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Weighted averages and order parameters for the infinite range Ising spin glass

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Abstract. The Sherrington–Kirkpatrick spin glass model is studied by replicas and by analysing the mean field equations of Thouless, Anderson and Palmer (TAP). We show that the standard order parameter defined by statistical mechanics is given by the *average* of all off-diagonal components of the matrix $q_{\alpha\beta}$. There is consequently no violation of the fluctuation dissipation theorem. We describe how to weight the different solutions of the TAP equations and argue that there is no entropy from solution degeneracy. This assumption is shown to be internally consistent. The square of a spin expectation value for a solution, averaged over solutions, is shown to be $q(1)$ if we make the Parisi–Sompolinsky ansatz for $q_{\alpha\beta}$.

1. Introduction

In the long search to establish a credible mean field theory for spin glasses the infinite range SK (Sherrington and Kirkpatrick 1975) Ising model has been particularly studied. The Hamiltonian of the SK model is given by

$$\mathscr{H} = -\sum_{i<j} J_{ij}\sigma_i\sigma_j - \sum_i h_i\sigma_i, \tag{1}$$

where $\sigma_i = \pm 1$ $(i = 1, \ldots, N)$ and the J_{ij} are independent random variables whose distribution has zero mean and width J/N, the same for all pairs of sites. We shall set Boltzmann's constant equal to one and in these units there is a transition in the thermodynamic limit at $T_c = J$. A crucial feature is that the mean field equations of TAP (Thouless *et al* 1977) have an enormous number of solutions (De Dominicis *et al* 1980, Bray and Moore 1980a, Tanaka and Edwards 1980). These equations are:

$$m_j^s = \tanh\left[\beta\left(\sum_k J_{jk}m_k^s + h_j - m_j^s \sum_k \beta J_{jk}^2[1-(m_k^s)^2]\right)\right], \tag{2}$$

where m_j^s is the average of σ_j for solution 's', and the corresponding free energy of each solution is given by

$$F\{m^s\} = -\sum_{i<j} J_{ij}m_i^s m_j^s - \tfrac{1}{2}\sum_{i<j} J_{ij}^2[1-(m_i^s)^2][1-(m_j^s)^2]$$
$$+\tfrac{1}{2}\sum_i \{(1+m_i^s)\ln[\tfrac{1}{2}(1+m_i^s)] + (1-m_i^s)\ln[\tfrac{1}{2}(1-m_i^s)]\} - \sum_i h_i m_i^s. \tag{3}$$

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Averages should be computed as sums over solutions with an appropriate (normalised) weight $P(s)$ which implies that there are many ways of defining an order parameter. For instance, we have

$$\langle\sigma_i\rangle_{\mathrm{T}} = m_i = \sum_s m_i^s P(s) \tag{4}$$

where $\langle \ldots \rangle_{\mathrm{T}}$ denotes the thermal average for a given set of interactions. The standard order parameter q, obtained from statistical mechanics, is then given by

$$q = \overline{\langle\sigma_i\rangle_{\mathrm{T}}^2} = \overline{\left(\sum_s m_i^s P(s)\right)^2}, \tag{5}$$

where the bar denotes an average over the random couplings.

Alternatively we obtain the EA (Edwards and Anderson 1975) order parameter, q_{EA}, by averaging $(m_i^s)^2$ over solutions, i.e.

$$q_{\mathrm{EA}} = \overline{\sum_s P(s)(m_i^s)^2}. \tag{6}$$

Clearly $q_{\mathrm{EA}} \neq q$ if many solutions contribute with significant weight. In order to have a non-zero value of q it is necessary for a symmetry breaking field to be applied. We shall take a uniform magnetic field, which can tend to zero if the thermodynamic limit is taken first (see e.g. Young and Kirkpatrick 1982).

The TAP equations still involve the full set of interactions J_{ij}, so most of the analytic work has instead centred on directly evaluating the statistical mechanics of the SK model by the replica method without going through the TAP equations. This involves making an ansatz for the matrix $q_{\alpha\beta}$ in replica space. The most successful such ansatz is due to Parisi (1979, 1980a, b, c, d, e) in which $q_{\alpha\beta}$ is a function of a single variable x, $0 \leqslant x \leqslant 1$. Furthermore, sums over distinct pairs of replicas become integrals over x, i.e.

$$\lim_{n\to 0} \frac{1}{n(n-1)} \sum_{\alpha\neq\beta} (q_{\alpha\beta})^k \equiv \int_0^1 q(x)^k \, \mathrm{d}x. \tag{7}$$

Since the field h_i couples to $\Sigma_\alpha \sigma_i^\alpha$ the local susceptibility χ_{ii} is given by $(nT)^{-1} \Sigma_\alpha \langle\sigma_i^{\alpha_0}\sigma_i^\alpha\rangle$ for fixed α_0, which for Parisi's ansatz becomes

$$T\chi_{ii} = 1 - \int_0^1 q(x)\, \mathrm{d}x, \tag{8}$$

whereas according to the fluctuation–dissipation theorem (FDT) one has

$$T\chi_{ii} = 1 - q. \tag{9}$$

By using dynamics instead of replicas Sompolinsky (1981) has produced a theory which involves, besides the order parameter $q(x)$, an anomaly $\Delta(x)$. These two functions are related by a gauge condition leaving a degree of arbitrariness for choosing $q(x)$ (or $\Delta(x)$) but $q(0)$, $q(1)$ and χ_{ii} are identical to Parisi's. In fact both ansatzes give identical results for the expectation value of all observables (De Dominicis *et al* 1982, Sommers 1983) although a rigorous proof (demonstrating the monotonic character of $\Delta'(x)/q'(x)$) is still missing. Like Parisi's, Sompolinsky's ansatz may also be given a direct replica derivation (De Dominicis *et al* 1981). However, the dynamic derivation gives in addition a physical interpretation of x in terms of a spectrum of time scales, all of which diverge in the thermodynamic limit (see also Mackenzie and Young

