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Random-bond Ising chain in a magnetic field at low temperatures

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The low-temperature behavior ($T \ll h, J$) of a random-bond Ising chain in a magnetic field is considered [$H = -(1/2)J\sum T_i\sigma_i\sigma_{i+1} - h\sum\sigma_i, \sigma_i = \pm 1$, $\{T_i\}$ is a fixed random sequence of numbers $+1$ and -1 with concentrations c_1 and $c_2 = 1 - c_1$, respectively]. The ground-state energy E_0, magnetization μ_0 and zero-point entropy S_0 are calculated exactly. It is shown that μ_0 and S_0 are discontinuous functions of magnetic field having jumps at $h = J/n$, $n = 1,2,\ldots$.

I. INTRODUCTION

Melting of heteropolymers is described by a one-dimensional two-component random Ising model.[1] Similar models are used for disordered linear magnetic systems and for ferromagnetic or antiferromagnetic linear systems in a random magnetic field. Also, it is hoped that such models will help us to understand more complicated problems with higher dimensionality. For these reasons random Ising chains have been a subject of interest over the last decade.[2-18]

A random Ising model does not allow an exact solution[19] (except for the special cases[2-4] when the magnetic field vanishes or when the chain breaks up into uncoupled segments). The problem can be reduced to an integral or functional equation which has to be solved numerically.[2,5-10] There are also several approximate analytic calculations[6,11-13] for the case h, $T \ll J$ [see Eqs. (1) and (2)]. In the present paper the low-temperature limit ($T \ll h, J$) is studied analytically.

The specific model to be considered is an Ising chain with random ferromagnetic and antiferromagnetic bonds (of equal strength) in a magnetic field. The Hamiltonian for this system is

$$H = -\tfrac{1}{2}J\sum_i T_i\sigma_i\sigma_{i+1} - h\sum_i \sigma_i\,, \tag{1}$$

where J, $h>0$, $\sigma_i = \pm 1$, $\{T_i\}$ is a fixed random sequence of numbers $+1$ and -1 with concentrations c_1 and $c_2 = 1 - c_1$, respectively. Let $\sigma_i = \tau_i$ be the ground state of the system at $h=0$, so that $T_i\tau_i\tau_{i+1} = +1$ for all i. Introducing new spin variables as $\sigma_i = \tau_i\sigma_i'$ we get

$$H = -\tfrac{1}{2}J\sum_i \sigma_i'\sigma_{i+1}' - h\sum_i \tau_i\sigma_i'\,. \tag{2}$$

This Hamiltonian represents a ferromagnet in a magnetic field statistically changing along the chain (a similar model is used for heteropolymer melting).

In the general case, the sequence $\{\tau_i\}$ is not random: there is a correlation between the neighboring links. Let w_{11} be the probability that $\tau_{i+1} = +1$ if $\tau_i = +1$, w_{21} the probability that $\tau_{i+1} = +1$ if $\tau_i = -1$, etc. Then it is easily understood that $w_{11} = w_{22} = c_1$ and $w_{12} = w_{21} = c_2$. (Note that the only case when the sequence $\{\tau_i\}$ is random is $c_1 = c_2 = 0.5$.)

Hamiltonians (1) and (2) are equivalent to each other. However, it proves more convenient to work with Eq. (2), and we shall use this form of the Hamiltonian in all calculations below.

