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LETTER TO THE EDITOR

Pure states in spin glasses

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Abstract. The question of the existence of multiple pure states in spin glasses and other disordered systems is considered. We show that the distribution of overlaps, $P(q)$, is an unreliable indicator of how many distinct pure states a system has. We discuss the definition of, and possible relations between, pure states. We also discuss the spin glass on a Bethe lattice and the infinite-range model, pointing out why their ordered phases are likely to be unlike that of realistic spin glass models. Various possibilities for the behaviour of finite-range spin glasses are discussed.

Much recent theoretical activity on spin glasses has been focused on the question of the existence of many distinct stable thermodynamic states at low temperatures and magnetic fields. This was primarily stimulated by an ansatz of Parisi for the solution of the infinite-range Sherrington-Kirkpatrick (SK) spin glass model [1], which indicates the existence of infinitely many states in a region of the magnetic field, H, and temperature T, plane [2]. On the other hand, recent work suggests that realistic spin glass models with finite-range interactions in a finite-dimensional space may well behave quite differently [3-5]. In a companion letter [6], we discuss the consequences of this picture for pure states in realistic spin glass models.

In this letter we discuss various general issues related to the question of pure states in spin glasses and other statistically translationally invariant (i.e. 'stationary') disordered systems. We first discuss the definition of pure states and possible relationships between distinct pure states, giving examples to illustrate the various possibiliites. We point out that the distribution of overlaps between replicas, $P(q)$ [2, 3], is not a very reliable indicator of the number of pure states in a system. We give examples in which $P(q)$ (*a*) ignores the presence of a physically important pure state and (*b*) gives the appearance of many states when only two are present.

Recent work has shown that the spin glass on a Bethe lattice behaves very much like the SK model [7]. We explain why the Bethe lattice model, although it only has short-range interactions, may behave very differently from spin glasses on finite-dimensional lattices. We also discuss how the SK model is only related to a rather unphysical limit of realistic spin glasses as the dimensionality of the lattice d, tends to infinity.

(*i*) *Definitions of states.* First we must define 'states' and 'pure states' [8]. We are interested in the states in a *single* realisation of the quenched disorder in an infinite system. A state is defined in terms of the correlation functions in all *finite* regions obtained as the thermodynamic limit of an infinite sequence of boundary conditions.

Thus each state can be selected by a boundary condition arbitrarily far away. The linear combination of any two states is also a state, since it is selected by a linear combination of boundary conditions. Therefore the set of all states is convex. For any given state the correlation functions (expectation values of operators O) in any finite region can be decomposed in the form

$$\langle O\rangle = \sum_{\alpha} \mu_\alpha \langle O\rangle_\alpha$$

in terms of the *pure* (*or extremal*) states, α, which are the extremal elements of the set of all states. Note that only the thermal average is being performed here, not an average over disorder. A system that has many states must have the property that, even in the thermodynamic limit, the deep interior of the system remains very sensitive to boundary conditions. A *ground state* is simply a pure state at zero temperature. Ground states have the property that their energies cannot be lowered by altering the configuration in any finite region of the system.

(*ii*) *Relationships between pure states.* If a system has more than one pure state then one should ask what are the differences between the states. Let us consider two different pure states, α and β. There exist several possibilities. (*a*) Globally congruent: α and β are simply related by a global symmetry of the system. This is the case for most familiar long-range ordered states, e.g. crystals, ferromagnets, etc. The opposite extreme is that α and β are not even *locally* related by symmetry. This may occur in two ways. (*b*) Dissimilar: α and β are unrelated by symmetry, and not even statistically similar. This occurs at many first-order phase transitions (e.g. liquid–vapour). (*c*) Similar but incongruent: α and β are unrelated by symmetry but have the same (up to a global, possibly statistical, symmetry) spatially averaged correlation functions. This highly non-trivial possibility occurs in the random-field Ising model ordered phase, where only a *statistical* symmetry is broken. (*d*) Regionally congruent: finally it is possible that α and β are not globally congruent due to the existence of domain walls or other defects, but are locally related by symmetry almost everywhere, i.e. in all but a vanishing fraction of regions of the system. This occurs for a lattice Ising ferromagnet with a domain wall present which is smooth (i.e. at temperatures below its roughening transition) and thus disrupts the order only near a particular lattice plane. In addition to these basic distinctions, more complicated possibilities also exist, such as coexistence between congruent and incongruent states separated by interfaces; we will not dwell on these here. Note that a rough domain wall does *not* constitute a distinct pure state because it cannot be forced through a particular location by infinitely far boundary conditions. This is true for the usual thermally rough domain wall, as well as for domain walls that are rough at $T=0$ due to disorder [9]. For any finite-size disordered ferromagnet in $d \leqslant 3$ (or $d<5$ if the disorder is strong enough) [9] a rough domain wall can be forced through the system for $T<T_c$. However, with a probability which tends to unity as $N\to\infty$, the domain wall will, for all boundary conditions, lie arbitrarily far away from any chosen point. Thus the correlation functions in any fixed finite region will be simply linear combinations of the up and down magnetised states.