1982) such that $x = 1$ is the shortest of these time scales and $x = 0$ is the longest. One naturally interprets these very long time scales in terms of fluctuations from one TAP equation to another (see e.g. Young 1981). With this assumption it follows *generally* that q_{EA}, defined by (6), is equivalent to the usual definition

$$q_{\mathrm{EA}} = \lim_{t\to\infty} \lim_{N\to\infty} \overline{\langle \sigma_j(0)\sigma_j(t)\rangle_{\mathrm{T}}}$$

which for the Sompolinsky ansatz gives

$$q_{\mathrm{EA}} = q(1). \tag{10}$$

On the other hand, statistical mechanics results are *in general* obtained on time scales longer than the largest relaxation time, i.e.

$$q = \lim_{N\to\infty} \lim_{t\to\infty} \overline{\langle \sigma_j(0)\sigma_j(t)\rangle_{\mathrm{T}}}$$

so, according to Sompolinsky,

$$q = q(0). \tag{11}$$

From (8), (9) and (11) it is clear that Sompolinsky's results violate the FDT. Recently Sommers (1982) has given a different argument for (11) based on replicas.

The violation of the FDT implied by (11) seems unsatisfactory to us, so we have studied in more detail the various order parameters in the SK model both in replica and TAP frameworks. Our main results are as follows.

(i) We give a simple replica argument (§ 2) that

$$q = \lim_{n\to 0} \frac{1}{n(n-1)} \sum_{\alpha\neq\beta} q_{\alpha\beta} \tag{12}$$

or in Parisi's ansatz

$$q = \int_0^1 q(x)\,\mathrm{d}x \tag{13}$$

so, comparing (8) and (9), we see that there is no violation of FDT in Parisi's theory if correctly interpreted. Other statistical mechanics averages are also obtained as *averages* over all replicas rather than one particular set.

(ii) We argue that the weight $P(s)$ for a TAP solution is given by

$$P(s) = \exp(-\beta F\{m^s\})/Z \tag{14}$$

where

$$Z = \sum_s \exp(-\beta F\{m^s\}) \tag{15}$$

and $F\{m^s\}$ is the free energy of the solution (3). We conjecture that with this weight there is no extensive contribution to the entropy due to solution degeneracy. A simple argument (§ 3) then leads to the FDT without using replicas.

(iii) We compute averages with the weight $P(s)$ by reducing the system to a one-site problem and using replicas. We show that the assumption of no solution degeneracy is consistent because it leads to the original SK Hamiltonian in terms of only the matrix $q_{\alpha\beta}$ for $\alpha \neq \beta$ (§ 4).

(iv) As an additional bonus we obtain a self-consistent equation for q_{EA} in (6), which is just $q_{\alpha\alpha}$ in replica language and has no analogue in the SK Hamiltonian. If we make the Parisi or Sompolinsky ansatz for $q_{\alpha\beta}$ ($\alpha \neq \beta$) we find that our equation for $q_{\alpha\alpha}$ is satisfied if $q_{EA} = q(1)$ which agrees with Sompolinsky in this case (see equation (10)). We also verify using the Parisi–Sompolinsky ansatz for $q_{\alpha\beta}$ ($\alpha \neq \beta$) that the free energy is equal to the weighted average of solution free energies (which is equivalent to there being no entropy due to solution degeneracy).

The only missing item to complete the argument for absence of entropy due to solution degeneracy is a stability analysis of our replica ansatz. We hope that this problem can be reduced to the one already explored (De Dominicis and Kondor 1983, Goltsev 1982) of the SK functional of $q_{\alpha\beta}$. Our conclusions are discussed in § 5 and some technical details are given in the appendix.

2. Connection between statistical mechanics averages and replicas

In this section we shall evaluate the statistical mechanics order parameter $q = \overline{\langle\sigma_i\rangle_T^2}$ (equation (5)) by a simple replica argument and show that it is given by (12). The definition of q is equivalent to

$$q = \overline{\frac{\mathrm{Tr}_1\, \sigma_i^1\, \mathrm{e}^{-\beta H_1}}{Z}\, \frac{\mathrm{Tr}_2\, \sigma_i^2\, \mathrm{e}^{-\beta H_2}}{Z}}, \tag{16}$$

where we label the spins in the first trace by '1' and the second trace by '2'. It is difficult to carry out the average over the disorder in (16) because the random interactions appear in the numerator and denominator. The replica trick gets around this by multiplying numerator and denominator by Z^{n-2} and letting $n \to 0$. Hence

$$q = \lim_{n\to 0} \overline{\left(\prod_{\alpha=1}^{n} \mathrm{Tr}_\alpha\right) \sigma_i^{\alpha_0}\sigma_i^{\beta_0} \exp\left(-\beta \sum_{\alpha=1}^{n} H^\alpha\right)} \tag{17}$$

since the denominator is just 1. Altogether there are n replicas and that labelled by '1' in (16) can be any one of these and that labelled by '2' can be any other. Thus the replicas α_0 and β_0 in (17) can be *any* distinct pair. By definition of $q_{\alpha\beta}$ one then has

$$q = q_{\alpha_0\beta_0}. \tag{18}$$

There is now an apparent paradox in situations where replica symmetry is broken, since one appears to get different results depending on the choice of replicas. This is not so, however, because of the following argument, which though simple does not seem to have appeared before in the spin glass literature.

