Properties of a random bond Ising chain in a magnetic field*†

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The Ising chain with random bonds in a magnetic field $\mathcal{H} = -\Sigma_i J_i \sigma_i \sigma_{i+1} - h\Sigma_i \sigma_i$, where $J_i = \pm 1$ at random, and $\Sigma_i J_i = 0$, represents a model of a magnetic glass, or of heteropolymer melting. Calculations of the thermodynamic properties of the chain as a function of field strength and temperature have been performed by Monte Carlo techniques. These results are compared with perturbation calculations for small and large values of h/T. The Monte Carlo results show, in agreement with the perturbation calculations, that the field-induced magnetization is generally smaller for the random bond model than for a chain of noninteracting spins. As $T \to 0$ the magnetization approaches the result for noninteracting spins.

I. INTRODUCTION

The Ising chain with random ferromagnetic and antiferromagnetic nearest-neighbor bonds (of equal strength) is equivalent to the simple one-dimensional Ising model, which is exactly soluble. In the presence of a magnetic field, however, the model cannot be solved in closed form. The Hamiltonian for this system is

$$\mathcal{H} = -\sum_i J_i \sigma_i \sigma_{i+1} - h \sum_i \sigma_i, \tag{1}$$

with $\sigma_i = \pm 1$, $J_i = \pm 1$ at random and $\sum_i J_i = 0$. The random nature of the bond is clearer if we define a new operator T_i, where $T_i = \pm 1$ at random, and $J_i = T_i J$. The Hamiltonian is then

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

In this form the chain represents a model for a one-dimensional magnetic glass. In addition, a simple transformation shows that this is also equivalent to the Hamiltonian for a ferromagnet in a random magnetic field

$$\mathcal{H} = -J \sum_i \sigma_i \sigma_{i+1} - h \sum_i T_i \sigma_i, \tag{3}$$

which has been shown to provide a model for heteropolymer melting.[1] We report here the results of calculations of the thermodynamic properties of a system governed by the Hamiltonian (2). There has been considerable theoretical work[2-6] on random systems similar to the one considered in this paper. The Monte Carlo calculations discussed here provide "experimental" results which can be compared with detailed theoretical calculations, and they should be useful in this context.

II. PERTURBATION CALCULATION

The partition function for this model with a given distribution of bonds is

$$Z(T_1, \ldots, T_N) = \sum_{(\sigma_i = \pm 1)} \exp\left(\beta \sum_i (T_i J \sigma_i \sigma_{i+1} + h\sigma_i)\right), \tag{4}$$

and the free energy for this distribution is

$$F(T_1, \ldots, T_N) = -\beta^{-1} \ln Z(T_1, \ldots, T_N).$$

The physical properties of the system are found by averaging the free energy over all possible configurations:

$$\{F\} = \sum_{(T_i = \pm 1)} P(T_1, \ldots, T_N) F(T_1, \ldots, T_N),$$

where $P(T_1, \ldots, T_N)$ is the probability of occurrence of the arrangement $T_1, \ldots, T_N$ of bonds. If the bonds occur completely at random,

$$P(T_1, \ldots, T_N) = [(N/2)!]^2/N!,$$

and

$$\{F\} = \sum_{(T_i = \pm 1)} F(T_1, \ldots, T_N) \frac{[(N/2)!]^2}{N!}. \tag{5}$$

The calculations reported in this paper are for this particular choice of P, but the Monte Carlo technique is easily adapted, if desired, to more complex choices of P.

It is possible to carry out straightforward perturbation-theoretic calculations of $\{F\}$ in the limits of small βh or small βJ. To do this we write $\mathcal{H} = \mathcal{H}_0 + V$, where we consider either

$$\mathcal{H}_0 = -J \sum_i T_i \sigma_i \sigma_{i+1}, \quad V = -h \sum_i \sigma_i; \tag{6a}$$

or

$$\mathcal{H}_0 = -h\sum_i \sigma_i, \quad V = -J\sum_i T_i\sigma_i\sigma_{i+1}. \tag{6b}$$

In either case, Eqs. (5) and (4) can be expanded to yield

$$\{F\} = \{F_0\} - \tfrac{1}{2}\beta\{\langle V^2\rangle\} - \tfrac{1}{24}\beta^3\{[\langle V^4\rangle - 3\langle V^2\rangle^2]\} + \cdots, \tag{7}$$

where

$$\langle A\rangle = \mathrm{Tr}(e^{-\beta\mathcal{H}_0}A)/\mathrm{Tr}\,e^{-\beta\mathcal{H}_0},$$

and

$$F_0 = -\beta^{-1}\ln \mathrm{Tr}\,e^{-\beta\mathcal{H}_0}.$$

The assumption of the specific form for $P(T_1,\ldots,T_N)$ mentioned above assures that averages of odd-order terms in V, e.g., $\{\langle V^3\rangle\}$, will vanish, so they have not been included in Eq. (7).

