Invariant geometry of spin-glass states

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(Received 7 July 1986)

We study how the geometry of spin-glass states changes under redefinitions of the metric. We show that in mean-field theory the property of ultrametricity is robust. We present numerical evidence suggesting that in the more realistic $D=2$ and $D=3$ spin-glass models a stronger result may hold, namely that the choice of metric is to a large extent unique.

Much of the recent progress in understanding the nature of the spin-glass phase has focused on the geometry of the space of thermodynamic equilibrium states. A striking feature of this space in mean-field theory is its ultrametric structure,[1] implying a hierarchical organization of states in clusters.

Ultimately, the importance of this ultrametric property will be determined by the extent to which it proves universal. Is it, for instance, a robust property of finite-dimensional spin glasses,[2] in which case it would be experimentally relevant, and of other complex frustrated systems,[3] in which case it may furthermore find applications in combinatorial optimization. And does it also imply a hierarchy of energy barriers, thereby leading to simple models of dynamical relaxation?[4]

Such questions are, in general, hard to address. In this paper we study one aspect of the universality of ultrametricity which can, however, be conclusively verified, namely its invariance under redefinitions of the metric in the space of states. The distance between two spin-glass states a and b has so far been taken to be a measure of the variation in local magnetization[5]

$$d_{ab}^2=\sum_{\text{site } i=1}^{N}\frac{1}{N}(m_i^a-m_i^b)^2\equiv 2(q_{\text{EA}}-q_{ab})\ , \tag{1}$$

where q_{ab} is their overlap, and the self-overlap q_{EA} is state independent. Though natural, this definition is not unique. By analogy with (1) we could define

$$(d_{ab}^{(O)})^2=\sum_i\frac{1}{N}(O_i^a-O_i^b)^2\equiv 2(q_{\text{EA}}^{(O)}-q_{ab}^{(O)}) \tag{2}$$

for any other observable density O_i, such as the local molecular field, a coarse grained magnetization, the energy density, etc.

Now the local details of how one chooses to define the distance between states should not matter, if ultrametricity is to be a meaningful concept, because (i) in real experiments, the precise density measured by a given probe may well be ambiguous (for instance, neutron diffraction experiments with less than perfect resolution would presumably measure a coarse-grained magnetization) and (ii) in most complex frustrated systems (such as the problem of close-packing randomly-shaped tiles, a model for amorphous materials) there is no *a priori* natural definition of the distance between states.

Our results are as follows: (a) We will show explicitly in mean-field theory that the property of ultrametricity is invariant under metric redefinitions, and (b) we will present numerical evidence that in the more realistic $D=2$ and 3 Ising spin-glass models not only is ultrametricity, if present, preserved, but a much stronger result apparently missed by mean-field theory may hold, namely that a wide variety of locally defined metrics are identical up to an overall scale factor. In this sense, the metric in the space of spin-glass states is almost unique, and the geometry universal.

The mean-field theory of spin glasses is described by the long-range Sherrington-Kirkpatrick[6] Hamiltonian

$$\mathscr{H}=-\sum_{i,j=1}^{N}J_{ij}\sigma_i\sigma_j-H\sum_{i=1}^{N}\sigma_i\ , \tag{3}$$

where the σ_i are Ising spins and the J_{ij} are independent quenched random variables with a symmetric Gaussian distribution of variance $1/\sqrt{N}$. The property of ultrametricity was demonstrated[1] by calculating the average probability that three states a, b, and c have mutual magnetization overlap z_1, z_2, and z_3. Using the replica trick this can be written

$$P(z_1,z_2,z_3)=\lim_{n\to 0}\operatorname*{Tr}_{\sigma}\prod_{i<j}\int_{-\infty}^{\infty}dJ_{ij}\sqrt{N/2\pi}\exp\left[-\frac{NJ_{ij}^2}{2}\right]\exp\left[-\beta\sum_{e=1}^{n}H(\sigma_i^e)\right]$$
$$\times\delta[q_{ab}(\sigma)-z_1]\delta[q_{bc}(\sigma)-z_2]\delta[q_{ca}(\sigma)-z_3]\ , \tag{4}$$

