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X Ciclo

Investigation of the hidden structure of states in spin glasses

An entropic approach

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Io rifletto,
il panico dell'insetto.

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I. Introduction

There are mean field models for spin glasses whose structure of the states cannot be studied by means of the usual methods of equilibrium statistical mechanics, so that this structure remains hidden to standard investigations. Among these models a leading role is played by the p-spin spherical model, which is the subject of this thesis.

The main question is: Why the structure of the states in such a model is hidden ? The answer is that the p-spin spherical model, and probably many other physical systems which exhibit a glassy behaviour, has a temperature phase where a new and anomalous definition of equilibrium must be adopted: within this definition, equilibrium states *have not* equilibrium free energy density. This anomaly has serious consequences on our standard definitions of thermodynamic weights, dominant states and so on, so that the standard methods fail in detecting the whole structure.

The reason of this anomalous equilibrium is exquisitely entropic. We can explain the problem in the following way: The low temperature phase of the p-spin spherical model is characterized by the presence of many different states, with different free energy densities. The important thing is that the number $\mathcal{N}$ of states with a given free energy density is not simply large, but *exponentially large*, that is it grows as an exponential of the size N of the system

$$\mathcal{N} \sim e^{N\Sigma}$$

where Σ is called *complexity* and plays a crucial role in the physics of glassy systems. In these conditions, in order to define equilibrium states we must take into consideration the fact that the entropy has two different contributions, an intra-state contribution S_{in} which comes from the configurations belonging to the same state and a collective contribution coming from the fact that there is an exponentially high number of states with the same free energy density. This second contribution is Σ. The total entropy density is thus

$$S = S_{in} + \Sigma$$

This means that the *individual* free energy density of a single state is

$$f = E - TS_{in}$$

while the *global* free energy density of the system is

$$\phi = E - TS = f - T\Sigma(f)$$

where we have grouped together states with the same free energy density f. Equilibrium is obtained by minimizing the global free energy, so that we must find the minimum of ϕ with respect to f: equilibrium is given by those states which optimize the balance between their free energy and their complexity, so that equilibrium states are not simply the ones with the lowest free energy, but those whose free energy density f gives the minimum of ϕ.

Moreover, it is clear that

$$\phi_{eq} = f_{eq} - T\Sigma_{eq} < f_{eq}$$

that is, equilibrium states have a free energy density f_{eq} which is *higher* than the global equilibrium free energy density ϕ_{eq} of the system, as we stated at the beginning. Besides, there are many states, both with free energy densities lower and higher than f_{eq}, which do not minimize ϕ: all these states must be considered as metastable.

It is known that a common feature of mean field models for disordered systems is to have many states and there are cases where an exponentially high number of metastable states is also present. So why this situation is not ubiquitous ? The reason is that in general the value f minimizing ϕ lies outside the region of the existing states, so that equilibrium is given by the lowest lying states. In this case equilibrium is not anomalous. This happens also for the p-spin spherical model when the temperature is very low: the free energy which minimizes ϕ lies below the free energy of the lowest states, which therefore will be the equilibrium ones. Yet, increasing the temperature the complexity becomes more and more important, until a temperature T_s is reached where the minimum of ϕ enters in the region of the existing states and the scenario described above takes place. T_s is the static transition temperature of the system.

The generalized free energy of the system ϕ is a fully collective quantity: singularly taken there is no real difference between an equilibrium and a metastable state, so that the same concept of equilibrium has to be interpreted as a collective effect. This fact has the important consequence that all the states, both metastable and equilibrium, have a thermodynamic weight which is vanishing in the thermodynamic limit. We shall talk a lot of this point in chapter II, but in this context we can understand this fact in a simple way: the difference between the extensive free energy of a single state, Nf, and the global equilibrium extensive free energy, $N\phi_{eq}$, is *extensive too* and it is roughly equal to $N\Sigma_{eq}$. This means that, no matter which are the small differences in free energy densities between the states, their thermodynamic weight is normalized by an extra factor $e^{N\Sigma}$, which brings the weight to zero. Metastable states are locally as much important as equilibrium states.

