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Thouless-Anderson-Palmer Approach to the Spherical p -Spin Spin Glass Model

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Abstract. — We analyze the Thouless-Anderson-Palmer (TAP) approach to the spherical p -spin spin glass model in zero external field. The TAP free energy is derived by summing up all the relevant diagrams for $N \rightarrow \infty$ of a diagrammatic expansion of the free energy. We find that if the multiplicity of the TAP solutions is taken into account, there is a first order transition in the order parameter at the critical temperature T_c higher than that predicted by the replica solution T_{RSB} , but in agreement with the results of dynamics. The transition is of “geometrical” nature since the new state has larger free energy but occupies the largest volume in phase space. The transition predicted by the replica calculation is also of “geometrical” nature since it corresponds to the states with smallest free energy with positive complexity.

The understanding of the low temperature phase of spin systems with random couplings, namely spin glasses (SG), is still an open and interesting problem. The main feature is the complex free energy landscape made of many minima, separated by very high barriers, not related by any symmetry one to another. This is responsible for the non-trivial behavior of these systems, even at the mean field level which is usually the first step towards the understanding of the phases [1, 2].

Recently a simple mean-field model [3, 4] has been introduced to investigate the static and dynamical properties of these systems. This is an infinite range spherical SG model with p -spin interactions. For any $p > 2$ the model possesses a non-trivial low-temperature and low-field phase. Within the Parisi scheme of replica symmetry breaking the most general solution for any temperature T and field is obtained with only one step of breaking (1RSB). In this paper we shall consider the system without external field. In this case the replica approach predicts a first-order transition in the order parameter at the critical temperature T_{RSB} where the order parameter jumps discontinuously from zero (high temperature) to a finite value (low temperature). The free energy, nevertheless, remains continuous. The study of the dynamics yields a similar scenario but with a first-order transition at a higher critical temperature $T_c > T_{RSB}$, and a slightly different low temperature phase. This surprising result was first noted in reference [5] in a soft-spin version of the model. The reason why the two

approaches led to two different results is that in the replica approach the transition was obtained by the requirement of largest replica free energy, while in dynamics it follows from marginality. The two conditions are equivalent for the continuous transition in a field, but not for the discontinuous one [3,4].

In an attempt to understand this result Kurchan, Parisi and Virasoro [6] proposed a Thouless-Anderson-Palmer (TAP) free energy for this model and showed that, in the absence of magnetic field, the 1RSB solution was a solution of the TAP equations. However, strangely enough, this solution does not correspond to an extremum of the proposed TAP free energy. Moreover, at any temperature, the replica symmetric solution leads to a lower value of this free energy. Therefore, it is not clear why there should be any transition.

We have derived the TAP free energy from a diagrammatic expansion of the free energy by summing up all the relevant diagrams in the $N \rightarrow \infty$ limit. We show that taking into account the degeneracy of the TAP solutions, usually called "complexity", then in the thermodynamic limit $N \rightarrow \infty$ this naturally leads to a transition in agreement with the results of dynamics. Moreover it gives the constraint under which the TAP free energy for the 1RSB is minimal. A similar behaviour has been found in the Potts glass with $p > 4$ [7].

The p -spin spherical SG model consists of N continuous spins σ_i interacting via quenched Gaussian couplings. The Hamiltonian is a p -body interaction

$$H(\sigma) = \frac{r}{2} \sum_{i=1}^N \sigma_i^2 - \sum_{1 \leq i_1 < \dots < i_p \leq N} J_{i_1, \dots, i_p} \sigma_{i_1} \dots \sigma_{i_p} - \sum_{i=1}^N h_i \sigma_i \quad (1)$$

where we have included an external field h_i and a parameter r to control the spin magnitude fluctuations. The couplings are Gaussian variables with zero mean and average $\overline{(J_{i_1, \dots, i_p})^2} = p!/(2N^{p-1})$. The scaling with N ensures a well-defined thermodynamic limit [8]. This formulation is slightly different from the one given in references [3,6]. In the large N limit the free energy per spin f of the original spherical model [3,6] and that of model (1), ϕ , are related by

$$f(J, T, h) = \phi(r, J, T, h) - r/2 \quad (2)$$

where r is the value which makes the r.h.s. of equation (2) stationary. This corresponds to imposing the global constraint $\sum_{i=1}^N \sigma_i^2 = N$ on the amplitude of the spins [3,6].

