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LETTER TO THE EDITOR

Finite size effects in spin glass overlap functions

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Abstract. The Parisi overlap functions $P(q)$ and $P(q_1, q_2, q_3)$, and the function $\Pi(Y)$, which measures sample to sample fluctuations, are calculated for the one-dimensional Ising spin glass in the temperature range in which the correlation length is of the order of the length of the system. The functions $P(q)$ and $\Pi(Y)$ are strikingly similar to those of the SK model but the topology of the space of states is not ultrametric.

In recent years great progress has been made towards a complete understanding of spin glasses at the mean-field level, i.e. in the model of Sherrington and Kirkpatrick (SK, 1975). The SK model is characterised by the existence of many pure states (Parisi 1983) whose free energies are close to the minimum free energy and which behave as independent random variables with an exponential distribution (Mézard *et al* 1985). More precisely, all the pure states have in the thermodynamic limit the same free energy per spin ($\lim_{N\to\infty} F_\alpha/N$). The corrections to the free energy per spin (f_α/N) act as independent random variables. The probability associated with each state is

$$P_\alpha = \exp(-\beta f_\alpha) \Big/ \sum_\gamma \exp(-\beta f_\gamma). \tag{1}$$

Strong correlations exist between the site magnetisations m_i^α ($=\langle S_i\rangle$ in state α) of different pure states. These can be investigated with the Parisi overlap functions (Parisi 1983, Mézard *et al* 1984a, b), the simplest of which is

$$P_J(q) = \sum_{\alpha,\beta} P_\alpha P_\beta \delta(q - q_{\alpha\beta}). \tag{2}$$

$q_{\alpha\beta}$ is the overlap, $N^{-1}\sum_i m_i^\alpha m_i^\beta$. We shall denote a thermal average by $\langle\ \rangle$ and averages over bonds J_{ij} by $(\overline{\ \ })$. $P(q) \equiv \overline{P_J(q)}$ is found in the low-temperature phase at zero field to be of the form

$$P(q) = (y/2)[\delta(q - q_{EA}) + \delta(q + q_{EA})] + \tilde{P}(q), \tag{3}$$

where

$$y = \bar{Y} \qquad Y = \sum_\alpha P_\alpha^2 \qquad q_{EA} = N^{-1}\sum_i (m_i^\alpha)^2.$$

$\tilde{P}(q)$ is a smooth function (i.e. free of delta functions), such that $\tilde{P}(q) = \tilde{P}(-q)$, which vanishes for $|q| > q_{EA}$ (Mézard *et al* 1984a, b). The distribution function $\Pi(Y)$ has been calculated (Mézard *et al* 1985, Derrida and Toulouse 1985).

Higher overlap functions such as

$$P_J(q_1, q_2, q_3) = \sum_{\alpha,\beta,\gamma} P_\alpha P_\beta P_\gamma \delta(q_1 - q_{\alpha\beta})\delta(q_2 - q_{\beta\gamma})\delta(q_3 - q_{\gamma\alpha}) \tag{4}$$

are of interest as $P(q_1, q_2, q_3) = \overline{P_J(q_1, q_2, q_3)}$ reveals the existence of ultrametric topology in the space of the pure states. It is zero unless $|q_1| = |q_2| = |q_3|$ or $|q_1| > |q_2| = |q_3|$ (plus permutations).

In practice, $P_J(q)$ and $P_J(q_1, q_2, q_3)$ are calculated without reference to pure states from their equivalent definitions (Parisi 1983)

$$P_J(q) = \left\langle \delta\left(q - N^{-1} \sum_i S_i^1 S_i^2\right)\right\rangle \tag{5}$$

where the thermal average is taken with the doubly replicated Hamiltonian $H = H\{S_i^1\} + H\{S_i^2\}$, and

$$P_J(q_1, q_2, q_3) = \left\langle \delta\left(q_1 - N^{-1} \sum_i S_i^1 S_i^2\right) \delta\left(q_2 - N^{-1} \sum_i S_i^2 S_i^3\right) \delta\left(q_3 - N^{-1} \sum_i S_i^3 S_i^1\right)\right\rangle \tag{6}$$

with the thermal average taken with the triply replicated Hamiltonian $H = H\{S_i^1\} + H\{S_i^2\} + H\{S_i^3\}$.