When the conditions described above occur it is not surprising that standard equilibrium methods fail in the investigation of the structure of the states. The best we can hope is that they catch the collective contribution correctly, giving the global free energy ϕ, but we cannot expect they are able to discriminate among states whose thermodynamic weight is zero: states are too much and too light.

Our next question is then: This really seems a very pathologic scenario. Why should we study models of this kind ? The answer is that this scenario gives a very good reference frame for the description of many features which are often encountered in the study of glassy systems.

The most important property of the p-spin spherical model, consequence of the strong role metastability has, is the presence of a dynamical transition at a temperature T_d which is higher than the static transition temperature T_s: at T_d relaxation times diverge and metastable states become determinant, even if standard equilibrium quantities do not show any anomaly. It is not difficult to understand that this peculiarity is strongly related to the scenario we have described above: the dynamics remains freezed by the presence of this huge number of metastable states, which singularly do not contribute to the static of the system, so that the transition is disregarded by equilibrium thermodynamics.

The presence of a dynamical transition is the main reason why these kind of models are considered as good mean field candidates for the description of real glasses. Within a mean field theory, barriers surrounding metastable states are infinite, so that at T_d relaxation times diverge. The most natural thing we can imagine (and hope) to happen out of mean field is that the global structure of the states is conserved, but that the average lifetime of metastable states becomes finite. In this context T_d would represent a crossover temperature, rather than a transition, where times start becoming very large, much larger than the laboratory times. This gives a good frame for the description of glasses, where a dramatic slowing down of the dynamics occurs without any divergence of thermodynamic quantities. Moreover, the dynamics of the p-spin spherical model is described by equations which are formally very similar to the Mode Coupling equations for super-cooled liquids, suggesting once again that this model has deep relations with the nature of the glassy phase.

From what explained above it is clear that a deep knowledge of the geometrical structure of the states for these kind of models is very important. This structure is hidden to standard methods, as we shall widely show in chapter II, so that we must introduce and develop some new methods to perform this investigation.

Our first necessity will be to demonstrate that a non-trivial structure of the states, worth of investigation, actually exists in the p-spin spherical model. This starting point is not trivial, since the results coming from the standard methods seem to suggest that there is no structure at all of the states. Chapter III is dedicated to prove that this last conclusion is not true.

In chapter IV we shall introduce a method which will lead us to a quite deep description of the geometrical structure of the states for this model. Our strategy will be purely entropic: given that all the most important features of this model have an entropic origin, we will completely disregard the equilibrium thermodynamic weight of the states, describing their geometrical organization simply in terms of their *number*. We shall define in this way a quantity which represents the main result of our work, which is the *constrained complexity*.

Most of the results exposed in this thesis are original. In particular, great part of chapter III and the entirety of chapter IV are fruits of the works done together with Irene Giardina and Giorgio Parisi. Nevertheless, there is no original result which is not influenced by discussions with other people. In our case many of these discussion have been determinant for the understanding and the advance of our work, so that we want to thank Alain Barrat, Jean-Philippe Bouchaud, Premi Chandra, Leticia Cugliandolo, Silvio Franz, Jorge Kurchan, Marc Mézard, Rémi Monasson, Heiko Rieger, Felix Ritort, Juan Jesús Ruiz-Lorenzo, David Ruelle, David Sherrington and Miguel Angel Virasoro.

I especially thank Giorgio, who taught me all of this and I neither understood how.

II. The known results

We expose in this chapter the most important known results on the p-spin spherical model and we introduce many concepts which are essential to the description of disordered systems. The results related to the statics of this model have been mainly obtained by means of two standard methods, the replica method and the TAP method. We shall analyze in details the nature of the anomalous equilibrium which occurs in this model, giving a general discussion of these standard results that will clarify the motivations of our next investigation. We end the chapter with a non-standard hypothesis on the nature of the paramagnetic state in this model.