Since the effective Hamiltonian in the replica formalism, given by

$$\exp(-\beta H_{\mathrm{eff}}) = \overline{\exp\left(-\beta \sum_{\alpha=1}^{n} H^\alpha\right)},$$

is replica symmetric it follows that for every solution $q_{\alpha\beta}$ there are other equivalent solutions obtained by permuting the replicas. If these solutions are distinct from the original one they must be included as well. In more mathematical terms one must sum over all equivalent saddle points. One should therefore evaluate $q_{\alpha_0\beta_0}$ for fixed

α_0 and β_0 but sum over all distinct solutions *which restores replica symmetry*†. For Parisi's ansatz (and we would argue for any physically acceptable solution) the number of inequivalent solutions formally tends to unity as $n \to 0$. Hence the correct procedure is to *average* over all distinct solutions, which is clearly equivalent to taking one solution and averaging over all distinct pairs of replicas, i.e.

$$q = \lim_{n\to 0} \frac{1}{n(n-1)} \sum_{\alpha\neq\beta} q_{\alpha\beta} \tag{12}$$

where the $q_{\alpha\beta}$ are for one solution. With Parisi's ansatz this becomes equation (13).

Other statistical mechanics averages can be evaluated in the same way. For instance:

$$q^{(2)} = \overline{\langle\sigma_j\sigma_k\rangle_{\mathrm{T}}^2} \qquad (j \neq k)$$

becomes

$$\lim_{n\to 0} \frac{1}{n(n-1)} \sum_{\alpha\neq\beta} (q_{\alpha\beta})^2 \equiv \int_0^1 q^2(x)\, \mathrm{d}x. \tag{19}$$

This is consistent with the linear response theory result that $q^{(2)} = 1 - 2T|U(T)|/J^2$ (Bray and Moore 1980b) where $U(T)$ is the energy per spin, since Parisi shows that $\int_0^1 q^2(x)\,\mathrm{d}x = 1 - 2T|U(T)|/J^2$.

It appears to us that Sommers' (1982) argument for $q = q(0)$ neglects the existence of many solutions. However G Parisi (private communication) has suggested that $q(0)$ may be obtained if the Hamiltonian H_1 and H_2 in (16) have different magnetic fields h_1, and h_2 since this breaks the replica symmetry in the analogue of (17). The difference $h_1 - h_2$ may, as usual, tend to zero after the thermodynamic limit has been taken. This leaves strict statistical mechanics averages with the above answer (12), but could lead to Sompolinsky's answer for 'time-dependent' magnetic fields.

3. The TAP equations: a conjecture

There is a general consensus that the SK model has many minima in phase space, corresponding to TAP solutions, with barriers between them whose height diverges in the thermodynamic limit (Sompolinsky 1981, Mackenzie and Young 1982, Young 1981, Hertz 1983a, b, Toulouse 1982). Indeed, it appears impossible to understand the model without this picture. At a given temperature and field there are consequently pockets of phase space which are inaccessible from each other. One can therefore, in principle at least, carry out restricted statistical sums separately in each portion of phase space. The quantitiy $\Sigma^s \exp[-\beta H\{\sigma\}]$, where Σ^s denotes a sum over all states accessible from each other in the minimum corresponding to TAP solution 's', is just the exponential of (minus β times) the corresponding free energy. In other words

$$\exp(-\beta F\{m^s\}) = \sum{}^s \exp(-\beta H\{\sigma\}). \tag{20}$$

† The order parameter $q_{\alpha_0\beta_0}$ (for instance, Parisi's ansatz) breaks the symmetry with respect to permutations of replica indices and the 'time reversal' symmetry (explicitly broken by the magnetic field). Only the permutational symmetry is restored (with a distinct Parisi ansatz for each distinct saddle point). In strictly zero field, saddle points generated by 'time reversal' also contribute, the symmetry is fully restored and the order parameter vanishes.

The partition function Z involves an unrestricted sum over states so

$$Z = \sum_s \exp(-\beta F\{m^s\}) \tag{15}$$

and the normalised statistical weight for each solution is given by

$$P(s) = Z^{-1} \exp(-\beta F\{m^s\}). \tag{14}$$

Similarly $m_i = \langle\sigma_i\rangle_{\mathrm{T}}$ is given by

$$m_i = Z^{-1} \sum_s \sum{}^s \sigma_i \exp(-\beta H\{\sigma\}) = \sum_s P(s) m_i^s, \tag{4}$$

since m_i^s is defined by

$$m_i^s = \frac{\sum^s \sigma_i \exp(-\beta H\{\sigma\})}{\sum^s \exp(-\beta H\{\sigma\})}. \tag{21}$$

We could alternatively obtain m_i by differentiating $T \ln Z$ with respect to h_i. From (3) and (15) this also appears to lead to (4). However, there is a possible complication since we know that the *total* number of solutions is of the form $\exp[N\alpha(h, T)]$, where α is a function of field and temperature, so we might expect another contribution to (4) coming from differentiating the solution degeneracy with respect to h_i. Since (4) must be correct as it stands (it is just another way of writing the definition of m_i), we require that the number of solutions *with significant statistical weight* does not give an extensive entropy.