Evaluation of these averages is straightforward, and we find:

Case A: Low fields (including fourth-order terms in βh):

$$\left\{\frac{F}{N}\right\} = -\frac{1}{\beta}\ln[2\cosh(\beta J)] - \frac{\beta h^2}{2} + \frac{\beta^3 h^4}{12}[3\cosh^2(\beta J) - 2], \tag{8}$$

$$\{M\} = \beta h - \frac{\beta^3 h^3}{3}[3\cosh^2(\beta J) - 2], \tag{9}$$

$$\left\{\frac{U}{N}\right\} = -kJ\tanh(\beta J) - \beta h^2 + \frac{\beta^3 h^4}{3}[3\cosh^2(\beta J) - 2] + \beta^3 h^4\cosh^2(J/kT) - \frac{\beta^4 h^4}{2}J\cosh(\beta J)\sinh(\beta J). \tag{10}$$

Case B: high fields (including second-order terms in βJ)

$$\left\{\frac{F}{N}\right\} = -\frac{1}{\beta}\ln[2\cosh(\beta h)] - \frac{\beta J^2}{2}[1 - \tanh^4(\beta h)], \tag{11}$$

$$\{M\} = \tanh(\beta h) - 2(\beta J)^2\tanh^3(\beta h)\,\mathrm{sech}^2(\beta h), \tag{12}$$

$$\left\{\frac{U}{N}\right\} = -h\tanh(\beta h) + 2h(\beta J)^2\tanh^3(\beta h)\,\mathrm{sech}^2(\beta h). \tag{13}$$

III. MONTE CARLO CALCULATIONS

In order to study the intermediate region where neither type of interaction is much stronger than the other, we have carried out Monte Carlo calculations on a ring of 1000 spins with equal numbers of randomly arranged ferromagnetic (F) and antiferromagnetic (AF) bonds. The method used was an importance sampling technique similar to that used for the Ising square lattice except that the "reference" spin was chosen randomly. The details of the method have been reported elsewhere.[7] The effect of finite size on the properties of rings is quite small, since the correlation length does not diverge at any finite temperature. From earlier work on small rings[8] and from our preliminary Monte Carlo studies we find that even rings as small as 50–100 spins should have negligible finite size effects. In order to study the average behavior of all such rings with different "random" bond distributions one can either study many short rings with different distributions or one long ring which would include all such distributions along its length. We have chosen the latter method.

Both Monte Carlo calculations and perturbation expansion evaluations were made over a range of field and temperature with the coupling constant $J = 1$. Results from the two methods at low temperatures are significantly different, as shown in Fig. 1. This is not surprising since the perturba-

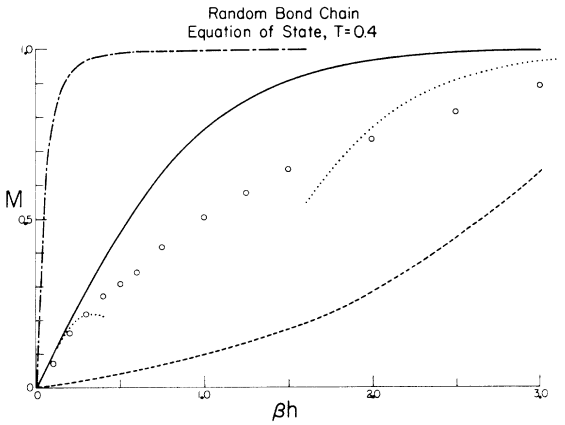

FIG. 1. Magnetization vs reduced field for $T = 0.4$ noninteracting case ————; ferromagnetic interactions ——— - ——— - ———; antiferromagnetic interactions -----; perturbation expansion for random bonds ···; Monte Carlo data for random bonds ○.

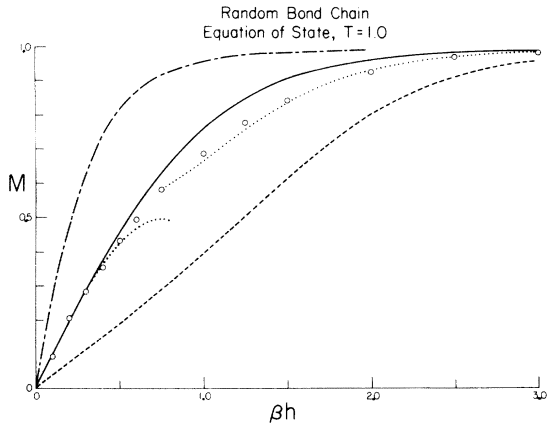

FIG. 2. Magnetization vs reduced field for $T=1.0$ noninteracting case ————; ferromagnetic interactions ——— - ——— - ———; antiferromagnetic interactions ------; perturbation expansion for random bonds •••; Monte Carlo data for random bonds ○.

