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1984 J. Phys. A: Math. Gen. 17 L307

(http://iopscience.iop.org/0305-4470/17/5/017)

J. Phys. A: Math. Gen. **17** (1984) L307–L312. Printed in Great Britain

LETTER TO THE EDITOR

On the interplay of replicas and metastable states in spin glasses

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Received 21 December 1983

Abstract. For the Ising Sherrington–Kirkpatrick (SK) spin glass we study the constraints imposed on the distributions $P(q, \{J_{ij}\})$, $P(U, M, \{J_{ij}\})$ for the overlap q, energy U and magnetisation M of the underlying metastable states, by the general nature of current replica symmetry breaking schemes. We confirm that whilst $P(q, \{J_{ij}\})$ shows significant sample to sample variations the thermodynamic energy and field cooled magnetisation are well behaved. For both the Edwards–Anderson order parameter and the Minimum overlap the case is less clear.

In recent years the Sherrington–Kirkpatrick (SK) (1975), spin glass model has received a great deal of attention. The once mysterious breaking of replica symmetry which led to the intriguing solution of Parisi (1979), is now known to be associated with the existence of a large number of metastable states (or distinct thermodynamic phases) at low temperatures. For the Ising spin glass, Parisi (1983) has recently demonstrated that the important distribution function $P(q, \{J_{ij}\})$ for the overlap between metastable states of magnetisation $\{m_i^s\}$

$$P(q, \{J_{ij}\}) = \sum_{s,s'} p(s)p(s')\, \delta\left(q - \frac{1}{N}\sum_{i=1}^{N} m_i^s m_i^{s'}\right) \tag{1}$$

is closely related to the spin glass order parameter $Q^{\alpha\beta}$ of the replica description, via

$$\bar{P}(q) = \overline{P(q, \{J_{ij}\})} = L_y^{-1}\left(\lim_{n\to 0} \frac{1}{n(n-1)} \sum_{\alpha \neq \beta}^{n} \exp(-yQ^{\alpha\beta})\right). \tag{2}$$

Here $p(s)$ is the occupation probability for a state s, the operator L_y^{-1} denotes an inverse Laplace tranform and $\overline{\cdots}$ refers to the usual disorder average. Now the function $P(q)$ is observable by Monte Carlo simulation either directly (Young 1983) or through moments such as the local field cooled susceptibility χ^l(FC), so for macroscopic samples ($N \gg 1$) one would hope that $P(q)$ is self averaging; $P(q) = \bar{P}(q)$. Surprisingly however it has recently been shown by Young *et al* (YBM) (1983) that even in the macroscopic limit there are significant sample to sample (different disorders) variations in $P(q)$. In this letter we study the influence of replica symmetry breaking on $P(q)$ and other distributions associated with the internal energy and magnetisation. We concentrate on the properties of the 'replica equivalent' ansätze which satisfy

$$\sum_{\gamma=1}^{n} (f(Q^{\alpha\gamma}) - f(Q^{\beta\gamma})) = 0, \qquad M^\alpha = M_p \tag{3}$$

0305-4470/84/050307+06$02.25

for all $\alpha, \beta = 1, 2, \ldots n$ and any function f. Here $Q^{\alpha\beta}$, M^{α} are respectively the spin glass and ferromagnetic order parameters. Naturally the Parisi (1979) and Sompolinsky (1981) replica ansätze satisfy (3). We present simple arguments which confirm that whilst $P(q, \{J_{ij}\})$ is not self averaging, the energy U, magnetisation M, Edwards–Anderson order parameter q_{EA} and minimum overlap q^* are. Working directly with the distribution functions we clarify some aspects of the YBM paper, emphasising in particular the role of the cluster property discussed by Parisi (1983). Specialising to the replica ansätze associated with Parisi (1979), Sompolinsky (1981) we present expressions both for $\bar{P}(q)$ and the distribution function $\overline{P(q)P(p)}$.

Our starting point is the observation of Parisi (1983), de Dominicis and Young (1983) that the existence of metastable states implies that a statistical mechanical expectation value $\langle \cdots \rangle$ must be decomposed according to

$$\langle \cdots \rangle = \sum_s p(s) \langle \cdots \rangle_s \qquad \sum_s p(s) = 1. \tag{4}$$

where $\langle \cdots \rangle_s$ denotes the average appropriate to a pure thermodynamic phase (Ruelle 1969). In each pure state all the connected correlations functions vanish at large distances (clustering), so for the SK model at fixed disorder we have

$$\langle \alpha_{i_1} \sigma_{i_2} \ldots \sigma_{i_k} \rangle = \langle \sigma_{i_1} \rangle \langle \sigma_{i_2} \rangle \ldots \langle \sigma_{i_k} \rangle \tag{5}$$