The free energy (per link) for our system is given by

$$F = -L^{-1}\, T\ln Z\,, \tag{3}$$

where

$$Z = \sum_{\sigma_i=\pm 1} \exp\frac{1}{T}\left(\tfrac{1}{2}J\sum_i \sigma_i\sigma_{i+1} + h\sum_i \tau_i\sigma_i\right) \tag{4}$$

and L is the number of links in the chain. (In this paper we assume $L\to\infty$.) At low temperatures ($T \ll h, J$) we can write

$$F = E_0 - TS_0 + O(e^{-J/T}, e^{-h/T})\,, \tag{5}$$

since there is a finite gap of order h or J between the ground state and the first excited state (except for the case when $|J - nh| \lesssim T$ with $n = 1, 2, \ldots$). Here $E_0 = L^{-1}\min(H)$ is the ground-state energy and $S_0 = L^{-1}\ln D$ is the entropy at $T=0$, D is the degeneracy of the ground state. We shall calculate E_0 and S_0 exactly using the method developed in Refs. 12–15. The magnetization is then found from

$$\mu = -\left(\frac{\partial F}{\partial h}\right)_T\,. \tag{6}$$

We shall see that at $T=0$ the magnetization μ_0 is a discontinuous function of the magnetic field. (In agreement with Refs. 7 and 18, where numerical calculations have been used) $\mu_0(h)$ has jumps at $h = J/n$, where $n = 1, 2, \ldots$. The density of jumps becomes infinite as $h\to 0$. The zero-point entropy S_0 has jumps at the same values of h. This gives rise to a phenomenon similar to the magnetic cooling.

II. GENERAL FORMULAS

The ground state of the Hamiltonian (2) is a sequence of sections with $\sigma=+1$ and $\sigma=-1$. We shall call them u sections and d sections, respectively. By definition, u sections neighbor with d sections on both sides and vice versa. If we want to talk about parts of u and d sections, we shall call them u and d segments, respectively.

Let $i=\mu_j$ and $i=\nu_j$ be the beginning and the end of the jth u section. The necessary conditions for the points μ_j and ν_j are easily formulated[11,12] in terms of the functions

$$n(M)=\sum_{i=1}^{M}\tau_i \tag{7}$$

and

$$n(M,M')\equiv n(M)-n(M'). \tag{8}$$

If (μ,ν) is a u section, then (a) $n(\mu,\nu)\geq N$, where $N\equiv J/h$, (b) it has no segments with $n<-N$ inside it, and (c) $n(\mu)\leq n(M)\leq n(\nu)$ for $\mu<M<\nu$. If (μ,ν) is a d section, then (a′) $n(\mu,\nu)\leq -N$, (b′) it has no segments with $n>N$ inside it, and (c′) $n(\mu)\geq n(M)\geq n(\nu)$ for $\mu<M<\nu$. One can easily verify that any violation of these conditions increases the energy of the system.

The conditions (a)–(c′) are illustrated by Fig. 1 where n is plotted as function of M. (The origins for n and M can be chosen arbitrarily.) We have d segments to the left of μ_1 and to the right of ν_2 and a u segment (μ_2,ν_1). Segments (μ_1,μ_2) and (ν_1,ν_2) can be u segments or d segments as well. Thus, we have four possible choices of a u section: (μ_1,ν_1), (μ_1,ν_2), (μ_2,ν_1), and (μ_2,ν_2). This means that the ground state is degenerate.

According to the discussion in Sec. I,

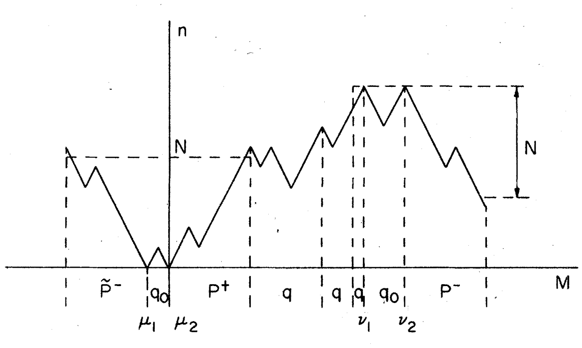

FIG. 1. Typical graph of the function $n(M)$ for a section of the chain. Division of this section into segments of types $\tilde{p}^-$, $\tilde{q}_0$, etc., is shown by dashed lines.

the graph of $n(M)$ can be thought of as representing a "Brownian motion" of a fictitious particle, n playing the role of coordinate and M the role of time. The particle makes a step in the same direction as its previous step with probability c_1 and in the opposite direction with probability c_2, $c_1+c_2=1$. The ground state energy E_0 and zero-point entropy S_0 can be expressed in terms of the probabilities of certain trajectories of such a particle.

