

Mean-Field Spin Glass in the Observable Representation

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The state space for the N -spin mean-field (Sherrington-Kirkpatrick) spin glass—nominally an N -cube—is embedded in a low dimensional continuous space in such a way that metastable and stable phases can easily be discerned, a concept of nearness of configurations defined, and peaks in the Parisi q -parameter overlap distribution identified. The dynamical and partly hierarchical interrelation of these phases can be directly imaged.

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The mean-field (Sherrington-Kirkpatrick) spin glass [1] continues to be an active focus of research both for its own sake and for the light it can cast on the short-range spin glass [2–7]. Nevertheless, problems remain. Among these is the difficulty of visualizing its state space. One would like to have an idea of the energy landscape, the absolute and local minima, an image of what states are “near” those minima and perhaps even get a handle on the elusive notion of pure state in finite systems. It would be especially convenient if phases, metastable or stable, could be identified and well localized on this landscape. A geometric picture in which at least some of these goals can be achieved is the object of the present article.

For systems evolving under stochastic dynamics there is an embedding, known as the *observable representation* (OR) [8,9], of the state space into continuous spaces of various dimension. In it the features just mentioned stand out, with phases identified as extrema of a certain convex set and with a distance inherited from the dynamics. This provides a direct image of the interrelationship between phases and of the hierarchical structure of passage from phase to phase. The notion of metastable phase—problematic in infinite volume systems—is natural in this context. Finally, there is no restriction of our method to mean field models, the only issue being whether lattice models exhibit structure for systems small enough for our technique to be applied.

The OR provides an abstract definition of phase (stable and metastable) and can be used to see the relation of phases to the Parisi overlap parameter [10], “ q .” In addition, the temporal flow of child phases into parents can be displayed. In this Letter I use as the state space all 2^N configurations. As I will show, reduction in the state space is possible, opening the door to extensive use of this method.

I first recall the definition of the OR. Then I offer evidence for structure in the 12-spin system (those less troubled by state-space size have not looked at such small systems). Then I get to the main point, which is to show how structure is displayed in the observable representation. I close with a discussion of prospects.

The observable representation and associated notation.—States are $x, y, z \in X$, with X a finite set. The

system moves in discrete time according to an (assumed) irreducible stochastic matrix R : $R_{xy} = \text{Pr}[z(t+1) = x | z(t) = y]$. For a spin glass, R satisfies detailed balance (although Refs. [8,11] are more general). The eigenvalues of R are therefore real and can be written $1 = \lambda_0 > |\lambda_1| \geq |\lambda_2| \dots \geq 0$. λ_0 is associated with the stationary distribution: $Rp_0 = p_0$; the eigenvalue relation for the associated left eigenvector, $A_0(x) \equiv 1$, expresses conservation of probability. Left eigenvectors are designated A_k (same k as in $\{\lambda_k\}$) and right eigenvectors p_k . They satisfy $\langle A_k | p_j \rangle = \delta_{kj}$ and are normalized by $\max_x |A_k(x)| = 1$.

The m -dimensional *observable representation* is the set (an embedding of X in \mathbb{R}^m)

$$\mathcal{A}_m \equiv \{ \mathbf{A} \in \mathbb{R}^m \mid \mathbf{A} = (A_1(x), \dots, A_m(x)), x \in X \}. \quad (1)$$

To visualize, write the first m left eigenvectors as row vectors, one atop the other. The points of \mathcal{A}_m are then the *columns*:

$$\begin{array}{ccccccc} & \mathbf{A}(x_1) & \mathbf{A}(x_2) & \mathbf{A}(x_3) & \dots & & \\ & \downarrow & \downarrow & \downarrow & & & \\ A_1 \rightarrow & A_1(x_1) & A_1(x_2) & A_1(x_3) & \dots & & \\ A_2 \rightarrow & A_2(x_1) & A_2(x_2) & A_2(x_3) & \dots & \dots & \\ \vdots & \vdots & \vdots & \vdots & & & \\ A_m \rightarrow & A_m(x_1) & A_m(x_2) & A_m(x_3) & \dots & & \end{array} \quad (2)$$

In [8] we established the properties of \mathcal{A}_m when there is a phase transition, which corresponds [11] to eigenvalue near degeneracy for the largest eigenvalues. If λ_m is close to 1, while λ_{m+1} is not, \mathcal{A}_m is a simplex with points belonging to the phases located at the vertices. Interior points are not in phases, but their barycentric coordinates with respect to the extrema are the probabilities that these points evolve towards the corresponding phase.