where Tr_σ stands for a summation over all spin configurations of the n replicas and the magnetization overlap of two real replicas is

$$q_{ab}(\sigma)=\frac{1}{N}\sum_i \sigma_i^a\sigma_i^b \ . \tag{5}$$

Using standard saddle-point integrations, this is rewritten as

$$P(z_1,z_2,z_3)=\lim_{n\to 0}\frac{1}{n(n-1)(n-2)} \times \sum_{a\neq b\neq c}\delta(Q_{ab}-z_1)\delta(Q_{bc}-z_2)\delta(Q_{ca}-z_3)\ , \tag{6}$$

where Q_{ab} is the $n\times n$ matrix that minimizes the free energy. Below the transition temperature, it has the hierarchical form obtained by Parisi[7] and best described by the homogeneous tree shown in Fig. 1, and a *monotone nonincreasing* and *positive* (for nonvanishing magnetic field H) sequence q_i. It follows immediately from the hierarchical form of Q_{ab}, and Eq. (6), that $P(z_1,z_2,z_3)$ vanishes unless the two smaller overlaps coincide. Thus all triangles in the space of pure states have their two bigger sides equal with probability one, which is the statement of ultrametricity.

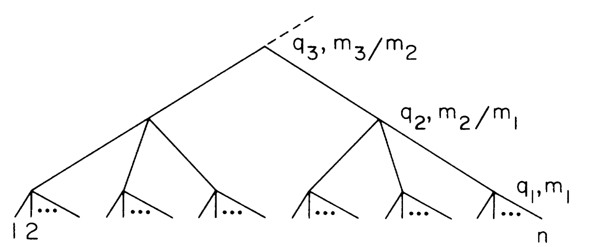

FIG. 1. The tree describing Parisi's hierarchical replica symmetry breaking ansatz. Then entry $Q_{ab}=q_i$ depends only on the level i of the nearest common ancestor of a and b. The bifurcation number of all branches at the ith level is m_i/m_{i-1}.

We are now ready to show that the property of ultrametricity is robust under redefinitions of the metric, of type (2).[8] Instead of a general proof, which would be tedious and not particularly illuminating, we will restrict ourselves here to two examples where the observable O_i is (a) the local molecular field, and (b) the energy density; these can then be readily generalized.

(a) *Local molecular field.* The field overlap of two real replicas is defined as

$$q_{ab}^{(h)}\equiv\frac{1}{N}\sum_i\left[\sum_j J_{ij}\sigma_j^a\right]\left[\sum_k J_{ik}\sigma_k^b\right] .$$

To calculate the average probability that three states a, b, and c have mutual field overlaps z_1, z_2, and z_3, we substitute $q_{ab}^{(h)}$ for q_{ab} in Eq. (4), and then replace in turn J_{ij} and $q_{ab}(\sigma)$ (for $a\neq b$) by their saddle-point values $(\beta/N)\sum_{i=1}^n \sigma_i^e\sigma_j^e$ and Q_{ab}, respectively. The result is the same as Eq. (6), but with the saddle-point matrix Q replaced by

$$Q^{(h)}=\beta^2(Q+\mathbf{1})^3\ ,$$

where $\mathbf{1}$ is the identity matrix. Now matrices of the Parisi form are closed under addition and multiplication, as can be easily seen by inspection. That monotonicity of q_i is preserved under multiplication follows from the trivial inequality $x\tilde{x}+y\tilde{y}\geq x\tilde{y}+\tilde{x}y$ if $x\geq y$ and $\tilde{x}\geq\tilde{y}$. Thus the matrix of field overlaps $Q^{(h)}$ has the same hierarchical form as the saddle-point matrix Q, which suffices to establish ultrametricity in the new metric.