Let us denote $p^+(p^-;\ \tilde{p}^-;\ q;\ q_0;\ \tilde{q}_0)$ the probability that the particle, starting from the point $n=0$ will for the first time get to the point $n>[N]$ $(n<-[N];\ n<-[N];\ n=1;\ n=0;\ n=0)$ without leaving the domain $1\leq n\leq[N]$ $(-1\geq n\geq -[N];\ -1\geq n\geq -[N];\ 0\geq n\geq -[N];\ -1\geq n\geq -[N];\ 1\leq n\leq [N])$, the last step before the particle starts being down (up; any; up; up; down). Here $[N]$ denotes the whole part of N and we assume that $N\neq[N]$. Note that our definitions of probabilities are different from those in Refs. 12–15. It is easily seen that

$$\tilde{q}_0=q_0,\quad p^+=p^-,\quad p^-+q_0=c_2, \tag{9}$$

$$q=c_1\sum_{K=0}^{\infty}q_0^K=c_1(1-q_0)^{-1},\quad \tilde{p}^-=(2c_2)^{-1}p^-. \tag{10}$$

Each u section has a segment of type $\tilde{p}^-$ on its left, then $\tilde{m}_0$ segments of type $\tilde{q}_0$, a segment of type p^+, then m segments of type q, m_0 segments of type q_0, and finally a segment of type p^- ($\tilde{m}_0$, m, and m_0 are arbitrary positive integers). The probability that an arbitrarily chosen link of the chain is the beginning of such section equals

$$P(\tilde{m}_0,m,m_0)=\tilde{p}^-p^-p^+\tilde{q}_0^{\tilde{m}_0}q^mq_0^{m_0}. \tag{11}$$

The energy difference between the u and d states of such section (including the surface energy) is

$$\Delta\mathcal{E}(m)=-2h(m+\delta N), \tag{12}$$

where

$$\delta N=[N]-N+1. \tag{13}$$

The ground-state energy can now be written

$$E_0=E_-+\sum_{\tilde{m}_0=0}^{\infty}\sum_{m=0}^{\infty}\sum_{m_0=0}^{\infty}P(\tilde{m}_0,m,m_0)\Delta\mathcal{E}(m), \tag{14}$$

where E_- is the energy (per link) of the chain with all spins down ($\sigma_i=-1$):

$$E_-=-\tfrac{1}{2}J+L^{-1}h\sum_i\tau_i=-\tfrac{1}{2}J. \tag{15}$$

In the last equation we made use of the fact that $\Sigma\tau_i=0$. Omitting the unimportant additive constant $-\frac{1}{2}J$ and using Eqs. (9) and (10) we get

$$E_0=-2h\tilde{p}^-(p^-)^2(1-q_0)^{-2}(1-q)^{-2}[q+(1-q)\delta N]. \tag{16}$$

Similarly, the entropy at $T=0$ can be expressed as

$$S_0=\sum_{\tilde{m}_0=0}^{\infty}\sum_{m=0}^{\infty}\sum_{m_0=0}^{\infty} P(\tilde{m}_0,m,m_0)\ln[(\tilde{m}_0+1)(m_0+1)]$$
$$=2\tilde{p}^-(p^-)^2(1-q)^{-1}(1-q_0)^{-1}\sum_{\kappa=0}^{\infty} q_0^{\kappa}\ln(\kappa+1). \quad (17)$$

Thus, the problem results in calculation of the probabilities $\tilde{p}^-, p^-$, q, and q_0.