tion method is really a high-temperature expansion. The Monte Carlo data show that the magnetization for the random bond chain lies clearly below the curve for the chain of noninteracting spins, and between the results for pure ferromagnetic and antiferromagnetic chains, which are shown for comparison. The same behavior is seen in the higher-temperature data shown in Figs. 2 and 3. In addition, as the temperature increases, the accuracy of the perturbation expansion improves, although for all temperatures in the intermediate region between low and high fields the results become unreliable. As the temperature increases the behavior of the magnetization approaches that of the noninteracting chain. This can be seen quite

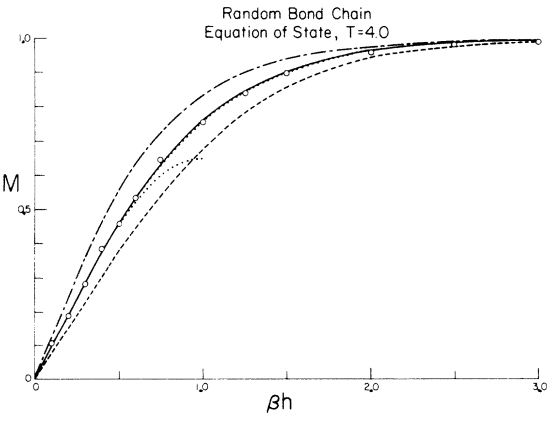

FIG. 3. Magnetization vs reduced field for $T=4.0$ noninteracting case ————; ferromagnetic interactions ——— - ——— - ———; antiferromagnetic interactions -----; perturbation expansion for random bonds •••; Monte Carlo data for random bonds ○.

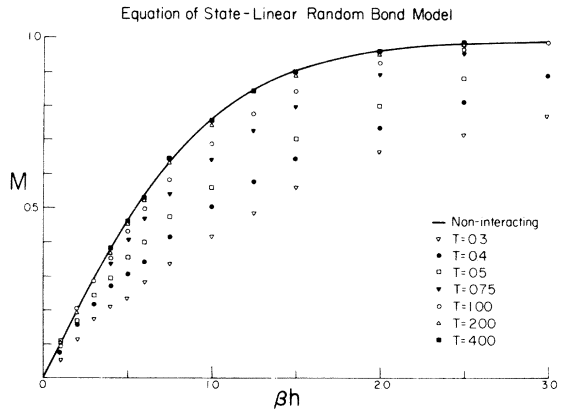

FIG. 4. Magnetization vs reduced field for the random-bond model at constant temperature.

clearly from the Monte Carlo data shown in Fig. 4.

The depression of the magnetization below that for the noninteracting case is easily understood in terms of the elementary excitations of the system. In a noninteracting Ising model in a field the elementary excitations are single-spin flips. All such single flips are equivalent and are split by $\Delta = 2h$ from the ground state. In the random bond model the elementary excitations are still single-spin flips but are no longer all equivalent. Those spins with two nearest-neighbor bonds will now require $\Delta = 2h + 4J$ to overturn whereas for those with two AF bonds $\Delta = 2h - 4J$, and for those with one F bond and one AF bond $\Delta = 2h$. Since the Boltzmann population is nonlinear in the temperature, those excitations involving a spin with two AF bonds will be more likely than those involving two F bonds so that the mean energy of the excitations will be lower than for the case of a noninteracting chain. In Fig. 5 we show the internal energy for $T=1.0$. The differences in the internal energy between the ran-

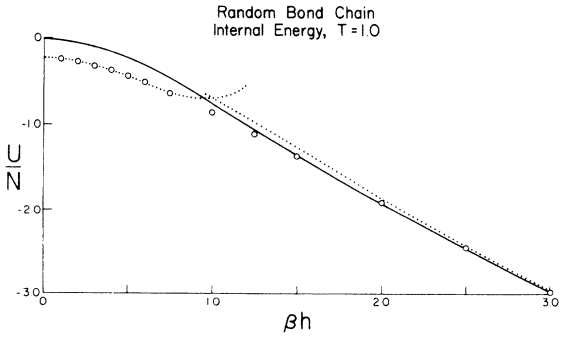

FIG. 5. Internal energy vs reduced field for $T=1.0$ noninteracting case ————; perturbation expansion for random bonds •••; Monte Carlo data for random bonds ○.

dom bond model and the noninteracting chain are pronounced for small fields, whereas the two are quite close at high fields. The Monte Carlo data presented here describe the thermodynamic behavior of a simple but unsolved model. Because the method can be extended to more complex Hamiltonians, it is well adapted to the quantitative study of the properties of other random systems which cannot be described by exact theories. Simple examples include models with more distant neighbor interactions, or variable g values.

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