At the present time it is unclear whether ultrametric topology or a non-trivial $P(q)$ exists in three-dimensional spin glasses. It is not yet certain whether there is even a finite temperature phase transition (McMillan 1985, Bray and Moore 1985, Ogielski and Morgenstern 1985, Bhatt and Young 1985). These numerical studies do not fully rule out the possibility that the lower critical dimension of Ising spin glasses is three with a phase transition temperature $T_c = 0$.

Very little is currently known about $P(q)$ and $P(q_1, q_2, q_3)$ in three-dimensional spin glasses. As these functions are not readily accessible to experiment they will probably have to be determined by numerical methods. Numerical work is always affected by finite size effects so we thought it would be useful to examine finite size effects on $P(q)$ and $P(q_1, q_2, q_3)$ in the context of exactly soluble models.

The soluble models studied were the one-dimensional Ising ferromagnet and the one-dimensional Ising spin glass. Their Hamiltonians are

$$H = -\sum_{i=1}^{N} J_i S_i S_{i+1}, \qquad S_i = \pm 1 \tag{7}$$

with $J_i = J$ for the ferromagnet while for the spin glass the $\{J_i\}$ are drawn from a continuous distribution $P_B(J)$, such that $P_B(J) = P_B(-J)$ and $P_B(0) \neq 0$. Of course, neither of these models has a finite temperature phase transition. However, they do have a correlation length ξ which grows to infinity as the temperature T is lowered towards zero, i.e. $T_c = 0$. For finite values of $\alpha(\approx L/\xi)$, but for $L \to \infty$ (L, the linear dimension of the sample, equals N in one dimension), we found rich structure in both $P(q)$ and $P(q_1, q_2, q_3)$ (which disappears as $\alpha \to \infty$). While the detailed form of these functions obtained below is specific to one dimension (and our results are modified just by going to periodic boundary conditions†) our calculations suggest that finite systems with a zero-temperature phase transition will generally have interesting correlations between low-lying states. Thus complex forms for $P(q)$ and $P(q_1, q_2, q_3)$ due to finite size effects should appear in certain versions of the travelling salesman problem (Kirkpatrick and Toulouse 1985), the two-dimensional random field Ising model, and two- (and possibly three-) dimensional spin glasses. It would also seem probable that finite size effects give non-trivial structure to the overlap functions at a finite temperature phase transition.

† Toulouse (1983) has discussed $P(q)$ for ferromagnetic and antiferromagnetic Ising rings.

We begin by calculating $P(q)$ for the spin glass case using the definition of (5). To this end we introduce the function $F_J(y)$, such that

$$P_J(q)=\int_{-i\infty}^{i\infty}\frac{dy}{2\pi i}e^{-yq}F_J(y) \tag{8}$$

and

$$F_J(y)=\left\langle \exp yN^{-1}\sum_i S_i^1S_i^2\right\rangle. \tag{9}$$

$F_J(y)$ is easily found using transfer matrices

$$T_i(S_i^1,S_i^2;S_{i+1}^1,S_{i+1}^2;y)=\exp\{\beta J_i(S_i^1S_{i+1}^1+S_i^2S_{i+1}^2)+\tfrac{1}{2}yN^{-1}(S_i^1S_i^2+S_{i+1}^1S_{i+1}^2)\} \tag{10}$$

then

$$F_J(y)=\mathrm{Tr}\prod_{i=1}^{N}T_i(S_i^1,S_i^2;S_{i+1}^1,S_{i+1}^2;y)\Big/\mathrm{Tr}\prod_{i=1}^{N}T_i(S_i^1,S_i^2;S_{i+1}^1,S_{i+1}^2;0). \tag{11}$$