Under general conditions the free energy ϕ can be derived from a variational principle [9]. To this end, we introduce the magnetization $m_i = \langle \sigma_i \rangle$ and the connected spin-spin correlation function $G_{ij} = \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle$ of (1) for fixed couplings, and perform a double Legendre transform of the free energy to obtain a functional of m_i and G_{ij} . We will use the formulation of references [10,11]. The free energy ϕ can then be written as

$$\beta N \phi(r, J, T, h) = \beta H(m) + \frac{1}{2} \text{Tr} \ln G^{-1} + \frac{1}{2} \text{Tr} \mathcal{D}^{-1}(m) G - \Gamma_2(m, G) + \text{const.} \quad (3)$$

where $\mathcal{D}^{-1}(m) = \partial^2 H(\sigma) / \partial \sigma_i \partial \sigma_j$, evaluated for $\sigma_i = m_i$. The functional $\Gamma_2(m, G)$ is given by the sum of all two-particle irreducible vacuum graphs in a theory with vertices determined by equation (1) and propagators set equal to G_{ij} . The m_i and G_{ij} are evaluated at the stationary point of the r.h.s. of equation (3).

By taking into account only the diagrams which contribute to the averaged free energy in the thermodynamic limit [12] (see Fig. 1), we obtain

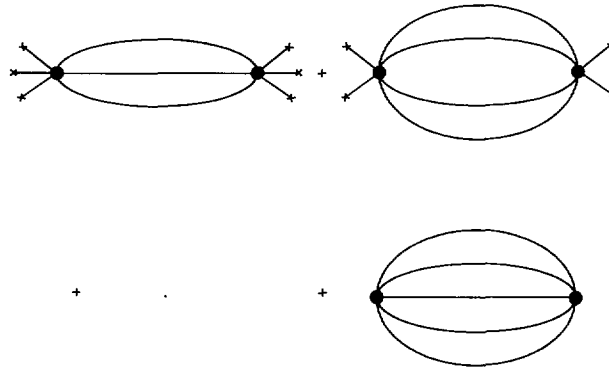


Fig. 1. — The two-particle irreducible diagrams which contribute in the limit $N \rightarrow \infty$ to $\Gamma_2(m, G)$. Each vertex has p lines and gives a contribution $-\beta J_{i_1, \dots, i_p}$. Each line joining two vertices gives a factor $G_{i,j}$, while each “dead-line” gives a factor m_i .

$$\begin{aligned} \phi(q, g, E, r) = \frac{r}{2}(q + g) &- \frac{1}{N}q^{1/2} \sum_i h_i \hat{m}_i + q^{p/2} E \\ &- \frac{T}{2} \ln g - \frac{\beta}{4} [(q + g)^p - q^p - pqg^{p-1}] \end{aligned} \quad (4)$$

where $Nq = \sum_i m_i^2$, $m_i = q^{1/2} \hat{m}_i$, $Ng = \text{Tr } G$ and $E = -(1/Np!) \sum J_{i_1, \dots, i_p} \hat{m}_{i_1} \dots \hat{m}_{i_p}$. The details are reported in Appendix A. In general, E is a random variable which depends on both the realization of couplings and the orientation of vector $\mathbf{m} = (m_1, \dots, m_N)$. In equation (4) we did not include the constant term which comes from the normalization of the trace over the spin variables [3] since it does not change the stationary point. Equation (4) is a variational principle for the free energy since, for any value of h , r and T , the m_i , or equivalently q and \hat{m}_i , and g are determined by the stationary point of (4).

We shall now consider only the zero external field case. From equation (4) we see that if $h_i = 0$ all situations with the same E will lead to the same free energy. Consequently, to have a defined problem, we consider E as given and study the solution as function of E . This corresponds to dividing the phase space into classes according to the value of E , and summing over all the states in one class. This is a statistics by classification [13], and corresponds to summing over the different TAP solutions [14–16].