Contents:

1. The model and some basilar definitions.

The p-spin spherical model is defined by the following Hamiltonian [1,2,3]

$$H(s) = - \sum_{1 \leq i_1 < \ldots < i_p \leq N} J_{i_1 \ldots i_p} s_{i_1} \ldots s_{i_p} \quad , \quad p \geq 3 \tag{1.1}$$

where the spins s are not Ising-like variables (± 1), but real numbers satisfying a spherical constraint necessary to keep finite the energy

$$\sum_{i=1}^{N} s_i^2 = N \tag{1.2}$$

and N is the total number of spins. The couplings J which encode the disorder are Gaussian variables with zero mean and variance $p!/2N^{p-1}$, so that their probability distribution is given by

$$\mathcal{D}P(J) = \prod_{i_1 < \ldots < i_p} \sqrt{\frac{N^{p-1}}{\pi p!}} \exp(-J^2_{i_1 \ldots i_p} N^{p-1}/p!) \; dJ_{i_1 \ldots i_p} \; . \tag{1.3}$$

A non-spherical Ising version of the p-spin model has been introduced long ago in [1], where it was shown that in the limit $p \to \infty$ the model was solved exactly by a first step of the Parisi replica symmetry breaking scheme (1RSB) [4,5,6]. In a subsequent work [7] it was found that for the same model there was a range of temperature where the 1RSB gives the correct solution for any $p \geq 3$. Therefore, it has been immediately clear that this model was a good candidate for a better understanding of the replica symmetry breaking mechanism. Successively, in the seminal paper of Kirkpatrick and Thirumalai [2] it has been taken into consideration a soft-Ising spin version of the model. Here, for the first time, appeared one of the most important features of this model, i.e. the presence of a dynamical transition, that is a breaking of the ergodicity with consequent freezing of the dynamics, at a temperature which is *larger* then the static transition temperature defined by means of equilibrium quantities. Therefore, for the first time it was recognized that the existence of metastable states in this model played a crucial role in determining its dynamical behaviour. In [3] it has been introduced the spherical version of the p-spin model and its static properties have been deeply analyzed by means of the Parisi replica symmetry breaking scheme. Here it has been fully demonstrated that the model is exactly solved for any $p \geq 3$ by a one step replica symmetry broken solution of the saddle point equations. We shall summarize in section 2 the results of this analysis. Finally in [8] it has been performed the TAP analysis of this spherical model, which we shall take into consideration in section 3.

Many things have to be noted on this model. First of all this is a mean field model, since the sum over the interactions is extended to all the spins of the system. Therefore in the limit $N \to \infty$ the saddle point approximation for the computation of the partition function must provide the exact solution.

Secondly, each term of Hamiltonian (1.1) is a p-bodies interaction. This has to be compared with the case of the Sherrington-Kirkpatrick [9] model where a two bodies interaction is present. The p-bodies interaction contributes in some sense to increase the degree of frustration of the system. We can understand this fact in the simple case of a non-disordered Ising-like version of the model: let us consider

$p = 3$ and the ferromagnetic couplings

$$J_{i,k,l} = 1 \qquad \text{for each} \quad i,k,l \ . \tag{1.4}$$

Each triplet of spins tends to give a sign + to lower the global energy (1.1). Yet we see that this can be achieved by one of the four configurations

$$\begin{array}{c} +++ \\ +-- \\ -+- \\ --+ \end{array} \tag{1.5}$$

We see that there is a degeneration of the minimum local energy, with consequent frustration of the system which can choose among many possibilities. In the case of a two body interaction $p = 2$ we would have only the two possibilities $++$ or $--$, which are related by the spin flip transformation. Note that in this example we do not have the contribution to the frustration coming from the disorder, which normally prevent each spin to satisfy simultaneously all the interactions. Moreover, we see from (1.5) that the magnetization of the first configuration is $m = 3$, while the other three configurations have $m = 1$, so that there is a degeneration of this low magnetization value. This means that at low temperature the global ferromagnetic state $s_i = +1$ with total magnetization $M \sim N$ is energetically favoured, but there is a large entropic contribution of the paramagnetic state with $M \sim 0$ due to the degeneration we stated above. Therefore we can imagine that the paramagnetic state will be favoured also at temperatures lower than the formation of the ferromagnetic state, which will be thus a metastable state. This is exactly what happens for the ferromagnetic p-spin spherical model: the ferromagnetic state appears at a temperature T_1, but due to its very low entropy is metastable. At temperature $T_2 < T_1$ the ferromagnetic energy is so low to overcome the free energy gap with the paramagnetic state, so that a first order transition from the paramagnetic to the ferromagnetic state occurs. Note how important is the role of the entropy in this transition: the ferromagnetic state has an energy which is *always* lower than the paramagnetic one, so that the metastability has exclusively an entropic origin. From this very simple case it is thus possible to forecast that even in the disordered case, the $p \geq 3$-bodies interaction will be a source of degeneration of the states, with a consequent strong role of metastability.

