Do Classical Spin Systems with the Same Metastable States Have Identical Hamiltonians?

I. Kanter and R. Gotesdyner
Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel
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The question whether systems having the same set of metastable states have identical Hamiltonian and hence identical dynamics is addressed and examined for various classical spin systems. The answer depends on the number of metastable states and on the distribution of the local fields for small fields. The rule that static properties determine dynamical properties is found to be applicable for a large class of random systems, almost any random system in the mean-field limit and many random systems in finite number of dimensions.

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Statistical mechanics of classical systems has developed into a field of growing interest during the second half of this century and it continues to be a source of new ideas for many interdisciplinary fields. It is constructed mainly from two major subfields, equilibrium statistical mechanics and nonequilibrium statistical mechanics. The former subfield is older and has achieved much progress in comparison to the latter. In general, equilibrium and nonequilibrium properties of physical systems are treated separately. The investigation of each one of these fields requires different analytical methods and concentrates on a different set of important physical quantities. For instance, for equilibrium statistical mechanics at low temperatures essentially only the ground states are relevant, whereas the dynamical properties of a state far from equilibrium are sensitive to other quantities, such as local minima, barrier heights, etc.

To illustrate, consider a ferromagnetic (FM) Ising spin system in the mean-field (MF) limit. The ground states of the system are the FM states where all spins occupy the same state, and the average magnetization as a function of the temperature is also well known. It is clear that this comprises the complete equilibrium information regarding this system. Can one conclude from this that two systems having the same equilibrium macroscopic properties consist of identical Hamiltonians?

For this illustrative example the answer is *no*. Assume that the distribution of the FM weights (interactions) in the two systems have on the average the same first and second moments. It is clear that the two systems have the same equilibrium properties, but different dynamical behavior. Since the weights are different, starting from the same initial configuration, the two systems evolve differently.

For the class of spin glass (SG) systems [1], it is true that the static properties (fixed points of the dynamics at zero temperature) alone give a clue as to the average characteristic behavior of the dynamics. The existence of many metastable states (MS) (together with the assumption of huge barriers) leads to long relaxation times. This dynamical behavior is common to any SG system, as is the fact that short relaxation times characterize any FM system, but clearly do not uniquely identify the system.

In this work we do not claim to solve explicitly the dynamics of any system. However, we address the question of whether static properties and dynamical properties are in general fully conjugate. More precisely, we ask whether systems with the same MS necessarily have the same weights. It is clear that systems which are described by the same Hamiltonian also have identical average macroscopic dynamical properties under any type of detailed balance dynamics, and furthermore have the same microscopic evolution when the systems are subject to the same noise.

Illustratively, one may consider the following example. Assume that two sandpiles have exactly the same locations of local minima. Does this information necessarily indicate that the surfaces of these two sandpiles are identical? In a similar manner one may ask a question regarding two polymers or any two physical systems having the same phase space.

Surprisingly, we will show that static properties determine dynamical properties for a large class of systems. The answer to the question of whether systems with the same MS have identical Hamiltonians depends in general on the number of MS and the distribution of the local fields in these states. The following two fundamental questions are also discussed below: (a) Is it possible to find a classical spin system with any number of local minima? (b) Is the distribution of the local fields in the MS a function of their number? Is it possible to construct a random system with any shape of the distribution of the local fields?

The first system examined is a pure Ising SG system in the MF limit and with binary weights described by the Hamiltonian

$$H = -\sum_{(ij)} J_{ij} S_i S_j \equiv -\sum_i S_i h_i. \qquad (1)$$

The summation is over all pairs of Ising spins, $S_i = \pm 1$, h_i is the local field on the ith spin and the distribution of the weights is given by

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$$P(J_{ij}) = \tfrac{1}{2}\,\delta(J_{ij} - 1/\sqrt{N}) + \tfrac{1}{2}\,\delta(J_{ij} + 1/\sqrt{N}), \tag{2}$$

where N is the size of the system [2]. The following two main results were obtained in the early days of SG regarding this model: (a) The number of MS was calculated analytically and found to scale exponentially with the size of the system, $\exp(AN)$ with $A \sim 0.199$ [3,4]. (b) The internal field distribution, $P(|h|)$, in the ground states was suggested by Anderson to be proportional to h^α for small fields with $\alpha \geq 1$. In numerical simulations, $P(|h|)$ was actually found to saturate the lower bound, $\alpha = 1$ [5]. These results are not sufficient. Further preliminary results regarding this model have to be obtained in advance before we will be ready to examine the main goal of this work, whether static properties determine the dynamical behavior.