To see how this can arise, let us replace the sum over solutions in (15) by an integral over free energy, i.e.

$$Z = \int g(\hat{F})\, \mathrm{e}^{-\beta\hat{F}} \,\mathrm{d}\hat{F}, \tag{22}$$

where $g(\hat{F})$ is the degeneracy of solutions of a given free energy $\hat{F}$. From Bray and Moore (1980a) we know that $g(\hat{F}) \propto \exp[N\alpha(\hat{f})]$ where $\hat{f} = \hat{F}/N$ and $\alpha(\hat{f})$ is zero for $\hat{f}$ less than $f_{\min}$, the minimum free energy. Hence (22) becomes

$$Z \propto \int_{f_{\min}} \exp[N(\alpha(\hat{f}) - \beta\hat{f})] \,\mathrm{d}\hat{f}, \tag{23}$$

which, for $N \to \infty$, is dominated by $\hat{f} = f^*$, the value of $\hat{f}$ which maximises the exponent. Then f^* is given either by $f^* = f_{\min}$ or the solution of $\alpha'(f^*) = \beta f^*$ depending on the form of $\alpha(\hat{f})$. The free energy is given by

$$f = f^* - T\alpha(f^*). \tag{24}$$

We shall *assume* that $f^* = f_{\min}$ and that $\alpha(f^*) = 0$ so that (24) becomes

$$f = f^* (= f_{\min}). \tag{25}$$

Indeed, we argued above that $\alpha(f^*) = 0$ is necessary, otherwise differentiation of the free energy with respect to h_i will not give the correct value of m_i (equation (4)). It also seems clear that we can consistently neglect any change in the number of solutions when performing higher derivatives over h or T, although we have not succeeded in giving a rigorous proof of this. In particular, one more derivative of (4) with respect to h_j gives

$$T\chi_{ij} = T\overline{\sum_s \frac{\partial m_j^s}{\partial h_j} P(s)} + \left\{\overline{\sum_s (m_j^s)^2 P(s)} - \overline{\left(\sum_s m_j^s P(s)\right)^2}\right\}. \tag{26}$$

The local susceptibility of a single solution is given by (Bray and Moore 1979)

$$T\, \partial m_j^s/\partial h_j = 1 - (m_j^s)^2 \tag{27}$$

which is just the FDT applied to the *states in one of the valleys* in phase space. The 'anomalous' terms in brackets in (26), which represent the extra response due to changing the solution probabilities, are actually just what is needed to make the FDT work for *averages over all of phase space*, i.e.

$$T\chi_{ij} = 1 - q \tag{9}$$

where q is given by (5). Our result for q disagrees with a recent TAP calculation by Dasgupta and Sompolinsky (1983), who find $q = q(0)$, as in Sompolinsky's (1981) dynamical theory. Like us, they assume that only states with $f = f_{\min}$ are important and that $\alpha(f_{\min}) = 0$. However, their approach seems to need several additional assumptions about the overlap of solutions which are not necessary in our method.

4. Equivalence to the original SK Hamiltonian

The partition function (15) can be written

$$Z = \int_{-1}^{1} \prod_j \left[\mathrm{d}m_j\, \delta\left(\frac{\partial \beta F\{m\}}{\partial m_j}\right)\right] \Delta\{m\} \exp(-\beta F\{m\}) \tag{28}$$

where $\Delta\{m\} = |\det \partial^2 \beta F/\partial m_i\, \partial m_j|$ normalises the delta functions to unity. It is convenient to use an integral representation of the δ function, i.e.

$$Z = \int_{-1}^{1} \prod_j \mathrm{d}m_j \int_{-\infty}^{\infty} \mathrm{d}\hat{m}_j \exp\left(\mathrm{i} \sum_j \hat{m}_j \frac{\partial \beta F}{\partial m_j}\right) \Delta\{m\} \exp(-\beta F). \tag{29}$$

Differentiating with respect to h_j gives

$$m_j = \langle m_j + \mathrm{i}\hat{m}_j \rangle \tag{30}$$

where the average is over the integrand in (29) divided by Z†. Clearly for consistency we need $\langle \hat{m}_j \rangle = 0$, which is just the mathematical expression for the absence of an extensive entropy due to solution degeneracy as discussed in § 3. Defining

$$Q = \frac{1}{N}\sum_j \langle m_j m_j \rangle, \qquad g = \frac{1}{N}\sum_j \langle \mathrm{i}\hat{m}_j m_j \rangle, \qquad \hat{q} = \frac{1}{N}\sum_j \langle (\mathrm{i}\hat{m}_j)^2 \rangle \tag{31}$$

then the condition that $\langle \hat{m}_j \rangle = 0$ for all h_j implies $\langle \partial \hat{m}_j \rangle / \partial h_j = 0$ so

$$g + \hat{q} = 0 \tag{32}$$

and $N^{-1} T\, \Sigma_j\, \chi_{jj} = \Sigma_j\, \partial \langle m_j \rangle / \partial h_j$ is given by

$$N^{-1} T \sum_j \chi_{jj} = N^{-1} \sum_j (Q + g - \langle m_j \rangle^2)$$

† We hope there is no confusion in using the same symbol m_j, both for the expectation value and the variable of integration in (28). This allows us to keep a simple notation in the following developments.

