

Remanence and non-exponential relaxation in an Ising chain with random bonds

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We study the time-dependent properties of an Ising chain with random bonds Gaussianly distributed. We obtain some exact as well as Monte Carlo (MC) results. Remanence, as well as a seemingly logarithmic long-time decay of the magnetization and of the energy towards their equilibrium values is observed at low temperatures by means of MC simulation. The remanent values of the magnetization ($\frac{1}{3}$, starting with all spins up) and of the energy are derived. A simple and explicit physical picture of the mechanism behind remanence and the logarithmic relaxation emerges. The equilibrium value of $q(t) = \langle \langle \sigma_i(0) \sigma_i(t) \rangle \rangle_J$ is obtained via the MC technique; it also seems to relax logarithmically for low temperatures. In contrast with the two- and three-dimensional cases, it is shown how any MC calculation can start immediately from an "equilibrium state" in this model, a very convenient feature for very-low-temperature MC computations. We show that if H is switched on at $t=0$, then $[\partial m(H,t)/\partial H]_{H=0} = (1/kT)[1 - q(t)]$ holds exactly in any number of dimensions, where m is the magnetization per spin. A time-dependent susceptibility $\chi(H,t)$ is defined and shown to vanish (as $H \rightarrow 0$) for low enough temperatures and finite t . The MC results for χ are in accord with this result and, if graphed versus T , show a hump at a time-dependent temperature. Finally, we compare the exact equilibrium specific heat, C , for this model with the results obtained by MC simulation of calorimetric measurements. Thus, a simple explicit case is exhibited of the difficulties which may arise in measurements of C in spin-glasses due to long-time effects.

I. INTRODUCTION

After a magnetic field applied to a spin-glass is switched off, a *remanent* magnetization, which decays non-exponentially (perhaps logarithmically) is always observed.¹ Monte Carlo (MC) studies^{2,3} of the spin-glass model proposed by Edwards and Anderson⁴ show similar behavior in two and three dimensions. Approximate solutions have recently been obtained.⁵

In order to obtain a clear picture of the mechanism behind remanence and its non-exponential relaxation, we study, in this paper, what we believe is the simplest possible model which exhibits such behavior: the nearest-neighbor Ising model in one dimension,

$$H = - \sum_{i=1}^N J_i \sigma_i \sigma_{i+1} - H \sum \sigma_i; \quad \sigma_i = \pm 1, \quad (1.1)$$

where each J_i is random, and distributed according to

$$P(J) \propto \exp[-\frac{1}{2} J^2 (\Delta J)^2].$$

As shown below, this model is simple enough so that some exact results are readily obtained (not only thermodynamic quantities for $H=0$, but some non-equilibrium quantities as well), and yet, in spite of its simplicity, MC computer experiments yield remanence and subsequent seemingly logarithmic in

time relaxation (for $kT \leq 0.5\Delta J$) which is typical of spin glasses. Due to the simplicity of the model, the mechanism behind such time-dependent effects becomes transparent.

In Sec. II we briefly derive the thermodynamic properties of the model for $H=0$. We then give the recipe for an "equilibrium state" which can be used as the initial state for MC calculations of equilibrium time-dependent correlation functions [such as $\langle \sigma_i(0) \sigma_i(t) \rangle$]. Lack of such a recipe makes such calculations unfeasible at low temperatures in two or three dimensions.

In Sec. III, we first discuss the magnetization and energy relaxations (starting with all spins up) as obtained from our MC computer experiments. We then derive the following results: in the zero-temperature limit, the magnetization decays to a remanent value of $\frac{1}{3}$ (it remains constant thereafter) and the energy decays to a remanent value of 86% of the ground-state energy. A very simple semiquantitative picture of the mechanism behind such time-dependent behavior emerges. From this picture, one can easily see why no logarithmic decay would be observed if each J were allowed to take only the discrete values $\pm J_0$. The absence of such logarithmic decay has already been observed by Kirkpatrick⁶ in two and three dimensions, and follows exactly in one dimension

from the work of Glauber.⁷

In Sec. IV we consider the *equilibrium* time-dependent autocorrelation function

$$q_T(t) = \langle \langle \sigma_i(0) \sigma_i(t) \rangle \rangle_J, \quad (1.2)$$

where the outer brackets denote average over all the allowed values of each J_j , and the inner brackets denote thermal average. The limiting value, $q_T(t \rightarrow \infty)$, is the spin-glass order parameter,⁴ which, of course, vanishes in one dimension.⁸

We define a time-dependent susceptibility $\chi(H, T, t)$ (H is switched on at $t=0$, and the magnetization is measured at time t), and show that

$$\chi(H=0, T, t) = \beta[1 - q_T(t)] \quad (1.3)$$

is *exactly* satisfied for any random bond Ising model as long as $P(J)$ is even in J (for any dimensionality).⁹ Monte Carlo results for $q_T(t)$ are given. They show a long-time, seemingly logarithmic, time decay for low enough temperatures ($kT \lesssim 0.5\Delta J$). Curves of $\chi(T, t)$ vs T are exhibited for a few values of t . These curves, which are not too different from the ones obtained by Bray *et al.*,³ exhibit humps, whose location depends on time. Indeed, whereas the equilibrium zero-field susceptibility (χ_0), defined by

$$\chi_0 \equiv \lim_{t \rightarrow \infty} \chi(H \rightarrow 0, T, t), \quad (1.4)$$

satisfies (see Sec. II)

$$\chi_0 = 1/kT, \quad (1.5)$$

the following contrasting result is shown to hold exactly

$$\lim_{t \rightarrow \infty} \lim_{T \rightarrow 0} \chi(H \rightarrow 0, T, t) = 0. \quad (1.6)$$

Equation (1.6) clearly shows that χ_0 as computed by the MC technique will vanish for low enough T , since t is of necessity finite. Our equilibrium results are in agreement with Eq. (1.6).