if $i_p \neq i_q$ for all $p, q = 1, 2 \ldots, k$. Furthermore by definition

$$m_i^s \equiv \langle \sigma_i \rangle_s. \tag{6}$$

Using this property one finds directly that the generating function $G(y)$ associated with $P(q, \{J_{ij}\})$ satisfies

$$G(y) \equiv \int \mathrm{d}q \, \mathrm{e}^{-yq} P(q, \{J_{ij}\}) = \left\langle\!\!\left\langle \exp\left(-\frac{y}{N} \sum_i^N \sigma_i^1 \sigma_i^2 \right) \right\rangle\!\!\right\rangle_{k=2} \tag{7}$$

where $\langle\!\langle \cdots \rangle\!\rangle_k$ refers to a statical mechanical average with respect to an SK model with a replicated Hamiltonian

$$H_k \equiv \sum_{r=1}^k H_{\mathrm{SK}}(\{\sigma_i^r\}) = -\sum_{r=1}^k \left(\sum_{i,j} J_{ij} \sigma_i^r \sigma_j^r + h \sum_i \sigma_i^r \right). \tag{8}$$

On the other hand we may use the replica trick to rewrite (7) in the form

$$G(y) = \lim_{n \to 0} \frac{1}{n(n-1)} \sum_{\alpha \neq p}^n \left[\mathop{\mathrm{Tr}}_{\{\sigma^\alpha\}} \left(\exp\left(-\frac{y}{N} \sum_{i=1}^N \sigma_i^\alpha \sigma_i^\beta - \beta H_n \right) \right] \tag{9}$$

which allowing us to perform the *disorder average*, leads following Sherrington and Kirkpatrick (1975) directly to Parisi's result

$$\bar{G}(y) = \lim_{n \to 0} \frac{1}{n(n-1)} \sum_{\alpha \neq \beta}^n [\exp(-yQ^{\alpha\beta})]. \tag{10}$$

Inverting this relation, using (7) gives then the quoted expression (1) for $\bar{P}(q)$.

An extension of this analysis provides insight into the influence of the replica ansatz (3) on other important distributions. We shall consider the distribution function

$$P(U, M, \{J_{ij}\}) = \sum_s p(s) \, \delta\left(U + \frac{1}{N} \left(\sum_{i \neq j}^N J_{ij} m_i^s m_j^s + h \sum_i^N m_i^s \right) \right) \delta\left(M - \frac{1}{N} \sum_i^N m_i^s \right) \tag{11}$$

from which we may calculate for example:

(a) the internal energy

$$U(\{J_{ij}\}) = \int \mathrm{d}U\, U \int \mathrm{d}M\, P(U, M, \{J_{ij}\}) = \frac{1}{N}\left(\sum_{i\neq j}^{N} J_{ij}\langle\sigma_i\sigma_j\rangle + h\sum_{i}^{N}\langle\sigma_i\rangle\right) \tag{12}$$

or

(b) the magnetisation

$$M(\{J_{ij}\}) = \int \mathrm{d}M\, M \int \mathrm{d}U\, P(U, M, \{J_{ij}\}) = \frac{1}{N}\sum_{i}^{N}\langle\sigma_i\rangle. \tag{13}$$

As above, using the clustering property (5), we find the associated generating function $G(x, z)$ defined by

$$G(x, z) = \int \mathrm{d}U \int \mathrm{d}M \exp(-xU - zM) P(U, M, \{J_{ij}\}) \tag{14}$$

satisfies the relation

$$G(x, z) = \left\langle\!\!\left\langle \exp\left(\frac{x}{N}\sum_{i\neq j} J_{ij}\sigma_i^1\sigma_j^1 + (hx - z)\frac{1}{N}\sum_i \sigma_i^1\right)\right\rangle\!\!\right\rangle_1. \tag{15}$$

Using the replica trick, we may recast (15) in the form

$$G(x, z) = \lim_{n\to 0}\frac{1}{n}\sum_{\alpha}^{n}\left(\operatorname*{Tr}_{\{\sigma^\alpha\}}\left(\exp\left(\frac{x}{N}\sum_{i\neq j} J_{ij}\sigma_i^\alpha\sigma_j^\alpha + (hx - z)\frac{1}{N}\sum_i \sigma_i^\alpha - \beta H_n\right)\right)\right)$$

whereupon the disorder average can be performed, leading for $N \gg 1$ to the expression

$$\bar{G}(x, z) = \lim_{n\to 0}\frac{1}{n}\sum_{\alpha=1}^{n}\exp\left(\frac{1}{2}\beta x\left(1 + \sum_{\beta\neq\alpha}^{n}(Q^{\alpha\beta})^2 + (hx - z)M^\alpha\right)\right). \tag{16}$$

For the 'replica equivalent' ansantz (3), the argument of the exponential is independent of α implying

$$\bar{G}(x, z) = \exp\left(\tfrac{1}{2}\beta x\left(1 + \lim_{n\to 0}\left(\frac{1}{n}\sum_{\alpha\neq\beta}^{n}(Q^{\alpha\beta})^2\right)\right) + (hx - z)M_p\right) \tag{17}$$

and whence on inversion the trivial distribution

$$\bar{P}(U, M) = \delta\left(U + \tfrac{1}{2}\beta\left(1 + \lim_{n\to 0}\frac{1}{n}\sum_{\alpha=\beta}^{n}(Q^{\alpha\beta})^2\right) + hM_p\right)\delta(M - M_p) \tag{18}$$

only if (3) is satisfied ($f(x) \sim x^2$).