In [8] we distinguished which assertions remain true if λ_{m+1} is not small. The convex hull of \mathcal{A}_m need not be a simplex, but there still are extrema, and points dynamically close and in a phase cluster about the extrema. The relation between dynamical proximity and closeness in \mathcal{A} also holds for nonextrema [9]. Let $D(x, y; t) \equiv \sum_u |(R^t)_{ux} - (R^t)_{uy}| / \sqrt{p_0(u)}$. $(R^t)_{ux}$ is the probability that starting at x

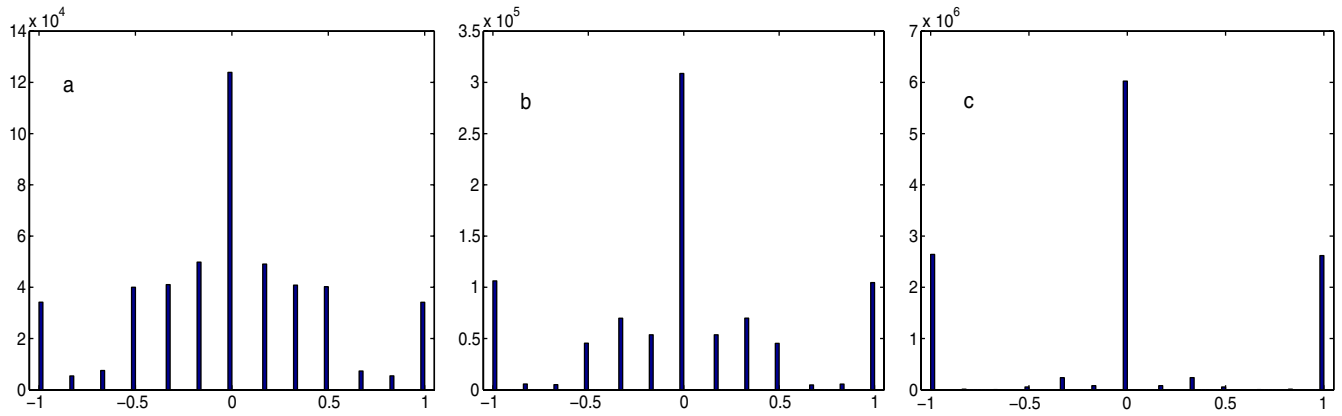


FIG. 1 (color online). Histogram of the distribution function for “ q ,” for the same quench, for a succession of times. $T = 0.2T_c$ and $t = 100, 200,$ and 3000 . The central peak does not correspond to an absence of ordering. Rather the phases break into pairs, with half the pairwise products, $x^{(j)}x^{(k)}$, being zero. Fig. 1c is close to the infinite-time distribution, $\sum_{x,y} p_0(x)p_0(y)\delta(q - q_{xy})$.

one arrives at u in t time steps. Then $D(x, y; t)/|\lambda_m|^t \geq [\sum_{\alpha=1}^m |A_\alpha(x) - A_\alpha(y)|^2]^{1/2}$. Points whose distributions merge are spatially close in \mathcal{A} .

Small mean-field models.—For N as small as 12 there are structures associated with slow relaxation to more stable phases. The energy is $E = -\sum J_{jk}\sigma_j\sigma_k/2\sqrt{N}$, with $J_{jk} = \pm 1$ the quenched bonds and $\sigma_j = \pm 1$ the spins. The temperature- T , transition probability from $x \equiv (\sigma_1, \sigma_2, \dots, \sigma_N)$ to $x' \neq x$ is $R(x', x) = \exp\{-[E(x') - E(x)]/T\}/N$, when $E(x') > E(x)$; otherwise it is $1/N$. I permit only single spin flips.