In Sec. V, we discuss how the slow-time relaxation of the energy at low temperatures may affect the interpretation of calorimetric measurements in spin-glasses. In particular, the experimentally observed specific heat seems to vanish at a finite temperature,¹⁰ which may appear to be consistent with a gap in the energy spectrum.¹¹ Instead, remanence of the energy is shown to produce such an effect.

Finally, in Sec. VI, we make some comments on the results obtained. In particular, we elaborate on the point that, although the model studied here has no frustration,¹² it exhibits the most prominent time-dependent features found in spin-glasses. The relevance of the distribution of J values to the effects observed is also discussed. We also discuss how frustration causes $\chi(H \rightarrow 0, T, t)$ not to satisfy Eq. (1.6) in more than one dimension.

II. EQUILIBRIUM

The thermodynamic quantities for zero external field are obtained in this section. We also point out that, in contrast to the *two-* or *three-* dimensional Ising models, it is possible to give a simple algorithm (in one dimension if $H=0$) to generate an "equilibrium state" of the system, which may be used as the initial state in MC calculations of equilibrium properties. Thus, we can compute (see Sec. IV) equilibrium quantities, such as $\langle \sigma_i(0) \sigma_i(t) \rangle$, at any temperature. In contrast, in MC calculations of spin-glass models in two or three dimensions, one must first wait for equilibrium to be reached, and it is far from clear that equilibrium is obtained within the time elapsed in the usual MC computer experiments.³

The thermodynamic functions of the model are easily derived for $H=0$. First note that any state of a chain of spins (with the two end spins free, say) can be specified *either* by giving the state of each spin, *or* alternatively by specifying one end spin plus the state of each bond. The partition function for one single bond of strength J_i is $e^{\beta J_i} + e^{-\beta J_i}$, and since the energy of the system is the sum of the bond energies, it follows that the partition function for a system of N bonds is given by

$$Z = 2 \prod_{i=1}^N 2 \cosh(\beta J_i), \quad (2.1)$$

where the 2 in front is due to the two states of one end spin which are necessary, in addition to the state of each bond, to specify completely the state of the system. It follows that, in the $N \rightarrow \infty$ limit, the free energy per spin (or bond) is given by

$$f = -kT \int dJ P(J) \ln[2 \cosh(\beta J)] \quad (2.2)$$

An alternative derivation of this expression can be given using the transfer matrix method,¹³ by noting that all the transfer matrices are diagonalized simultaneously if $H=0$. The entropy and energy expressions follow immediately.

To obtain the zero-field susceptibility χ_0 , note that

$$\chi_0 = \frac{\beta}{N} \sum_{ij} (\langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle), \quad (2.3)$$

and (see Sec. IV, or Ref. 9.),

$$N^{-1} \sum_i \langle \sigma_i \sigma_{i+n} \rangle = \delta_{n,0},$$

for $P(J) = P(-J)$, whence we have

$$\chi_0 = \beta, \quad (2.4)$$

since⁸ $\langle \sigma_i \rangle = 0$ in one dimension.

To obtain the algorithm to generate an "equilibrium state" (if $H=0$), first note that the state of each bond in the chain can be specified independently of

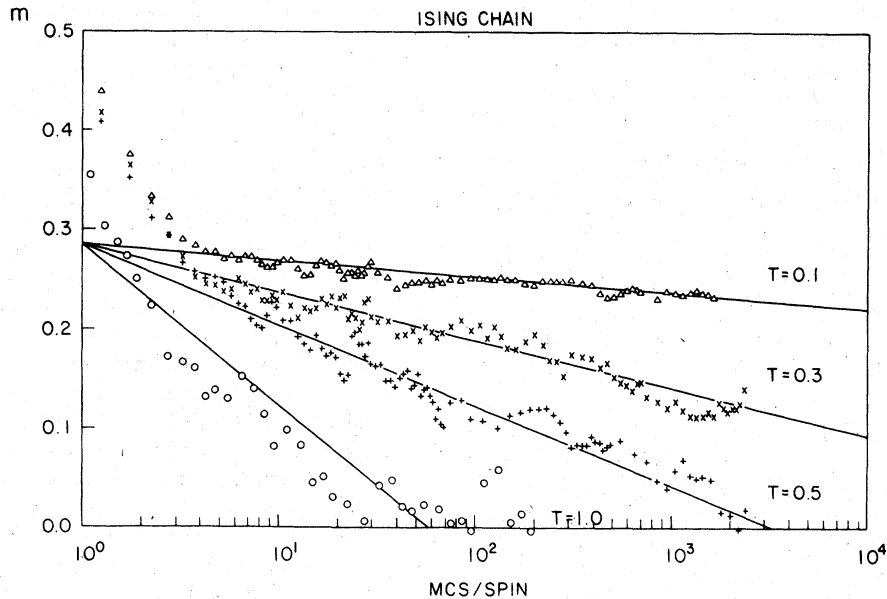


FIG. 1. Magnetization m vs the number of Monte Carlo steps (MCS) per spin is shown for different temperatures T expressed in units of ΔJ . All spins point up initially. The values shown are averages over the times elapsed between adjacent points shown. The straight lines come from Eq. (3.1).

the rest of the system, and the energy of the system is the sum of the bond energies if $H=0$; therefore, the probability that the i th bond be broken is given by

$$P_b = \exp(-|\beta J_i|) / [\exp(-\beta J_i) + \exp(\beta J_i)] \quad (2.5)$$

The probability P_f that it be fulfilled is, of course, given by $P_f = 1 - P_b$. What we call an "equilibrium state" is generated by first choosing a spin at the end of a chain to be up or down arbitrarily and each successive spin down the chain is set pointing up or down randomly with the probability just given. It is now clear why we call the state thus generated an "equilibrium state," for repetition of this process *ad infinitum* will generate a *canonical* distribution of the states of the chain.