III. CALCULATION OF PROBABILITIES

Calculation of the probability q results in the problem of Brownian motion of a particle between two absorbing boundaries: $n=1$ and $n=-[N]-1$. Corresponding equations are[15]

$$\begin{aligned}\phi^1_{M,n}&=c_1\phi^1_{M-1,n+1}+c_2\phi^2_{M-1,n+1},\\ \phi^2_{M,n}&=c_1\phi^2_{M-1,n-1}+c_2\phi^1_{M-1,n-1},\end{aligned} \quad (18)$$

with boundary conditions

$$\phi^1_{M,0}=0, \quad \phi^2_{M,-[N]}=0 \quad (19)$$

and initial conditions

$$\phi^1_{0,n}=0, \quad \phi^2_{0,n}=\delta_{0n}. \quad (20)$$

Here $\phi^1_{M,n}$ ($\phi^2_{M,n}$) is the probability that at "time" M the particle has "coordinate" n, its last step being down (up). q is given by

$$q=\sum_{M=1}^{\infty}\phi^2_{M,1}. \quad (21)$$

Introducing

$$\phi^{1,2}_n\equiv\sum_{M=1}^{\infty}\phi^{1,2}_{M,n}, \quad (22)$$

and summing Eqs. (18) and (19) over M from $M=1$ to infinity, we get a system of equations for $\phi^{1,2}_n$:

$$\phi^1_n=c_1\phi^1_{n+1}+c_2\phi^2_{n+1} \quad (-[N]-1\le n\le -2), \quad (23a)$$
$$\phi^2_n=c_1\phi^2_{n-1}+c_2\phi^1_{n-1} \quad (-[N]+1\le n\le 1), \quad (23b)$$
$$\phi^1_{-1}=c_1\phi^1_0+c_2\phi^2_0+c_2, \quad (23c)$$
$$\phi^1_n=0 \quad (n\ge 0), \quad (23d)$$
$$\phi^2_n=0 \quad (n\le -[N]). \quad (23e)$$

The general solution of Eqs. (23a) and (23b) is

$$\left.\begin{aligned}\phi^1_n&=A_1+Bn\\ \phi^2_n&=A_2+Bn\end{aligned}\right\} \quad (-[N]\le n\le -1), \quad (24)$$

where A_1, A_2, and B are constants and

$$c_2(A_1-A_2)=B. \quad (25)$$

From Eqs. (23c)–(23e) we find

$$\begin{aligned}&A_1=c_2/c_1, \quad A_2=B[N],\\ &B=c_2^2c_1^{-1}(1+c_2[N])^{-1},\end{aligned} \quad (26)$$

and

$$q=c_1(1+\phi_0^2)=(c_1+c_2[N])/(1+c_2[N]). \quad (27)$$

The probabilities q_0, p^-, and $\tilde{p}^-$ can be found from Eqs. (9) and (10):

$$\begin{aligned}&q_0=c_2^2[N]/(c_1+c_2[N]), \quad p^-=c_1c_2/(c_1+c_2[N]),\\ &\tilde{p}^-=c_1/2(c_1+c_2[N]).\end{aligned} \quad (28)$$

IV. RESULTS

Substituting Eqs. (27) and (28) in Eqs. (16) and (17) we get

$$E_0=\frac{c_1c_2J-c_1(1+2c_2[N])h}{(c_1+c_2[N])(1+c_2[N])} \quad (29)$$

and

$$S_0=\frac{c_1^2c_2}{(c_1+c_2[N])^2}\sum_{\kappa=0}^{\infty}q_0^{\kappa}\ln(\kappa+1), \quad (30)$$

where q_0 is given by Eq. (28) and $N=J/h$. Note that Eq. (30) becomes ambiguous when $h>J$ and $q_0=0$. However, from the derivation of Eq. (17) it is obvious that in this case $S_0=0$. Since S_0 vanishes at $h\to 0$ ($S_0\sim h^2$), it must have a maximum in the interval $0<h<J$.