Structure was observed in the time-dependent distribution of the Parisi overlap parameter, “ q ” [4,5,10]: For fixed J , two random initial conditions ($x^{(l)}$) are taken. They evolve separately under the stochastic dynamics and the overlap $q \equiv x^{(1)}x^{(2)}/N \equiv (1/N)\sum_{k=1}^N \sigma_k^{(1)}\sigma_k^{(2)}$ is calculated. Values of q are collected for many times and many initial conditions. In the distribution function for q , peaks represent persistence in pairs of metastable phases, and the time dependence of the distribution reflects relaxation.

For $N = 12$ there is structure. Figure 1 shows histograms for a specific quench, J_{ij} (to be called \hat{J}), for three run times. For a few hundred time steps the system gets

caught in metastable phases whose importance gradually lessens (space limitations preclude more figures) until about time 3000. This time scale is confirmed by $\{\lambda_k\}$. Note that the central peak does *not* indicate an absence of structure (see the caption).

Visualizing structure in the OR.—Fig. 2 shows \mathcal{A}_2 and \mathcal{A}_3 for the R associated with \hat{J} . The first few eigenvalues of $1 - R$ are: $0, (2.1, 7.1, 8.3) \times 10^{-6}, (5.58, 5.62, 11.19, 11.20) \times 10^{-4}, (7.92, 7.93, 10.84, 10.86) \times 10^{-3}$. By the criteria of [8], there are many phases.

The following features can be identified. The four “corner” states in \mathcal{A}_2 are absolute minima. The clusters of nearby points constitute the ground states, and as in [8] (Fig. 3), contain more points than is evident to the eye. The prominent points near $A_1 = 0$ (at large $|A_2|$) support metastable phases (they are extrema in higher dimension), but do not evolve to unique target phases. A state at one of these positions will ultimately find itself with near 50–50 probability on one side or the other. This statement is not based on simulation (although it can be so verified), but rather on the “barycentric” theorem quoted earlier. The prominent points near $A_2 = 0$ (with large $|A_1|$) have similar properties and asymptotics.

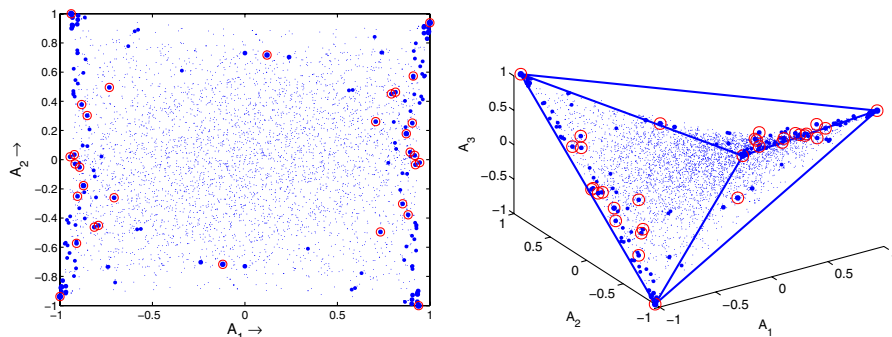


FIG. 2 (color online). \mathcal{A}_2 and \mathcal{A}_3 for \hat{J} . Symbol size increases with equilibrium weight (hence lower energy). Circles indicate local minima in energy. For \mathcal{A}_3 the convex hull (a tetrahedron) has been outlined. The vertical lines of large-weight points on the left and right sides of \mathcal{A}_2 are at approximately right angles to one another in \mathbb{R}^3 .