(*iii*) $P(q)$. The Parisi solution of the SK model ordered phase [2] has been interpreted as indicating the existence, in the thermodynamic limit where the number of spins $N\to\infty$, of many states, each labelled by an index α and having total free energy F_α. The special properties of the Parisi solution [2] depend on an infinite set of states, each of which contributes a non-zero weight $\mu_\alpha \propto \exp(-F_\alpha/T)$ to the unrestricted Boltzmann average. In order for this to occur, the total free energy of each of these states must differ from the lowest by only a *finite* amount in the thermodynamic limit.

The properties of the states of the SK model have been probed by studies of the distribution of overlaps between two exact copies or replicas, a and b, of the same system [2]. The overlap between the configurations of the two replicas is

$$q^{ab} = (1/N) \sum_i S_i^a S_i^b$$

where the sum runs over all N pairs of spins, $S_i^{a,b} = \pm 1$. The distribution of these overlaps is $P(q) = [\langle \delta(q - q^{ab}) \rangle]$, where the angular brackets here denote independent Boltzmann averages over each system and the square brackets denote a configurational average over the disorder. For the Parisi solution of the SK model, $P(q)$ is, for $T < T_c$, the sum of a continuous part and two delta functions, as shown in figure 1(a), which is interpreted as indicating the existence of infinitely many states with a continuous distribution of overlaps between states [2]. However, $P(q)$ arises from a Boltzmann average, so does not contain information about possible physically relevant pure states that have the same free energy *per spin* as the lowest free energy state but whose total excess free energy diverges (less rapidly than N) as $N \to \infty$. Thus, even if $P(q)$ consists of just one or two delta functions for a given system, as has been suggested for realistic spin glasses [3-5], this by itself does not rule out the existence of many states. (Note that differences in total free energy of states are not in general well defined; they depend on how the thermodynamic limit is taken.)

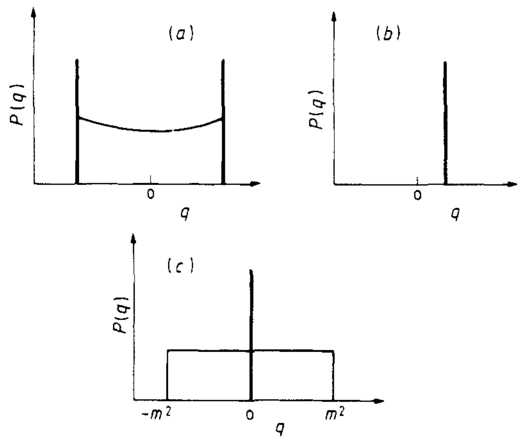

Figure 1. The form of the distribution $P(q)$ of overlaps q for (a) the SK model ordered phase, (b) a random-field Ising model for all finite temperatures, $T \geq T_c$ or $T < T_c$, and (c) an Ising ferromagnet with antiperiodic boundary conditions in all directions for $T < T_c$ and *either* $T < T_R$ *or* $T \geq T_R$. The bold vertical lines denote delta functions.

