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Spin-Glass Energy Landscape

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We consider a nearest-neighbor-interaction $\pm J$ Ising spin glass in a square lattice. Inspired by natural evolution, we design a dynamic rule that includes *selection*, *randomness*, and *multibranch exploration*. Following this rule, we succeed in walking along the space of states between local energy maxima and minima alternately. During the walk, we store various information about the spin states corresponding to these minima and maxima for later statistical analysis. In particular, we plot a histogram displaying how many times each minimum (or maximum) energy is visited as a function of the corresponding density value. Through finite-size scaling analysis, we conclude that a nonvanishing fraction of bonds remains unsatisfied (satisfied) at these energy minimum (maximum) states in the thermodynamic limit. This fraction measures the degree of unavoidable frustration of the system. Also in this limit, the width of these histograms vanishes, meaning that almost all metastable states occur at the same energy density value, with no dispersion.

KEY WORDS: Spin glasses; complexity; landscapes.

In the Edwards–Anderson spin glass on the square lattice with interactions $\pm J$ between nearest neighbors, each site is surrounded by zero to four unsatisfied bonds ($J_{\langle ij \rangle} S_i S_j = +J$ for $S_i = \pm 1$) which contribute to the total energy. We simulate here the energy of the whole lattice by orienting consecutively each spin such that each spin flip lowers the energy, according to a dynamic rule defined later. In this way, we get into a local, not necessarily the global, minimum of the energy in the spin distribution space. After storing the relevant information concerning this minimum for later statistical analysis, we search now for a local energy maximum following the same rule. Now, each spin flip increases the energy. We then store

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also the information concerning this maximum, and restart the process, again searching another minimum, and so on, performing a walk on the space of states.

Each step in this walk corresponds to a single mutation, only one spin being flipped at a time. We also introduce randomness in the dynamic process. We scan the lattice site by site. If a spin flip on the current site will lower the energy, then we perform this mutation with only 50% probability when looking for local minima. The same probability is adopted for the search for local maxima. In this way, our system evolves through *random* mutations, under a *nonrandom* selection rule (the energy lowering or increasing), according to evolution theory.[1-4] The other fundamental feature of evolution, the *multibranched search*, is also taken into account by including an infinitesimal magnetic field in order to deal with free spins. First this field points up. So if the current site is surrounded by just two unsatisfied bonds, its spin will be forced to point up after the 50% probability tossing. We scan the whole lattice many times until convergence, with no more spins to be flipped. Then we reverse the field to down orientation, and restart the process until a new convergence, always decreasing (increasing) the energy when looking for a minimum (maximum). Then, the field is reversed to up again, and so on. The process stops when the energy cannot be further decreased (increased) by further field reversing.

The repeated reversing-field procedure was introduced before[5] in looking for the ground states of the diluted Ising antiferromagnet in a uniform magnetic field. The advantage of its inclusion in our problem can be understood as follows. Suppose we adopted only the naive dynamic rule of flipping all spins with three or four surrounding unsatisfied bonds until reaching a locked state S_0. This state is certainly a "local energy minimum" in the sense that its energy is smaller than or at most *equal* to each one of its N neighboring states. Suppose S_0 has just n spins with two surrounding unsatisfied bonds. Then there are just n neighboring states with the *same* energy. Unlike S_0, however, it is *not* true that these n states are also necessarily "local energy minima." Some of them may have neighboring states (second neighbors of S_0) corresponding to equal or even lower energies. The same may occur also to some of the neighbors of these neighbors (third neighbors of S_0), and so on. In this case, S_0 is not a truly metastable state, i.e., it is not a state from which any further minimization can be achieved only by large jumps through energy barriers. On the contrary, starting from S_0, one can explore this multibranched network of possibilities, looking for deeper energy valleys along the space of states, *always* through single-spin mutations and *never* increasing the energy. Our repeated reversing-field procedure is a way to do just that. Its power is illustrated by Fig. 1, showing the potential number of spins to be flipped