By eliminating g and r from the stationary point of equations (2) and (4)

$$g = 1 - q \quad (5)$$

$$\beta r = \frac{1}{1 - q} + \frac{\beta^2 p}{2} (1 - q^{p-1}) \quad (6)$$

we are led to the following variational principle for the free energy per spin of the spherical p -spin SG model

$$f(q, E, T) = q^{p/2} E - \frac{T}{2} \ln(1 - q) - \frac{\beta}{4} [1 + (p - 1)q^p - pq^{p-1}] \quad (7)$$

which, for any T and E , has to be stationary with respect to q . Equation (6), for $\bar{r}(q) = \beta r - \beta^2 p/2$, is the equation of state first derived in reference [4] from the study of dynamics. Here r disappears, being replaced by the free energy.

The functional $f(q, E, T)$ is related to the generating functional of one-particle irreducible graphs, and hence the stationary point is a minimum of f . Equation (7) is the TAP free energy proposed by Kurchan *et al.* [6] and obtained by adding to the “naive” mean-field free energy, the first two terms in equation (7), the Onsager reaction term, the last term in (7), for the Ising p -spin SG model [17].

The stationary point of equation (7) gives, [6],

$$(1 - q)q^{p/2-1} = zT \quad (8)$$

where

$$z = \frac{1}{p-1} \left[-E \pm \sqrt{E^2 - E_c^2} \right], \quad E_c = -\sqrt{2(p-1)/p}. \quad (9)$$

It is easy to understand that, for any temperature T , and z low enough, there are two solutions of the saddle point equation (8), one corresponding to a maximum and one to a minimum. For $z > z_c = z(E_c)$ the stable solution leads to an unphysical q decreasing with temperature. Therefore, in equation (9) we take the “minus” sign. For $z < z_c$, and T low enough, the stable solution is the largest one, $q \geq 1 - 2/p$. The condition $z \leq z_c$ is equivalent to the non negativity of the relevant eigenvalue of the replica saddle point [3]. This confirms the assumption made in reference [6] on the stability of the TAP solution. Here, it comes naturally from the analysis of the saddle point.

The results discussed so far are valid for any fixed $E \leq E_c$. For values larger than E_c there are no physical solutions. The residual dependence of the free energy on E follows from the fact that we have summed only over all states within the class selected by the given E . Consequently, equation (7) represents the free energy of that class. To have the full partition function we have to sum $\exp(-\beta f)$, the partition function of the class E , over all classes, including the degeneracy factor [14–16]. In the thermodynamic limit the sum can be done by saddle point, so we have

$$f_J = \min_{E_J} \left[f(E_J, T) - \frac{T}{N} \ln \mathcal{N}(E_J) \right] \quad (10)$$

where the subscript “ J ” denotes that all this has to be done for fixed couplings. In other words, the minimum has to be taken over all allowed values of E for the given realization of couplings. In equation (10), $\mathcal{N}(E_J)$ is the volume, or density of states, of the class. In general $\mathcal{N}(E_J)$ is a random function which depends on the disorder only through the value of E_J . This follows from the fact that for fixed temperature f depends only on the value of E_J .

By definition f_J is a function of the realization of disorder. However, the free energy is self-averaging. This means that for $N \rightarrow \infty$ the overwhelming majority of sample will give the same free energy $\bar{f}(T)$, i.e.,

$$\text{for } N \rightarrow \infty \quad f_J(T) = \bar{f}(T) \quad \text{with probability 1.}$$

As a consequence, $\bar{f}(T)$ can be obtained by just averaging equation (10) over disorder. Due to the selfaveraging of E_J , this means replacing the second term by $\ln \mathcal{N}(E)$ and taking the minimum over all allowed values of E .

We have calculated $\mathcal{N}(E)$ following the lines of references [14,17]. The details are reported in Appendix B. The explicit calculation reveals that $g(E) = \ln \mathcal{N}(E)/N$ for $N \rightarrow \infty$ is given by

$$g(E) = \frac{1}{2} \left(\frac{2-p}{p} - \ln \frac{pz^2}{2} + \frac{p-1}{2} z^2 - \frac{2}{p^2 z^2} \right), \quad z \leq z_c. \quad (11)$$