An example where $P(q)$ is insensitive to the existence of an important pure state is a three-dimensional random-field Ising model at low temperatures, with a random field strength that is weak enough so that there is long-range ferromagnetic order [10]. With either free or periodic boundary conditions the similar but incongruent 'up' and 'down' magnetised states of this system differ in free energy by $O(N^{1/2})$ due to fluctuations in the random fields. Hence, for $N \to \infty$, only one of them enters in $P(q)$, which is thus (even before configurational averaging) a delta function at

$$q = N^{-1} \sum_i \langle S_i \rangle^2$$

at *all* temperatures, as shown in figure 1(b), with no qualitative change in its form at the ordering transition. In this example $P(q)$ completely ignores the appearance of a new pure state.

Not only can the function $P(q)$ miss physically important states, it can also give the appearance of there being many states when there are not. An example is an exactly solvable two-dimensional Ising ferromagnet on a square lattice with antiperiodic boundary conditions in both directions. This system is uniformly frustrated on a global scale, much as the spin glass is randomly frustrated on local scales. For $T < T_c$, this system orders with magnetisation $\pm m$ everywhere except near a fluctuating domain wall which runs along one of the two diagonals of the lattice. For $N \to \infty$, as illustrated in figure 1(c), $P(q)$ consists of the sum of a delta function at $q = 0$ with weight $\frac{1}{2}$, due to overlaps between configurations with domain walls oriented differently, and a continuous part running from $-m^2$ to $+m^2$, due to configurations with parallel domain walls. This $P(q)$ is qualitatively similar to that of the SK model order phase, although there are only the two distinct pure states with $\pm m$ magnetisation. For the analogous three-dimensional system $P(q)$ will have precisely the same form both *above* the domain wall roughening temperatures, T_R (but $T < T_c$) where there are only two pure states, and *below* T_R where there are an infinite number of pure states corresponding to different positions of the smooth domain wall.

The reason why $P(q)$ gives potentially misleading information in these examples is that it is too global a measurement. Therefore it is sensitive to the *total* free energy and misses completely stable and physically important pure states whose total excess free energy over the minimum free energy state diverges for $N \to \infty$. Because $P(q)$ only looks at the *total* overlap it is also not sensitive to the difference between a small overlap due to domain walls being present and a small overlap due to the two replicas being in incongruent states. Finally, in general, $P(q)$ depends crucially on how the thermodynamic limit is taken (e.g. on the boundary condition). Note that it may be possible to eliminate pathologies such as that for the antiperiodic Ising model by modifying the definition of $P(q)$. However, there may not be any limiting procedure short of using the exact states themselves which yields in the thermodynamic limit a mixture of the up and down states in the random-field Ising model. The same difficulty is likely to occur for any other system which exhibits similar but incongruent pure states.

(*iv*) *Bethe lattice.* A spin glass on the Bethe lattice has recently been shown to exhibit many statistically similar pure states [7] and we show below that these states are generally incongruent. We argue that the presence of many pure states is due to the peculiarities of the Bethe lattice, and therefore should not be taken as an indication that many states are present on finite-dimensional lattices. To illustrate why there are many states for the Bethe lattice model, let us focus on the behaviour of a given pair of nearest-neighbour spins, S_i and S_j. The entire Bethe lattice may be broken into two parts, one containing site i and the other containing site j. These two parts are only connected by the bond between sites i and j (note that no physically realistic lattice with $d \geq 2$ has this property). We assume fixed-spin boundary conditions arbitrarily far away. By summing over all configurations of the spins in each part of the lattice for each orientation of S_i and S_j, we obtain effective fields on each spin which are functions of the particular boundary conditions, B. From this we obtain an effective

Hamiltonian for the spins we are focusing on: $H_{eff} = -J_{ij}S_iS_j - h_i(B)S_i - h_j(B)S_j$ where the effective fields $h_{i,j}(B)$ are independent. The distribution of effective fields can, in principle, be obtained as in [7] and is non-trivial for $T < T_c$. For $0 < T < T_c$ the correlation function $\langle S_iS_j \rangle$ therefore depends on the boundary conditions for all pairs of spins. (For $T = 0$ this dependence may be confined to a non-zero fraction of such pairs.) Thus for two typical uncorrelated boundary conditions $\langle S_iS_j \rangle$ will differ for all pairs of spins. This demonstrates the system's extreme sensitivity to distant boundary conditions and shows that states with different boundary conditions are generally incongruent. It is clear that the peculiarities of the Bethe lattice are instrumental in allowing this sensitivity.