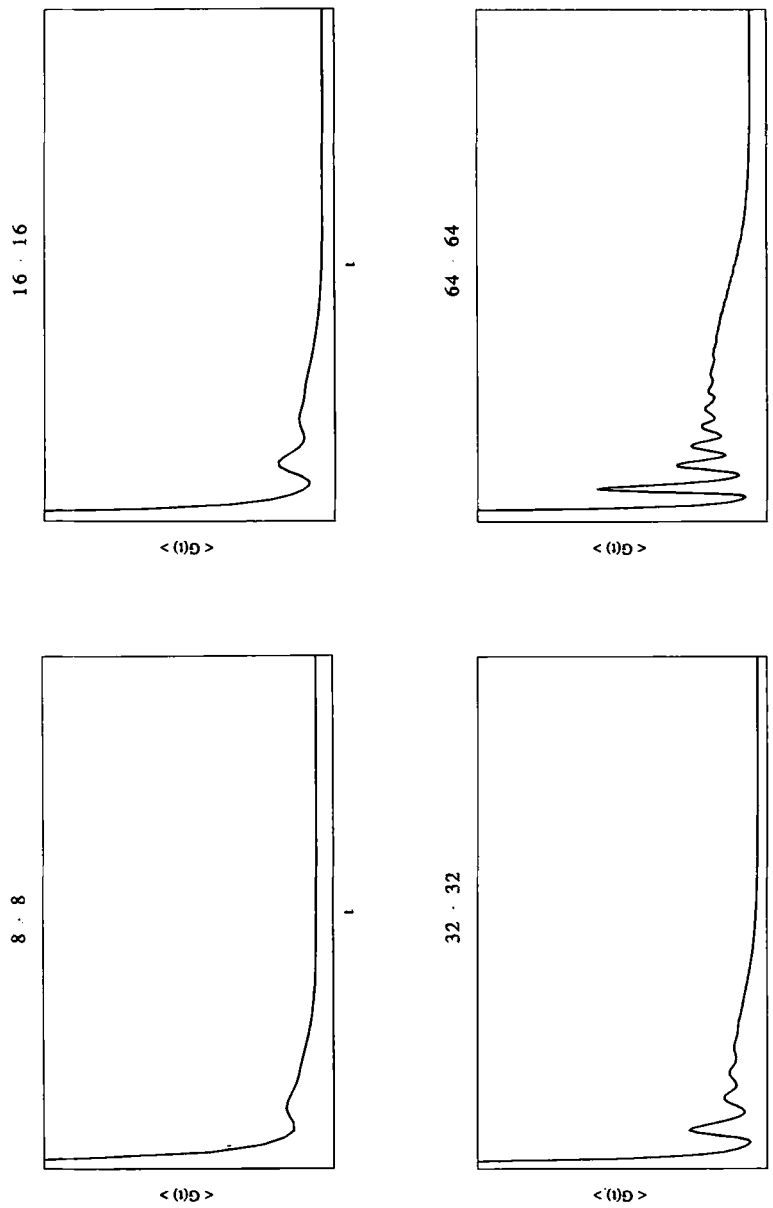

Fig. 1. Averaged number $\langle G(t) \rangle$ of spins able to be flipped (before performing the 50% tossing), measured from one maximum to the next minimum (and vice versa).

(before the 50% tossing) as a function of time t (number of whole lattice updates). The successive peaks on the plots correspond to successive field reversing. The rounded behavior is due to averaging, taking into account many maximum–minimum trajectories. For only one such a trajectory, the plots would touch the horizontal axis just before each field reversing, growing again just after, like a saw. As one can see by comparing the plots, the larger the lattice, the more efficient is the reversing-field procedure.

We normalize the energy per site into the unit interval. Thus, $\mathscr{E} = 0$ means no unsatisfied bonds, whereas $\mathscr{E} = 1$ corresponds to all bonds being unsatisfied. We will call *state* the spin distribution which is the dynamical variable. On the other hand, we will call *configuration* the $\pm J$ bond distribution on the lattice, which is quenched. A typical histogram of $\mathscr{E}$ consists of two sharp peaks, one for the visited energy minima and the other for maxima. The interesting features about such plots are their widths decreasing for increasing system sizes, and also the positions of their averaged values $\langle \mathscr{E}_{\max} \rangle$ ($\langle \mathscr{E}_{\min} \rangle$) increasing (decreasing) for increasing system sizes. Two questions can be formulated.

