On the TAP approach to the Spherical p-spin SG Model

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(June 7, 1994)

Abstract

In this letter we analyze the 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 $N \to \infty$ of a diagrammatic expansion of the free energy. We find that if the multiplicity of the TAP solutions is taken into account, then 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.

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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 possess a non-trivial low temperature and 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. The free energy, nevertheless, remains continuous. The study of the dynamics yields a similar scenario but with a first order transition at an higher critical temperature \( T_c > T_{RSB} \), and a slightly different low temperature phase. This surprising result was first noted in Ref. [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 TAP free energy for this model and showed that in the absence of magnetic field the 1RSB solution is 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 $N \to \infty$ limit. In this letter we show that taking into account the degeneracy of the TAP solutions, usually called “complexity”, then in the thermodynamic limit $N \to \infty$ 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. All details will be reported elsewhere.

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

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

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 $(J_{i_1, \ldots, i_p})^2 = p!/(2N^{p-1})$. The scaling with $N$ ensures a well defined thermodynamic limit [7]. This formulation is slightly different from the one given in Refs. [3,6]. In the large $N$ limit the free energy per spin $f$ of the original spherical model [3,6] and that of the model (1), $\phi$, are related by

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

where $r$ is the value which makes the r.h.s. of (2) stationary. This corresponds to impose 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 $\phi$ can be derived from a variational principle. 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. Then following Refs. [8,9] the free energy $\phi$ can be written as

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

where $T \mathcal{D}^{-1}(m) = \partial^2 H(\sigma)/\partial \sigma_i \partial \sigma_j$ 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 (I) and propagator set equal to $G_{ij}$. The $m_i$ and $G_{ij}$ are evaluated at the stationary point of the r.h.s. of (II).

By taking into account only the diagrams which contribute to the averaged free energy in the thermodynamic limit [10], see Fig. I, we obtain

$$\phi(q, g, E, r) = \frac{r}{2}(q + g) - \frac{1}{N} q^{1/2} \sum_i h_i \hat{m}_i + q^{p/2}E$$

$$- \frac{T}{2} \ln g - \frac{\beta}{4} \left[ (q + g)^p - q^p - pgq^{p-1} \right]$$

(4)

where $Nq = \sum_i m_i^2$, $m_i = q^{1/2} \hat{m}_i$, $Ng = \text{Tr} G$ and $E = -(1/N!) \sum J_{i_1, \ldots, i_p} \hat{m}_{i_1} \cdots \hat{m}_{i_p}$. The details will be reported elsewhere. In (II) we did not included the constant term which comes from the normalization of the trace over the spin variables [3] since it does not change the stationary point. In general $E$ is a random variable which depends on both the realization of couplings and on the orientation of the vector $\mathbf{m} = (m_1, \ldots, m_N)$. 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 (II).

We shall now consider only the zero external field case. From (II) 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 divide the phase space into classes according to the value of $E$, and sum over all the states in one class. This is a statistics by classification [11].

By eliminating $g$ and $r$ from the stationary point of equations (I) and (II)

$$g = 1 - q$$

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

(5)

(6)

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

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

(7)
which, for any $T$ and $E$, has to be stationary with respect to $q$. Equation (6), for $\tau(q) = \beta r - \beta^2 p/2$, is the equation of state first derived in [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 (6), the Onsager reaction term, the last term in (6), for the Ising $p$-spin SG model [12].

The stationary point of equation (7) gives, c.f.r. [6],

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

where

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

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 solutions leads to an unphysical $q$ decreasing with temperature. Therefore, in (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 Ref. [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 eq. (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. In the thermodynamic limit the sum can be done by saddle point, so we have
\[ f_J = \min_{E_J} \left[ f(E_J, T) - \frac{T}{N} \ln \mathcal{N}(E_J) \right] \]  

(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 (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 \(N \to \infty\) the overhalming majority of sample will give the same free energy \(\overline{f}(T)\), i.e.,

\[
\text{for } N \to \infty \quad f_J(T) = \overline{f}(T) \quad \text{with probability 1.}
\]

As a consequence \(\overline{f}(T)\) can be obtained just averaging eq. (10) over disorder. Due to the selfaveraging of \(E_J\) this means to replace 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 Refs. [13,12]. The details will be reported elsewhere. The explicit calculation reveals that \(g(E) = \ln \mathcal{N}(E)/N\) for \(N \to \infty\) is given by

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

(11)

This function is an increasing function of \(E\) which takes its maximum at the extremum \(E = E_c\) and is zero for \(E = E_{RSB} < E_c\). In figure 2 we report the behavior of \(g(E)\) as a function of \(E\) for \(p = 3\) where 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 \(E < E_{RSB}\) the volume \(\mathcal{N}(E)\) is exponentially small in \(N\). Consequently, in looking for the minimum in (10) we have to restrict ourselves to values of \(E\) in the range \(E_{RSB} \leq E \leq E_c\).

Collecting all the results we have that for \(N \to \infty\) there exists a critical temperature \(T_c\) below which the thermodynamics of the spherical \(p\)-spin SG model is described by the free energy.
\[
\overline{f}(T) = f(q, E, T) - T \, g(E) - \frac{T}{2} \left[ 1 + \ln(2\pi) \right]
\]  
(12)

where \( q \) is given by eq. (8) and \( E \) is the value which for the given temperature makes the r.h.s of (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 \( \overline{f}(T) \) 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 (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 \( T < T_{RSB} \) we have \( E = E_{RSB} \). We note that while for temperatures in the range \( T_{RSB} \leq T \leq T_c \) the free energy (12) is numerically equal to that of the replica symmetric solution, for \( T < T_{RSB} \) 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 \( \exp(N \, g(E)) \) 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 restrict to \( E = E_c \) and we get the free energy (12) with \( E \) replaced by \( E_c \) for which

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

The energy defined by the thermodynamic relation \( E = \partial\beta \overline{f}(T)/\partial\beta \) 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],
\[ \mathcal{E} = -\frac{\beta}{2} (1 - q^p + m q^p) \] (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 Fig. 3 we report \( f(T) \) 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 \textit{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 [14].

\section*{ACKNOWLEDGMENTS}

AC thanks the Sonderforschungsbereich 237 for financial support and the Universität-Gesamthochschule of Essen for kind hospitality, where part of this work was done.
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FIGURES

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

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.

FIG. 3. $\mathcal{F}(T)$ eq. (12) as a function of $T$ for $p = 15$ and different values of $E$: (a) $E = E_c$; (b) $E_{RSB} < E < E_c$; (c) $E = E_{RSB}$; (d) the replica symmetric (high temperature) free energy.