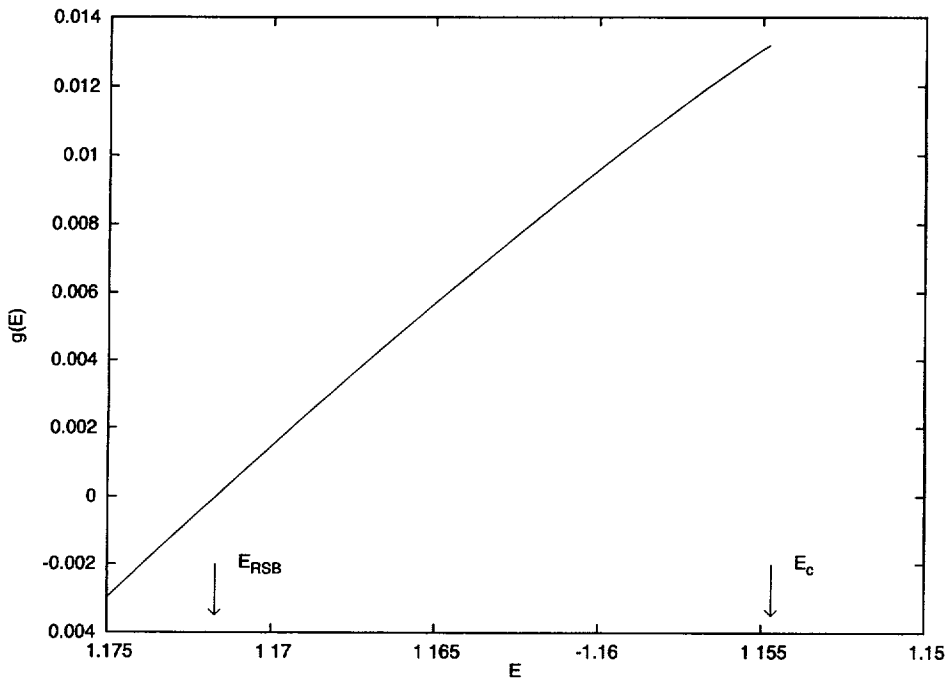


Fig. 2. — $g(E)$ as a function of E for $p = 3$. The range of E is restricted to $E \leq E_c$. The value E_{RSB} denotes the 1RSB solution.

This function is an increasing function of E which takes its maximum at the extremum $E = E_c$ and is zero for $E = E_{\text{RSB}} < E_c$. In Figure 2 it is shown the behavior of $g(E)$ as a function of E for $p = 3$, the corresponding values of E_c and E_{RSB} are indicated. For $E > E_c$ there are no physical solutions, i.e., $\mathcal{N}(E) = 0$. For $E < E_{\text{RSB}}$ the volume $\mathcal{N}(E)$ is exponentially small in N . Consequently, in looking for the minimum in equation (10), we have to restrict ourselves to values of E in the range $E_{\text{RSB}} \leq E \leq E_c$.

Collecting all the results we have that for $N \rightarrow \infty$ there exists a critical temperature T_c below which the thermodynamics of the spherical p -spin SG model is described by the free energy

$$\bar{f}(T) = f(q, E, T) - T g(E) - \frac{T}{2} [1 + \ln(2\pi)] \quad (12)$$

where q is given by equation (8) and E is the value which for the given temperature makes the r.h.s of equation (12) minimal. The last term, not included before, comes from the normalization of the trace over the spins and represents the entropy of the system at infinite temperature [3].

The critical temperature T_c is the largest temperature where $\bar{f}(T)$ is equal to the free energy of the replica symmetric solution $q = 0$ (high temperature solution), and is obtained for $E = E_c$. This corresponds to the critical temperature derived from dynamics from marginality. Indeed for $E = E_c$ we have $z = z_c$, i.e., the marginal condition [4].

