Dynamic properties of a spin-glass model at low temperatures

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We present a semiphenomenological calculation of the low-temperature dynamic properties of a spin-glass model which is a two-dimensional Ising model with Gaussian random nearest-neighbor interactions. The distribution of the low-lying energy levels of the system is studied with the aid of a numerical program. The results of this investigation suggest a simple picture of independent spins and small-size clusters of spins flipping in a frozen-random-background field. This picure is similar to the phenomenological description of amorphous materials in terms of two-level systems. Distributions of the quantities which characterize a low-lying energy state in this picture are obtained numerically. A crude analytic calculation of these distributions is also included. These distributions are then used to calculate various low-temperature dynamic properties such as the time-dependent susceptibility, relaxation of the magnetization in an external magnetic field, and the remanent magnetization. We find that this simple description provides qualitative explanations of a large number of results obtained in previous Monte Carlo simulations.

I. INTRODUCTION

A convenient definition of a spin glass is a system of spins each of which, in the absence of an external field, has a nonzero time average and such time average differs from spin to spin in a random way so that the sum of all spins becomes zero. At the infinite-time limit, it corresponds to the spin-glass phase defined by Edwards and Anderson.[1] The literature on this subject is vast.[2,3] However, a satisfactory theoretical understanding has been lacking. The existence or nonexistence of the spin-glass phase at the infinite-time limit has not been clarified. Recently, in addition to experiments, there have been extensive Monte Carlo simulations with spin-glass models[4–8] and many results are waiting for explanation. To provide a qualitative understanding of these results and other important features of the spin glass, we present a semiphenomenological study of a spin-glass model.

The model we study is an Ising model in two dimensions with randomly distributed nearest-neighbor interactions. We are concerned with dynamic (time-dependent) properties at very low temperatures. No attempt is made to understand properties near the transition temperature or the infinite-time limit. Our work includes a study of the low-energy spin configurations, in particular the energy minima, or the metastable states. These energy minima are probed with the aid of a computer program. The distribution of energy minima and the heights of barriers separating them are compiled. Approximate analytic calculations are also included to derive the qualitative features of these distributions. The results are then used as inputs to kinetic equations for calculating various properties. At low temperatures [$T \ll$ (typical interaction energy between a pair of spins)], only barrier heights and energy changes comparable to T are involved. We find that the dynamics is adequately described by the flipping of a small number of spins and spin clusters of small sizes. This picture is very similar to the two-level system picture in the phenomenological theory of glasses.[9,10]

We outline the paper and summarize the major results as follows: In Sec. II, we define our model as the Ising model with Gaussian-distributed random interations on a 20×20 square lattice. We describe the program which samples the energy minima and determines various characteristics of them, the energy barriers between them, as well as the distribution of local fields (i.e., effective field seen by a spin as provided by neighbors). These properties are those of the "energy surface" defined on the phase space. They are geometrical properties, from which dynamical properties can be calculated. An important result is that the energy minima separated by low barriers can be described as configurations which differ from each other by the reversal of a small number of small-size clusters (of two or three spins). Thus, these energy minima can be characterized by the distribution of small clusters. We have also performed similar analysis of a model with interactions whose magnitudes are Gaussian distributed, but having no "frustration."[11] We obtained qualitatively the same results. Thus an important conclusion is that frustration does not play an important role in determining the low-temperature, finite-time behavior of this model.

Section III provides a crude analytic study of low-temperature properties to gain a qualitative under-

standing. From the simple cluster picture borne out in Sec. II, we derive static and dynamic properties at low temperatures. The time variations of physical quantities are typically proportional to $t^{-\alpha T}$, where t is the time, T is the temperature, and α a constant depending on the physical quantity involved and on the initial state of the clusters. Geometrical quantities obtained by simple approximations fit the results of Sec. II reasonably well.

Section IV gives a more detailed analysis of a range of dynamic properties by solving the kinetic equations using direct data obtained in Sec. II. Results obtained are found to be in good qualitative agreement with those observed in previous Monte Carlo simulations.[5,6,8]

A few concluding remarks are made in Sec. V.

II. STATISTICS OF LOW-LYING ENERGY LEVELS

In our numerical study of the properties of the low-lying energy states of a spin galss, we considered the Edwards-Anderson model[1] with Ising spins on a 20×20 square lattice with periodic boundary condition. The Hamiltonian for this system is given by

$$H = -\sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j \ , \tag{2.1}$$

where $\langle ij \rangle$ represents a pair of nearest-neighbor lattice sites, σ_i's are Ising spins which take on the values ± 1, and each J_{ij} is an independent random variable with a Gaussian probability distribution

$$P(J_{ij}) = \frac{1}{(2\pi)^{1/2}J} e^{-J_{ij}^2/2J^2} \ . \tag{2.2}$$

We took J to be equal to one. The computer was used to generate several random configurations of the J_{ij}'s distributed according to Eq. (2.2). Since the sample size was rather small, special care had to be taken to ensure that the J_{ij}'s for a particular random configuration indeed satisfied the probability distribution given by Eq. (2.2). For each random configuration of the J_{ij},'s we calculated $\langle J_{ij} \rangle$, $\langle J_{ij}^2 \rangle$, and $\langle J_{ij}^4 \rangle$. We also determined the number and the locations of the "frustrated" squares (a square is "frustrated" if the product of the four J_{ij}'s on its four sides is negative). For a bond distribution that is truly Gaussian, one should have $\langle J_{ij} \rangle = 0$, $\langle J_{ij}^2 \rangle = 1$, and $\langle J_{ij}^4 \rangle = 3$. Also, for such a distribution, half of the total number of squares should be frustrated, and the frustrated squares should be distributed randomly on the lattice. We used only those configurations for which all these properties were satisfied to a high degree of approximation.

A. Properties of the "ground states"

After having generated a random configuration of the J_{ij}'s the next step was to locate a "ground state" of the system for this particular configuration of the exchange constants. For a spin glass, the concept of a ground state is not quite well defined. Previous studies[4,7] indicate that a spin-glass system has a very large number of low-lying local ground states which are approximately degenerate in energy. Kirkpartrick[4] has estimated the ground-state degeneracy of an Ising spin glass with $J_{ij} = \pm J$ to be as high as 2^{CN} where N is the total number of spins and $C \sim 0.1$. For the model that we are considering here, one does not expect such a high degeneracy, essentially because of the fact that, for a Gaussian bond distribution, finite clusters which can be turned over with no energy cost at all form a set of measure zero. However, the degeneracy may still be quite substantial. Also, it is an impossible task to numerically locate a "global" ground state, because one would need prohibitively large amounts of computer time to prove that no better ground state exists. For these reasons, we did not attempt to locate a global energy minimum. Instead, we took a low-lying local minimum of the energy surface in phase space to be our working definition of a ground state. Such a state was located in the following way.