(b) *Energy density.* The energy overlap of two replicas is

$$q_{ab}^{(E)}(\sigma)=\sum_i\left[\sum_j J_{ij}\sigma_i^a\sigma_j^a\right]\left[\sum_k J_{ik}\sigma_i^b\sigma_k^b\right] .$$

Going through the same steps as before, we arrive at the joint probability of mutual energy overlaps of a triplet given by Eq. (6) with Q now replaced by

$$Q_{ab}^{(E)}=\beta^2\sum_{c,d=1}^{n}(Q+1)_{ac}(Q+1)_{bd}M_{abcd}\ ,$$

where M_{abcd} is the one-site average[9]

$$M_{abcd}=\left[\mathop{\mathrm{Tr}}_{\sigma}\sigma^a\sigma^b\sigma^c\sigma^d\exp\left[\tfrac{1}{2}\sum_{e,f}Q_{ef}\sigma^e\sigma^f\right]\right]\Big/\left[\mathop{\mathrm{Tr}}_{\sigma}\exp\left[\tfrac{1}{2}\sum_{e,f}Q_{ef}\sigma^e\sigma^f\right]\right] .$$

To show that $Q^{(E)}$ has the same hierarchical structure as Q, note that the invariance group of the latter is the direct product of the permutation groups of m_{i_A}/m_{i_A-1} branches at each branching point A on the tree:

$$Q_{ab}=Q_{\pi(a)\pi(b)};\quad \pi\in\bigotimes_{\substack{\text{branching}\\ \text{point } A}}P_{m_{i_A}/m_{i_A}-1}\ .$$

When a runs over all n replicas so does $\pi(a)$ and hence, by a change of dummy variables it follows that $Q^{(E)}$ has the same symmetry group, and thus also the same hierarchical structure as the Parisi matrix. It remains to prove that its entries are larger the more they are nested. This can be shown with the use of lengthy to prove but straightforward inequalities[10] for the ferromagnetic hierarchical model with Hamiltonian $H=\frac{1}{2}\sum_{a,b}Q_{ab}\sigma^a\sigma^b$ which is a generalization of the long-range Dyson ferromagnet. The positivity of Q_{ab} is crucial here.

The above examples can be easily generalized to other gauge-invariant definitions of the metric. The invariance of ultrametricity is a consequence of the fact that the distance $d_{ab}^{(O)}$ of two states is a (monotone increasing) function of their magnetization distance alone: $d_{ab}^{(O)}=f^{(O)}(d_{ab})$. (Note that such a functional relationship does not exist among the various overlaps of arbitrary spin configurations.) In mean-field theory the functions $f^{(O)}$ are, in general, complicated.

We will now present numerical evidence that in the more realistic two- and three-dimensional spin-glass models (a) $d_{ab}^{(O)}$ are still monotone functions of d_{ab}, and (b) for several Z_2-odd densities O_i these functions appear to be, surprisingly, straight lines. Hence, such changes of metric amount to a simple rescaling that preserves not only the notion of ultrametricity, but all other geometric features (such as the distribution of overlaps) as well.

Our numerical simulations were done on the IBM 3081 at SLAC. We studied models (3), with J_{ij} being ± 1 with equal probability for nearest neighbors on a $D=2$ square, and $D=3$ cubic lattice, and zero otherwise. We used periodic boundary conditions on lattices whose size varied from 16^2 to 54^2 and from 8^3 to 14^3. We slowly (~ 5000 lattice sweeps) cooled several replicas, typically 50, of the same sample down to some low temperature, that ranged from $\beta=0.8$ to 3.0, and then in each replica we measured the densities of magnetization (m_i), molecular field (h_i), energy (E_i), coarse-grained magnetization (m_i^c), and a composite operator (c_i), where m_i^c is the average magnetization over an elementary square of cube of the lattice with i at its lower left corner, and for the composite operator we took

$$c_i = \left\langle \frac{1}{2D} \left[\sum_{\substack{\text{nearest} \\ \text{neighbors } j}} J_{ij}\sigma_j \right]^2 \sigma_i \right\rangle .$$

The averages were taken over a few hundred Monte Carlo sweeps. Finally we measured the distances $d^{(O)}$ between each replica and some randomly chosen fixed replica, for each of the above densities O, as well as the self-overlaps $q_{\mathrm{EA}}^{(O)}$.