III. REMANENCE

In this section we first discuss some results of relaxation towards equilibrium of an Ising chain of 1000 spins, as obtained by the application of the standard MC method² (a spin is first selected at random without bias; then it is flipped if the energy of the system is thereby lowered ($\Delta E < 0$), but if $\Delta E \geq 0$, then the spin is flipped only if a random number ($0 \leq R \leq 1$) generated without bias satisfies $R \leq \exp(-\beta \Delta E)$. The exact values of the remanent magnetization and energy are derived and compared with the MC results.

The evolution of the magnetization in time obtained in the MC computer experiment is exhibited

in Fig. 1. We start from an initial state with all spins up ($m=1$), with no external field present ($H=0$). At low temperatures ($kT \leq 0.5\Delta J$) two distinct regimes can clearly be observed in the curves: (a) an initial fast decay, from $m=1$ down to $m \approx 0.3$; (b) a slow decay towards the equilibrium value ($m=0$). The latter part is satisfactorily fitted by the logarithmic-decay equation,

$$m \approx 0.285 - 0.07(kT/\Delta J) \ln(t/\tau) \quad (3.1)$$

where τ is the time of a MC step per spin. The constants 0.285 and 0.07 are peculiar to our particular choice of 1000 values for the exchange constants in the Ising chain. As we will see below, the value 0.285 would go into $\frac{1}{3}$ for an *infinite* chain.

Figure 2 shows the relaxation of the *energy* towards equilibrium from an initial state with all spins up. Again, the curves show two distinct regimes at low temperatures ($kT \leq 0.5\Delta J$); after the rapid decay, the remanent value seems to relax logarithmically. The energy reaches its equilibrium value faster than the magnetization does.

Visual inspection of Figs. 1 and 2 shows that remanent values are only defined exactly in the $T \rightarrow 0$ limit. Accordingly, we shall now derive the values of the magnetization and energy after the initial fast relaxation (remanent values) for $kT \ll \Delta J$.

It is convenient to take the following approach: instead of considering the spins, look at the bonds. In Fig. 3, we have a histogram representing the *absolute* value of the coupling constants of a section of the

chain. There are three kinds of bonds: (a) tops; (b) steps, and (c) bottoms. Any bond which is broken will be marked with a dot. Each broken bond contributes to the energy by exactly twice its height. As time elapses, the dots move through the chain following the rules: (1) a dot can jump from a bond to the next; (2) if two dots meet in the same bond they annihilate each other; (3) pairs of dots may be created in adjacent bonds.

Now, one can easily understand why there is remanence in the system. Consider first the $T \rightarrow 0$ limit. The energy must decrease in every process, and consequently the dots (energy defects) can only descend to the bottoms where they arrive after only a few steps per spin. Thereafter, the dots are trapped and can move no further. Thus, the system gets into a metastable state and cannot reach true equilibrium (no dots). For small but finite temperature ($0 < kT \ll \Delta J$), the dots have a nonzero probability of escaping their traps, and consequently, a slow evolution towards equilibrium ensues after the first rapid decay.

We now obtain the value of the remanent energy. First note that the probability that a bottom bond be broken at the end of the rapid relaxation is $\frac{1}{2}$, as follows from the fact that the probability that a bottom bond be broken initially (i.e., the probability that it be antiferromagnetic, since all spins are up initially) is $\frac{1}{2}$. Thus, half the bonds sandwiched in between bonds of higher strength will remain broken thereafter in the $T \rightarrow 0$ limit. To see how much en-

ergy this configuration amounts to, note first that the probability density that a bond be of strength J , and that it be a bottom bond, is given by

$$P_{b0}(J) = P(J) \left[2 \int_{|J|}^{\infty} P(J') dJ' \right]^2, \quad (3.2)$$

Now, since the defect energy associated with a broken bond of strength J is $2|J|$, it follows that the mean *remanent defect energy* per bond is given by

$$\Delta E_0 = \frac{1}{2} \int_{-\infty}^{\infty} 2|J| P(J) \times \left[2 \int_{|J|}^{\infty} P(J') dJ' \right]^2 dJ. \quad (3.3)$$

Integrating by parts, it becomes

$$\Delta E_0 = \frac{8}{3} \int_0^{\infty} dJ \left(\int_J^{\infty} P(J') dJ' \right)^3, \quad (3.4)$$

which yields

$$\Delta E_0 \approx 0.112 \Delta J. \quad (3.5)$$

For comparison, note that the ground-state energy is

$$E_0 \approx -0.798 \Delta J, \quad (3.6)$$

as follows from Eq. (2.2).