For a given random configuration of the bonds, we started with a random configuration of the spins. We then applied a deterministic descent procedure to reach a local minimum of the energy surface. In this procedure, the first step was to calculate the local exchange energy $h_i (= -\sigma_i \sum_{\langle j \rangle} J_{ij}\sigma_j$, where $\sum_{\langle j \rangle}$ means a sum over nearest neighbors) for each spin in the starting configuration. The spin with the highest positive h_i was then flipped, and the local energies were recalculated. This process was continued until the system reached a metastable configuration. (A configuration is, by definition, metastable if all the h_i's are negative, so that every single spin flip increases the energy of the system.) The first such metastable state obtained from a random starting configuration was, in general, found to have rather high energy. We then "warmed up" the system slightly, in order to get it out of this metastable state. The warming up procedure that we used was a simple modification of the standard (Metropolis) Monte Carlo flipping routine. A Monte Carlo step (MCS) in our flipping routine consisted of choosing a spin at random, calculating the total energy E_{tot} of the state that would be obtained by flipping this spin, and flipping it if $E_{\text{tot}} < E_0 + \Delta E$, where E_0 is the total energy of the starting metastable state, and ΔE is an adjustable energy increment. This flipping routine generated a subset of all the states with total energy less than $E_0 + \Delta E$ and thus, corresponds to representing the system in the microcanonical ensemble. This pro-

cedure allowed us to probe directly the structure of the energy surface in phase space. We found that if we let the system evolve for a few MCS/spin with $\Delta E \sim 5$, and then applied the descent procedure, the system dropped into a different metastable state. This indicated that the system has a very large number of metastable configurations, and the single-spin-flip barriers separating one such configuration from a neighboring one are, in general, not very high. This process of warming up and the cooling down was repeated 25 times and the metastable state with the lowest energy obtained in this sequence was taken to be a ground state of the system. For a given configuration of the J_{ij}'s we located five different ground states by starting from five different random configurations. This procedure was repeated for ten different random configurations of the J_{ij}'s. All of the 50 ground states obtained in this way had energy per spin in the interval between -1.23 and -1.26. This is in good agreement with the Monte Carlo result of Stauffer and Binder,[7] who found the ground-state energy per spin for this system to be close to -1.25. We also found that two ground states obtained from two different initial random configurations are very nearly orthogonal to each other in the sense that they differ from each other by the reversal of $\sim\frac{1}{2}N$ spins. Similar results have been obtained by Stauffer and Binder.[7]

In Fig. 1, we show our result for $P_1(|h|)$, the distribution of local exchange energies averaged over the 50 ground states. Since all these states are metastable, $h_i = -|h_i|$ for all i. It is seen that $P_1(|h|)$ peaks at $|h| \simeq 2$, and approaches a nonzero value as $|h| \to 0$. These features are in qualitative agreement with the results obtained by Binder[6] from his Monte Carlo simulations at low temperatures. In the inset of Fig. 1, we have plotted $P_1(|h|)$ for very small $|h|$. It appears that $P_1(|h|)$ is roughly constant at a value of about 0.12 for $|h| \lesssim 0.3$. The distribution shown in Fig. 1 is quite different from the prediction of Klein's mean-random-field theory[12] according to which $P_1(|h|)$ should be a Gaussian centered at zero and with a width proportional to the Edwards-Anderson order parameter.[1]

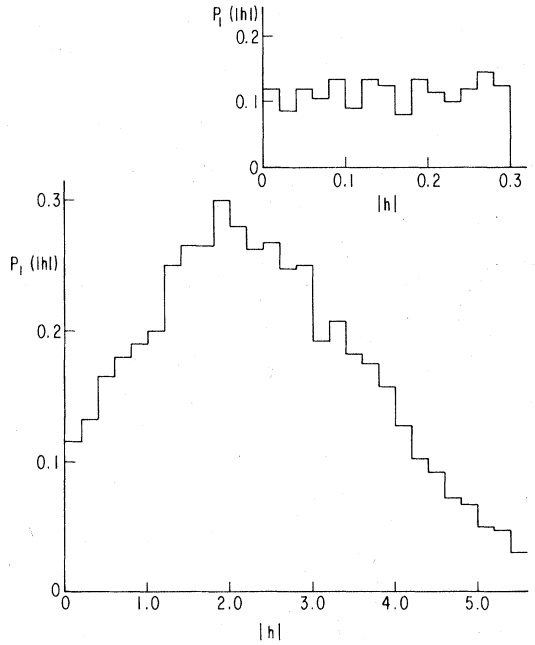

FIG. 1. Distribution of local exchange energies, $P_1(|h|)$, averaged over the 50 ground states. Upper inset: Distribution of $P_1(|h|)$ for small h.

B. Properties of the two-level clusters

After having located a ground state, we then proceeded to study the properties of the energy surface in its vicinity. We started with the system in a ground state, and then let it evolve in time according to the Monte Carlo flipping routine described above. As mentioned before, this procedure generated a subset of all states with total energy less than $E_0 + \Delta E$, where E_0 is the total energy of the ground state and ΔE is an appropriately chosen energy increment. At regular intervals along the time evolution of the system, we applied the descent procedure to search for new local minima. After each descent, time evolution was resumed from the configuration from which the descent was started. We repeated this procedure for several runs, using different random numbers for generating the sequence of attempted spin flips. The number of new local minima discovered in this way gave us an indication of the total number of local minima which are separated from the initial one by energy barriers with height less than ΔE. We started with $\Delta E = 2$ and increased ΔE in steps. For $\Delta E = 2$, a new local minimum was being discovered in about 20 attempts. All these new minima were found to differ from the initial one by flips of one or two small clusters of spins. As we increased ΔE, the number of new local minima encountered in a given number of attempts also increased in a roughly linear fashion until, for $\Delta E \sim 20$, a new local minimum was being found in almost every attempt. The typical phase-space separation between a new local minimum and the original one (measured by the number of spins which have to be turned over in order go to from one to the other) also increased with ΔE. A closer inspection of the distant local minima showed that most of these differed from the initial one by the reversal of several disconnected small clusters of spins. Most of these clusters were found to consist of two and three spins. We also kept track of the number of times a particular spin got flipped during the time evolution

of the system. For small values of ΔE, we found that the spins that got flipped formed small isolated groups. These groups grew larger as ΔE was increased, and finally, at $\Delta E \sim 20$, almost every spin in the sample was getting flipped. These observations suggest the following description for the low-lying energy states of our spin-glass system.

The energy surface of the system in phase space has a very large number of local minima (metastable states). A local minimum differs from its neighboring one typically by the reversal of a small (two or three-spin) cluster. The local minima are separated from one another by single-spin-flip activation barriers. The barrier separating two neighboring local minima is, in general, not very high, so that thermally activated transition from one of them to the other can take place. (Since our system is classical, we do not consider quantum-mechanical tunneling between the two metastable states.) However, if the temperature is very low and the observation time is not very long, the transition from a local minimum to another one that differs from the first one by the reversal of a large cluster is extremely unlikely. This is quite plausible because the reversal of a large cluster of spins will either require high energy, or have low entropy (because it would involve a coordinated motion of many spins), and, therefore, will be a very rare event, especially at low temperatures. Thus, the finite-time behavior of the system at low temperatures can be obtained from the properties of these small clusters which, by flipping, take the system from one metastable state to another.

Such a cluster corresponds to what is known in the literature as a two-level system (TLS). The reason for calling it a two-level system should be clear from Fig. 2 in which we have schematically shown a section of the energy surface along a generalized coordinate, x, that describes the flipping of the cluster. The two minima of Fig. 2 correspond to the two metastable states which are connected by the reversal of the cluster. These two states are separated from each other by a single-spin-flip energy barrier. The existence of such two-level systems in disordered materials was postulated by Anderson *et al.*[9] and by Phillips[10] some time ago. Theories based on this postulate have been quite successful in explaining many of the low-temperature properties of ordinary and metallic glasses. However, a precise microscopic understanding of the nature of these two-level systems in glasses is not yet available. By contrast, the two-level systems in our spin-glass model are quite precisely defined, and this makes a direct microscopic study of their properties possible. In general, the two states of a two-level system have different energies, ϵ_1 and ϵ_2. We characterize a two-level system by the energy difference $|\epsilon|(=|\epsilon_1-\epsilon_2|)$ between the two levels, and the barrier height, r, measured from the higher of the two levels. The barrier height, v, measured from the lower of the two levels is the sum of $|\epsilon|$ and r. We should mention here that this characterization is far from complete. For a more complete description, one has to take into account such things as the number of alternative paths which connect the two levels, the barrier heights associated with these paths, the phase-space separation between the two levels, etc. However, we will not go into these complications here. Both $|\epsilon|$ and r are random quantities whose distributions are expected to be correlated. Let $P_n(|\epsilon|,r)\Delta|\epsilon|\Delta r$ be the probability that a n-spin cluster is a two-level system with energy difference between $|\epsilon|$ and $|\epsilon|+\Delta|\epsilon|$, and barrier height between r and $r+\Delta r$. This joint probability distribution is related to the number, $N_n(|\epsilon|,r)\Delta|\epsilon|\Delta r$, of such two-level clusters in the following way:

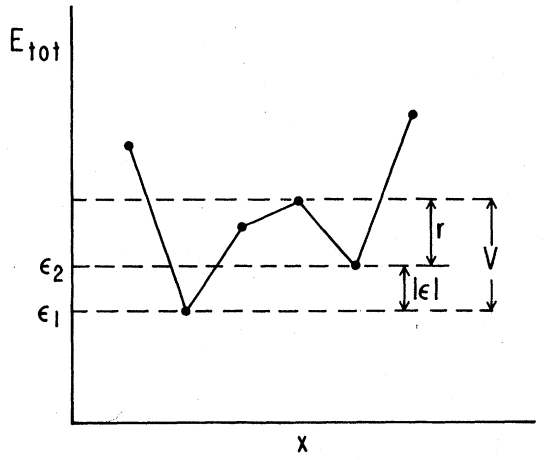

FIG. 2. Energy surface along a generalized coordinate x, that describes the flipping of a two-level cluster.

$$N_n(|\epsilon|,r) = C_n L^2 P_n(|\epsilon|,r) \ , \tag{2.3}$$

where L^2 is the total number of spins in the system, and C_n is the number per spin of distinct n-spin clusters. If these joint probability distributions, $P_n(|\epsilon|,r)$, are known, then the low-temperature properties of the system can be calculated from the two-level system picture.

We have numerically calculated the probability distributions, $P_n(|\epsilon|,r)$, for two- and three-spin two-level clusters. This is, to our knowledge, the first direct calculation of these distribution functions. We started with the system in one of its ground states. We then looked at every possible two- and three-spin cluster and checked whether the new state obtained by flipping the cluster was also a metastable state or not. If the new state was metastable, then the cluster corresponded to a two-level system. The energy difference between the two states gave $|\epsilon|$. In more

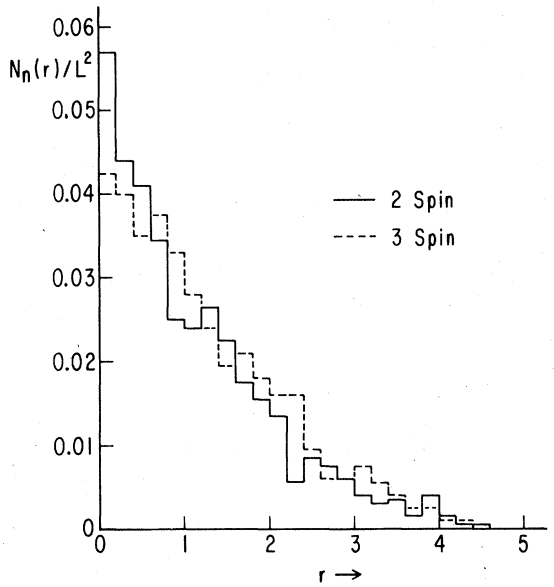

FIG. 3. Distributions of barrier height r, measured from the higher of the two levels, for two- and three-spin two-level clusters.

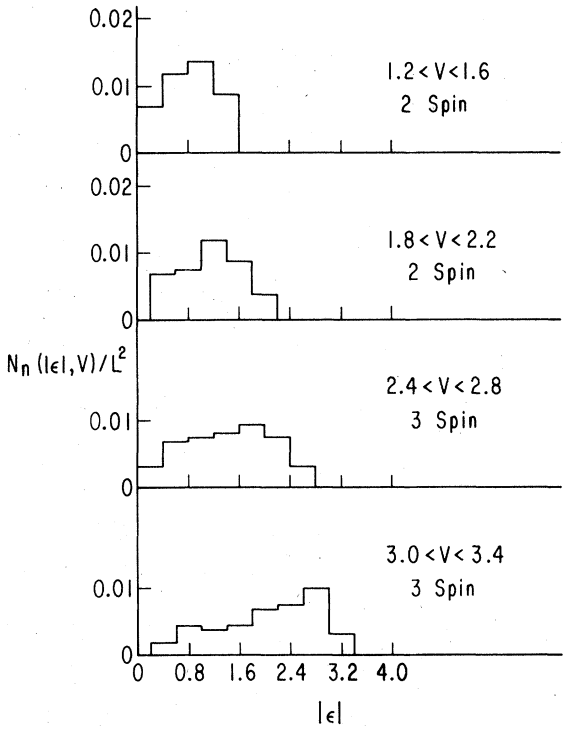

FIG. 5. Distributions of the energy difference $|\epsilon|$ for different values of the barrier height v.

than 95% of the cases, we found that the new state had higher energy than the original one. This confirmed that the local ground state was indeed a very low-lying energy state. In order to determine the barrier heights r and v, we generated all possible sequences in which the spins in the cluster could be flipped, and calculated the energies associated with these flips. We then took r and v to be the barrier heights for the sequence that corresponded to the lowest-energy path between the two metastable states. This procedure was carried out for all 50 ground states. The number of both two- and three-spin two-level systems was found to vary between 25 and 35 as we went from one ground state to another. We also looked at some four-spin two-level clusters.

For most of these clusters, we found that the lowest-energy path between the two levels passed through an intermediate metastable state which corresponded to a reversal of two of the four spins. This observation lends further support to our contention that it is sufficient to consider only two- and three-spin clusters if the observation time is not very long.

Our numerical results for the various distribution functions are shown in Figs. 3–6. Figure 3 shows the distributions of the barrier height r for two- and three-spin clusters. Here, $N_n(r)\Delta r$ represents the

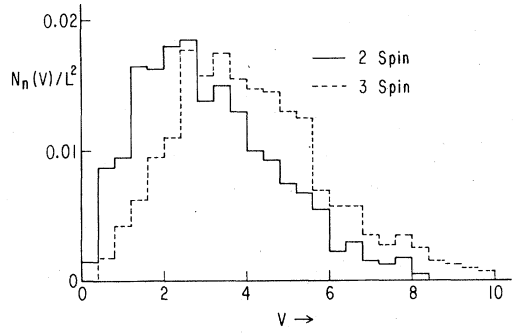

FIG. 4. Distributions of barrier height v, measured from the lower of the two levels, for two- and three-spin two-level clusters.

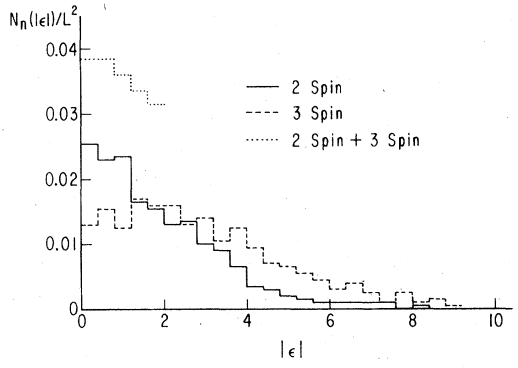

FIG. 6. Distributions of the energy difference $|\epsilon|$ for two- and three-spin clusters.

number of n-spin two-level clusters with barrier height between r and $r+\Delta r$. $N_n(r)$ is related to the joint number distribution, $N_n(|\epsilon|,r)$, defined above in the following way:

$$N_n(r)=\int_0^\infty N_n(|\epsilon|,r)\,d|\epsilon| \ . \tag{2.4}$$

For both $n=2$ and $n=3$, the distribution functions are peaked near $r=0$, and they fall off rather steeply as r is increased. The fall-off for $n=2$ is faster than that for $n=3$. In Fig. 4, we have shown the probability distributions of the barrier height v measured from the lower of the two levels. For both $n=2$ and $n=3$, $N_n(v)$ increases sharply as v is increased from zero, then reaches a plateau, and finally falls off for large v. The value of v at which the plateau of the distribution is reached is higher for $n=3$ than for $n=2$. The fact that the distributions for r and v are quite different indicates that the barrier height v and the energy difference $|\epsilon|$ are strongly correlated. It is obvious from the form of $N_n(r)$ that most of the two-level systems have $|\epsilon|$ rather close to v. This tendency can be clearly seen in Fig. 5 where we have shown the distributions of $|\epsilon|$ for different values of v. Figure 6 shows the distributions of the energy difference $|\epsilon|$ for $n=2$ and $n=3$. It can be seen that the sum of $N_2(|\epsilon|)$ and $N_3(|\epsilon|)$ is roughtly constant for small values of $|\epsilon|$. This confirms the hypothesis of Anderson *et al.*[9] that the distribution of $|\epsilon|$ is more-or-less flat for small $|\epsilon|$.