which, together with (4), (5) and (9), gives

$$g = 1 - Q. \tag{33}$$

We wish to average our results over the bond distribution which in practice necessitates replicas. The quantities Q, g and q in (31) then become matrices $q_{\alpha\beta}$, $g_{\alpha\beta}$ and $\hat{q}_{\alpha\beta}$ respectively where, for instance,

$$q_{\alpha\beta} = N^{-1} \sum_j m_{j\alpha} m_{j\beta}. \tag{34}$$

We shall be carrying out a saddle point integration for which the $q_{\alpha\beta}$ take their expectation values (see (41)), so the absence of an average on the RHS of (34) compared with (31) is of no significance. The variables introduced in (31) when averaged over the J_{ij} now become diagonal components, e.g.

$$\bar{Q} = q_{\alpha\alpha}. \tag{34a}$$

To see this, take the definition of the average $\langle m_j m_j \rangle$ (given below (30)), multiply by Z^{n-1} and (following § 2) let $n \to 0$. We shall only consider solutions which are replica symmetric along the diagonal (i.e. $q_{\alpha\alpha}$ etc independent of α), so we do not have to average (34a) over equivalent saddle points as is necessary for off-diagonal components (see § 2). From (6), (31) and (34a) one obtains

$$q_{\alpha\alpha} = q_{\mathrm{EA}}. \tag{35}$$

The conditions corresponding to (32) and (33) now read

$$g_{\alpha\alpha} = 1 - q_{\alpha\alpha}, \qquad \hat{q}_{\alpha\alpha} = -(1 - q_{\alpha\alpha}). \tag{36}$$

For $\alpha \neq \beta$ we have $g_{\alpha\beta} = \overline{\langle m_j \rangle \langle \mathrm{i}\hat{m}_j \rangle}$ and $\hat{q}_{\alpha\beta} = \overline{\langle \mathrm{i}\hat{m}_j \rangle^2}$ which should both vanish since $\langle \mathrm{i}\hat{m}_j \rangle = 0$. As discussed in § 2, this really implies that $\Sigma_{\alpha\neq\beta}\, g_{\alpha\beta} = \Sigma_{\alpha\neq\beta}\, \hat{q}_{\alpha\beta} = 0$ in a replica symmetry broken situation, but we shall make the ansatz that all off-diagonal elements separately vanish, i.e.

$$g_{\alpha\beta} = \hat{q}_{\alpha\beta} = 0 \qquad (\alpha \neq \beta). \tag{37}$$

The calculation proceeds by replicating (28) n times, introducing Grassmann variables η_j to evaluate the determinant and averaging over the J_{ij} as described in De Dominicis *et al* (1980). We find

$$-\beta f = \lim_{n \to 0} \frac{1}{n} \max(A + \ln C) \tag{38}$$

where

$$A = \mathrm{Tr}[\mathrm{i}(\tilde{q}q + \tilde{\hat{q}}\hat{q} + \tilde{g}g + \tilde{n}n) - (J^2/2T^2)(q\hat{q} + \tfrac{1}{2}q^2 + 2gq + g^2 - n^2)]$$
$$+ \sum_\alpha (J^2/T^2)[\tfrac{1}{4}(1 - q_{\alpha\alpha})^2 + (n_{\alpha\alpha} - g_{\alpha\alpha})(1 - q_{\alpha\alpha})] \tag{39a}$$

and

$$C = \int \prod_\alpha \left(\mathrm{d}m_\alpha \frac{\mathrm{d}\hat{m}_\alpha}{2\pi} \right) \det[(1 - m^2)^{-1}\mathbb{1} - \mathrm{i}\tilde{n}]\, \mathrm{e}^L \tag{39b}$$

with

$$L = \mathrm{i}\,\mathrm{Tr}[\tilde{q}mm + \tilde{g}(\mathrm{i}\hat{m}m) + \tilde{\hat{q}}(\mathrm{i}\hat{m}\mathrm{i}\hat{m})]$$
$$+ \sum_\alpha [h(m_\alpha + \mathrm{i}\hat{m}_\alpha) - \tfrac{1}{2}\ln(1 - m_\alpha^2) - (m_\alpha + \mathrm{i}\hat{m}_\alpha)\tanh^{-1} m_\alpha]. \tag{39c}$$

The trace is over replica labels, $n_{\alpha\beta}$ is related to the Grassmann variables by

$$n_{\alpha\beta} = \frac{1}{N}\sum_j \eta^*_{j\alpha}\eta_{j\beta}, \tag{40}$$

the tilded variables are used to enforce constraints and we have assumed the same magnetic field on each site. The determinant in (39*b*) is of an $n \times n$ matrix and '$\mathbb{1}$' refers to the unit matrix. Equation (38) is to be maximised with respect to $q_{\alpha\beta}$, $g_{\alpha\beta}$, $\hat{q}_{\alpha\beta}$, $n_{\alpha\beta}$ and the corresponding constraint variables. Strictly speaking we should also include the antisymmetric variables

$$p_{\alpha\beta} = \frac{1}{N}\sum_j \eta_{j\alpha}\eta_{j\beta}, \qquad p^*_{\alpha\beta} = \frac{1}{N}\sum_j \eta^*_{j\alpha}\eta^*_{j\beta}.$$

There is certainly a stationary point with $p_{\alpha\beta} = p^*_{\alpha\beta} = 0$ which is the one we choose. A stability analysis would be necessary to verify that this is the correct choice.

