta J$.

First we calculate the partition function Z using the transfer-matrix method.[6] Then

$$Z(\beta\{J\}_N, \beta H; N) = \mathrm{Tr}\prod_{i=1}^{N} T(J_i) \quad , \tag{3}$$

where

$$T(J_i) = \begin{pmatrix} e^{\beta(J_i+H)} & e^{-\beta J_i} \\ e^{-\beta J_i} & e^{\beta(J_i-H)} \end{pmatrix} \quad , \tag{4}$$

where $\beta = 1/kT$, k is the Boltzmann constant, and N the number of bonds in the chain.

Note that for $H = 0$ the partition function for the one-dimensional model under consideration is equal to the ordinary one-dimensional Ising-model partition function.[7] However, that is not the case for $H \neq 0$; the partition function has not been obtained analytically in this case.

We perform numerically the N-matrix multiplication shown in (4) to obtain Z for different values of H, β, and ΔJ for $N = 4000$. The entropy follows from $S = \partial(kT \ln Z)/\partial T$ (performed numerically). Figure 1 shows the entropy per spin, S/k, vs T/J_0 for $H = 2.0J_0$ and $H = 1.5J_0$ and various values of ΔJ ($\Delta J/J_0 = 0$, 0.1, and 0.3). Note that S fails to vanish in the $T \rightarrow 0$ limit only for $\Delta J = 0$, in agreement with Kirkpatrick's[4] results, but $S = f(H, \Delta J)T$ for $kT << \Delta J$ when $\Delta J \neq 0$.

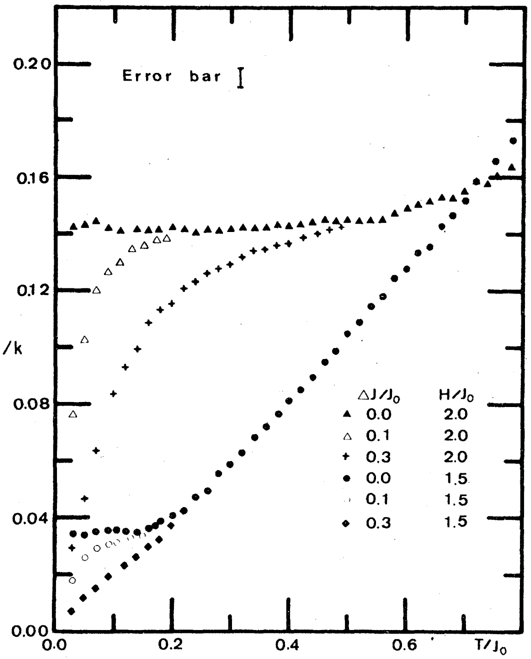

FIG. 1. Entropy per spin vs the temperature (in units of J_0) is shown for different values of ΔJ (the uncertainty in J), and of the external field (H) in units of J_0.

To get a simple picture for the mechanism behind this result, consider first the ground state for $J_0 < H < 2J_0$ and $\Delta J = 0$. A moment's reflection shows that any two adjacent spins in the chain connected by a ferromagnetic bond point up in the ground state (since $H > J_0$). The only possible ground-state degeneracy must, therefore, come from chainlets of two or more consecutive antiferromagnetic (A) bonds sandwiched in between ferromagnetic (F) bonds. Furthermore, it is easily seen that for chainlets with an even number of A bonds there is no degeneracy, since $H < 2J_0$ and the two end spins are up. On the other hand, for chainlets with an odd number (larger than one) of A bonds, one of these bonds must necessarily be broken (just as closed so called *frustrated*[8] chainlets in two or three dimensions); it is not too difficult to realize that the broken bond can only occur at $n+1$ places in an $(2n+1)$-A-bond chainlet. The number of chainlets with $2n+1$ A bonds in a chain with N bonds is $(\frac{1}{2})^{2n+3}N$ (N is the total number of bonds in the chain), and therefore

$$\frac{S}{k} = \sum_{n=1}^{\infty} (\tfrac{1}{2})^{2n+3} \ln(n+1) \ ,$$

which yields $S/k \cong 0.0340$, in agreement with the $T \to 0$ limit shown in Fig. 1 for $H = 1.5J_0$ and $\Delta J = 0$.