It is clear from Figs. 3, 4, and 6 that the three-spin clusters have, on the average, higher values of $|\epsilon|$, r, and v than the two-spin clusters. This indicates that both the barrier height and the energy difference increase with the cluster size. This trend is confirmed by our preliminary results for four-spin clusters. This observation provides us with further justification for considering only two- and three-spin clusters in our description of the low-temperature, finite-time behavior of the system.

In order to determine the extent to which frustration effects are important in determining the properties of the two-level systems, we carried out the above program for a model with no frustration. The Hamiltonian of this model has the same form as Eq. (2.1). However, the J_{ij}'s in this model are distributed according to

$$J_{ij}=|K_{ij}|\tau_i\tau_j \ , \tag{2.5}$$

where each K_{ij} is an independent random variable with a Gaussian distribution of the form given in Eq. (2.2), and the τ_i's are also independent random variables taking on the values ± 1. This model does not have any frustration because the product of the four J_{ij}'s around a square is always positive. The system has a unique ground state in which $\sigma_i=\tau_i$ for all i. The energy per spin of this ground state is $-4/(2\pi)^{1/2}\simeq -1.6$. Our numerical study showed that this sytem also has a very large number of metastable excited states. The low-lying metastable states obtained by using the procedure outlined above had their energies between -1.45 and -1.50. The properties of these metastable states were found to be quite similar to those in the frustrated system. In particular, we found that the distribution functions $P_1(|h|)$ and $P_n(|\epsilon|,r)$ are of the same general form as those obtained before. These results indicate that the low-temperature, finite-time behaviors of the two systems will be quite similar. In the infinite-time limit, however, the two systems may behave quite differently. The unfrustrated system has a unique ground state, and given enough time, it will find its way to this ground state. The geometrical properties of the energy surface in the vicinity of this ground state are expected to be quite different from those near a typical ground state of the frustrated system. However, this ground state will be extremely inaccessible because of the presence of a very large number of metastable excited states. For this reason, the finite-time behavior of the system will be determined by the properties of the metastable excited states. Since the relevant distribution functions for these metastable states are of the same general form in the two systems, we expect them to exhibit similar low-temperature properties if the observation time is not very long.

III. ANALYTIC STUDY

A. Dynamics at low temperatures

Based on the above results, a qualitative phenomenological calculation can be made for properties at very low temperatures. At $T=0$, there will be no thermal agitation, and the system will stay in a metastable state, i.e., one of the energy minima, for good. For nonzero but low temperatures ($T \ll 1$), there will be transitions to other states with excitation energy comparable to T. These transitions will involve climbing over barriers of heights comparable to T. The path representing the time evolution of the system will traverse a small region in phase space bounded by energy barriers much higher than T. Beyond these high barriers there can be energy minima lying lower than the minima in the region. Of course, if the period of observation is infinitely long, there would be a finite probability of climbing over barriers of any height, and the path would eventually find its way to the lowest-energy minimum to spend most of its time near there. This infinite-time limit is not of our concern here. The analysis below is restricted to finite times not long enough for climbing over barriers much higher than T.

This section is devoted to a simple analytic study, which will illustrate qualitatively the main results and estimate roughly numerical values of various quanti-

ties. A more detailed numerical calculation will be presented in Sec. IV.

For simplicity assume the following dynamics. A spin has a flip rate $1/\tau$ if the state after the flip has a lower energy, and $(1/\tau)e^{-\epsilon/T}$ if the flipped state has an energy higher by ϵ. We shall choose τ as the unit of time, i.e., $\tau=1$. For the moment, the distribution of the single-spin excitation energy $N_1(\epsilon)$, and that of barrier height and excitation energy of two-level clusters $N(\epsilon,r)$ defined above will be taken as known. They will be estimated later in this section.

Consider first the effect of single spin flips. Qualitatively, the number of spins involved at a low temperature T is of the order $TN_1(0)$ and the energy involved per spin is T. Thus the specific heat C is $\sim TN_1(0)/L^2$. More precisely,

$$C \approx \frac{1}{L^2}\frac{\partial}{\partial T}\int_0^\infty d\epsilon\, N_1(\epsilon) f(\epsilon)\epsilon \approx \frac{(\pi^2/6)N_1(0)\,T}{L^2} , \tag{3.1}$$

where

$$f(\epsilon)=\frac{1}{e^{\epsilon/T}+1} , \tag{3.2}$$

and L^2 is the total number of spins. The physical picture is a dilute gas of independently excited spins. It coincides with that of a free Fermi gas at low temperatures. $N_1(0)$ plays the role of the denisty of states. The magnetic susceptibility likewise assumes the form of a Pauli susceptibility

$$\chi=\frac{1}{L^2}\int_0^\infty d\epsilon\, N_1(\epsilon)2\frac{\partial}{\partial\epsilon}[1-2f(\epsilon)] \approx \frac{2N_1(0)}{L^2} . \tag{3.3}$$

The time required for reaching the equilibrium probability $f(\epsilon)$ for an excited spin is ~ 1.

Now consider the flip of a cluster of spins. The cluster is initially in state 1, which is one of the two energy minima of the cluster. The barrier separating state 1 and the second minimum 2 is r and the energy difference is $\epsilon_2-\epsilon_1=\epsilon$. One easily calculates the subsequent probability of finding the cluster in these states by solving the kinetic equation. The average value of any dynamic variable A over this probability is

$$A_1[1-f(\epsilon)]+A_2 f(\epsilon)+(A_1-A_2)f(\epsilon)e^{-\gamma t} , \tag{3.4}$$

$$\gamma=\tfrac{1}{2}e^{-r/T} . \tag{3.5}$$

Here A_1, A_2 are the values of A if the cluster is in state 1, and in state 2, respectively. From Eq. (3.4) we can obtain for example the change of total energy, $E_{\rm tot}$, in time: Set $A_1=0$, $A_2=\epsilon$, and sum over all clusters. One obtains

$$\Delta E_{\rm tot}(t)=\langle\Delta E_{\rm tot}\rangle+E'(0)\,t^{-\alpha_E T}/\alpha_E , \tag{3.6}$$

$$\langle\Delta E_{\rm tot}\rangle=\int_0^\infty dr\, E'(r) , \tag{3.7}$$

$$E'(r)=\int_{-\infty}^\infty d\epsilon\, N(\epsilon,r)f(\epsilon)\epsilon \approx \int_{-\infty}^0 d\epsilon\, N(\epsilon,r)\epsilon , \tag{3.8}$$

$$\alpha_E=-\left[\frac{dE'(r)}{dr}\Big/E'(r)\right]_{r=0} . \tag{3.9}$$

In Eq. (3.6), the time t is assumed to be much larger than 1 (e^{-t} dropped). Terms of $O(T)$ smaller are not kept. The power law $t^{-\alpha_E T}$ is not accurate beyond $T\ln t$, i.e., there are extra $T^2(\ln t)^2$ terms unless $E'(r)$ is strictly proportional to $e^{-\alpha_E r}$. Equations (3.6)–(3.9) show a very slow decay of energy via climbing over the barriers into lower minima. The quantity $\langle\Delta E_{\rm tot}\rangle$ in Eqs. (3.6) and (3.7) is the total energy (measured from the initial energy) when the clusters have reached equilibrium at temperature T. For very low T, it would be the energy when all clusters are in their lower states. $\langle\Delta E_{\rm tot}\rangle$ as well as α_E, depend crucially on $N(\epsilon,r)$, the initial distribution of cluster energies and barrier heights. If initially the clusters have an equilibrium distribution, then $\Delta E_{\rm tot}(t)$ would be simply zero. If initially the system is in a "ground state" prepared in the manner described in Sec. II, then there will be $\sim 5\%$ of the clusters in their higher states. The initial distribution can also be prepared by applying a magnetic field and then switching it off. The details of preparation will be elaborated further in Sec. IV.