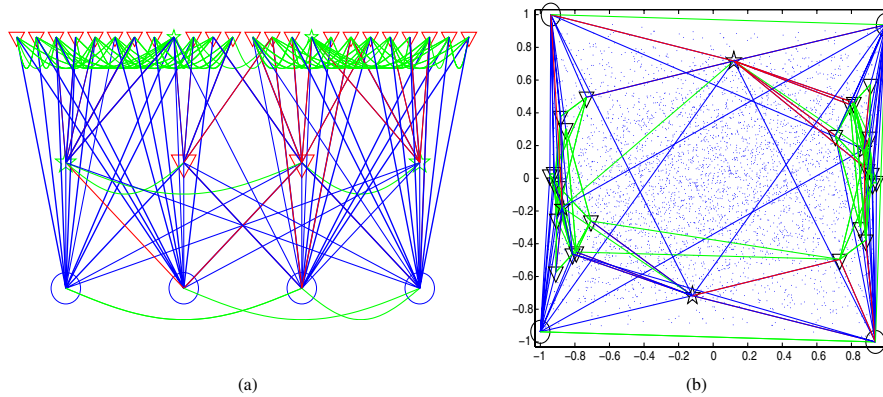


FIG. 3 (color online). Representations of the matrix \tilde{R} , as explained in the text. The quench is \hat{J} . The sequence of symbols (in order of declining amount) is circle, star, base-up triangle, base-down triangle. The sequence of colors is black, red, blue, green, cyan.

To study the hierarchy of temporal evolution I use the extrema of \mathcal{A} to identify phases. For \hat{J} there are 32 local minima and by \mathcal{A}_7 they are all extrema. I use them as the nuclei of the phases. Among J 's this is a relatively large number, but our results are unchanged when non-local-minimum extrema are used as nuclei. A significant aspect of phase identification is the positing of a distance on X . We have previously discussed several metrics [12,13] and I here use $d_t^2(x, y) \equiv \sum_{k \geq 1} |A_k(x) - A_k(y)|^2 |\lambda_k|^t$. t is an adjustable time scale. The results are not sensitive to this choice, nor to t .

Phases can now be defined: For a phase nucleus, x (an extremum in \mathcal{A}_m for appropriate m), the distance to the nearest other nucleus was found. All points within half that distance were associated with x and called its phase. This left points in “no man’s land”, which was formally treated as another phase. For \hat{J} they were about 40% of the points. Nevertheless, their total p_0 measure was only $\sim 2 \times 10^{-5}$.

The next step was to study the induced dynamics among the phases. An ensemble of points was started within each phase with the probability of being in a given state (within that phase) proportional to its p_0 measure [14]. I then checked the likelihood that on exiting this phase it went to a particular other phase. This coarse-grained matrix of transition probabilities is designated \tilde{R} .

It is in a diagrammatic representation of the flows in \tilde{R} that one can hope to see the hierarchical structure associated with relaxation through a succession of metastable phases. Figure 3 shows two such representations. In the first, the phases are sorted into 3 categories, long-, medium-, and short-lived. On the lowest level are the longest-lived, etc. The symbol and color correspond to the amount of inflow. A phase’s left-right position follows the A_1 values of that phase’s nucleus among phases at the same lifetime level. Lines indicate transition probabilities, with line width a monotonic function of transition probability. Blue lines are flow from higher (shorter lifetime) levels to lower, red go oppositely, and green are lateral transitions. A perfect hierarchical structure would be al-

most all blue and each node would flow to only one other node. This is clearly not the case, with the principal deviations related to the col-like metastable phases.

A second display is to superimpose the flows of \tilde{R} on the OR for R (putting a phase at the location of its nucleus). This is Fig. 3(b). Now the symbol reflects the energy of the nucleus of the phase, and its size the lifetime. Again the breakdown in tree structure arises principally from the quasicolts. The stable phases are in the corners, and metastable phases with flows to more than one side of the diagram have intermediate lifetime and $A_1 \approx 0$.

If one were to watch the time evolution of the system on this embedding, it would have the appearance of a random walk on a landscape of hills and valleys, as envisioned, for example, in Kobe and Krawczyk [15], who present images resembling ours. The advantage of using the OR is that I do not need to resort to hamming distance (which, can be a poor measure of dynamical proximity), but have a metric that is automatic and has physical significance.

The variation of these figures with quench can be seen in Fig. 4, illustrating \tilde{R} for a 13-spin system. There are no isolated local minima (there are equal energy pairs differing by a spin flip), nor do the local-minima exhaust the extrema used. Here a more treelike structure occurs. The cols (the most important being the base-down triangles at $A_1 \approx \pm 0.45$) are both of lesser weight and have larger $|A_1|$ values. This also is evident in Fig. 4(a), since the principal phases that feed both sides have relatively short lifetimes.