To obtain the remanent magnetization in the $T \rightarrow 0$ limit (all dots must descend in this limit), consider first any spin which is *not* next to a top bond. To show that the probability that it will finish pointing down is $\frac{1}{2}$, note that: (a) it will do so if the number

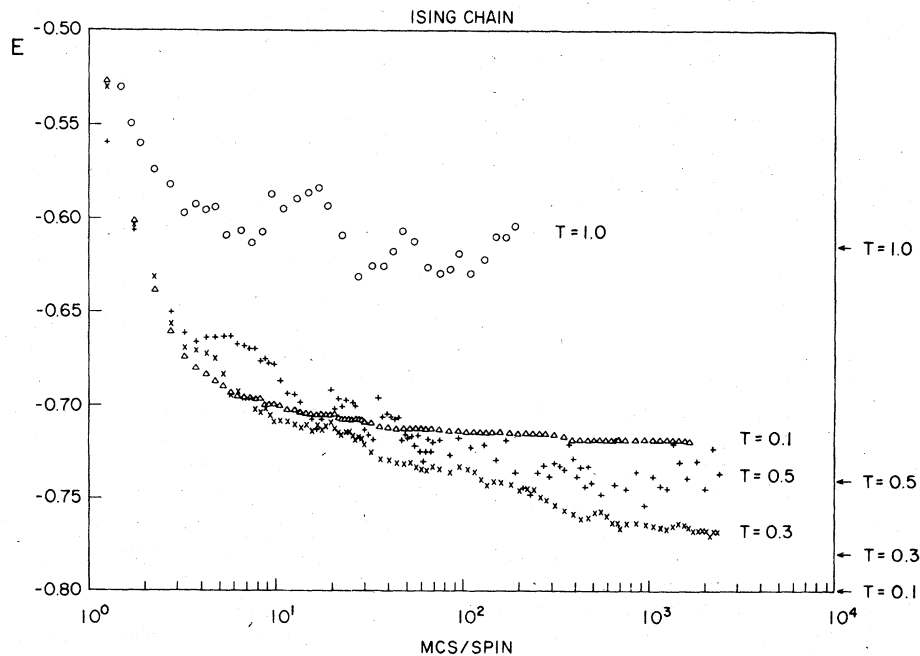


FIG. 2. Energy vs MCS per spin is shown for different temperatures T expressed in units of ΔJ . The arrows at the right indicate equilibrium values. The values shown are averages over the time elapsed between adjacent points shown.

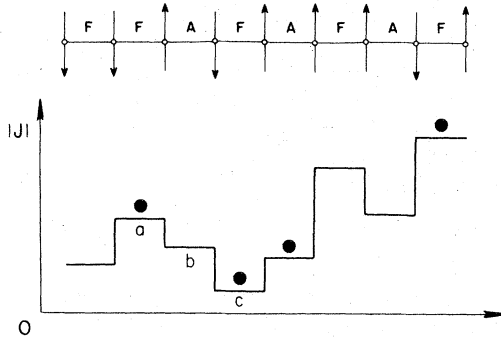


FIG. 3. Two alternative ways to describe a state of the Ising chain for $H=0$. The letters A and F indicate whether a bond is antiferromagnetic or ferromagnetic, respectively. Each broken bond is shown in the diagram below by a dot. The diagram below exhibits the strength of each bond, $|J|$. Bonds with an a , b , or c below them are called tops, steps, or bottoms, in the text.

of dots passing through it is odd; (b) all the dots passing through will come from the same side (where the higher strength bond lies); (c) that the probability that the higher strength bond next to it have a dot on it initially is $\frac{1}{2}$. A bit of reflection shows that the spins will finish pointing down with probability $\frac{1}{2}$.

We next consider all the other spins, i.e., all pairs of spins connected by top bonds. Note that if a top bond is initially broken, then one of the two spins will flip, for the dot on the bond will fall. On the other hand, all the pairs of spins joined by bonds which are initially fulfilled (all the ferromagnetic bonds) will stay up, since in the $T \rightarrow 0$ limit no dot can move up to a top bond. Therefore, the remanent magnetization m is equal to twice the fraction of ferromagnetic bonds which are tops. Now, the probability that a J bond be in between two bonds of lower strength is given by

$$\left(\int_{-|J|}^{|J|} P(J') dJ' \right)^2,$$

therefore,

$$\Delta m = 2 \left[\frac{1}{2} \int_{-\infty}^{\infty} P(J) dJ \left(\int_{-|J|}^{|J|} P(J') dJ' \right)^2 \right]$$

which becomes,

$$\Delta m = \frac{8}{3} \left(\int_0^{\infty} P(J) dJ \right)^3, \quad (3.7)$$

since $P(J) = P(-J)$. It follows that

$$\Delta m = \frac{1}{3},$$

which is the desired result.

The remanent magnetization and energy derived were checked by MC computations at $T=0$. The average values (over 13 different chains of 10^3 spins each) obtained are: $\Delta m = 0.33 \pm 0.01$ and $\Delta E_0/\Delta J$

$= 0.112 \pm 0.003$, in complete accord with our derived values.

A very rough argument showing why the remanent magnetization and energy decay close to logarithmically to their equilibrium value is given next. Clearly, there will be energy defects only at or near the bottoms of valleys after the initial rapid relaxation at low temperatures. As follows from the above derivation of remanent values, half of the valleys will then be occupied. The system must shed some of these energy defects to reach equilibrium. Different energy defects in the system must surmount *different* barrier heights to meet other energy defects and be annihilated in pairs. To estimate the relaxation of the magnetization, recall that the spins to be flipped are the pairs joined by ferromagnetic tops, and any such pair will flip when an energy defect climbs over the top. Consequently, the rate of change of the magnetization is proportional to the rate at which tops are being jumped over, therefore,

$$\frac{dm}{dt} \approx -\lambda m, \quad (3.8)$$

which using the solution becomes

$$\frac{dm}{dt} \approx -m_0 \lambda e^{-\lambda t} \quad (3.9)$$

for a barrier with a given jump over rate λ , where m_0 is the "initial" magnetization. By averaging over different barriers, Eq. (3.9) becomes,

$$\frac{d}{dt} \langle m \rangle_J \approx -\frac{1}{3} \int_0^{\infty} \lambda P(\lambda) e^{-\lambda t} d\lambda, \quad (3.10)$$