Now let us note that in model (1.1) the spins are real variables: due to this each spin is less frustrated then the case $s_i = \pm 1$, since it can choose among a continuous spectrum of values to satisfy its local field. As a consequence of this balance between the p-bodies interaction (higher frustration) and the continuity of the variables (lower frustration) one can show that the spherical model with $p = 2$ has a quasi-trivial static behaviour, in the sense that there is the formation of only two states in the low temperature phase, so that the system does not exhibit a fully glassy phenomenology [10].

An important geometrical consequence of the spherical constraint is that the phase space of this model is an $(N-1)$-dimensional sphere, embedded in an N dimensional space. Each configuration can be viewed as a vector of length $\sqrt{N}$ on this sphere. In this context it arises a natural definition of the the distance between two different configurations in the phase space. Given two configurations s^a and s^b, we define the *overlap* $q_{s^a s^b}$ between them as

$$q_{s^a s^b} = \frac{1}{N}\sum_{i=1}^{N} s_i^a s_i^b \tag{1.6}$$

which is exactly the cosine of the angle between the two configurations on the sphere. With this definition, two configurations have the maximum distance when their overlap is zero, i.e. when they are orthogonal. On the other hand, we note that $q_{s^a s^b} = 1$ does not necessarily implies that two configurations are coincident. Indeed, all the results we will obtain have to be understood in the thermodynamic limit $N \to \infty$, therefore it is sufficient that two configurations differ for a number of spins which is finite or which grows as N^α with $\alpha < 1$, to get $q_{s^a s^b} = 1$.

The overlap gives also a measure of the similarity between different *states*, intended as different component of the Boltzmann measure. We can write [11]:

$$\langle s_i \rangle = \sum_\alpha w_\alpha \langle s_i \rangle_\alpha \tag{1.7}$$

where the sum is extended over all the different states α of the system and w_α is their thermodynamic weight, defined as

$$w_\alpha = \frac{e^{-\beta N f_\alpha}}{Z} = \frac{Z_\alpha}{Z} \ . \tag{1.8}$$

Here f_α is the free energy density of state α and Z the total partition function. The overlap $q_{\alpha\beta}$ between two states is defined as

$$q_{\alpha\beta} = \frac{1}{N}\sum_{i=1}^{N} \langle s_i \rangle_\alpha \langle s_i \rangle_\beta \tag{1.9}$$

To understand in an intuitive way the meaning of the overlap between states we can proceed in the following way. We write the thermodynamic average $\langle s_i \rangle_\alpha$ as an average over all the configurations which *belongs* to state α:

$$\langle s_i \rangle_\alpha = \frac{1}{Z_\alpha}\sum_{[s^\alpha]} s_i^\alpha e^{-\beta H(s^\alpha)} \quad , \quad Z_\alpha = e^{-\beta N f_\alpha} \tag{1.10}$$

There is no formal way to define configurations s^α, but we stress that this is only an intuitive approach. In this way we have for the overlap between two states:

$$q_{\alpha\beta} = \frac{1}{Z_\alpha Z_\beta}\sum_{[s^\alpha, s^\beta]} \frac{1}{N}\sum_{i=1}^{N} s_i^\alpha s_i^\beta \ e^{-\beta H(s^\alpha)} \ e^{-\beta H(s^\beta)} = \frac{1}{Z_\alpha Z_\beta}\sum_{[s^\alpha, s^\beta]} q_{s^\alpha s^\beta} \ e^{-\beta H(s^\alpha)} \ e^{-\beta H(s^\beta)} \ . \tag{1.11}$$

We see that the overlap between states is the average of the overlap between all the configurations belonging to them, that is their average distance on the sphere. The overlap between two states is a measure of their similarity and can be viewed as the inverse distance which separates the states. For this reason we will often use the term *distance* instead of *overlap* when talking about the structure of the states.