On the other hand, the situation is qualitatively different for $\Delta J \neq 0$. Again, consider the fairly representative case in which H is in the neighborhood of $1.5J_0$, but now with $0 < \Delta J << J_0$. In this case ($\Delta J \neq 0$) each of the $n+1$ different positions for the broken bond in chainlets with $2n+1$ A bonds corresponds to a different energy in general; thus, the degeneracy is lifted. For instance, a three-A-bond chainlet with exchange constants $-J_0 + \delta J_1$, $-J_0 + \delta J_2$, and $-J_0 + \delta J_3$ has two levels separated by the energy $2|\delta J_3 - \delta J_1|$. The average entropy of a system of m energy levels distributed randomly and uniformly in an energy interval $2\Delta J$ is

$$\bar{S}_m = \int_0^{2\Delta J} d\epsilon_m\, P(\epsilon_m) \int_0^{2\Delta J} d\epsilon_{m-1}\, P(\epsilon_{m-1}) \cdots \int_0^{2\Delta J} d\epsilon_1\, P(\epsilon_1) S_m(\epsilon_1, \epsilon_2, \ldots, \epsilon_m) \ ,$$

where

$$S_m(\epsilon_1, \epsilon_2, \ldots, \epsilon_m) = \frac{\partial}{\partial T}\left\{ kT \ln \sum_{i=1}^{m} e^{-\beta\epsilon_i} \right\} \ ,$$

and $P(\epsilon_i)$ is the probability distribution of the energy of the ith level. Equivalently,

$$\bar{S}_m = m! \int_0^{2\Delta J} d\epsilon_m\, P(\epsilon_m) \int_0^{\epsilon_m} d\epsilon_{m-1} P(\epsilon_{m-1}) \cdots \int_0^{\epsilon_2} d\epsilon_1\, S(\epsilon_1, \epsilon_2, \ldots, \epsilon_m) P(\epsilon_1) \ .$$

Now, for $kT << 2\Delta J/m$, only the two lowest levels contribute significantly; therefore,

$$\bar{S}_m = \frac{m}{2}\frac{kT}{\Delta J}\int_0^{\infty} dx [\ln(1+e^{-x}) + x(1+e^{x})^{-1}] \ ,$$

whence,

$$\bar{S}_m \simeq 0.82 mkT/\Delta J \quad \text{for } mkT << 2\Delta J \ . \qquad (5)$$

Since the number of chainlets with $2n+1$ A bonds is $N(1/2)^{2n+3}$ and each of them contributes with $n+1$ energy levels, the total mean entropy per spin is

$$\frac{S}{k} \cong 0.82 \frac{kT}{\Delta J} \sum_{n=1}^{\infty} (n+1)(\tfrac{1}{2})^{2n+3} \ ,$$

which yields

$$S/k \cong 0.0797 kT/\Delta J \ ,$$

in agreement with the low-temperature results shown in Fig. 1 for $kT << \Delta J$.

Figure 2 shows S/k vs H/J_0 for various temperatures and $\Delta J = 0$. Note that s depends on H in the $T \to 0$ limit, showing singular values at $H/J_0 = 2/m$ ($m = 1, 2, 3, \ldots$). For an insight into the origin of the peaks at $H/J_0 = 2/m$, consider the case of $H/J_0 = 2$; in contrast with the $J_0 < H < 2J_0$ case, where only chainlets with an odd number of A bonds have degeneracy in the ground state, the chainlets with an even number of A bonds do contribute for $H = 2J_0$. Consider, for instance, two A bonds sandwiched between two F bonds. Clearly, the spin in the middle can either be up or down with no change in energy.