where $P(\lambda)$ is the probability density that the jump-over rate of a barrier be λ , and the factor $\frac{1}{3}$ is the mean "initial" value of $\langle m \rangle_J$, that is, its remanent value. To evaluate Eq. (3.10), note that,

$$\lambda \approx (1/\tau) \exp(-\beta \Delta E), \quad (3.11)$$

where ΔE is the activation energy (i.e., the energy necessary to climb the barrier), and τ is the order of the time of an MC step per spin. Substitution of Eq. (3.11) into

$$P(\lambda) \left| \frac{d\lambda}{d(\Delta E)} \right| = P(\Delta E) \quad (3.12)$$

yields

$$\beta \lambda P(\lambda) = P(\Delta E). \quad (3.13)$$

Crudely, $P(\Delta E)$ is about constant for $\Delta E \lesssim \Delta J$, therefore

$$\frac{d}{dt} \langle m \rangle_J \approx -\frac{kT}{3\Delta J} \int_{\lambda_1}^{1/\tau} e^{-t\lambda} d\lambda, \quad (3.14)$$

where

$$\lambda_1 = (1/\tau) e^{-\Delta J/kT}. \quad (3.15)$$

Now, for t such that $\exp(-t/\tau) \ll 1$ and $\exp(-\lambda_1 t) \approx 1$, that is, for

$$t/\tau \geq 1 \text{ and } \ln(t/\tau) \leq \Delta J/kT, \quad (3.16)$$

Eq. (3.14) becomes

$$\langle m \rangle_J \approx \frac{1}{3} - (kT/3\Delta J) \ln(t/\tau), \quad (3.17)$$

where the integrating constant was fixed using the calculated value ($\frac{1}{3}$) of the remanent magnetization [see Fig. 1, or Eq. (3.7)]. Equation (3.17) is not too different from Eq. (3.1), which is based on our MC results; there is a discrepancy of a factor of about 5 in front of the logarithm, which is not too surprising in view of our very crude derivation.

IV. SELF-CORRELATION FUNCTION AND TIME-DEPENDENT SUSCEPTIBILITY

The Edwards-Anderson⁴ order parameter is

$$q = \langle \langle \sigma_i \rangle^2 \rangle_J, \quad (4.1)$$

where the inner brackets indicate a thermal average and the outer ones indicate an average over the random exchange constants in H . It does not vanish only in the spin-glass phase. Note that

$$q = \lim_{t \rightarrow \infty} \langle \langle \sigma_i(0) \sigma_i(t) \rangle \rangle_J, \quad (4.2)$$

assuming that the system is mixing,¹⁴ i.e., that

$$\langle \sigma_i(0) \sigma_i(t) \rangle \xrightarrow{t \rightarrow \infty} \langle \sigma_i(0) \rangle \langle \sigma_i(\infty) \rangle. \quad (4.3)$$

To obtain Eq. (1.3), first note that

$$\langle \langle \sigma_i(0) \sigma_j(t) \rangle \rangle_J = 0 \text{ if } i \neq j, \quad (4.4)$$

and if $P(J) = P(-J)$, as follows from the following simple argument: let $\langle \sigma_j(t) \rangle_\phi$ be the mean value of σ_j at time t , provided the system was initially in state ϕ ; now, let $\sigma_i \rightarrow -\sigma_i$ in the initial state ϕ , and let $J_{ik} \rightarrow -J_{ik}$ for every k . Clearly, $\langle \sigma_j(t) \rangle_\phi$ is unchanged for any $i \neq j$, if $H = 0$, for an Ising or classical Heisenberg model as long as the time evolution of the system depends only on H (as it certainly does in MC simulations). That is,

$$\langle \sigma_i(0) \sigma_j(t) \rangle_\phi \rightarrow -\langle \sigma_i(0) \sigma_j(t) \rangle_\phi; \quad i \neq j \quad (4.5)$$

under the transformation $\sigma_i \rightarrow -\sigma_i$ and $J_{ik} \rightarrow -J_{ik}$ for every k . A bit of reflection shows that Eq. (4.4) follows if $P(J) = P(-J)$.

We now define $\chi(H, T, t)$. Let H be switched on at $t = 0$, and $M(H, T, t)$ be the magnetization at time t ; then

$$\chi(H, T, t) = \frac{\partial m(H, T, t)}{\partial H}. \quad (4.6)$$

The system is in thermal equilibrium at temperature T for $t < 0$, and it evolves in time for $t > 0$ according to the MC scheme. Note that our definition of χ is not the usual one; in our case $H = \text{constant}$ for $t > 0$, whereas usually $H \propto \delta(t)$.

To finally arrive at Eq. (1.3), we now use the linear-response theory equation,¹⁵

$$\chi(t) = \beta \sum_{ij} [\langle \sigma_i(0) \sigma_j(0) \rangle - \langle \sigma_i(0) \sigma_j(t) \rangle],$$

which becomes Eq. (1.3) after taking averages over all J 's and using Eq. (4.4).

With the connection between $q_T(t)$ and $\chi(H, T, t)$ provided by Eq. (1.3), in mind, we now examine the time evolution of $q_T(t)$. Our MC results are shown in Fig. 4 for a few temperatures. For low temperatures, $kT \leq \Delta J$, the curves show a seemingly logarithmic approach to its $t \rightarrow \infty$ asymptotic value. The curves for $q_T(t)$ do not show the initial rapid relaxation of the energy and magnetization (Figs. 1 and 2).

Figure 5 shows an MC run of the time evolution of the magnetization after a small field ($H = 0.15 \Delta J$) is applied. The continuous line represents the result of Eq. (1.3) using a smoothed $q_T(t)$ taken from Fig. 4.