Now let us consider an initial distribution with a finite total magnetization. Suppose that single-spin flips have brought the system to an energy minimum. We concentrate on the further decay of the total magnetization due to the flipping of clusters;

$$M_{\rm tot}(t)=\overline{M}_{\rm tot}+M'(0)\,t^{-\alpha_M T}/\alpha_M , \tag{3.10}$$

where

$$\overline{M}_{\rm tot}=\int_0^\infty dr\int_{-\infty}^\infty d\epsilon\,\langle m\rangle(\mathrm{sgn}\,\epsilon)N(\epsilon,r) ,$$
$$M'(r)=\int_{-\infty}^0 d\epsilon\, 2\langle m\rangle N(\epsilon,r) , \tag{3.11}$$
$$\alpha_M=-\left[\left(\frac{dM'}{dr}\right)\Big/M'(r)\right]_{r=0} .$$

Here $\langle m\rangle$ is the spin per cluster averaged over the $N(\epsilon,r)\,d\epsilon\,dr$ clusters. As just mentioned above, the distribution $N(\epsilon,r)$ depends on how the system was prepared. So, the form of the decay of the total magnetizaiton is determined by the history of the system.

The susceptibility defined as $\chi(t)=(1/L^2)\partial M_{\rm tot}(t)/\partial H$ can be deduced from Eqs.

(3.10) and (3.11). The application of a small field H changes $N(\epsilon,r)$ slightly, by

$$\left(\frac{\partial N}{\partial \epsilon}\frac{\partial \epsilon}{\partial H}+\frac{\partial N}{\partial r}\frac{\partial r}{\partial H}\right)H \ .$$

We find

$$\chi(t)=\bar{\chi}+\hat{\chi}t^{-\alpha_M T}+\bar{\chi}'(0)\,t^{-\alpha T}/\alpha \ , \tag{3.12}$$

$$\bar{\chi}=\frac{1}{L^2}\int_0^\infty dr\, 4\langle m^2\rangle N(0,r) \ , \tag{3.13}$$

$$\hat{\chi}=-\frac{1}{L^2}\int_{-\infty}^0 d\epsilon\, 2\langle m^2\rangle N(\epsilon,0) \ , \tag{3.14}$$

$$\bar{\chi}'(r)=-\frac{1}{L^2}2\langle m^2\rangle N(0,r) \ ,$$

$$\alpha=-\left(\frac{d\chi'(r)}{dr}\Big/\chi'(r)\right)_{r=0} \ . \tag{3.15}$$

Since $\hat{\chi}, \bar{\chi}' < 0$, the susceptibility $\chi(t)$ increases with time.

The exponent coefficients α_E, α_M, and α depend only on $N(\epsilon,r)$ for r very small, i.e., only clusters with barrier heights comparable to T contribute. However, if the time t is very large, larger r would play a part, and the power law would be modified.

B. Approximate calculation of distributions

The distributions of spin excitation energies and cluster barrier heights studied above can be calculated directly from the model definitions. A quantitative calculation would be rather involved. We shall only make an estimate of various distributions based on simple arguments and crude approximations.

First, we estimate the energy of metastable states. The energy for a spin configuration $\{\sigma\}$ is

$$H[\sigma]=-\sum_{\langle ij\rangle}J'_{ij} \ ,$$

$$J'_{ij}\equiv\sigma_i\sigma_j J_{ij} \ . \tag{3.16}$$

For $\{\sigma\}$ to be an energy minimum, or a metastable state, it must satisfy

$$\epsilon_i\equiv 2\sum_j J'_{ij}>0 \tag{3.17}$$

for every site. This makes the calculation difficult. Let us simplify it by considering only the seven bonds joined to two nearest-neighbor spins as shown in Fig. 7 and calculate the probability distribution $P(J')$ for the bond in the middle. The two sites must satisfy Eq. (3.17), i.e.,

$$J'+J'_1+J'_2+J'_3>0 \ ,$$
$$J'+J'_4+J'_5+J'_6>0 \ . \tag{3.18}$$

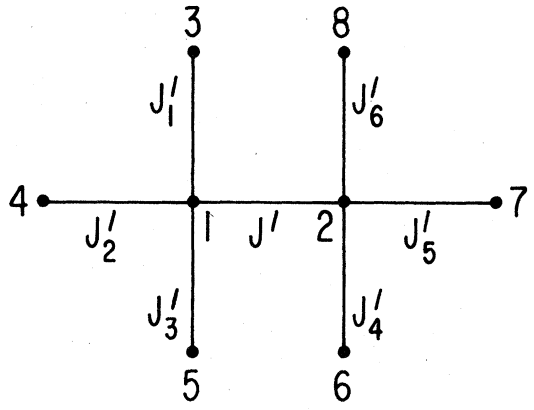

FIG. 7. Group of seven bonds joined to two nearest-neighbor spins in a two-dimensional square lattice.

Without these conditions, $P(J')$ would be just a Gaussian distribution $e^{-J'^2/2}$. With these conditions, we have

$$P(J')\propto\int\theta(J'+J'_1+J'_2+J'_3)\,\theta(J'+J'_4+J'_5+J'_6)\times e^{-J'^2/2}\prod_{i=1}^{6}e^{-J_i'^2/2}dJ'_i$$

$$\propto e^{-J'^2/2}\left(\int_{-J'/\sqrt{3}}^{\infty}dx\, e^{-x^2/2}\right)^2 \ . \tag{3.19}$$

This distribution has a maximum at

$$\bar{J}\approx 0.65 \ . \tag{3.20}$$

For our purpose of qualitative analysis, it is sufficient to use the approximation

$$P(J')\approx\frac{1}{(2\pi)^{1/2}}e^{-(J'-\bar{J})^2/2} \ . \tag{3.21}$$

Since $-J'$ is the energy in a bond, $P(J')$ gives the local energy distribution for a metastable state. The mean energy per spin is $-2\bar{J}=-1.3$, which is in reasonable agreement with that found in Sec. II.

The distribution of single-spin excitation energy, namely, $N_1(\epsilon)$, can be estimated from $P(J')$. The excitation energy of a given spin is

$$\epsilon=2(J'_1+J'_2+J'_3+J'_4)>0 \ ,$$

where 1, 2, 3, and 4 label the four bonds joining at the site of that spin. The distribution for ϵ is

$$\frac{N_1(\epsilon)}{L^2}=\int\delta(\epsilon-2|J'_1+J'_2+J'_3+J'_4|)\prod_{i=1}^4P(J'_i)\,dJ'_i$$

$$=(32\pi)^{-1/2}(e^{-(\epsilon/4-2\bar{J})^2/2}+e^{-(\epsilon/4+2\bar{J})^2/2}) \ . \tag{3.22}$$

We have approximated the joint probability distribu-

tion of $J_1', \ldots, J_4'$ by the product of the four distributions of single J'. $N_1(\epsilon)$ calculated from Eq. (3.22) shows a maximum at $\epsilon \simeq 4.8$. This result is in fair agreement with that shown in Fig. 1. (Note that the variable $|h|$ in Fig. 1 is $\frac{1}{2}\epsilon$.) Of special interest is $N_1(0)$. Equation (3.22) gives

$$\frac{N_1(0)}{L^2} = 0.085 \ . \tag{3.23}$$

This corresponds to $P_1(0) \simeq 0.17$, which is somewhat higher than the value obtained in Sec. II.