For both $P(q, \{J_{ij}\})$ and $P(I, M, \{J_{ij}\})$ the limitations of the self averaging assumption are reflected directly by the distribution functions

$$\bar{C}_k(\{x_i\}) \equiv \overline{\prod_{i=1}^{k} P(x_i, \{J_{ij}\})} \tag{19}$$

where x denotes q or (U, M). Analysing $P(q, \{J_{ij}\})$ in this way we first observe that from the above ((7) *et seq*), generating function $\bar{G}_k$ associated with $\bar{C}_k$ satisfies

$$\bar{G}_k(\{y_i\}) \equiv \overline{\prod_{i=1}^{k} G(y_i)} = \lim_{n\to 0}\left(\frac{k!}{n!}\right)\sum_{\substack{\{\alpha_i,\beta_i\}\\ \text{All distinct}}}^{n}\exp\left(-\sum_{i=1}^{k} y_i Q^{\alpha_i\beta_i}\right). \tag{20}$$

Considering the first few cases in turn, we reproduce (10) for $k=1$

$$\bar{G}_1(y)=\bar{G}(y)=\lim_{n\to 0}\frac{1}{n(n-1)}\sum_{\alpha\neq\beta}^{n}\exp(-yQ^{\alpha\beta}) \tag{21}$$

whilst for $k=2$ we find

$$\bar{G}_2(x,z)=\lim_{n\to 0}\frac{1}{n(n-1)(n-2)(n-3)}\sum_{\alpha\neq\beta\neq\gamma\neq\delta}^{n}\exp(-xQ^{\alpha\beta}-zQ^{\gamma\delta}). \tag{22}$$

It is interesting to rewrite (22) in the form

$$\begin{aligned}\bar{G}_2(x,z)=\lim_{n\to 0}\frac{1}{n(n-1)(n-2)(n-3)}&\left\{\left(\sum_{\alpha\neq\beta}^{n}\exp(-xQ^{\alpha\beta})\right)\left(\sum_{\alpha\neq\delta}^{n}\exp(-zQ^{\gamma\delta})\right)\right.\\&+2\sum_{\alpha\neq\beta}^{n}\exp(-(x+z)Q^{\alpha\beta})-4\sum_{\alpha}^{n}\left(\sum_{\beta\neq\alpha}^{n}\exp(-xQ^{\alpha\beta})\right)\\&\left.\times\left(\sum_{\gamma\neq\alpha}^{n}\exp(-zQ^{\gamma\alpha})\right)\right\},\end{aligned} \tag{23}$$

for it is then clear that the 'replica equivalence' condition implies

$$\bar{G}_2(x,z)=\tfrac{1}{3}\bar{G}(x+z)+\tfrac{2}{3}\bar{G}(x)\bar{G}(z). \tag{24}$$

Inverting (21), (2) we are therefore led to the interesting result

$$\overline{P(q)P(p)}=\tfrac{1}{3}\delta(q-p)\bar{P}(p)+\tfrac{2}{3}\bar{P}(p)\bar{P}(q) \tag{25}$$

which confirming the breakdown of self averaging seen by YBM, also allows us to discuss the nature of the sample to sample variations we might expect in $P(q,\{J_{ij}\})$ (see below). In sharp contrast to this conclusion the distribution function $P(U,M,\{J_{ij}\})$ is certainly self averaging. We simply observe that for a 'replica equivalent' ansatz the generating function

$$\begin{aligned}\bar{G}_k(\{x_i,z_i\})&=\overline{\prod_{i=1}^{k}G(x_i,z_i)}\\&=\lim_{n\to 0}\left(\frac{k!}{n!}\right)\sum_{\substack{\{\alpha_i\}\\ \text{All distinct}}}\exp\left(\sum_{i=1}^{k}\tfrac{1}{2}\beta x_i\left(1+\sum_{\beta\neq\alpha_i}^{n}(Q^{\alpha_i\beta})^2\right)+(nx_i-z_i)M^{\alpha_i}\right)\end{aligned} \tag{26}$$

factorises (see (16) *et seq*), leading on inversion to the expression

$$\overline{\prod_{i=1}^{k}(P(U_i,M_i,\{J_{ij}\})-\bar{P}(U_i,M_i))}=0 \tag{27}$$

for all k, or $\bar{P}(U,M)=P(U,M,\{J_{ij}\})$. Of course since $P(U,M)$ is trivial (18), it is natural to consider instead the thermodynamic averages for the internal energy (12) and magnetisation (13) as directly self averaging.