The mechanism behind the logarithmic decay of the magnetization and of the energy, discussed in Sec. III, can also account qualitatively for the long-time behavior of $q_T(t)$. At equilibrium and low temperatures, the energy defects are mostly on bottom bonds (see Fig. 3), and the spins within any given valley will only lose memory of their initial position after an energy defect either leaves or comes into the valley over a barrier. The *distribution* of different barrier heights produces the close to logarithmic decay in time, as shown in Sec. III.

On the other hand, at higher temperatures one may assume that a spin loses memory of its initial direction after flipping once. In this case, one can consider each spin σ_i approximately independent of its neighbors. There are four different initial possibilities for the adjacent bonds; each one with its own transition rate W_α , that depends on the coupling constants J', J'' ($|J'| < |J''|$). These four possibilities are: (i) both bonds broken; then, $W_1 = \tau^{-1}$; (ii) no broken bonds; then $W_2 = \tau^{-1} \exp[-2\beta(|J'| + |J''|)]$; (iii) only J' broken, then $W_3 = \tau^{-1} \exp[-2\beta(|J''| - |J'|)]$; (iv) only J'' broken, then $W_4 = \tau^{-1}$. For each initial possibility, the relaxation of the spin is exponential $\sim \exp(-2W_\alpha t)$. By weighing each initial possibility α with its probability $P_\alpha(J', J'')$, calculated from Eq. (2.5), and by taking the average over the configuration of J one gets

$$q_T(t) = \sum_{\alpha} \langle P_{\alpha}(J', J'') e^{-2W_{\alpha} t} \rangle_J. \quad (4.7)$$

This formula was used to compute the solid lines shown in Fig. 4. For $kT \leq 0.5\Delta J$, the independent spin approximation fails.

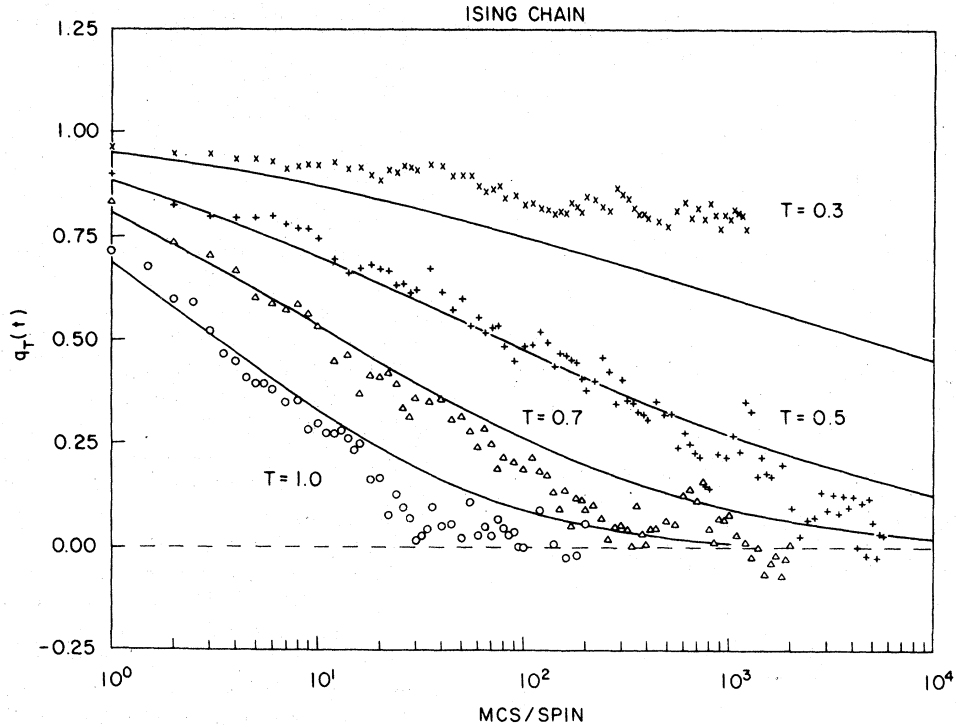


FIG. 4. Equilibrium value of the time-dependent self-correlation function, $q_T(t) = N^{-1} \sum_i^N \sigma_i(0) \sigma_i(t)$, is shown for different temperatures. The temperature (T) is in units of ΔJ . The full lines follow from Eq. (4.7), valid for $kT \geq \Delta J$.

For low temperatures, our MC results show that the time it takes $q_T(t)$ to reach its zero asymptotic value is of the order of $\exp(2\beta\Delta J)^2$. Therefore, from Eq. (1.3) it follows that the susceptibility $\chi(H=0, T, t)$, obtained by the MC procedure, with a fixed running time t , must decrease (for $kT \ll \Delta J$) as T decreases. Figure 6 shows $\chi(0, T, t)$ vs T for some fixed values of t [as obtained from Eq. (1.3), having computed $q_T(t)$]. According to Bray *et al.*,³ the susceptibility peak seen in two or three dimensions is also a non-equilibrium effect, as it clearly is in this one-dimensional model.

We will now show that for any finite running time the zero-field susceptibility must vanish as $T \rightarrow 0$ for the one-dimensional model studied here. More precisely, Eq. (1.6) will be derived.