Recent work on the ordered phase of short-range Ising spin glass models on finite-dimensional lattices has emphasised the role of droplet [4] and domain wall [11] excitations and their energetics. The free energy cost to pass a domain wall across a finite hypercubic sample of size $N = L^d$ spins appears to scale as $L^\theta = N^{\theta/d}$ for $N \to \infty$, with $\theta > 0$ for $d \geqslant 3$ [11]. From the above discussion it is clear that a domain wall can be passed across an infinite Bethe lattice at *finite* energy cost by passing it through only one bond. Therefore we see that the analogous exponent satisfies $(\theta/d) \leqslant 0$ for the Bethe lattice. This is important in allowing different boundary conditions to stabilise many different states, as discussed above.

Another important scale is the energy cost of flipping the lowest energy droplet of N spins in a particular region of the interior of a much larger system [4]. For finite-dimensional lattices we expect this droplet energy to scale as $N^{\theta'/d}$, with $\theta' = \theta$, since the domain wall surrounding the droplet is very similar to the domain walls across finite systems discussed in the previous paragraph [4]. We have argued that $\theta'/d < \frac{1}{2}$, which via an Imry–Ma [10] argument implies that there is no spin glass order in the presence of a magnetic field, i.e. no de Almeida–Thouless [12] transition [4]. For the Bethe lattice, on the other hand, the energy cost to produce a droplet excitation of N spins is clearly much more than that of passing a domain wall across a finite lattice of N spins, since the former domain wall must cross more than N bonds, while the latter may cross only one. Thus we expect $\theta'/d > \theta/d$. A simple calculation, similar to those in [7], shows that the average energy to flip N connected spins, allowing nearby relaxations, is proportional to N, i.e. $\theta'/d = 1$. This means that, in some sense, the system has a surface tension. It is consistent with the presence of a de Almeida–Thouless transition [7]. Therefore we find that the energies of low-lying excitations for the spin glass on a Bethe lattice behave very differently from what we expect for spin glasses on finite-dimensional lattices, even in the limit $d \to \infty$. The difference is not surprising, since finite-dimensional lattices have frustration loops on all length scales, while the Bethe lattice does not have any loops at all and is only frustrated due to the boundary conditions.

(*v*) *SK model.* It is also worthwhile considering the relationship between the SK model [1] and spin glasses with short-range interactions in the limit $d \to \infty$. The SK model consists of N spins, all pairs of which interact with identically distributed couplings. A physical representation of this is N spins forming a single 'hypertetrahedron' (all spins equidistant from one another) in a $d = (N-1)$-dimensional space. Such hypertetrahedral units may be packed to form a hypertetrahedral lattice (for $d = 2$, the triangular lattice; for $d = 3$, the FCC lattice, etc) on which a spin glass model with only nearest-neighbour interaction may be considered. The nature of the long-range spin glass order that might occur on such a lattice is determined by correlations between spins separated by many hypertetrahedral lattice units. Thus it is clear that the SK model, being a model of a single isolated unit of size one lattice spacing, does not model the *long*-range order that is present at low temperatures in spin glasses with short-range interactions for $d \to \infty$. It is only a model of possible *short*-range order on length scale one lattice spacing. Note that it might already be helpful to understand the behaviour for the length *two* lattice spacings for $d \to \infty$.

One might object to the previous paragraph on the grounds that infinite-range models give correct descriptions of ordered phases in all well understood models. However, for mean-field theories of ferromagnets, for example, we can consider the coordination number z and the system size, N, to be large *independently* so that with $N \gg z \gg 1$ a *large* high-dimensional system is modelled. In this case the same limit is reached for bulk properties, *independent* of how the limit $N \to \infty$, $z \to \infty$ is taken. For spin glasses, on the other hand, there is no reason to believe that this is the case. Indeed the nature of frustration in spin glasses suggests the contrary. Even for conventional systems infinite-range models miss any spatial structure of ordered states. Examples are domain walls in Ising models and defects and textures in XY or Heisenberg ferromagnets. The analogous low-lying excitations, namely droplet excitations and spin waves, respectively, are also absent in an infinite-range model. Since the differences between incongruent pure states in short-range spin glasses (if they exist) must be precisely such domain walls, defects and textures [13], one has reason to believe that the SK model is not a reliable indicator of how many pure states exist in realistic spin glasses. The infinite-range models *do* give the correct critical behaviour for large *d*, however, and there is no indication that this does not remain true for spin glass models (although one might worry about the influence of Griffiths' singularities). If it is true, it is presumably because spatial fluctuations are unimportant at the fixed point governing the critical behaviour for large *d*. For the spin-glass *ordered* phase, on the other hand, there is competition due to frustration on all length scales which, we argue [4, 6], results in a non-trivial behaviour for all d that is not captured, even in the limit $d \to \infty$, by the SK model. For example, if there are many pure states in the SK model, the distinction between incongruent and regionally congruent states as defined above does not even exist due to the lack of a sensible definition of 'locally'.