The denominator in (11) equals $4\,\Pi_{i=1}^{N}(2\cosh\beta J_i)^2$. At this stage it is convenient to perform the bond average to calculate $F(y)=\overline{F_J(y)}$. Let

$$\tilde{\mathbf{T}}=\overline{(\mathbf{T}/4\cosh^2\beta J_i)}=\tfrac{1}{4}[\exp\tfrac{1}{2}yN^{-1}(\sigma_i+\sigma_{i+1})][1+\overline{\tanh^2\beta J}\,\sigma_i\sigma_{i+1}], \tag{12}$$

where $\sigma_i=S_i^1S_i^2$. We shall always work in the very low temperature region where

$$\overline{\tanh^2\beta J}\equiv 1-\overline{\mathrm{sech}^2\beta J}=1-2TP_B(0) \qquad \text{as } T\to 0$$

$$=1-2\alpha N^{-1}, \qquad \text{with } \alpha=NP_B(0)T. \tag{13}$$

We take α to be of order one which implies that the temperature itself is of order $1/N$. Then

$$F(y)=\tfrac{1}{4}\sum_{\sigma_1,\sigma_{N+1}}\ \sum_{S_1^1,S_2^1,\ldots,S_{N+1}^1}\tilde{\mathbf{T}}^N=\tfrac{1}{2}\sum_{\sigma_1,\sigma_{N+1}}\tilde{\tilde{\mathbf{T}}}^N, \tag{14}$$

where, to $O(1/N)$

$$\tilde{\tilde{\mathbf{T}}}=2\tilde{\mathbf{T}}=\begin{pmatrix}1+\dfrac{y-\alpha}{N}, & \dfrac{\alpha}{N}\\[2ex] \dfrac{\alpha}{N}, & 1-\dfrac{(y+\alpha)}{N}\end{pmatrix}. \tag{15}$$

Hence

$$F(y)=\tfrac{1}{2}\sum_{\sigma_1,\sigma_{N+1}}[\lambda_1^N\langle\sigma_1|\lambda_1\rangle\langle\lambda_1|\sigma_{N+1}\rangle+\lambda_2^N\langle\sigma_1|\lambda_2\rangle\langle\lambda_2|\sigma_{N+1}\rangle]. \tag{16}$$

The eigenvalues λ_1 and λ_2 of $\tilde{\tilde{\mathbf{T}}}$ are

$$\lambda_{1,2}=1-N^{-1}[\alpha\pm(\alpha^2+y^2)^{1/2}]. \tag{17}$$

By finding the eigenvectors $\langle\sigma|\lambda_1\rangle$ and $\langle\sigma|\lambda_2\rangle$ and using the identity

$$\lim_{N\to\infty}(1+xN^{-1})^N=e^x$$

one obtains

$$F(y)=\tfrac{1}{2}e^{-\alpha}\left[\left(1+\frac{\alpha}{(\alpha^2+y^2)^{1/2}}\right)\exp(\alpha^2+y^2)^{1/2}+\left(1-\frac{\alpha}{(\alpha^2+y^2)^{1/2}}\right)\exp[-(\alpha^2+y^2)^{1/2}]\right]. \tag{18}$$

The calculation for the ferromagnetic case is even simpler and *exactly* the same result is obtained provided one redefines α as

$$\tanh^2 \beta J = 1 - 2\alpha N^{-1} \tag{19}$$

i.e. work on a temperature scale $T \sim J/\log N$. In other words, finite size corrections will decrease logarithmically slowly with increasing system size in the ferromagnetic case (and a similar situation would be expected for the case of other systems at their lower critical dimension). Note that for both the ferromagnet and the spin glass the temperature scale is so low that thermally activated hopping between spin states will vanish when $N \to \infty$ with α finite.

It is revealing to express α in terms of L/ξ. For the ferromagnet

$$\langle S_i S_j \rangle = (\tanh \beta J)^{|i-j|} = \exp(-|i-j|/\xi), \tag{20}$$

where $\xi = -(\ln \tanh \beta J)^{-1}$. Hence using (19) one sees that as $N \to \infty$, $\alpha = L/\xi$. For the spin glass, a correlation length can be defined from

$$\overline{\langle S_i S_j \rangle^2} = (\overline{\tanh^2 \beta J})^{|i-j|} = \exp(-|i-j|/\xi), \tag{21}$$

so $\xi = -(\ln \overline{\tanh^2 \beta J})^{-1} \approx L/2\alpha$ as $N \to \infty$, so $\alpha = L/2\xi$. On scaling grounds one would expect for all systems at or below their lower critical dimension that $P(q)$ could be expressed as

$$P(q) = P(q, L/\xi) \tag{22}$$

and (18) demonstrates this explicitly.