Let some \bar{J} be such that

$$kT \ll \bar{J} \ll \Delta J, \quad (4.8)$$

which can only be defined for very low temperatures. Now, any spin which is going to flip within a time

$$t \equiv \tau \exp(2\bar{J}/kT), \quad (4.9)$$

must be in between coupling constants J_1 and J_2 such that

$$|J_1| + |J_2| \leq \bar{J}, \quad (4.10)$$

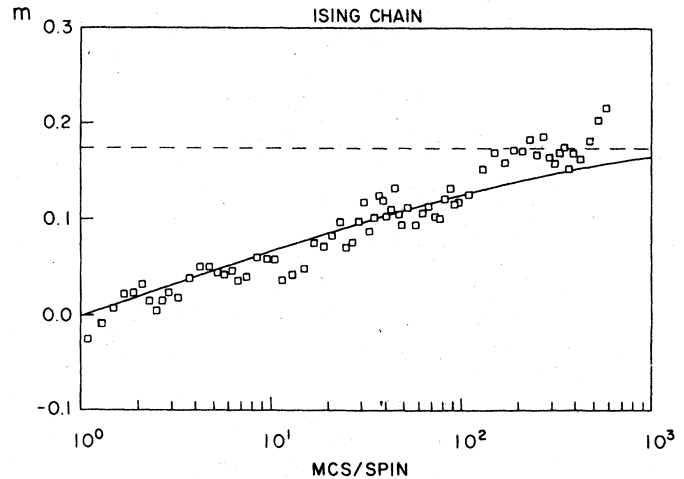


FIG. 5. It illustrates the validity of Eq. (1.3). The squares \square show evolution in time (MCS per spin) of the magnetization after a small field ($H=0.15$) is applied to the system which was previously in equilibrium at temperature $T=0.7$. Both T and H are in units of ΔJ . The full line is obtained by smoothing $q_T(t)$ as shown in Fig. 4 for $T=0.7$ and then using Eq. (1.3). The dotted line indicates the equilibrium value of m for $H=0.15$, computed by the transfer matrix method for our particular chain of 10^3 fixed exchange constants. The values shown are averages over the times elapsed between adjacent point shown.

if the system is in equilibrium. The fraction f of spins fulfilling this condition is given by

$$f \approx (1/\pi)(\bar{J}/\Delta J)^2, \quad (4.11)$$

since $\bar{J} \ll \Delta J$. But $2f \geq 1 - q(t)$, whence

$$1 - q(t) \leq (2/\pi)(\bar{J}/\Delta J)^2. \quad (4.12)$$

Equivalently, it follows from Eq. (4.9) that

$$1 - q(t) \leq \frac{1}{2\pi} \left(\frac{kT}{\Delta J} \right)^2 \left[\ln \left(\frac{t}{\tau} \right) \right]^2, \quad (4.13)$$

subject to the condition

$$1 \ll \ln(t/\tau) \ll \Delta J/kT, \quad (4.14)$$

as follows from condition (4.8). Clearly, Eqs. (4.13), (4.14), and (1.3) imply Eq. (1.6), which is the desired result.

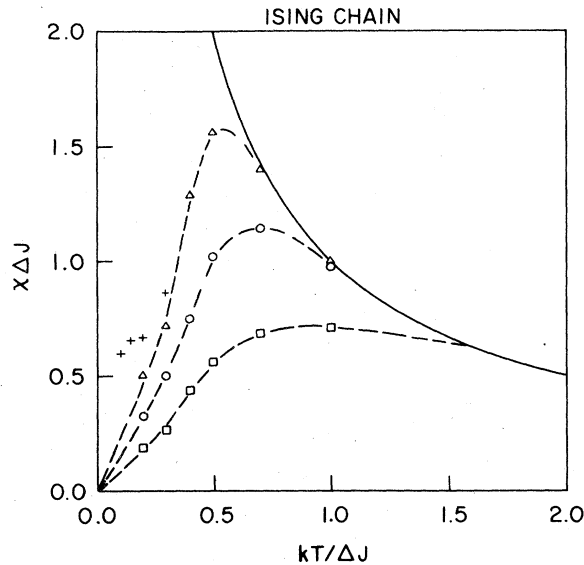


FIG. 6. Zero-field time-dependent susceptibility $\chi(H=0, T, t)$, defined in Sec. IV, is shown for the following running times: Δ for 10^3 MCS per spin; \circ for 10^2 MCS per spin; and \square for 10 MCS per spin. Equation (1.3) was used to obtain χ from the computer generated equilibrium values of $q_T(t)$. The points marked by crosses (+) were obtained similarly, except that the values used for $q_T(t)$ were not true equilibrium values, rather $q_T(t)$ was generated as follows: the system was allowed to "age" (evolve in time, starting from an initial state with all spins up) for 10^3 MCS per spin, and $q_T(t)$ was obtained subsequently, letting the system evolve for an additional 10^3 MCS per spin. The full line shows the equilibrium value of the susceptibility.

V. SPECIFIC HEAT AND THE RESIDUAL ENTROPY

The specific-heat measurements are also affected by the slow relaxation in our model. When the temperature is changed, the logarithmic relaxation of the energy makes the measured energy difference smaller than the equilibrium one, and consequently, a smaller specific heat results. Figure 7 shows the results of our MC calculations of the specific heat. For each temperature, an initial equilibrium state was used. The energy of that state was obtained by averaging over 800 MC steps; then the temperature was changed and the new energy was obtained by averaging over the next 800 MC steps. The specific-heat values so obtained are shown as bars in Fig. 7. For comparison, the solid line shows the equilibrium specific heat computed by the transfer matrix method,¹³ for the particular configuration of J 's used in the MC calculation.

The slow relaxation effect appears for $kT \ll 0.7\Delta J$. Note that the MC result vanishes for $kT \ll \Delta J$, whereas the equilibrium value is proportional to T for $kT \ll \Delta J$. A similar behavior appears in the two- and three-dimensional MC results.² Of course, the exact results for the specific heat are not known in these cases, and no comparison can be made.