As the temperature is decreased, the value of E which minimizes equation (12) decreases until it reaches the lower bound E_{RSB} . This happens at the critical temperature T_{RSB} , the same as found in the replica approach. From this point on the value of E cannot be decreased further since for lower values the number of solutions is exponentially small in N . Therefore for

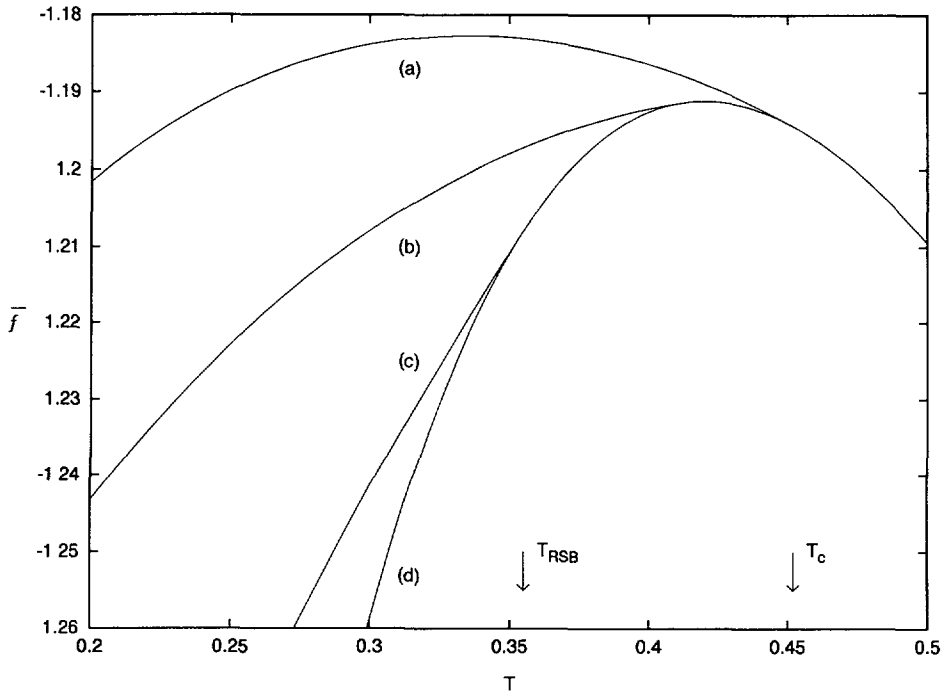


Fig. 3. — $\bar{f}(T)$ (Eq. (12)) as a function of T for $p = 15$ and different values of E : a) $E = E_c$; b) $E_{\text{RSB}} < E < E_c$; c) $E = E_{\text{RSB}}$; d) the replica symmetric (high temperature) free energy.

$T < T_{\text{RSB}}$ we have $E = E_{\text{RSB}}$. We note that while for temperatures in the range $T_{\text{RSB}} \leq T \leq T_c$ the free energy (12) is numerically equal to that of the replica symmetric solution, for $T < T_{\text{RSB}}$ it is larger. Nevertheless it is the lowest free energy among all the accessible states.

Similarly, in a dynamical calculation we have to restrict to the states with an energy corresponding to the largest volume in the phase space where the systems spends most of the time in its evolution. In our case the volume is proportional to $\exp(Ng(E))$, which is maximal for $E = E_c$, and all other permitted states have exponentially small volume compared to this. This means that the time to visit the other states is exponentially large in the system size. Therefore in the thermodynamic limit we have to limit to $E = E_c$ and we get the free energy (12) with E replaced by E_c for which

$$g(E_c) = -\frac{1}{2} \left[\ln(p-1) - 2 \frac{p-2}{p} \right]. \quad (13)$$

The energy defined by the thermodynamic relation $\mathcal{E} = \partial\beta\bar{f}(T)/\partial\beta$ is not affected by the complexity (13) since it does not depend on temperature. Moreover, it turns out that the energy so defined is *equal* to the energy derived from the dynamical calculation [4],

$$\mathcal{E} = -\frac{\beta}{2} (1 - q^p + m q^p) \quad (14)$$

where the parameter m following from the “quasi fluctuation dissipation theorem” is obtained from the marginal condition: $m = (p-2)(1/q-1)$ with q given by (8) with $z = z_c$.

We note that the free energies calculated in this paper for different E are all higher than free energies calculated in the replica approach for different m . They coincide only for the 1RSB solution. In Figure 3 we report $\bar{f}(T)$ as a function of T for $p = 15$ and different values of E . The free energies calculated in the replica approach are all below the 1RSB free energy. The free energy computed in this paper for the marginal solution corresponds to the correct free energy of the dynamical solution. It gives, in fact, the correct dynamical energy \mathcal{E} , while the corresponding quantity derived from the replica free energy for the marginal m gives a much lower energy.