The estimate of cluster distributions can be made along the same lines, but is more involved. Here we shall only discuss two-spin clusters.

Consider the two neighboring spins, 1 and 2, as shown in Fig. 7. We begin with the joint probability distribution for ϵ_1, ϵ_2, and $|J|$

$$P(\epsilon_1, \epsilon_2, |J|) = \int \delta(\epsilon_1 - 2(|J| + J_1' + J_2' + J_3')) e^{-J^2/2}/(2\pi)^{1/2} \delta(\epsilon_2 - 2(|J| + J_4' + J_5' + J_6')) \prod_{i=1}^{6} P(J_i')\, dJ_i' \ . \tag{3.24}$$

If these two spins form a two-level cluster, then, by definition, a new energy minimum is reached after flipping both spins. This is possible only if $|J|$ is sufficiently large to dominate over interaction energies in the other bonds connected to the two spins:

$$|J| > |J_1' + J_2' + J_3'| \ ,$$
$$|J| > |J_4' + J_5' + J_6'| \ . \tag{3.25}$$

The joint distribution of the J''s is again approximated by a product of $P(J')$'s. Then we use Eq. (3.21) for $P(J')$. Now define the barrier height r and the cluster excitation energy ϵ as

$$r = \text{minimum of } (\epsilon_1, \epsilon_2, \epsilon_1 - \epsilon, \epsilon_2 - \epsilon) \ ,$$
$$\epsilon \equiv \epsilon_1 + \epsilon_2 - 4|J| \ . \tag{3.26}$$

By changing variables from ϵ_1, ϵ_2, J to r, ϵ, and $r' = (\text{next minimum above } r)$, and integrating over r', we obtain the distribution for r and ϵ

$$P(\epsilon, r) = A \exp[-\tfrac{5}{96}\epsilon^2 - \tfrac{1}{8}r^2 - \tfrac{1}{8}|\epsilon| r - (\tfrac{1}{4}r + \tfrac{1}{8}|\epsilon|) + \tfrac{1}{2}\bar{J}\epsilon] \ , \tag{3.27}$$

where $A \approx 0.0028$ is the normalization factor and $\bar{J} = 0.65$ as given by Eq. (3.20). The distribution of $|\epsilon|$ and r, as sampled in Sec. II, is [see Eq. (2.3)]

$$N_2(|\epsilon|, r) = 2L^2[P(|\epsilon|, r) + P(-|\epsilon|, r)] \ . \tag{3.28}$$

In obtaining Eq. (3.27), simplification was made by fitting a complicated function with a Gaussian. By integrating Eq. (3.27) over ϵ and $r > 0$, one obtains the probability of 3% that a pair of neighboring spins form a two-level cluster. This number is quite close to the result ($\sim$3.75%) obtained in Sec. II. Also, the forms of the distributions, $N_2(r)$ and $N_2(|\epsilon|)$, calculated from Eqs. (3.27) and (3.28) are in good agreement with the numerically obtained results shown in Figs. 3 and 6.

If we use the distribution $P(\epsilon, r)$ given by Eq. (3.27) as $N(\epsilon, r)/2L^2$ used in Eq. (3.8) through Eq. (3.15), we can compute the exponents α_E, α_M, and α in Eqs. (3.6), (3.10), and (3.13). We obtain

$$\alpha_E = 0.82, \quad \alpha_M = 0.54, \quad \alpha = 0.27 \ . \tag{3.29}$$

The distribution $P(\epsilon, r)$ given by Eq. (3.27) was calculated not by considering how the initial state was prepared, but via Eq. (3.24), which attempts to obtain $P(\epsilon, r)$ by picking energy minima at random. The numerical results obtained thus can serve only as order-of-magnitude estimates.

IV. NUMERICAL CALCULATION OF DYNAMIC PROPERTIES AT LOW TEMPERATURE

In this section, we present numerical calculations of some of the time-dependent properties of the spin-glass system at low temperatures. These calculations are based on the two-level system picture described in Sec. II. We assume that the low-temperature, finite-time behavior of the system can be described in terms of independent flips of single spins and small (two- or three-spin) two-level clusters. These flips are assumed to be uncorrelated, i.e., we do not consider the interactions among the two-level systems. This assumption is a reasonable one because a pair of two-level clusters will interact with each other only if they overlap, or if they are adjacent to each other. We also assume the simple dynamics of the kinetic Ising model, as described in Sec. III. The numerically determined distributions $P_1(|h|)$ and $P_n(|\epsilon|, r)$ are used as input data.

For the study of any time-dependent property, it is necessary to specify the initial state of the system. We assume that the initial state is a metastable state, characterized by the distributions $P_1(|h|)$ and $P_n(|\epsilon|, r)$. In addition, one has to specify whether a particular two-level system is in the higher or the lower of the two levels. Let ϵ be the difference in energy between the level the system is initially in and the other level. Thus, $\epsilon = |\epsilon|$ corresponds to the two-level system initially being in the lower level, whereas $\epsilon = -|\epsilon|$ corresponds to it being in the upper level at $t = 0$. If the initial metastable state is prepared by applying a magnetic field, then the populations of the two levels depend on the total spin of the two-level cluster. Let m be the total spin of the cluster when it is in the lower-energy state. We

can then characterize the initial metastable state by the distribution $N_n(m,\epsilon,r)$, where $N_n(m,\epsilon,r)\Delta\epsilon\Delta r$ is the number of n-spin two-level clusters with total spin m, energy difference between ϵ and $\epsilon+\Delta\epsilon$, and barrier height between r and $r+\Delta r$. This distribution is related to the probability distribution, $P_n(|\epsilon|,r)$, introduced in Sec. II [see Eq. (2.3)], in the following way:

$$N_n(m,\epsilon,r)=\frac{1}{2^n}L^2C_nK_n(m)P_n(|\epsilon|,r)\{\Theta(\epsilon)f(m,|\epsilon|,r)+[1-\Theta(\epsilon)][1-f(m,|\epsilon|,r)]\}\ , \tag{4.1}$$

where

$$\Theta(x)=\begin{cases}1, & \text{if } x\geq 0\\ 0, & \text{if } x<0\end{cases}\ ,$$

$K_n(m)$ is the number of distinct configurations of an n-spin cluster with total spin m (here we have assumed that all these configurations are equally probable), and $f(m,|\epsilon|,r)$ is the probability that the two-level system is initially at the lower-energy state. This probability function, $f(m,|\epsilon|,r)$, depends on the way the initial state is prepared, and cannot be determined in a simple way. In what follows, we will make simple approximations for f and then calculate the resulting time-dependent behavior.