1. Do the widths of these plots vanish in the thermodynamic limit? If so, this means that almost all metastable states occur at the same energy density, with no dispersion.
2. Do $\langle \mathscr{E}_{\min} \rangle$ and $\langle \mathscr{E}_{\max} \rangle$ approach 0 and 1, respectively, in the thermodynamic limit? This question can be reformulated as follows. Is the degree of unavoidable frustration a null measure set, with dimension smaller than the lattice dimensionality?

The main purpose of the present work is to answer these questions.

A histogram for eight distinct configurations with six distinct walks each is presented in Fig. 2, corresponding to 720,000 minima (and maxima) for a 16×16 lattice. An interesting effect appears: the histogram seems to be composed of two distinct ones, with shifted averaged values. The physical reason for this feature is the existence of two distinct classes of configurations, *even* or *odd*. The value of $\mathscr{E}$ gives simply the density of unsatisfied bonds on the lattice, i.e., the number $\mathscr{U}$ of unsatisfied bonds divided by the total number $2N$ of bonds. As each flipped spin changes this number $\mathscr{U}$ by 0, ± 2, or ± 4, it cannot be even for some state and odd for another one corresponding to the same configuration. So each configuration is categorized into two distinct classes, even or odd, according to the parity of the number of unsatisfied bonds it can hold. We considered four even and four odd configurations in our simulations leading to Fig. 2, showing a higher degree of frustration for the odd ones. On the other hand, for the 32×32 lattice (not shown), we obtain the opposite trend, taking also four even and four odd configurations. This behavior indicates that

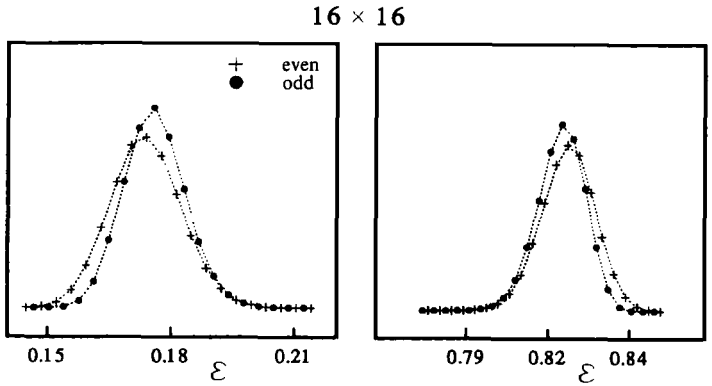

Fig. 2. 16 × 16 lattice histogram of energy minima (left) and maxima (right) for eight distinct configurations and six distinct walks each, corresponding to 720,000 minima or maxima. There are four even and four odd configurations (see text), leading to the two-peak appearence of the histogram. The lines are guides to the eye.

only-one-configuration histograms depend upon the particular configuration simulated. Thus, the measurement of averaged energies or widths may require many distinct random configurations. We profit from the comparison between results for even and odd configurations in order to control the statistical quality of all our results.

The whole process would be unfeasible (at least on our personal computers) by using canonical programming techniques. Instead, we adopted a multispin strategy.[6]

Table I shows the averaged values and peak widths of our histograms, from simulations on four different sizes of lattices, taking for each one an adequate number of distinct configurations, according to the desired numerical accuracy. The final three columns correspond to averages over only even, only odd, and both even and odd configurations, respectively. The coincidence of the most representative digits gives us confidence in them, according to our early discussion concerning Fig. 2. Thus, one can conceive that these *simulated* histograms must be equal (within this degree of numerical accuracy) to the *exact* histograms one could in principle determine by taking all metastable states from all possible configurations, for each lattice size. This may be true with regard to the horizontal scales (energy axis) of the histograms, but not for the vertical scales (number of metastable states). A third question can be formulated, besides the other two already quoted.

3. What is the behavior of the total number of metastable states (averaged over configurations) as a function of the lattice size?