Using extensive simulations we are able to expand our knowledge regarding this model and to obtain the following results. We verify that the number of MS grows exponentially as e^{AN} with $A \sim 0.19$ (see Fig. 1). The method used in the simulations was to build a table of distinct MS, using zero temperature Monte Carlo dynamics initiated from many random configurations. For each size of the system, a halting criterion was chosen following the rate of appearance of a new MS [6]. The lower bound obtained for A in the simulations is very close to the theoretical prediction [3,4]. This table of MS serves as the main database for the following investigations.

Second, the internal field distribution averaged over all MS is found to scale for small fields as $P(|h|) \propto h$, as for the ground states, but with a greater slope. Furthermore, the average probability for the minimal field $|h_{\min}| = 1/\sqrt{N}$ on each spin was found (see inset, Fig. 1) to scale as

$$P_N(|h_{\min}|) = 4.5/N. \tag{3}$$

This result can be understood using the following argument. For the case of continuous weights with Gaussian distribution [7] which will be discussed below,

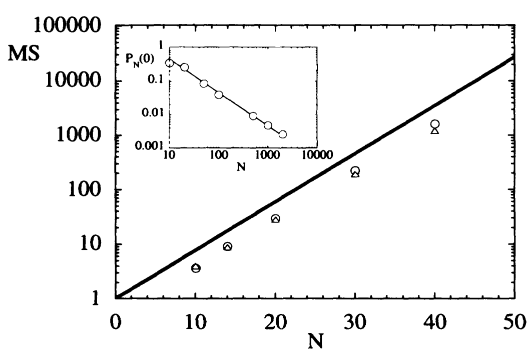

FIG. 1. Number of MS for pure SG (○) and for $c = 0.4$ (△). The line describes $2e^{0.19N}$. Inset: $h_{\min}$ vs $1/N$ for pure SG; the line describes $4.5/N$.

$$p(J) = \sqrt{\frac{N}{2\pi}}\,e^{-\frac{NJ^2}{2}}, \tag{4}$$

it was found in our simulations that $P(0) \propto 1/\sqrt{N}$, as was previously obtained for the ground states [5]. Hence, the weight of the local fields up to $1/\sqrt{N}$ is proportional to

$$\int_0^{1/\sqrt{N}} P(h)dh \propto \frac{1}{N}. \tag{5}$$

Since the behavior of continuous and discrete SG systems is expected to be the same in the MF limit, it is now clear that the relation between $P(|h|)$ for small fields in both cases is like the relation between a continuous function and a histogram.

It is important to note that Eq. (3) only indicates that in the ensemble of MS each spin on the *average* has a local field equal to $h_{\min}(4.5/N)e^{AN}$ times. The fluctuation of $P_N(|h_{\min}|)$ in different spins was examined and was found to be negligible in the leading order. Hence, all spins have the same probability in the leading order to be in a MS with $h_{\min}$. Details on the distribution of $h_{\min}$ will be given elsewhere [6].

The last question which has to be answered in advance is whether the frustration is distributed homogeneously over all the weights. In each MS of Eqs. (1) and (2) roughly one-half of the weights are frustrated, since the energy is an extensive quantity and the strength of the weights is $1/\sqrt{N}$. An important question is whether there are weights which are not frustrated (or frustrated) in *any* MS, or are all weights equally frustrated. In the case that the frustrated weights in each MS and among the MS are uncorrelated then the following Gaussian distribution, $P(x)$, for the number of times that a weight is frustrated is expected [i.e., each weight executes a random walk of length $\exp(AN)$]:

$$P(x) = Ce^{-(x-Be^{AN})^2/2e^{AN}}, \tag{6}$$

where C is a normalization constant, e^{AN} is the number of MS, and B is a constant which is expected to be equal to $1/2$ in the thermodynamic limit. Nevertheless, the correlations cannot be neglected even for the MS and the distribution is fit by form

$$P(x) = Ce^{-DN^2(x-Be^{AN})^2/2e^{2AN}}, \tag{7}$$

where D is a constant of order unity (for $N = 50, 100$, $D \sim 0.36$, $B \sim 0.4$, and $B \to 0.5$ as the system's size grows). Using Eq. (7) and the above analogy to random walks Eq. (6), we expect the standard deviation to vary as $p/\ln(p)$, where p is the number of examined MS; see Fig. 2 where each point is averaged over a few hundred samples. Furthermore, following Eq. (7), the minimal x with nonvanishing probability should be proportional to $[B - 2\sqrt{2\ln(N^2/2)/DN^2}]e^{AN}$. This was indeed confirmed in our simulations and the effect of a long tail can be neglected. Hence, one can say that although the ef-