Consistency checks included verifying that the internal energy of all our states agreed with previous simulations

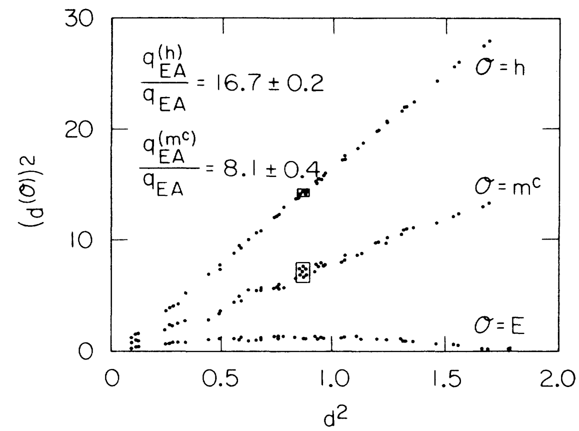

FIG. 3. Plots of $(d^{(h)})^2$, $(d^{(m^c)})^2$, and $(d^{(E)})^2$ versus d^2 for a typical $3D$ $12\times12\times12$ sample at $\beta=2.1$.

to within 1%,[11] and that self-overlaps are to a good approximation state independent and self-averaging; we used their fluctuations to estimate error bars. We made no attempt to establish the presence or absence of an equilibrium transition, for which much better data already exists;[12] for all we know our states could be metastable.

In Figs. 2 and 3 we present typical distributions of $(d_{ab}^{(O)2}, d_{ab}^2)$ with $O=h$ and c for a $D=2$ sample, and $O=h$ and m^c for a $D=3$ sample, at zero external field. The little squares indicate the area in which the points $(q_{aa}^{(O)}, q_{aa})$ fall for all replicas a. Assuming state-independent self-overlaps, the square sizes can be used as estimates of the corresponding error bars. Within these error bars, the distributions are (1) one-dimensional curves, rather than spread out over the plane, and (2) remarkably well fitted by straight lines. Due to the global Z_2 invariance, there is a reflection symmetry about the point $(q_{\mathrm{EA}}^{(O)}, q_{\mathrm{EA}})$; thus the slopes of the straight lines are the ratios of the corresponding self-overlaps, whose values

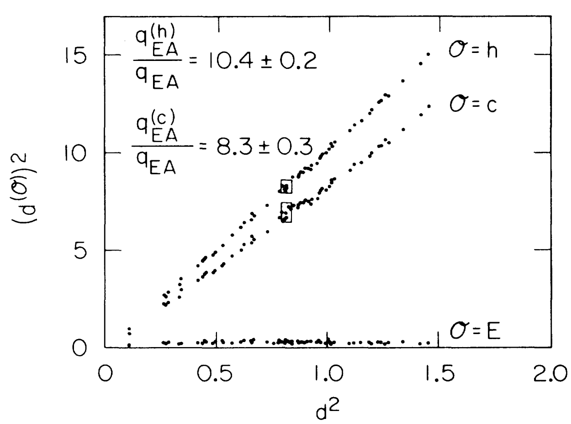

FIG. 2. Plots of $(d^{(h)})^2$, $(d^{(c)})^2$, and $(d^{(E)})^2$ versus the magnetization distance d^2, for 50 replicas of a typical $2D$ 24×24 sample at $\beta=2.1$. The little squares indicate where the corresponding self-overlaps for all 50 states fall. The slopes are the ratios of self-overlaps; the quoted errors are due to fluctuations from sample to sample. The energy fluctuations $(d^{(E)})^2$ may be vanishing in the thermodynamic limit.