First, let us consider the relaxation of the magnetization in an external magnetic field and the consequent time-dependent susceptibility. We assume that, at $t=0$, the system is in thermal equilibrium at a temperature T. The f for this initial state is given by

$$f(m,|\epsilon|,r)=1/(1+e^{-|\epsilon|/T})\ . \tag{4.2}$$

We then apply a small magnetic field, H. This changes the energy difference and the barrier height in the following way:

$$\begin{aligned}&\epsilon\rightarrow\epsilon(H)=(|\epsilon|+2mH)\,\mathrm{sgn}\,\epsilon\ ,\\ &r\rightarrow r(H)=r-mH\ ,\\ &v\rightarrow v(H)=v+mH\ .\end{aligned} \tag{4.3}$$

(Here, we have assumed that the energies of the intermediate states are not affected by the magnetic field.) This induces transitions between the two levels. Since these transitions involve climbing over energy barriers, the magnetization grows very slowly in time. A part of the magnetization, of course, comes from the flippings of single spins. However, this contribution does not show any interesting time-dependent behavior because the single spins reach equilibrium in a time of order unity. We have used Eq. (3.4) and the numerically determined distributions, $P_2(|\epsilon|,r)$ and $P_3(|\epsilon|,r)$, to calculate the time dependence of the magnetization due to the flippings of the two-level clusters. A typical growth of the magnetization per spin with time is shown in Fig. 8. The form of the $M(t)$ vs $\ln t$ curve is very similar to that observed by Kinzel[8] in his Monte Carlo simulation. It can be seen from Fig. 8 that the growth of the magnetization per spin can be described to a good degree of approximation by a logarithmic law of the form

$$M(t)=b+a\ln t \tag{4.4}$$

We have calculated the prefactor a for different values of the field H. The results are shown in Fig. 9. We find that a increases very sharply from zero as H is increased from zero, reaches a maximum at $H\simeq 1.0$, and then falls off as H is increased further. This behavior is in excellent agreement with Kinzel's[8] Monte Carlo result.

If we define the time-dependent susceptibility of the system as

$$\chi(t)=\lim_{H\rightarrow 0}\frac{M(t)}{H}\ , \tag{4.5}$$

then it follows from the above discussion that the susceptibility will also increase very slowly with time. Such a slow increase of the susceptibility with obser-

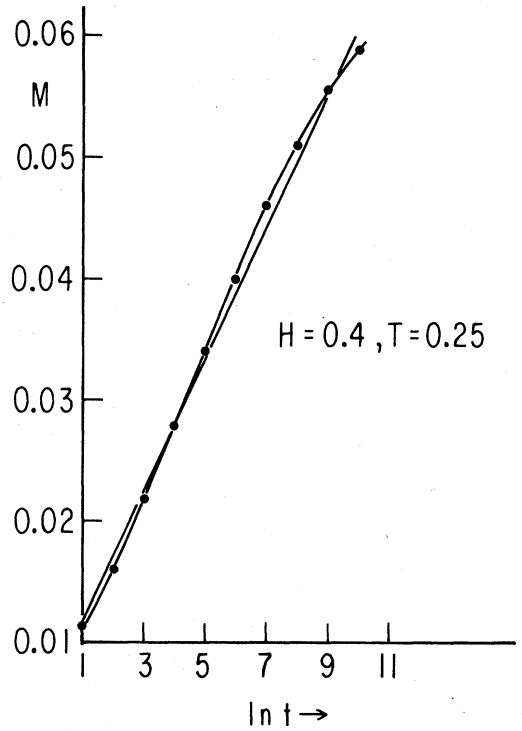

FIG. 8. Growth of the magnetization with time in an external magnetic field.

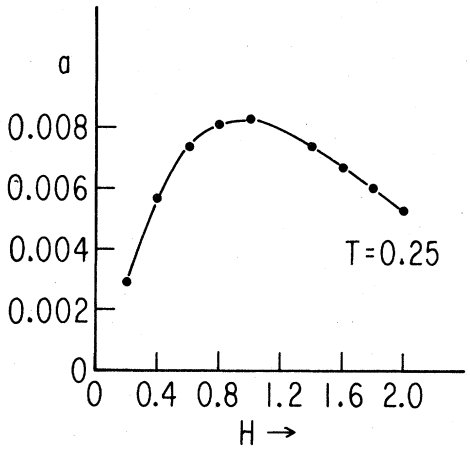

FIG. 9. Coefficient a of the fit $M \sim b + a \ln t$ as function of applied magnetic field.

vation time has recently been seen by Bray and Moore[5] in their Monte Carlo simulations. In Fig. 10, we have shown the results of our calculations of the low-temperature susceptibility (this includes the contribution of single spins) for three different observation times. The calculated values of $\chi(t)$ for $t = 1000$ units are in reasonable agreement with Monte Carlo results[5] for $t = 1000$ Monte Carlo steps/spin.

Spin glasses exhibit several interesting remanence properties at low temperatures. A recent Monte Carlo simulation of the two-dimensional Edwards-Anderson model with Ising spins has shown[8] that this model also exhibits remanence properties which are remarkably similar to those observed in experiments. A remanence state can be prepared in several different ways. The *field-cooled* or *thermoremanent magnetization* (TRM) is obtained by cooling the system slowly in an external magnetic field and then switching the field off. On the other hand, if one first cools the system down to a low temperature, applies a magnetic field for a short time Δt, and then switches the field off, one obtains what is known as the *isothermal remanent magnetization* (IRM). We have calculated various properties of these two kinds of remanent magnetization within the framework of our description in terms of the two-level system. In the TRM case, one starts from thermal equilibrium in an external field, H. We, therefore, assume that the probability function $f(m, |\epsilon|, r)$ for the initial metastable state for TRM is given by

$$f(m, |\epsilon|, r) = 1/(1 + e^{-(|\epsilon| + 2mH)/T}) \quad . \tag{4.6}$$

In the IRM case, one starts with a system which is in thermal equilibrium at zero field. We assume that the probability function for this state is given by Eq. (4.2). The application of the external field changes f. We use the kinetic equations to calculate this change in time Δt. The resulting probability function is used to characterize the initial metastable state for IRM. (The validity of these approximations for the remanence states is discussed at the end of this section.) We then use Eq. (3.4) to calculate the relaxations of the magnetization and the internal energy to their equilibrium values.

The results of our calculation are shown in Figs. 11–14. In Fig. 11, we have plotted the remanent magnetization per spin, averaged over 1000 time

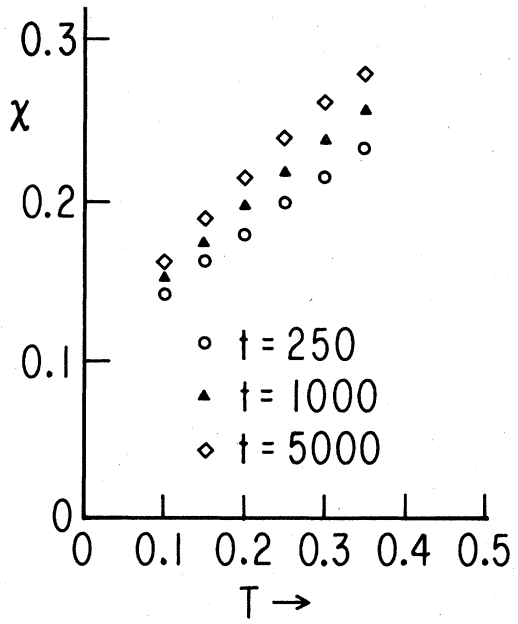

FIG. 10. Susceptibility vs temperature for different observation times.

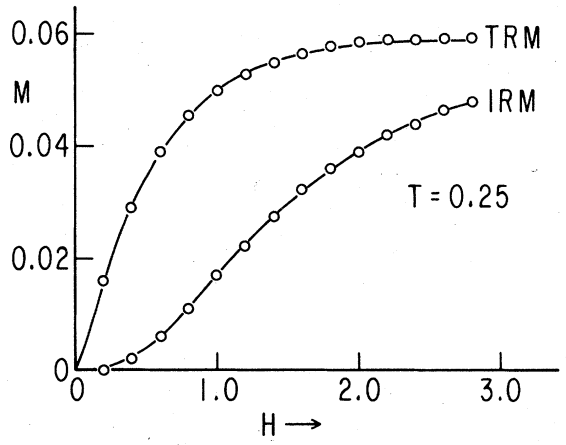

FIG. 11. Remanent magnetization averaged over 1000 time units for different values of the initially applied magnetic field H.