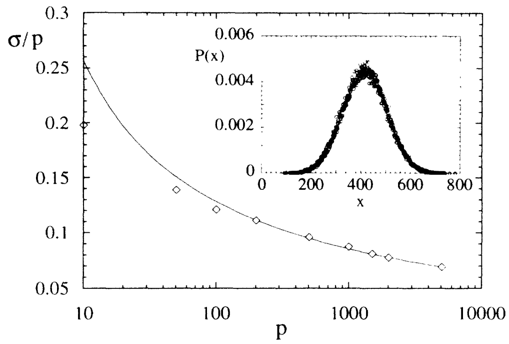

FIG. 2. σ is the standard deviation of $P(x)$ [see Eq. (7)] and p is the number of examined MS. The line describes $0.59/\ln(p)$. Inset: A typical distribution $P(x)$ for $N = 50$ and $p = 1000$; average $x \sim 420$ and $\sigma \sim 86 \sim 0.59p/\ln(p)$.

fect of correlations is visible, Eq. (7), in the leading order the number of times that each weight is frustrated is the same and equal to one-half of the number of MS.

Let us now prove in a negative way that there are no two different pure SG systems, Eq. (1), in the space of the weights (of size $2^{N(N-1)/2}$) which have an identical set of MS. Assume that the weight $\{J_{ij}^{\alpha}\}$ of system α and its set of MS of the size e^{AN} are given. Assume also that there exists a different system defined by $\{J_{ij}^{\beta}\}$ which has the same set of MS as system α. From Eq. (3) one can deduce that the average number of times that each spin has $h_{\min}$ in all MS is $\propto e^{AN}/N$. To move from $\{J_{ij}^{\alpha}\}$ to $\{J_{ij}^{\beta}\}$ one has to flip on the average some of the $N-1$ weights connecting each one of the N spins. On the average, one-half of these weights are frustrated and the processes that a weight moves from being frustrated $\leftrightarrow$ unfrustrated have the same probability. Since the spins are uncorrelated in the leading order with respect to different MS [4], the average probability that a spin with local field $h_{\min}$ in system α will remain stable after the flip of the weights is 1/2. (For instance, if the sign of an unfrustrated weight is flipped then a spin with $h_{\min}$ connected to this weight loses its stability.) The probability that this spin will remain stable at least in all MS where its field is equal to $h_{\min}$ (in α) is given by

$$[\tfrac{1}{2}]^{e^{AN}/N}. \tag{8}$$

This factor decreases to zero much faster than $2^{N^2/2}$, the number of different possibilities to system β. Hence, system β does not exist and the solution is unique. It is clear that the same argument holds even for the case where systems α and β differ in one weight only. In this case, Eq. (8) applies only to the two spins connecting this particular weight.

For a pure SG system with Gaussian weights, Eq. (4), the following results which characterize the MS are obtained, as was previously obtained also for the ground states [5]. (a) $P(h) \propto h$ for small fields. (b) $P(0)$ scales as $1/\sqrt{N}$.

The examination to determine whether there exist two different systems with the same set of MS should be modified in the case of continuous weights. Assume that in one system the strength of one of the weights is modified; $J \rightarrow J+\epsilon$ where $\epsilon \ll |J|$. Let us now estimate the probability that all MS do not lose their stability. The number of MS with local fields less than ϵ on a spin connected to the modified weight is proportional to

$$e^{AN}\int_0^{\epsilon} P(h)dh \quad \propto \quad \epsilon^2 e^{AN}. \tag{9}$$

Each one of these MS loses its stability after the modification with probability 1/2. Using a similar argument as for the binary case, Eq. (8), one can verify that the probability that all MS do not lose their stability is given by

$$[\rho]^{a\epsilon^2 e^{AN}}, \tag{10}$$

where a and ρ are constants of order unity. [Since $\sqrt{N}J$ is of $O(1)$ and the energy is an extensive quantity, a finite fraction of the weights are frustrated.] One can also verify that a similar probability holds when few weights are modified. This probability drops to zero (polynomial corrections due to $e^{-N^2\ln\epsilon}$, the size of space of weights under scale ϵ, are neglected) as long as

$$\epsilon \quad < \quad e^{-\sqrt{AN}} \tag{11}$$

in the leading order. Only systems whose weights differ by a constant of order $e^{-\sqrt{N}}$ may have the same MS. The actual modification may be even smaller, since Eq. (11) is only a necessary condition.

Let us now leave the details and return to our main goal, whether static properties determine the dynamics of pure SG with continuous weights. Assume that there are two systems having the same MS. Following Eq. (11), their microscopic evolution is identical (when they are subject to the same noise) on the average for times t,

$$t \quad < \quad e^{\sqrt{AN}}. \tag{12}$$

A simple way to understand this result is to imagine a Monte Carlo process of two such systems with the same initial conditions. It is clear that in the leading order the first time step in which at least one of the spins behaves differently in both systems is given by Eq. (12). In contrast to a SG system with discrete weights, for continuous weights static properties determine the dynamics up to some cutoff time. However, as long as the number of MS scales exponentially with N, this time diverges as $e^{\sqrt{N}}$.