The integral required to extract $P(q)$ from $F(y)$ has been performed by Bruce (1981) in a different context. The result is

$$P(q) = \tfrac{1}{2} e^{-\alpha}[\delta(q-1) + \delta(q+1)] + \tilde{P}(q), \tag{23}$$
$$\tilde{P}(q) = \tfrac{1}{2}\alpha\, e^{-\alpha}[I_0(x) + (\alpha/x) I_1(x)]\theta(1-q^2)$$

where $x = \alpha(1-q^2)^{1/2}$, $I_0(x)$ and $I_1(x)$ are Bessel functions, and θ is the usual step function. For $\alpha \to 0$, $\tilde{P}(q)$ is a constant equal to $\alpha/2$. As $\alpha \to \infty$, $P(q) \to \delta(q)$, the expected trivial result. Equation (23) is strikingly similar to (3), which gives the form of $P(q)$ for the SK model.

There is a simple way of understanding (23). We consider the ferromagnetic case only (although a similar argument is possible for the spin glass). The probability that the ferromagnet is in one of its two ground states (i.e. has all its spins up or down) is

$$\tfrac{1}{2} e^{N\beta J}/(2 \cosh \beta J)^N = \tfrac{1}{2} e^{-\alpha/2}.$$

Using the definition of (5) for $P(q)$ one sees that the delta function contribution arises from the overlaps of the ground states of each Hamiltonian in the doubly replicated Hamiltonian. That $\tilde{P}(q) \to \alpha/2$ as $\alpha \to 0$ arises from the overlap of a ground state of one Hamiltonian and a state containing one 'kink' in the other Hamiltonian. (A kink arises when all the spins are reversed beyond a given spin in the chain.) The probability of a kink occurring at a given site is $\alpha/4N$. The overlap of a kink at site t with a ground state is $(2t/N - 1)$. Summing over all kink positions (and types of kink) gives $\tilde{P}(q) \to \alpha/2$ as $\alpha \to 0$. Higher terms in the expression of $\tilde{P}(q)$ in powers of α represent the effects of inserting more and more kinks.

$P(q_1, q_2, q_3)$ can also be found by transfer matrix methods, but it is easier to use the kink picture directly

$$\begin{aligned} P(q_1, q_2, q_3) = {} & \tfrac{1}{4}\, e^{-3\alpha/2}\{\delta(q_1-1)\delta(q_2-1)\delta(q_3-1)+\delta(q_1-1)\delta(q_2+1)\delta(q_3+1) \\ & +\delta(q_1+1)\delta(q_2-1)\delta(q_3+1)+\delta(q_1+1)\delta(q_2+1)\delta(q_3-1)\} \\ & +\tfrac{1}{4}\, e^{-\alpha}(1-e^{-\alpha/2})\{\delta(q_1-1)\delta(q_2-q_3)+\delta(q_1+1)\delta(q_2+q_3) \\ & +\text{permutations}\} \\ & +\tfrac{1}{8}\, e^{-\alpha/2}(1-e^{-\alpha/2})^2\{\delta(q_1+|q_2-q_3|-1)+\delta(q_1-|q_2+q_3|+1) \\ & +\text{permutations}\}+\tilde{P}(q_1, q_2, q_3). \end{aligned} \tag{24}$$

This result holds for both ferromagnetic and spin glass models with the appropriate definition of α. For the ferromagnet the first term in (24) comes from the overlap of the ground states, i.e. when in (6) each Hamiltonian of the triply replicated Hamiltonian is in its ground state. The second term arises when two of the Hamiltonians are in their ground states, while the third term derives from the case when only one is in its ground state. The smooth function $\tilde{P}(q_1, q_2, q_3)$ is determined by the cases when none of the Hamiltonians are in their ground states and is a constant equal to $\alpha^3/64$ as $\alpha \to 0$. Equation (24) shows the existence of striking structure in $P(q_1, q_2, q_3)$ but that ultrametric topology is absent. The numerical attempts to determine $P(q_1, q_2, q_3)$ in two- and three-dimensional spin glasses (Bachas 1985, Sourlas 1984) are probably not of sufficient precision to distinguish appropriate generalisations of (24) from genuine ultrametric topology.