Making (38) stationary with respect to the constraint variables gives

$$q_{\alpha\beta} = \langle m_\alpha m_\beta\rangle, \qquad g_{\alpha\beta} = \langle \mathrm{i}\hat{m}_\alpha m_\beta\rangle, \qquad \hat{q}_{\alpha\beta} = \langle \mathrm{i}\hat{m}_\alpha \mathrm{i}\hat{m}_\beta\rangle, \tag{41}$$

where the expectation values here and in the rest of this section are with a weight given by the integrand in (39*b*) divided by C. We now impose the requirement that there is no entropy, due to solution degeneracy, by substituting (36) and (37) into (39). We also assume

$$n_{\alpha\beta} = (1 - q_{\alpha\alpha})\delta_{\alpha\beta} \qquad (= g_{\alpha\beta}). \tag{42}$$

This is obtained by requiring that the energy U is given by

$$U = \sum_s U\{m^s\}P(s)$$

with no extra contribution from solution degeneracy. One can show that this extra term vanishes if $n_{\alpha\beta} = g_{\alpha\beta}$. Minimising, we find that (36), (37) and (42) are stationary points and, choosing this solution, we have in addition

$$\mathrm{i}\tilde{q}_{\alpha\beta} = \mathrm{i}\tilde{\hat{q}}_{\alpha\beta} = \mathrm{i}\tilde{g}_{\alpha\beta}/2 = (J^2/2T^2)q_{\alpha\beta} \tag{43}$$

and

$$\tilde{n}_{\alpha\beta} = 0.$$

Using (43) and defining new variables $\hat{\mu}_\alpha$ by

$$\mathrm{i}\hat{\mu}_\alpha = \mathrm{i}\hat{m}_\alpha + m_\alpha \tag{44}$$

one obtains

$$A = \frac{J^2}{4T^2}\left(\sum_\alpha (1 - 2q_{\alpha\alpha}) - \sum_{\alpha\neq\beta} q^2_{\alpha\beta}\right) \tag{45}$$

and

$$L = \frac{J^2}{2T^2}\sum_{\alpha,\beta} q_{\alpha\beta}\mathrm{i}\hat{\mu}_\alpha\mathrm{i}\hat{\mu}_\beta + \sum_\alpha \mathrm{i}\hat{\mu}_\alpha\left(\frac{h}{T} - \tanh^{-1} m_\alpha\right) - \tfrac{1}{2}\ln(1 - m^2_\alpha) \tag{46}$$

so from (39) and (46)

$$C = \int_{-\infty}^{\infty} \prod_\alpha \left(\frac{\mathrm{d}\hat{\mu}_\alpha}{2\pi}\mathrm{d}X_\alpha\, 2\cosh X_\alpha\right)\exp\left[\frac{J^2}{2T^2}\sum_{\alpha,\beta} q_{\alpha\beta}\mathrm{i}\hat{\mu}_\alpha\mathrm{i}\hat{\mu}_\beta + \sum_\alpha \mathrm{i}\hat{\mu}_\alpha\left(\frac{h}{T} - X_\alpha\right)\right] \tag{47}$$

where

$$X_\alpha = \tanh^{-1} m_\alpha. \tag{48}$$

The integral over X_α in (47) just constrains the $i\hat{\mu}_\alpha$ to be ± 1 so we finally obtain

$$-\beta f = \lim_{n\to 0} \frac{1}{n} \max\left[\frac{J^2}{4T^2}\left(n - \sum_{\alpha\neq\beta} q_{\alpha\beta}^2\right) + \ln \sum_{\{S_\alpha=\pm 1\}} \times \exp\left(\frac{J^2}{2T^2} \sum_{\alpha\neq\beta} q_{\alpha\beta} S_\alpha S_\beta + \frac{h}{T}\sum_\alpha S_\alpha\right)\right] \tag{49}$$

which is just the replicated version of the SK model in terms of discrete Ising spins $S_\alpha(=\pm 1)$. Notice that $q_{\alpha\alpha}$ has dropped out of our final result (49) because of the length constraint on the spins. The length constraint also means that averages over the m's, i.e. $\langle m_\alpha m_\beta \ldots\rangle = \langle \tanh X_\alpha \tanh X_\beta \ldots\rangle$, can be replaced by the corresponding averages of $i\hat{\mu}$'s (or equivalently of S's) provided no two replicas are the same. For example

$$q_{\alpha\beta} = \langle m_\alpha m_\beta\rangle = \langle S_\alpha S_\beta\rangle \qquad (\alpha\neq\beta) \tag{50}$$

as required. This does not work if two identical replicas occur so

$$q_{\alpha\alpha} = \langle m_\alpha^2\rangle = \langle \tanh^2 X_\alpha\rangle \tag{51}$$

cannot be represented as averages over the S's. In terms of solution averages $q_{\alpha\alpha}$ is just q_{EA}, see (35).

The fact that we recover the original problem, whilst a hollow achievement from one point of view, nonetheless provides some justification for our ansatz, equations (36), (37) and (42) together with $p^*_{\alpha\beta} = p_{\alpha\beta} = 0$. Furthermore from (51) we obtain, as an additional bonus, an expression for q_{EA}, which has no analogue in the original formulation of the problem. Equation (51) is a rather complicated self-consistent expression for $q_{\alpha\alpha}$ because it involves all the off-diagonal elements $q_{\alpha\beta}$. In the appendix we show that if we make the Sompolinsky (or equivalently Parisi) ansatz for $q_{\alpha\beta}(\alpha\neq\beta)$ then (51) is self-consistently satisfied by

$$q_{\alpha\alpha}(=q_{\mathrm{EA}}) = q(1). \tag{10}$$

This result is also obtained from Sompolinsky's dynamical interpretation of the Parisi variable x.