In presence of an external field the scenario could be more complex since it is not *a priori* clear if there exists a consistent free energy corresponding to the dynamical state.

We conclude by noting that quite recently Marinari, Parisi and Ritort found, in a different model, numerical evidence of the scenario discussed in this paper [18].

Acknowledgments

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Appendix A

In this appendix we sketch the derivation of equation (4). The functional $\Gamma_2(m, G)$ is given by the sum of all vacuum diagrams of a theory with interactions determined by $\beta H_{\text{int}}(\sigma; m)$ and propagators G_{ij} . The interaction term is defined by the shifted Hamiltonian

$$H(\sigma + m) - H(m) - \sum_i \sigma_i \left. \frac{\partial H(\sigma)}{\partial \sigma_i} \right|_{\sigma_i = m_i} = \frac{T}{2} \sum_{i,j} \sigma_i \mathcal{D}_{ij}^{-1}(m) \sigma_j + H_{\text{int}}(\sigma; m). \quad (\text{A.1})$$

This procedure corresponds to a dressed loop expansion with vertices which depend on σ , and can exhibit non-perturbative effects even for small number of dressed loops. From (1) and (A.1) we obtain

$$\mathcal{D}_{ij}^{-1}(m) = r \delta_{ij} - (1 - \delta_{ij}) \frac{\beta}{(p-2)!} \sum_{k_1, \dots, k_{p-2}} J_{k_1, \dots, k_{p-2}, i, j} m_{k_1} \dots m_{k_{p-2}} \quad (\text{A.2})$$

and

$$\beta H_{\text{int}}(\sigma; m) = - \sum_{n=3}^p \frac{\beta}{n!(p-n)!} \sum_{\substack{k_1, \dots, k_{p-n} \\ h_1, \dots, h_n}} J_{k_1, \dots, k_{p-n}, h_1, \dots, h_n} m_{k_1} \dots m_{k_{p-n}} \sigma_{h_1} \dots \sigma_{h_n}. \quad (\text{A.3})$$

The interaction term contains $(p-2)$ vertices with $3, 4, \dots, p$ σ -leg and $p-3, p-4, \dots, 0$ m -leg, respectively. To evaluate $\Gamma_2(m, G)$ we have to consider all possible two-particle irreducible diagrams obtained joining together the σ -leg. The general structure is a series of “bubbles”.

We are interested in diagrams which contribute to the free energy in the thermodynamic limit $N \rightarrow \infty$. In this limit the leading contribution comes from the diagrams shown in Figure 1. For $N \rightarrow \infty$ we can replace J_{i_1, \dots, i_p}^2 by its average value, the correction being of order $O(1/N)$. Thus after some algebra the contribution of the diagrams of Figure 1 is:

$$\Gamma_2(m, G) = \frac{N\beta^2}{4} \left[(q+g)^p - q^p - p q^{p-1} g - \frac{p(p-1)}{2} q^{p-2} g^2 \right] \quad (\text{A.4})$$

where $Nq = \sum_i m_i^2$ and $Ng = \text{Tr } G$. From the stationarity of (3) with respect to variations of G_{ij} we get that G_{ij} obeys a Dyson-type equation

$$G_{ij}^{-1} = G_o^{-1} \delta_{ij} - \Sigma_{ij} \quad (\text{A.5})$$

with

$$G_o^{-1} = -\beta r - \frac{\beta^2 p}{2} [(p+q)^{p-1} - q^{p-1} - (p-1)q^{p-2}g] \quad (\text{A.6})$$

and self-energy

$$\Sigma_{ij} = \frac{\beta}{(p-2)!} \sum_{k_1, \dots, k_{p-2}} J_{k_1, \dots, k_{p-2}, i, j} m_{k_1} \cdots m_{k_{p-2}}. \quad (\text{A.7})$$