units, for different values of the initially applied magnetic field H. The TRM increases steeply with H and reaches a saturation value at $H \simeq 2$. The IRM increases less steeply and is smaller than the TRM. These qualitative features are in agreement with experiments[13] and Monte Carlo results.[8] Both experiments and Monte Carlo studies show a broad peak in the TRM as a function of H. Our calculations do not show such a peak. This is probably due to the crudeness of our approximation for the initial remanence state. The calculated initial values of both the TRM and the IRM are smaller than the values obtained in Monte Carlo simulations[8] by a factor of about 2. The initial values of the internal energy for TRM are in rough agreement with the Monte Carlo results of Kinzel.[8]

Both the TRM and the IRM decay very slowly in time. We found that this decay can be well approximated by a power law of the following form:

$$M_{\mathrm{TRM\ (IRM)}} \sim M_0 t^{-\alpha_{\mathrm{TRM\ (IRM)}}} \tag{4.7}$$

The internal energy per spin, E, in TRM was also found to show a similar power-law decay

$$E_{\mathrm{TRM}}(t) \sim E_0 t^{-\alpha_E} \tag{4.8}$$

Typical decays of M and E are shown in Fig. 12. This behavior is in agreement with the predictions made in Sec. III. Similar power-law decays have also been observed in Monte Carlo studies.[6,8] We have calculated the exponents α_{TRM}, α_{IRM}, and α_E for different values of H and T. Both α_{TRM} and α_E were found to increase with temperature in a roughly linear fashion. This is shown in Fig. 13. Similar results have been obtained in Monte Carlo simulations.[6,8] In Fig. 14, we have shown the variation of these exponents with the initially applied field H. The exponent α_{TRM} increases with H for small values of H, and then saturates at $H \simeq 2$. α_E also increases with H initially and then reaches a saturation value which is higher than that of α_{TRM}. The exponent, α_{IRM}, on the other

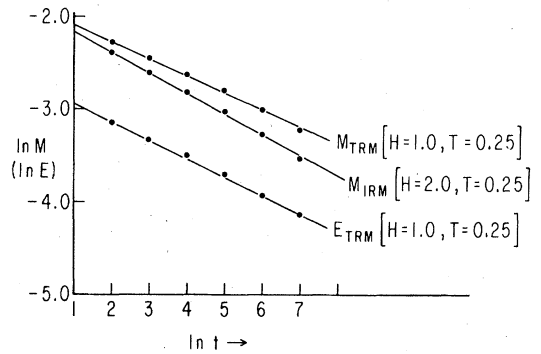

FIG. 12. Remanent magnetization and internal energy as a function of time on a log-log plot showing a power-law decay.

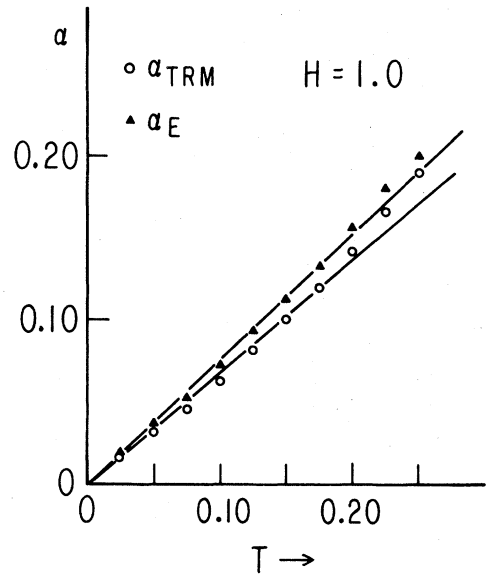

FIG. 13. Temperature dependence of the exponents α_{TRM} and α_E.

hand, decreases as the field is increased from zero, and then approaches a saturation value which is roughly equal to that of α_{TRM}. All these features are in qualitative agreement with the Monte Carlo results of Kinzel.[8] The calculated value of α_E is in fair agreement with Kinzel's result, and also with the value predicted in Sec. III. The values of α_{TRM} and α_{IRM} are higher than the values obtained in Monte Carlo simulations[8] by a factor of about 2.

Thus, we see that our simple description in terms of the two-level systems is able to reproduce, at least qualitatively, many of the interesting time-dependent properties of the spin-glass system at low tempera-

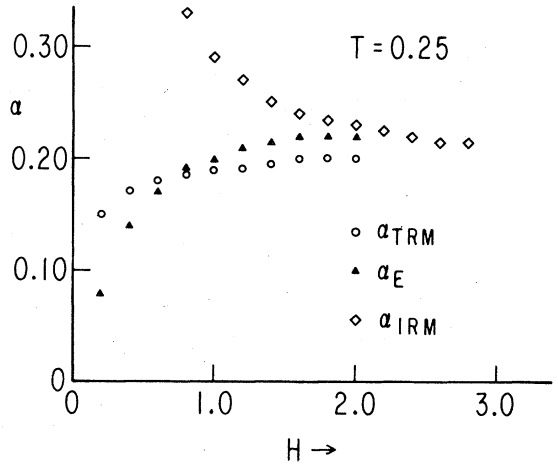

FIG. 14. Field dependence of the exponents α_{TRM}, α_{IRM}, and α_E.

tures. The quantitative results for the remanent magnetization are somewhat different from the results obtained in previous Monte Carlo studies. We believe that this discrepancy is due to the crudeness of our approximations about the remanence states. When a magnetic field is applied, a substantially large number of spins line up with the field. For this reason, the metastable state that is obtained when the magnetic field is switched off is not adequately described by the excitations of a few small clusters. A large cluster that is reversed by the application of a magnetic field relaxes back to equilibrium when the field is switched off by successive flips of small clusters. This adds to the magnetization a very slowly decaying component, which has the effect of increasing the remanent magnetization and decreasing the relaxation exponents α_{TRM} and α_{IRM}. Also, since the remanence states have rather high magnetization, the probability distributions for the two-level systems in these states are expected to be somewhat different from those calculated in Sec. II. Unfortunately, it is not clear how these effects can be taken into account in a quantitative way.

V. CONCLUDING REMARKS

The above calculations based on the simple description in terms of two-level clusters have been able to reproduce a wealth of results observed in previous Monte Carlo calculations. It seems evident that this simple picture is at least qualitatively correct and convenient for describing low-temperature behaviors of a spin glass. There is no need to cast the description in terms of the order parameter usually appearing in the literature on spin glasses, although it is clear in the cluster picture that the spins appear to be "frozen" (i.e., they have net time averages) at low temperatures if the observation time is not very long. An important theoretical question is whether or not the time average of a spin remains nonzero in the infinite-time limit. Our present study cannot answer this question. This is because our analysis in Secs. I–IV is limited not only to low temperatures, but also to sufficiently short times, $t \sim e^{1/T}$. For observation times much longer than $\exp(1/T)$, one would see improbable events leading to climbing over high-energy barriers and visiting distant regions of phase space. If one wants to describe these events in terms of reversals of clusters, one would have to study very large clusters as well as smaller ones. A more efficient description would be needed for this.

The behavior of the system over finite observation times is expected to show some qualitative changes at a temperature of the order of the typical barrier height of small two-level clusters. It is tempting to identify this temperature with the spin-glass transition temperature, T_c. Such a connection, however, is not very apparent from our calculations. As shown in Fig. 3, the distribution of the barrier height, r, for two- and three-spin clusters extends up to $r \simeq 4$, whereas the spin-glass transition temperature, T_c, is expected to be close to unity. Thus, it is not clear from our simple picture why the finite-time behavior of the system changes so dramatically at $T = T_c$. An explanation of this might go as follows. The distributions obtained in Sec. II are defined with respect to a "ground state" of the system and are relevant only if most of the two-level clusters are in their lower-energy states. As the temperature is increased, more clusters are excited and the effective distributions with respect to these excited configurations are expected to be somewhat different. Our numerical results indicate that the average barrier height decreases as the energy of the metastable state with respect to which the two-level systems are defined is increased. Thus, it may be possible to estimate T_c via the self-consistently determined distribution of the barrier height of small two-level clusters.

ACKNOWLEDGMENTS

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