It is easily verified that E_0 is a continuous function of h, while its derivative $\partial E_0/\partial h$ and the entropy S_0 have jumps at $h=J/n$ with $n=1,2,3,\ldots$.

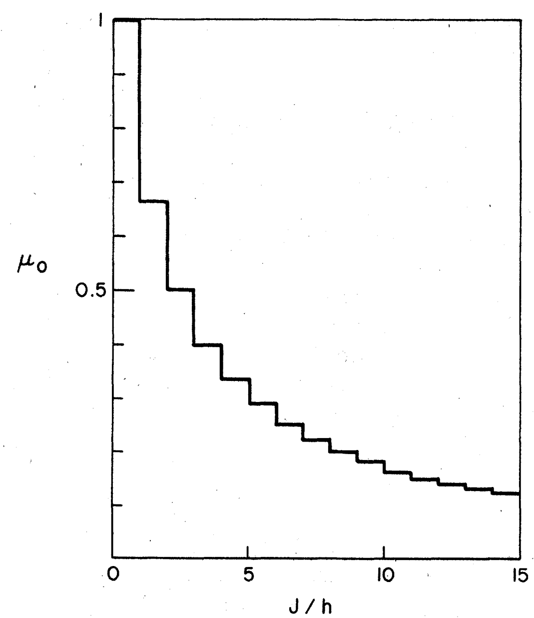

FIG. 2. Ground-state magnetization μ_0 as a function of the magnetic field h; $c_1=c_2=0.5$.

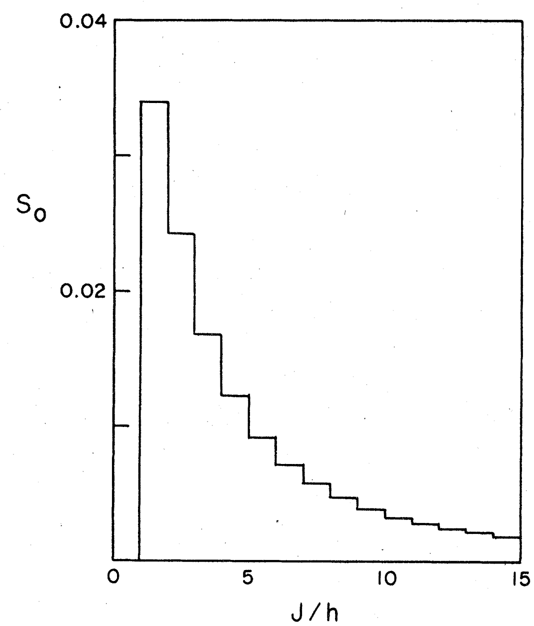

FIG. 3. Zero-point entropy S_0 as a function of the magnetic field h; $c_1=c_2=0.5$.

The density of jumps becomes infinite as $h\to 0$. For all values of h other than $h=J/n$, $\partial S_0/\partial h=0$ and Eq. (6) gives

$$\mu_0=-\frac{\partial E_0}{\partial h}=\frac{c_1(1+2c_2[N])}{(c_1+c_2[N])(1+c_2[N])}\,. \tag{31}$$

At small h, $\mu_0\approx 2c_1h/c_2J$. If $c_1=c_2=0.5$, Eq. (31) becomes particularly simple

$$\mu_0=2([N]+2)^{-1},\quad c_1=c_2=0.5\,. \tag{32}$$

This expression is in a quantitative agreement[20] with the numerical calculation of Ref. 18. The graphs of $\mu_0(h)$ and $S_0(h)$ are given in Figs. 2 and 3 for the case $c_1=c_2=0.5$.

Equations (30) and (31) are not valid in the vicinity of points $h=J/n$ where $|J-nh|\lesssim T$ and Eq. (5) is no longer a good approximation for F. At small but finite temperatures the vertical jumps of μ_0 and S_0 will be smoothed with a characteristic width $\delta h\sim T/n\sim Th/J$.