Table I. Averaged Values $\langle \mathscr{E} \rangle$ and Widths $\langle \Delta\mathscr{E} \rangle$ of Histograms for 8×8, 16×16, 32×32, and 64×64 Lattices[a]

		Only even	Only odd	Even and odd
8×8	$\langle \mathscr{E}_{min} \rangle$	0.17888	0.17887	0.17888
	$\langle \mathscr{E}_{max} \rangle$	0.82119	0.82110	0.82114
	$\langle \Delta\mathscr{E}_{min} \rangle$	0.02032	0.02044	0.02038
	$\langle \Delta\mathscr{E}_{max} \rangle$	0.02033	0.02044	0.02038
16×16	$\langle \mathscr{E}_{min} \rangle$	0.17435	0.17445	0.17440
	$\langle \mathscr{E}_{max} \rangle$	0.82563	0.82556	0.82560
	$\langle \Delta\mathscr{E}_{min} \rangle$	0.00991	0.00992	0.00992
	$\langle \Delta\mathscr{E}_{max} \rangle$	0.00993	0.00991	0.00992
32×32	$\langle \mathscr{E}_{min} \rangle$	0.16994	0.17013	0.17004
	$\langle \mathscr{E}_{max} \rangle$	0.83007	0.82989	0.82998
	$\langle \Delta\mathscr{E}_{min} \rangle$	0.00489	0.00490	0.00489
	$\langle \Delta\mathscr{E}_{max} \rangle$	0.00490	0.00489	0.00489
64×64	$\langle \mathscr{E}_{min} \rangle$	0.16643	0.16637	0.16640
	$\langle \mathscr{E}_{max} \rangle$	0.83358	0.83363	0.83360
	$\langle \Delta\mathscr{E}_{min} \rangle$	0.00252	0.00248	0.00250
	$\langle \Delta\mathscr{E}_{max} \rangle$	0.00252	0.00248	0.00250

[a] We take just one walk corresponding to 400 minima and 400 maxima for each configuration. The number of configurations adopted for each lattice size is, respectively, 10,000, 6000, 4000 and 2648 (approximately half even and half odd), corresponding to 4,000,000, 2,400,000, 1,600,000 and 1,059,200 minima or maxima, respectively. Averages are performed over only even, only odd, and both even and odd configurations, respectively.

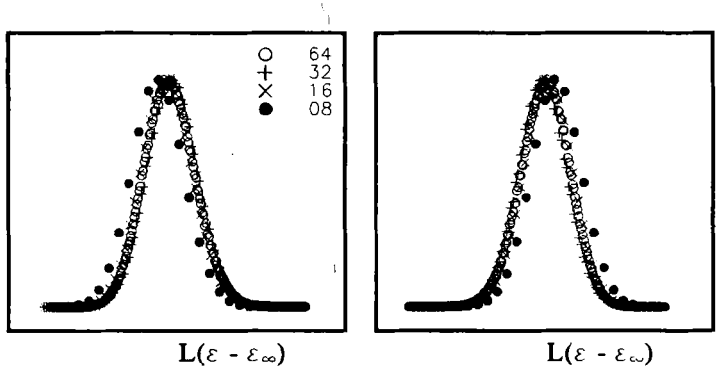

Fig. 3. Data-collapsing plots of histograms for 16×16, 32×32, and 64×64 lattices (same data corresponding to Table I), according to the scaling equation (1). Data for the tiny 8×8 lattice are also included.

Unfortunately, our simulations do not add much information (if any) about this point. See refs. 7 and 8.

Let us return to questions 1 and 2. Figure 3 shows data-collapsing plots obtained by fitting our simulated histograms for 16×16, 32×32, and 64×64 lattices to the form of a generalized homogeneous function[9]

$$H(l^a(\mathscr{E} - \mathscr{E}_\infty), l^{-1}L) = l^{-\Phi} H((\mathscr{E} - \mathscr{E}_\infty), L) \tag{1}$$