In the limit $N \rightarrow \infty$ the lines Σ_{ij} correlate only together, thus we can replace

$$\phi_o(G_o) = \text{Tr} \ln G^{-1} = \text{Tr} \ln(G_o^{-1} - \Sigma) \quad (\text{A.8})$$

by the partially averaged one over disorder $\overline{\phi_o(G_o)}$ for fixed G_o [12]. This leads to

$$\overline{\phi_o(G_o)} = -\frac{\alpha}{2} (\text{Tr } G)^2 - \ln(G_o^{-1} - \alpha \text{Tr } G) \quad (\text{A.9})$$

where the r.h.s has to be evaluated at the stationary point with respect to $\text{Tr } G$, and

$$\alpha = \frac{\overline{\Sigma_{ij}^2}}{2N} = \frac{\beta^2}{2N} p(p-1)q^{p-2} \quad (\text{A.10})$$

Similarly in the limit $N \rightarrow \infty$ we have

$$\text{Tr } G = \frac{N}{G_o^{-1} - \alpha \text{Tr } G}. \quad (\text{A.11})$$

Finally we have

$$\frac{\beta}{(p-2)!} \sum_{k_1, \dots, k_{p-2}, i, j} J_{k_1, \dots, k_{p-2}, i, j} m_{k_1} \cdots m_{k_{p-2}} G_{ij} = \text{Tr } \Sigma G = \frac{\alpha}{N} (\text{Tr } G)^2 \quad (\text{A.12})$$

Inserting equations (A.2), (A.4), (A.9) and (A.12) into (3) equation (4) follows. The resulting equation is stationary with respect to variations of m_i and g .

Appendix B

Here we derive equation (11) of the text. The TAP equations are obtained by differentiation of the free energy functional equation (7) with respect to m_i , and reads

$$\left[\frac{1}{1-q} + \mu(p-1)(1-q)q^{p-2} \right] m_i = \frac{\beta}{(p-1)!} \sum_{k_1, \dots, k_{p-1}} J_{k_1, \dots, k_{p-1}, i} m_{k_1} \cdots m_{k_{p-1}} + \beta h \quad (\text{B.1})$$

where we have included an external magnetic field, and $\mu = \beta^2 p/2$. The number of solutions $\mathcal{N}(q)$ of the TAP equations (B.1) for a given value of q is given by

$$\mathcal{N}(q) = N \int_{-\infty}^{\infty} \prod_i^N dm_i \prod_i \delta(G_i) |\det A| \delta(Nq - \sum_i m_i^2), \quad (\text{B.2})$$

where

$$G_i = \left[\frac{1}{1-q} + \mu(p-1)(1-q)q^{p-2} \right] m_i - \frac{\beta}{(p-1)!} \sum_{k_1, \dots, k_{p-1}} J_{k_1, \dots, k_{p-1}, i} m_{k_1} \cdots m_{k_{p-1}} - \beta h \tag{B.3}$$

and $A_{ij} = \partial G_i / \partial m_j$. We calculate $\overline{\mathcal{N}}(q)$, which means averaging over the bond distribution, following reference [14, 17]. We do not report all the details, the interested reader can find them in reference [17]. The final equation reads

$$\overline{\mathcal{N}} = c \int d\hat{q} dB d\Delta e^{N\Xi} \tag{B.4}$$

where c is a constant and

$$\Xi = i\hat{q}q - (B + \Delta)(1-q) + \frac{1}{\lambda}(B^2 - \Delta^2) + \ln \left(\frac{1}{1-q} + B \right) + \ln I \tag{B.5}$$

$$I = \int \frac{dm d\hat{m}}{2\pi} \exp \left\{ \frac{\mu q^{p-1}}{2} (i\hat{m})^2 + i\hat{m} \left[\left(\frac{1}{1-q} - \Delta \right) m - \beta h \right] - i\hat{q}m^2 \right\} \tag{B.6}$$

where $\lambda = 2\mu(p-1)q^{p-2}$. Performing the integrals on \hat{q} , B and Δ we finally have

$$\overline{\mathcal{N}}(q) = e^{N g(q)} \tag{B.7}$$

$$g(q) = -\ln(1-q) + \frac{1}{2} + \frac{1}{2} \ln q - \frac{1}{2} \ln(\mu q^{p-1}) + \frac{p-1}{2\mu p q^{p-2}} \left[\frac{1}{1-q} - \mu(1-q)q^{p-2} \right]^2 - \frac{1}{2\mu(1-q)^2 q^{p-2}}. \tag{B.8}$$

Equation (11) follows by eliminating q as a function of z through equation (8).

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