The effects of the slow relaxation of the energy

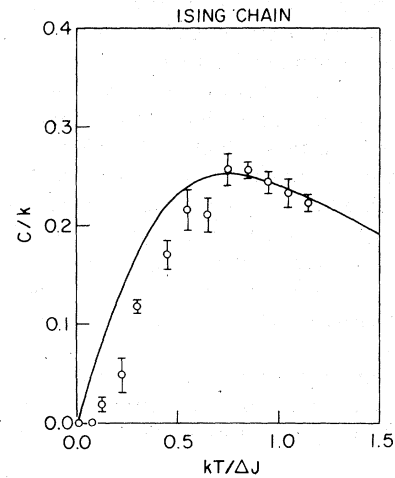


FIG. 7. Full line shows the equilibrium specific heat C . The points show values of C obtained by the following MC simulation: starting from an "equilibrium state," the energy is averaged over 800 MCS per spin, thus obtaining the equilibrium value $E_{eq}(T)$; then, without changing the state the system is in, the temperature is changed by ΔT , and the energy is averaged again over 800 MCS per spin, thus obtaining $\bar{E}(T + \Delta T)$, which is not an equilibrium value for low temperatures; finally, $C = [\bar{E}(T + \Delta T) - E_{eq}(T)]/\Delta T$. The values of C thus obtained are shown at $T + \frac{1}{2}\Delta T$.

have been observed experimentally. Nieuwenhuys and Mydosh¹⁶ showed that the heat flow in AuFe relaxes as t^{-1} ; thus the energy relaxes logarithmically. Furthermore, some specific-heat measurements show similar behavior to the MC results. For example, the extrapolation of the CuMn specific-heat data of Wenger and Keesom¹⁷ suggests that the measured specific heat would vanish for $T \leq 1$ K.

These long-time effects, on both calorimetric experiments and MC simulations, indicate that one should interpret any data so obtained with caution.¹⁸ For example, if one uses the specific heat of Fig. 7 and the high-temperature value of the entropy ($S_\infty = k \ln 2$) to calculate the entropy at $T=0$, one gets $S_0 \approx 0.2 S_\infty$, while the equilibrium value is in accord with Nernst's law, as follows from Eq. (2.2).

VI. COMMENTS

Note that:

(a) The system we treat has no frustration,¹² but shows remanence and subsequent logarithmic relaxation to equilibrium. Our analysis of Sec. III shows that the continuous distribution of J values, giving rise to a continuous distribution of barrier heights, is the fundamental ingredient leading to remanence and logarithmic relaxation. Thus, we can conjecture, for instance, that a Mattis¹⁹ model modified by letting the exchange constants take a continuous set of values, still an unfrustrated model, will exhibit remanence and logarithmic decay in any dimensions. On the other hand, a frustrated model with $J_{ij} = \pm J_0$ does not exhibit a logarithmic relaxation, as Kirkpatrick⁶ has found, although it shows remanence.

(b) We have shown that $\chi(H=0, T, t)$ vanishes as $T \rightarrow 0$ in one dimension. In contrast, MC work^{2,3} in two and three dimensions yields a nonvanishing χ in the $T \rightarrow 0$ limit, in agreement with experimental results.¹ As shown below, this difference is due to the fact that the systems in more than one dimension are frustrated (broken bonds are present even in the ground state).

To get the low-temperature behavior of $\chi(H=0, T, t)$, note that the argument leading from Eq. (4.8) to Eq. (4.14) must then be modified as fol-

lows: first, Eq. (4.10) becomes

$$0 \leq \sum_{i=1}^z |J_i| (-1)^{n_i} \leq \bar{J}, \quad (6.1)$$

where z is the coordination number $n_i = 0$ (-1) if the i th bond is fulfilled (broken). If $n_i = 0$ for all i , then

$$f \propto (\bar{J}/\Delta J)^z. \quad (6.2)$$

On the other hand, for a spin next to a number n of broken bonds, such that $1 \leq n < z$, it follows easily that

$$f \approx \text{const}(kT/\Delta J), \quad (6.3)$$

for $kT \ll \Delta J$, which leads to

$$1 - q(t) \leq \text{const}(kT/\Delta J) \ln(t/\tau), \quad (6.4)$$

again subject to condition (4.14). Spins with no broken bonds attached to them contribute with a higher power of T to Eq. (6.4), as follows from the relationship (6.2), and their contribution is therefore not included as it will vanish in the $T \rightarrow 0$ limit. Equations (6.4), (4.14), and (1.3) now yield

$$\lim_{T \rightarrow 0} \chi(H=0, T, t) \leq (\text{const}/\Delta J) \ln(t/\tau), \quad (6.5)$$

in agreement with the known results in two and three dimensions.

Note that the presence of broken bonds at $T=0$ is crucial to arrive at Eq. (6.5); indeed, $\chi \propto T^{z-1}$ if there were no broken bonds (as in the Mattis model), as follows from relationship (6.2). Broken bonds are present in more than one dimension because: (a) frustration, and (b) MC calculations do not quite simulate *equilibrium* (one would have to wait an infinite time in the $T \rightarrow 0$ limit for equilibrium to be reached). In our one-dimensional MC calculation, we know how to start right off from an equilibrium state, and hence we get a vanishing χ in the $T \rightarrow 0$ limit. On the other hand, when we started from a nonequilibrium state, we obtained a nonvanishing χ in the $T \rightarrow 0$ limit. This result is shown in Fig. 6 as crosses. The calculation of $q_T(t)$ [which yields χ , using (1.3)] started *after* allowing the system to decay for 10^3 MCS per spin (MCS, Monte Carlo steps) from an initial state with $m=1$.

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⁸It follows from Eqs. (1.3), (1.4), and (1.5) or by the usual arguments; see, for instance, G. Wannier, *Statistical Physics* (Wiley, New York, 1966), p. 337.

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