Returning to \hat{J} , I interpret the transients in Fig. 1. I have already noted that the central peak persists for long times because the product of points in the stable phases is zero for several combinations. In the time-200 histogram the largest peaks away from 0 or ± 1 are at $q = \pm 1/3$. Aside from combinations of low probability these involve *exclusively* the two phases at $(A_1, A_2) \approx \pm(0.12, 0.72)$, which are the stars in Fig. 3(b) (and are extrema of \mathcal{A}_6). Indeed, going to our lifetime data, there are only 4 phases with lifetimes on the order of hundreds. The others are at $(A_1, A_2) \approx \pm(0.87, 0.18)$ (referred to earlier as metastable

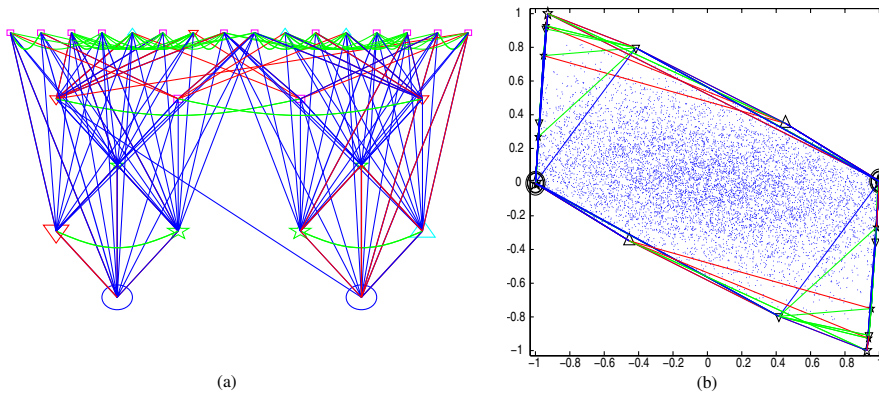


FIG. 4 (color online). Representations of the matrix \hat{R} for a 13 spin system, as explained in the text. The same symbols, etc., are used as in the previous figure.

phases). Their inner product with the stable states however is either 0 or ± 1 . I have thus identified the phases giving rise to a specific peak in the Parisi q distribution.

Summary and prospects.—The observable representation for the mean-field spin glass (and for other systems as well) provides a continuous embedding of a discrete state space. In the OR, the distance between points reflects dynamical proximity and the extrema of the convex hull correspond to phases, stable and metastable. Moreover, the barycentric coordinates of a point in the interior of the convex hull provide probabilities for the arrival of this point in one or another of the phases.

An obstacle to the implementation of this representation is the growth of the state space with N , the number of spins. There are two reasons, however, that it should prove possible to go well beyond the N 's used in this article. First, my own resources, both with respect to programming and hardware are modest. But more important is the possibility of focusing on the *significant* states. This is done, for example, in Ref. [15], where for the $4 \times 4 \times 4$ lattice spin glass (2^{64} spin states) they restrict themselves to the first 3 levels, comprising $1\,635\,796 \approx 2^{20.6}$ states, a reduction of more than 40 powers of 2. To test whether such a reduction would affect the OR, I restricted the matrix R

associated with \hat{J} to the first 4 energy levels. This gave 162 states in place of 4096. The associated OR is shown in Fig. 5. Comparison with Fig. 2 shows that the restriction has left the important information intact. This justifies optimism that the $3 \times 3 \times 3$ cube should yield to this analysis, and perhaps larger systems as well.

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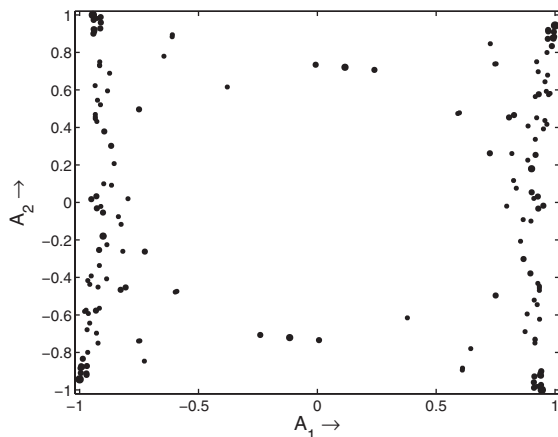


FIG. 5. Observable representation for the same quench (and the same temperature) as the left image of Fig. 2.

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