supposed to be valid for arbitrary values of l, and for large enough lattice sizes L. Here, a, $\mathscr{E}_\infty$, and Φ are parameters to be determined. They are related to questions 1, 2, and 3, respectively. As discussed above, we are not able to compare the vertical scales of distinct simulated histograms obtained from different lattice sizes. So we impose $\Phi = 0$ by normalizing our histograms to the same maximum height. The actual value of Φ would be related to the true maximum height $H_{\max} \sim L^{\Phi}$ of the exact histograms, and remains an open question. In Fig. 3, we used $a = 1$, and found $\mathscr{E}_\infty = 0.1633$ for energy minima histograms ($1 - \mathscr{E}_\infty = 0.8367$ for maxima). Considering the dimension $D = 2$ of our systems, and according to $a = 1 = D/2$, the width of these histograms vanishes as $1/\sqrt{N}$ in the thermodynamic limit $N \to \infty$. This behavior is characteristic of systems formed by N uncorrelated units, and may be a consequence of the lack of spin-glass long-range order in that dimension. In Fig. 3, we include also data for the tiny 8×8 lattice not collapsing very well onto the other three curves. This means that our sequence of sizes $L = 16$, 32, and 64 is not large enough to give us complete confidence on the last digits estimated for $\mathscr{E}_\infty$.

As a last remark, we do not claim that our minimum energies correspond to *ground* states. According to our evolutionary dynamic rule, we can only guarantee that they are *metastable* states in the sense extensively discussed above. One can devise two possible scenarios. First, the true ground states have a smaller energy density than our $\mathscr{E}_\infty$. In this case they are hidden in our simulations, being thus a null measure set compared to our metastable states (their number scaling as L^α, where $\alpha < \Phi$). Second, the energy density of the true ground states coincides with our $\mathscr{E}_\infty$. In this case, our "metastable" states are actually the true ground states. Considering what are supposed to be the true ground states, Monte Carlo estimates give $\mathscr{E}_\infty \cong 0.15$ (see, for instance, ref. 10), whereas theoretical topological arguments[11] give a lower bound of $\mathscr{E}_\infty = 0.125$, to be compared with our $\mathscr{E}_\infty = 0.1633$. Also, non-vanishing values for the entropy per site are reported, seeming to rule out the first scenario. For a recent discussion about this subject, see ref. 12.

In conclusion, we have studied the energy landscape of nearest-neighbor $\pm J$ square lattice Ising spin glasses through computer simulation.

In the thermodynamic limit, we measured a nonvanishing degree of unavoidable frustration, corresponding to a *precise* (vanishing dispersion) finite fraction of unsatisfied bonds. The search for minimum energy values is performed through single random mutations (single spin flips) repeated sequentially, following a nonrandom selective evolutionary process. Also, multibranched possibilities are explored in this search, through the inclusion of an infinitesimal magnetic field that is reversed iteratively. This multibranch exploration allows one to follow channels of nonstrict local minimum energies across the space of states until reaching true metastable states from which the energy cannot be minimized by single-step mutations.

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REFERENCES

1. C. Darwin, *The Origin of Species* (London, 1859).
2. S. A. Kauffman, in *The Economy as an Evolving Complex System*, P. W. Anderson, K. J. Arrow, and D. Pines (Santa Fe Institute Studies in the Sciences of Complexity, Addison-Wesley, New York, 1988).
3. S. A. Kauffman, *The Origin of Order* (Oxford University Press, Oxford, 1993).
4. R. Dawkins, *The Blind Watchmaker* (Norton, New York, 1987).
5. P. M. C. de Oliveira, S. M. Moss de Oliveira, and S. L. A. de Queiroz, *Physica A* **175**:345 (1991).
6. P. M. C. de Oliveira, *Computing Boolean Statistical Models* (World Scientific, Singapore, 1991).
7. J. P. Bouchaud, *J. Phys.* (Paris) **12**:1705 (1992).
8. J. P. Bouchaud, E. Vincent, and J. Hammann, preprint (1993).
9. H. E. Stanley, T. S. Chang, F. Harbus, and L. L. Liu, in *Proceedings of the International Summer School Enrico Fermi, Course LIX*, K. A. Müller and A. Rigamonti, eds. (North-Holland, Amsterdam, 1976).
10. K. Binder and A. P. Young, *Rev. Mod. Phys.* **58**:801 (1986).
11. J. Vannimenus and G. Toulouse, *J. Phys. C* **10**:537 (1977).
12. E. E. Vogel, J. Cartes, S. Contreras, and J. Villegas, *Phys. Rev. B* (1993), submitted.

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