More generally, to obtain the degeneracy (Ω_m) of a n-A-bond chainlet with the two end spins up (i.e., the spins at the positions zero and n are up), divide the states of the chainlet into two sets. In one set (set I), the spin at position 2 is up, while in the other set (set II), the spin at position 2 is down. Thus,

$$\Omega_n = \Omega_{n-2}(\mathrm{I})\,\Omega_2(\mathrm{I}) + \Omega_{n-2}(\mathrm{II})\,\Omega_2(\mathrm{II}) \ ,$$

where $\Omega_m(\mathrm{I})$ is the number of states of a chainlet of m A bonds with the two end spins up, and $\Omega_m(\mathrm{II})$ is the number of states of a chainlet of m A bonds with one end spin down and the other end spin up. Now, $\Omega_{n-2}(\mathrm{I}) = \Omega_{n-2}$ and $\Omega_2(\mathrm{I}) = \Omega_2$. Note now that if a spin is down, then its nearest neighbors are both up, in the ground state. Therefore,

$$\Omega_{n-2}(\mathrm{II}) = \Omega_{n-3}$$

and

$$\Omega_2(\mathrm{II}) = 1 \ .$$

Consequently,

$$\Omega_n = 2\Omega_{n-2} + \Omega_{n-3} \ ,$$

which, together with $\Omega_2 = 2$ and $\Omega_3 = 3$, can be used to generate the value of any Ω_n. Then the entropy per spin in the $T \to 0$ limit given by

$$\frac{S}{k} = \sum_{n=2}^{\infty} \left(\tfrac{1}{2}\right)^{n+2} \ln \Omega_n$$

yields $S/k = 0.143$, in agreement with the value shown in Figs. 1 and 2.

We thus conclude that Nernst's law is not fulfilled for $J_i = \pm J_0$ ($\Delta J = 0$), but if there is any uncertainty in J_0 ($\Delta J \neq 0$), then at very low temperatures, the system provides a concrete model of the Anderson *et al.*[9] mathematical two-level random model and, accordingly, s vanishes linearly with T, as exhibited in Fig. 1.

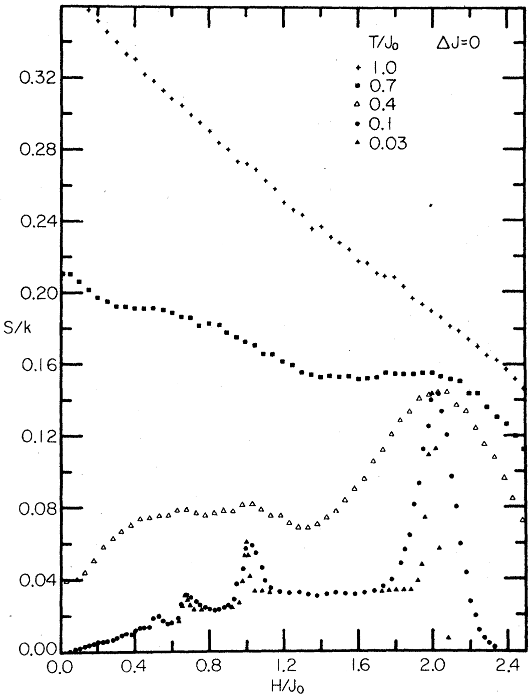

FIG. 2. Entropy per spin vs the applied field (H) in units of J_0 is shown for $\Delta J = 0$ and different values of the temperature (T) in units of J_0. Note that S depends nontrivially on H in the $T \to 0$ limit, against Nernst's law.

The error analysis we have performed follows closely the treatment of Ref. 5. There are two main sources of error: (a) the fact that calculation is performed for a finite chain, and (b) the fact that the results for a chain of N given J's are not averaged over an infinite set of chains with different distribution of J's. The resulting error is shown in Fig. 1.

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[7] For $H=0$, $T(J_i)$ commutes with $T(-J_i)$, and consequently, $Z=Z_n(-J)Z_{N-n}(J)$, where n is the number of J bonds, $Z_n(-J)$ is the partition function of n contiguous $-J$ bonds, etc.

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