As a final consistency check on our assumptions we show that the actual free energy f as given by (49) is equal to the average solution free energy f^*. Evaluating the weighted average of $f\{m_s\}$ along the same lines as the above calculation gives

$$-\beta f^* = \frac{J^2}{2T^2}\left(\sum_\beta (q_{\alpha\beta}^2 + g_{\alpha\beta}g_{\beta\alpha} + g_{\beta\alpha}g_{\alpha\beta}) + \tfrac{1}{2}(1-q_{\alpha\alpha})^2\right) - \langle m_\alpha \tanh^{-1} m_\alpha + \tfrac{1}{2}\ln(1-m_\alpha^2)\rangle. \tag{52}$$

We have been unable to evaluate this expression in general but in the appendix we show that $f^* = f$ for the Sompolinsky–Parisi ansatz. From (24) this shows that $\alpha(f^*) = 0$, as has been assumed all along.

Since we argue that only solutions with $f = f_{\min}$ contribute to the final results we could equivalently have replaced the $\exp(-\beta F)$ factor in (28) by a delta-function constraint on the free energy and eventually set $f = f_{\min}$. This approach has been pursued by Bray and Moore (1981). Indeed, if we impose (42) together with $\tilde{n}_{\alpha\beta} = 0$, and minimise (39) with respect to $q_{\alpha\beta}$, $g_{\alpha\beta}$ and $\hat{q}_{\alpha\beta}$, but do not yet impose (36) and (37), we obtain equation (11) of Bray and Moore (1981) if they set $u=-1$, where u is an auxiliary variable which imposes the delta-function constraint on the free energy. Our final ansatz, (36) and (37), corresponds in the Bray and Moore notation to $q=q_{\alpha\alpha}$, $2\Delta=8\lambda=J^2q_{\alpha\alpha}/T^2$, $\eta_{\alpha\beta}=4\eta^*_{\alpha\beta}=-2\rho_{\alpha\beta}=J^2q_{\alpha\beta}/T^2$. Bray and Moore obtain a different solution from this, which they show is equivalent to Parisi's to lowest order in T_c-T. In fact the values of u, Δ, λ etc in the two approaches are different even above the de Almeida–Thouless (AT, 1978) line in the h–T plane, although both give (correctly) the SK free energy. The difference arises because we calculate directly the free energy so solutions are weighted by $\exp(-\beta F)$, which automatically imposes $u=-1$. Bray and Moore on the other hand calculate the logarithm of the number of solutions and u is allowed to determine itself. Above the AT line where there is only one solution a 'white average' (i.e. equal weight to all solutions), which corresponds to $u=0$, will give correct results and this is the solution Bray and Moore find. Below the AT line the Bray–Moore solution has $u<0$ but with u tending to zero as the line is approached from below, whereas we have $u=-1$ always. Since the two solutions, though mathematically different, describe the same physics above the AT line, they may also be equivalent below the line but this has only been established to lowest order in T_c-T (where both give Parisi's solution).

5. Discussion

We have presented a consistent picture of the SK model in both TAP and replica frameworks. Our main assumption is that there is no solution degeneracy and we show that this is self-consistently satisfied. In our view there is no violation of the FDT if averages are consistently worked out by statistical mechanics. This agrees with earlier work by Young and Kirkpatrick (1982) and Hertz (1983a, b) but disagrees with Sompolinsky (1981), Dasgupta and Sompolinsky (1983) and Sommers (1982). We do, however, agree with Sompolinsky's result that $q_{\mathrm{EA}}=q(1)$.

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Appendix

We compute here the average value of $\phi(X_{\alpha_0})$ over the (normalised) weight given by the integrand in (48), i.e.

$$\langle\phi(X_{\alpha_0})\rangle=\frac{1}{C}\int\prod_\alpha \mathrm{d}X_\alpha\frac{\mathrm{d}\hat{\mu}_\alpha}{2\pi}\exp\left(\tfrac{1}{2}\sum_{\alpha\beta}q_{\alpha\beta}\mathrm{i}\hat{\mu}_\alpha\mathrm{i}\hat{\mu}_\beta+h\sum_\alpha\mathrm{i}\hat{\mu}_\alpha\right)$$
$$\times\prod_\alpha\exp(-\mathrm{i}\hat{\mu}_\alpha X_\alpha)(\mathrm{e}^{X_\alpha}+\mathrm{e}^{-X_\alpha})\phi(X_{\alpha_0}). \qquad \text{(A1)}$$

To compute this average we use the Sompolinsky ansatz as in De Dominicis *et al* (1981). We work out in detail the two-step case which generalises immediately.