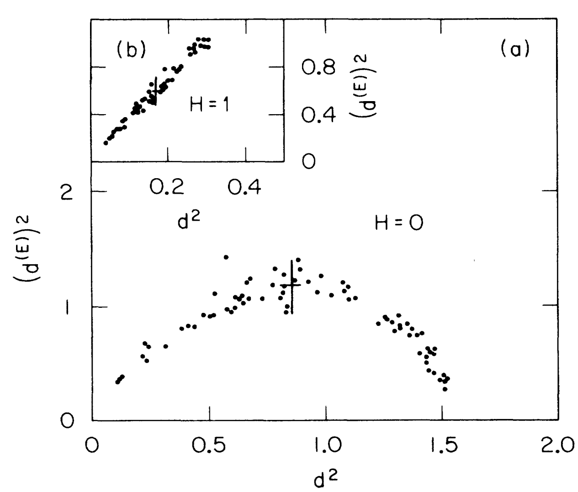

FIG. 4. (a) A typical $(d^{(E)})^2$ versus d^2 curve at external field $H=0$. In the insert, (b) a magnetic field $H=1$ has been switched on.

we found to be essentially independent of lattice size, cooling rate, sample, and to a good approximation temperature below $1/\beta = 1$; they are given on the figures. Note that if gauge noninvariant additions to the metric self-average to zero, one would expect $q_{EA}^{(m^c)}/q_{EA} = 8$ in three dimensions, which is consistent with the "experimental" value. Let us stress, that although our data shows no statistically significant deviations from linear laws, we know of no theoretical argument that would exclude such deviations.

In Figs. 2 and 3, on the same scale as $[d^{(h)}]^2$, we have also plotted $[d^{(E)}]^2$, to show that the energy-density fluctuations from one state to another are relatively small. A preliminary scaling analysis suggests that in $D = 2$ these fluctuations may actually vanish in the thermodynamic limit, an intriguing possibility. In $D = 3$, the $(d^{(E)})^2$ curves seem to converge to the symmetric shape shown in Fig. 4(a). The symmetry under reflections about $d = q_{EA}$ is due to the fact that E_i is Z_2 even, and can be lifted in the presence of a magnetic field, as shown in Fig. 4(b). Our statistics are not good enough to determine the functional form of these curves, although we can safely say that, up to reflections, they are monotone increasing and hence preserve the notion of ultrametricity.

In conclusion, we have presented analytic (in mean field theory) and numerical (in the $D = 2$ and 3 spin-glass models) evidence, that the notion of ultrametricity is invariant under redefinitions of the distance between states. We have also presented evidence that in the $D = 2$ and 3 models, the choice of metric may to a large extent be unique.

This work was supported by the Department of Energy under Contract No. DE-AC03-76SP00515.

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[8] For technical reasons, our method only applies to gauge-invariant definitions. At zero external field this is not a real restriction since, as one can argue by performing a random gauge transformation, any gauge noninvariant addition to the metric should self-average to zero.

[9] The reader unfamiliar with calculations in the framework of Parisi's replica symmetry breaking can consult, for instance: M. Mézard and M. Virasoro, J. Phys. (Paris) **46**, 1293 (1985); also J. R. L. De Almeida and E. J. Lage, J. Phys. C **16**, 939 (1982).

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[11] For a recent review see the contributions of K. Binder, W. Kinzel, and also I. Morgenstern and A. P. Young, at the Heidelberg Colloquium on Spine Glasses, edited by J. L. Van Hemmen and I. Morgenstern (Springer-Verlag, New York, 1983).

[12] There is wide consensus that no transition occurs in $D = 2$, see Ref. 14. In $D = 3$ recent high statistics simulations are by A. J. Ogielski and I. Morgenstern, Phys. Rev. Lett. **54**, 928 (1985); J. Appl. Phys. **57**, 3382 (1985); A. T. Ogielski, Phys. Rev. B 32, 7384 (1985); R. N. Bhatt and A. P. Young, Phys. Rev. Lett. **54**, 924 (1985).