The following discussion is devoted to examining the generality of the connection between static and dynamical properties. The two cornerstones of the abovementioned discussion are (a) e^{AN} MS and (b) no gap in $P(h)$ as $h \rightarrow 0$, where a gap in the discrete case means that $P(h_{\min}) = 0$.

Let us first discuss briefly why it is impossible to violate (b), to find a random system in the MF limit with exponentially many MS but with a gap. Assume that such a random system [$P(J_{ij})$ independent of $P(J_{kl})$] exists and the minimal nonvanishing $P(|h|)$ is $h^0 > h_{\min}$. Let us now flip [or modify following $P(J)$] the weights such that the sum of the absolute value of the modifications is Y and $\delta < Y < h^0$. It is clear that there are many such modified systems whose weight is greater than the weight of the original system and that these modifications cannot alter the stability of the MS. Nevertheless, these modifications weaken by δ_1 a finite fraction of the exponentially many local fields of the strength $h^0 < h < h^0 + \delta_2$, with $\delta_2 < \delta_1$. Hence, we end with a contradiction that $P(h) \neq 0$ for $h < h^0$. The idea behind this proof is to show an instability for $P(h)$ in the space of the weights.

The relation between static and dynamical properties seems to be sensitive to the number of MS and to the exact form of $P(h)$ for small h. For a discrete system with N^x MS, for instance, one can show that the solution is not unique for some $x \leq x_0$, where x_0 is a function of the shape of $P(h)$ [6]. It is therefore interesting to examine the following questions: Is it possible to construct a random system with any number of MS? What is the plausible interplay between the number of MS and the shape of $P(h)$? The two limit cases, FM (2 MS) and spin glass (e^{AN} MS), are known, but the intermediate region is in question. Surprisingly, there is no intermediate region. Following Ref. [7] we proved *analytically* that for a system as in Eq. (1) and with $P(J_{ij}) = (1-c)\delta(J_{ij} - 1/N) + c\delta(J_{ij} + 1/N)$ where $c = O(1)$, the number of MS in the leading order is the same as for the pure SG case [6]. The results of the numerical simulations for $c = 0.4$ and $N \leq 40$, for instance, are presented in Fig. 1 and indicate that indeed the number of MS scales as e^{AN} with $A > 0.18$. Furthermore, all the previously discussed properties of the pure SG case, such as the scale of $P(0)$ and the distribution of the frustration, also hold for the case $c \neq 1/2$. Hence, the conclusions regarding the relation between static and dynamical properties for both discrete and continuous weights hold also for the nonpure SG and even for systems with a FM ground state and short relaxation times. The pure FM system is a unique and exceptional system.

For MF Heisenberg SG, a gap in $P(h)$ is expected for the MS, as previously found for the ground states [5]. Nevertheless, since spins have continuous degrees of freedom the gap is meaningless in relation to our discussion, and small changes in weights lead to different MS. Hence, our results are expected to hold even for this model.

The number of MS in a two-dimensional square lattice with random ± 1 weights was previously found to be e^{AN} with $A \sim 0.14$ [1, 8]. We analyze a similar model where each spin is connected to three weights of strength ± 1 and to one weight of strength ± 1.1. This modification ensures a zero entropy at zero temperature and a unique solution to the strength of the weights connected to one of the spins if its state is known for all of the sixteen states of its four neighbors. It was found in the simulations that the exponentially many MS uniquely define all the weights, and hence static properties determine the dynamics. It is clear that this is not the case for this model with continuous weights. This model with RKKY weights [1,9], $J_{ij} = \pm |r_{ij}|^{-3}$, where r_{ij} is the distance between spins i and j, was also examined numerically. It is found that $P_N(0)$ decays much more slowly than $1/N$ (may be as $1/\ln N$) and it is therefore expected that our conclusions hold even for this model.

Finally, we briefly discuss the analogy between this work and the question of learning from random examples, one of the current areas of interest in the theory of neural networks [10]. On one hand, each spin in Eq. (1) behaves like an output of a perceptron with $N-1$ input units. However, there are many crucial differences: (a) Our system, Eq. (1), is a recurrent network and for that reason $P(h)$ is not Gaussian as for the perceptron. (b) The random examples are replaced by the MS which are a correlated subset of measure zero. This analogy raises the following interesting question. What is the number of pure SG systems having different sets of MS? Following Eq. (11) this number is bounded from below by $O(\exp(N^{2.5}))$, since the relevant scale of a weight is $O(e^{-\sqrt{N}})$, and an upper bound is given by $\exp(N^3)$, the number of Boolean functions which can be implemented by N independent perceptrons.

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