The matrix $q_{\alpha\beta}$ is divided into n/p_0 big blocks (indexed by $j_0=1,2,\ldots,n/p_0$) with p_0 replicas in each big block. Each big block is divided into p_0/p_1 small blocks (indexed by $j_1=1,2,\ldots,p_0/p_1$), each small block containing p_1 replicas indexed by α_1 ($\alpha_1=1,2,\ldots,p_1$). Thus $\alpha\equiv(j_0j_1\alpha_1)$. Using q_0, q_1 as values for the off-diagonal and diagonal small blocks belonging to each diagonal big block, and r_0, r_1 for the off-diagonal and diagonal small blocks belonging to each off-diagonal big block, one has

$$\sum_{\alpha\beta} q_{\alpha\beta}\mathrm{i}\hat{\mu}_\alpha\mathrm{i}\hat{\mu}_\beta \equiv r_0\Big(\sum_{j_0j_1\alpha_1}\mathrm{i}\hat{\mu}\Big)^2+(q_0-r_0)\sum_{j_0}\Big(\sum_{j_1\alpha_1}\mathrm{i}\hat{\mu}\Big)^2$$
$$+(r_1-r_0)\sum_{j_1}\Big(\sum_{j_0\alpha_1}\mathrm{i}\hat{\mu}\Big)^2+[(q_1-q_0)-(r_1-r_0)]\sum_{j_0j_1}\Big(\sum_{\alpha_1}\mathrm{i}\hat{\mu}\Big)^2 \tag{A2}$$

where $\mathrm{i}\hat{\mu}$ stands for $\mathrm{i}\hat{\mu}_{j_0j_1\alpha_1}$. Introducing z_0, z_{j_1} and $y_{j_0}y_{j_0j_1}$ to linearise and using

$$q_0-r_0=-\Delta_0'/p_0, \qquad q_1-r_1=-\Delta_1'/p_1, \tag{A3}$$

one may perform the X_α integration (i.e. trace over spins) except for $\alpha=\alpha_0(\equiv j_0^0j_1^0\alpha_1^0)$, namely

$$\langle\phi(X_{\alpha_0})\rangle=\int\frac{\mathrm{d}z_0}{\sqrt{2\pi}}\exp(-z_0^2/2)\int\prod_{j_0}\frac{\mathrm{d}y_{j_0}}{\sqrt{2\pi}}\exp\Big(-p_0\sum_{j_0}y_{j_0}^2/2\Big)$$
$$\times\Big[\int\prod_{j_1}\frac{\mathrm{d}z_j\,\mathrm{d}y_{j_0j_1}}{(2\pi)}\exp\Big(-\sum_{j_1}z_{j_1}^2/2-p_1\sum_{j_0j_1}y_{j_0j_1}^2/2+p_1{\sum_{j_0j_1}}'\ln 2\cosh U_{j_0j_1}\Big)$$
$$\times\exp[+(p_1-1)\ln 2\cosh U_{j_0^0j_1^0}]\Big]$$
$$\times\int\frac{\mathrm{d}\hat{\mu}_{\alpha_0}}{2\pi}\mathrm{d}X_{\alpha_0}\exp[\mathrm{i}\hat{\mu}_{\alpha_0}(U_{j_0^0j_1^0}-X_{\alpha_0})+2\ln 2\cosh X_{\alpha_0}]\phi(X_{\alpha_0}) \tag{A4}$$

where $\alpha_0\equiv(j_0^0j_1^0\alpha_1^0)$, the Σ' sum excludes $(j_0^0j_1^0)$, and

$$U_{j_0j_1}=(q_0)^{1/2}z_0+(q_1-q_0)^{1/2}z_j+(\Delta_0')^{1/2}y_{j_0}+(\Delta_1')^{1/2}y_{j_0j_1}. \tag{A5}$$

Integration over $\hat{\mu}_{\alpha_0}$ replaces $\phi(X_{\alpha_0})$ by $\phi(U_{j_0^0j_1^0})$. Saddle points over y variables as p_0 and p_1 tend to infinity ($p_0\gg p_1\gg 1$) are unaffected by the weight ϕ and one thus obtains

$$\langle\phi(X_{\alpha_0})\rangle=\int\frac{\mathrm{d}z_0\,\mathrm{d}z_1}{2\pi}\exp[-\tfrac{1}{2}(z_0^2+z_1^2)]\phi[U(z_0,z_1)], \tag{A6}$$

with

$$U(z_0,z_1)=(q_0)^{1/2}z_0+(q_1-q_0)^{1/2}z_1+\Delta_0'm_0(z_0)+\Delta_1'm_1(z_0,z_1). \tag{A7}$$

As in the standard case

$$y_{j_0}^c=(\Delta_0')^{1/2}m_0(z_0), \qquad y_{j_0j_1}^c=(\Delta_1')^{1/2}m_1(z_0,z_1), \tag{A8}$$

and the magnetisations m_0, m_1 are as in Sompolinsky stationarity conditions, with obvious generalisation to the general R-step case.

As a result:

(i) if $\phi \equiv \tanh^2 X_{\alpha_0}$ we have

$$q_{\alpha_0\alpha_0} = \int \prod_{r=0}^{1} \frac{dz_r}{\sqrt{2\pi}} \exp\left(-\tfrac{1}{2}\sum_{r=0}^{1} z_r^2\right) \tanh^2 U\{z_r\} \tag{A9}$$

in a form that generalises with $1 \to R$. This, in the continuum limit, is by definition $q(1)$ a result consistent with the implicitly made assumption in writing (A2);

(ii) if $\phi \equiv -X_{\alpha_0} \tanh X_{\alpha_0} + \ln 2 \cosh X_{\alpha_0} \equiv s$ we have

$$s = \sum_{r=0}^{1} (q_r \Delta'_r + q_r \Delta'_r) + \int \prod_{r=0}^{1} \frac{dz_r}{\sqrt{2\pi}} \exp\left(-\tfrac{1}{2}\sum_{r=0} z_r^2\right) \ln 2 \cosh U\{z_r\}. \tag{A10}$$

This allows us to compute $-\beta f^*$ as given by (53) and to verify that it is identical with the Sompolinsky free energy, thus proving that the solution entropy vanishes, i.e.

$$\alpha(f^*) = 0.$$

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