(*vi*) *Conclusion.* The natural possibilities for the existence of distinct pure states for realistic Ising spin glasses are as follows.

(*a*) A unique state for all $T > 0$ and magnetic field H.

(*b*) Exactly two states for $H = 0$ and $T < T_c$ which are globally related by a spin flip and therefore congruent. In this case we have previously argued [4] that there is a unique state for $H > 0$ because $\theta/d < \frac{1}{2}$.

(*c*) For $T < T_c$ and $H = 0$, many domain wall states which are regionally congruent, in which case again there is a unique state for $H > 0$, since $\theta/d < \frac{1}{2}$.

(*d*) Several, or many statistically similar but incongruent, states for $T < T_c$, in which case there could still be more than one state for sufficiently small non-zero H and thus a de Almeida–Thouless transition [12].

Possibility (*a*) is almost certainly correct for small *d*, particularly $d = 2$. In a companion letter [6], based on a simple scaling ansatz, we argue that possibility (*b*) is the most plausible for all d (presumably $d \geqslant 3$) for which $T_c > 0$. Unless possibility (*d*) obtains, however, the relationship between states in finite-range spin glasses will not be very different from that in more conventional systems, since possibility (*c*) obtains for, e.g., Ising ferromagnets at $T < T_R$.

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References

[1] Sherrington D and Kirkpatrick S 1975 *Phys. Rev. Lett.* **35** 1792

[2] Parisi G 1979 *Phys. Rev. Lett.* **43** 1574; 1983 *Phys. Rev. Lett.* **50** 1946
Mézard M, Parisi G, Sourlas N, Toulouse G and Virasoro M 1984 *Phys. Rev. Lett.* **52** 1156; 1984 *J. Physique* **45** 843
de Dominicis C and Young A P 1983 *J. Phys. A: Math. Gen.* **16** 2063

[3] Moore M A and Bray A J 1985 *J. Phys. C: Solid State Phys.* **18** L699

[4] Fisher D S and Huse D A 1986 *Phys. Rev. Lett.* **56** 1601

[5] Bovier A and Frohlich J 1986 *J. Stat. Phys.* **44** 347

[6] Fisher D S and Huse D A 1987 *J. Phys. A: Math. Gen.* **20** L1005

[7] Thouless D J 1986 *Phys. Rev. Lett.* **56** 1082
Chayes J T, Chayes L, Sethna J P and Thouless D J 1986 *Commun. Math. Phys.* **106** 41
Chayes J T and Chayes L private communication

[8] Ruelle D 1978 *Thermodynamic Formalism* (Reading, MA: Addison-Wesley)
Sinai Ya G 1982 *Theory of Phase Transitions: Rigorous Results* (Oxford: Pergamon)

[9] Nattermann T 1984 *Z. Phys.* B **54** 2708
Huse D A and Henley C L 1985 *Phys. Rev. Lett.* **54** 2708

[10] Imry Y and Ma S-K 1975 *Phys. Rev. Lett.* **35** 1399

[11] McMillan W L 1985 *Phys. Rev.* B **31** 340
Bray A J and Moore M A 1985 *Phys. Rev.* B **31** 631
Caflisch R G and Banavar J R 1985 *Phys. Rev.* B **32** 7617

[12] de Almeida J R L and Thouless D J 1978 *J. Phys. A: Math. Gen.* **11** 983

[13] Henley C L 1984 *Ann. Phys., NY* **156** 368