For the spin glass model we can also study the sample-to-sample fluctuations which lead to the 'lack of self-averaging' familiar from the SK model (Young *et al* 1984, Mézard *et al* 1984a, b) and the 'random energy model' (Derrida 1980, Derrida and Toulouse 1985). A central quantity is the probability distribution $\Pi(Y)$, where Y is the total amplitude of the delta function contributions to $P_J(q)$. These contributions are due to 'self-overlap' of states, $Y = \Sigma_\alpha W_\alpha^2$, $W_\alpha = \exp(-\beta E_\alpha)/\Sigma_{\alpha'} \exp(-\beta E_{\alpha'})$, where α now labels microscopic spin states, giving

$$Y = \frac{\mathrm{Tr}\, e^{-2\beta H}}{(\mathrm{Tr}\, e^{-\beta H})^2} = \prod_{i=1}^{N} (1 - \tfrac{1}{2}\,\mathrm{sech}^2\, \beta J_i). \tag{25}$$

(Here we have included only one state from each pair of states generated by time reversal symmetry.) At temperatures of O(1) the product over i in (25) reduces Y to zero for $N \to \infty$. However, in the temperature range of interest here, $T = O(1/N)$, low-lying states, which have excitation energies of $O(1/N)$, have Boltzmann weights which are of order unity, but which vary from sample to sample, leading to sample-to-sample fluctuations in Y. (Note that this is the same mechanism which leads to sample-to-sample fluctuations in the SK model.)

The average of Y over samples is $y \equiv \bar{Y} = \{1 - \tfrac{1}{2}\overline{\mathrm{sech}^2\, \beta J}\}^N = (1 - \alpha N^{-1})^N = e^{-\alpha}$ for $N \to \infty$. In a similar way all the moments of $\Pi(Y)$ can be evaluated:

$$\overline{Y^n} = e^{-2\alpha I_n} = y^{2I_n}$$

$$I_n = \int_0^\infty dx[1 - (1 - \tfrac{1}{2}\,\mathrm{sech}^2\, x)^n].$$

To first order in α (i.e. to first order in $1 - y$) the moments are identical to those obtained from the SK model. It is convenient to work with the variables $1-Y$, whose moments are given by

$$\overline{(1-Y)^n}=\frac{(n-1)!}{(2n-1)!!}\alpha+\mathrm{O}(\alpha^2), \qquad n\geq 1. \tag{26}$$

This agrees with the moments obtained by Mézard *et al* (1985) for the SK model. Also the behaviour of $\Pi(Y)$ for $Y\to 1$ is strikingly similar to that of the SK model. From the behaviour of I_n for large positive n, $I_n=\frac{1}{2}[\ln(2n)+\gamma+\mathrm{O}(1/n)]$, where γ is Euler's constant, one infers

$$\Pi(Y)\sim(\mathrm{e}^{-\gamma\alpha}/2^\alpha\Gamma(\alpha))(1-Y)^{\alpha-1}, \qquad Y\to 1, \tag{27}$$

which agrees with the SK model to leading order in α (i.e. leading order in $1-y$) (Mézard *et al* 1985). The physical origin of this 'superuniversal' behaviour for $\alpha\to 0$ is that in this limit the space of states may be truncated to the two lowest states. Including just the ground state and the lowest energy kink state yields, using the distribution $P(|J_{\min}|)=2NP_B(0)\exp(-2NP_B(0)|J_{\min}|)$ for the strength of the weakest bond (Bray and Moore 1984), the closed form expression

$$\Pi(Y)=\frac{\alpha}{(1-Y)(2Y-1)^{1/2}}\left(\frac{1-(2Y-1)^{1/2}}{1+(2Y-1)^{1/2}}\right)^\alpha, \qquad \tfrac{1}{2}<Y<1,$$

and $\Pi(Y)=0$ otherwise. This expression generates both the moments (26) and the $Y\to 1$ limit (27) correct to leading order in α.

In a future work, we hope to analyse finite size effects in the low-temperature phase of a spin glass where $T_c\neq 0$.

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