V. DISCUSSION

(i) The unusual behavior of magnetization and entropy shown in Figs. 2 and 3 allows a simple explanation. Formation of a u section requires energy $\Delta\epsilon=2(J-nh)$, where $n=\sum_{i=\mu}^{\nu}\tau_i$, $i=\mu$ and $i=\nu$ are the beginning and the end of the section. [Similarly, $\Delta\epsilon=2(J+nh)$ for a d section.] Obviously, n is an integer. New u sections appear in the ground state when $\Delta\epsilon=0$, i.e., $J-nh=0$. This means that the magnetization changes by leaps at $h=J/n$.

As it was shown in Sec. II, the boundaries of the u sections are not uniquely determined, i.e., the ground state is degenerate. If we start from $h=0$ when the ground state is unique and $S_0=0$ (strictly speaking, the ground state is doubly degenerate), and increase the magnetic field, new d and u sections appear, the degeneracy of the ground state increases and the entropy grows. However, it is easily understood from Fig. 1 that increase in h leads to a decrease in the degeneracy associated with already existing sections [segments of type q_0 split into u and d segments at $h=J/n$, where n is the maximal variation of $n(M)$ in the segment]. The first process dominates at small h and the second at $h\sim J$. At $h>J$ all the spins are aligned with the magnetic field, the ground state is nondegenerate and $S_0=0$.

(ii) A random-bond Ising chain studied in this paper exhibits a phenomenon similar to the magnetic cooling. Let $\tilde{S}(T)$ be the entropy associated with nonmagnetic degrees of freedom (which are absent in our model), e.g., vibrations. The total entropy is then given by $S=S(h)+\tilde{S}(T)$. [We assume that $T\ll h$, J, and the temperature dependence of $S(h)$ can be neglected.] If the system is thermally isolated and we change the magnetic field adiabatically, the total entropy must remain constant, and we get $\Delta\tilde{S}=-\Delta S$. If $\Delta S>0$, the temperature must decrease: $T_2<T_1$. A difficulty arises if the initial temperature is very low, so that $\tilde{S}(T_1)<\Delta S$. In this case one can speculate that to thermalize the system, we have to introduce some interactions (which can be very small) allowing transitions between various ground states. These interactions will remove the degeneracy, the characteristic splitting being of order Δ (the strength of the interaction). If T drops lower than Δ, Eq. (30) for the entropy is no longer correct and the paradox does not arise.

(iii) Equations (29) and (30) with $c_1=c_2=0.5$ hold for the case of a ferromagnetic chain in a random magnetic field described by Hamiltonian (2). Magnetization in this case is equal to zero. [Equation (32) does not hold since μ_0 is not equal to $-\partial E_0/\partial h$.]

(iv) It should be noted that a discontinuous dependence of μ_0 on h is not a specific property of the one-dimensional random system studied in this paper, but rather a general feature of disordered Ising systems with arbitrary dimensionality and with finite-range interactions. Above some critical value of h (corresponding to flipping of one spin in the most energetically unfavorable configuration) all the spins are aligned with the magnetic field. Below this value the magnetization changes by jumps corresponding to flipping of several spins. The density of jumps becomes infinite as $h \to 0$.

Note added in proof: Puma and Fernandez[21] have demonstrated that at $J/h = n$ with $n = 1, 2, \ldots$ the zero-point entropy has special values $S_0(n)$ which are greater than $S_0(n-0)$ and $S_0(n+0)$. For $J/h \neq n$, the numerical calculations of Puma and Fernandez agree with the results of the present paper. I am grateful to Dr. Fernandez for sending me his paper before publication and for his remarks which helped me to eliminate a numerical error in the paper.

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[19] In this paper we consider only the quenched situation when randomness is frozen in and does not change with temperature or magnetic field.

[20] Note that our J corresponds to $2J$ in notations of Ref. 18.

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