To elucidate further the structure of the distribution function $P(q,\{J_{ij}\})$ we are now finally forced to consider the Parisi (1979) and Sompolinsky (1981) solutions in greater detail. Considering first the Sompolinsky ansatz (see de Dominicis *et al* 1982), we find that the generating function $\bar{G}(y)$ (10) is of the form

$$\bar{G}_s(y)=\int_0^1 \mathrm{d}x\left(\mathrm{e}^{-y\bar{q}_{\mathrm{EA}}}-y\left(\frac{\mathrm{d}\Delta}{\mathrm{d}x}\right)\mathrm{e}^{-yq(x)}\right) \tag{28}$$

where $\Delta(x)$, $q(x)$, $x\in(0,1)$ are the Sompolinsky order parameters (Elderfield 1983) and we have identified the Edwards–Anderson order parameter $\bar{q}_{\mathrm{EA}}$. Inverting (20) we find

$$\bar{p}_s(q)=(-\partial\Delta/\partial q)\,\delta(q-\bar{q}^*)+(1+\partial\Delta/\partial q)\,\delta(q-\bar{q}_{\mathrm{EA}})-(\partial^2\Delta/\partial q^2) \tag{29}$$

where $\bar{q}^*=\min(q(x))$. The Parisi (1983) form can be easily recovered as a special case by choosing $\Delta'(x)=-xq'(x)$ (de Dominicis *et al* 1982), whereupon we find

$$\bar{P}_{\mathrm{PARISI}}(q)=x^*\,\delta(q-\bar{q}^*)+(1-x_m)\,\delta(q-\bar{q}_{\mathrm{EA}})+(\partial x/\partial q) \tag{30}$$

Here x^*, x_m are respectively the lower and upper breakpoints of the Parisi (1979) solution. At least for the Ising SK model it appears at present that $\bar{P}_s(q)$ and $\bar{P}_{\mathrm{PARISI}}(q)$ are indistinguishable. We learn from (29), (30) that $\bar{P}(q)$ is typically characterised by a smooth function $\partial^2\Delta/\partial q^2$ (or $\partial x/\partial q$) and the weights/positions of two singular contributions, so re-examining (25) it seems that whilst $P(q,\{J_{ij}\})$ is certainly not self averaging the underlying parameters $\bar{q}^*$, $\bar{q}_{\mathrm{EA}}$ are.

To conclude, we have demonstrated above the importance of the clustering property (Parisi 1983) *and* the notion of a 'replica equivalent' ansatz in determining the structure of the SK model. We confirm the observations of YBM, who studying the Parisi solution showed that whilst $P(q,\{J_{ij}\})$ is non self averaging, the internal energy $U(h,T)$ and magnetisation $M(h,T)$ certainly are. For the Edwards–Anderson order parameter $\bar{q}_{\mathrm{EA}}$ the situation is less clear, for the clustering property alone is insufficient to relate

$$q_{\mathrm{EA}}(\{J_{ij}\})\equiv\sum_s p(s)\left(\frac{1}{N}\sum_{i=1}^{N}(m_i^s)^2\right) \tag{31}$$

to a replica computation. Our computation of $\bar{P}(q)$, $\overline{P(q)P(q)}$ and extensions to the higher functions $\bar{C}_k(k>2)$ (19), certainly suggests that both $q_{\mathrm{EA}}(\{J_{ij}\})$ and $q^*(\{J_{ij}\})$ (29) are self averaging. By contrast YBM who study directly the first few moments

$$\hat{q}(\{J_{ij}\})\equiv\frac{1}{N}\sum_{i=1}^{N}\langle s_i\rangle^2=\int \mathrm{d}q\,P(q,\{J_{ij}\})q$$

and (32)

$$\hat{q}^{(2)}(\{J_{ij}\})\equiv\frac{1}{N^2}\sum_{i,j}\langle s_is_j\rangle^2=\int \mathrm{d}q\,P(q,\{J_{ij}\})q^2$$

showing that for the Parisi solution

$$\overline{(\hat{q}(\{J_{ij}\})-\bar{q})^2}>0 \qquad \overline{(\hat{q}^{(2)}(\{J_{ij}\})-\bar{q}^{(2)})^2}>0 \tag{33}$$

or equivalently $\bar{P}(q)\neq P(q)$, lose precisely the information needed to draw this conclusion.

I would like to thank Professor D Sherrington, and Dr P Young for valuable discussions and the SERC for financial support.

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