Note that in this intuitive context we can write

$$Z_\alpha = \sum_{[s^\alpha]} \ e^{-\beta H(s^\alpha)} \tag{1.12}$$

If we compute the overlap of a state with itself, we have

$$q_{\alpha\alpha} = \frac{1}{N}\sum_{i=1}^{N}\langle s_i\rangle_\alpha\langle s_i\rangle_\alpha \tag{1.13}$$

which is called *self-overlap* and gives the average largeness of the state. Obviously, by virtue of the spherical constraint, configurations have a self-overlap equal to one. Note that the self-overlap of a state can be written as

$$q_{\alpha\alpha} = \frac{1}{N}\sum_{i=1}^{N}(m_i^\alpha)^2 \tag{1.14}$$

where m_i^α is the local magnetization of state α in the site i. In this form one can understand why the self-overlap is often considered as the order parameter for spin glasses and for disordered systems in general: due to the disorder each single site has a different local magnetization also in the low temperature phase, so that the global magnetization is zero and it is not a good order parameter. Thus one resorts to compute the self-overlap. In [12] it has been introduced for the first time a quantity similar to the self-overlap: the original definition of the Edward-Anderson order parameter was

$$q_{EA} = \overline{\frac{1}{N}\sum_{i=1}^{N} m_i^2} \tag{1.15}$$

where the bar indicates an average over the disorder J. By means of equation (1.7) q_{EA}, can be written as

$$q_{EA} = \overline{\sum_{\alpha,\beta} w_\alpha w_\beta \; q_{\alpha\beta}} \; . \tag{1.16}$$

Note the difference with definition (1.13): q_{EA} mixes together the self-overlaps and the mutual overlaps of *all* the states. Obviously these two definitions are coincident when there is just one thermodynamic state, as it happens in the high temperature paramagnetic phase of a system.

We note here a thing which will be important in the following. We have seen that two configurations are coincident in the thermodynamic limit if their mutual overlap is equal to one, which is the self-overlap of each configuration. For the states we can give a similar definition. Given two states with the *same* self-overlap q_{self}, the maximum value of their mutual overlap q is exactly

$$q = q_{self} \; . \tag{1.17}$$

In other words, we are saying that two states are coincident if their mean distance is equal to their largeness. Again we stress that this definition has to be interpreted only in the limit $N \to \infty$: if two states are separated by energy barriers which grows as $N^\alpha, \alpha < 1$, we are not able to say which configurations belong to one state or to the other, so that these two states would fulfill equation (1.17). Thus we shall often refer to such states as not well separated states. When two states have different self-overlap, we can generalize the above discussion giving the following definition of well separated states:

$$\frac{q_{12}}{\sqrt{q_1 q_2}} < 1 \tag{1.18}$$

where q_1, q_2 are the self-overlaps of the two states and q_{12} is their mutual overlap.

Once we have defined the overlap between states we can introduce the overlap distribution function $P(q)$

$$P(q) = \overline{\sum_{\alpha,\beta} w_\alpha w_\beta \ \delta(q - q_{\alpha\beta})} \tag{1.19}$$

where the bar indicates the average over the disorder J. The distribution $P(q)$ simply gives the probability that, drawn two states with probability equal to their thermodynamic weight, their mutual overlap is q. This quantity gives a very important structural information on the mutual disposition of the states in the phase space [11]. By means of $P(q)$ we can write the Edward-Anderson order parameter as

$$q_{EA} = \overline{\int dq \ P(q) \ q} \tag{1.20}$$

that is the mean value of the overlap q. Nevertheless, it is common to indicate with q_{EA} the genuine self-overlap of the states, as defined in (1.13). In the following of this thesis we shall use as much as possible the term self-overlap to indicate this quantity, even if sometimes q_{EA} will be also used as a synonymous of self-overlap.

The last thing we want to state on the overlap concerns a very special value of it, that is $q = 0$. Normally the paramagnetic state is associated to the property of ergodicity of the system: the self-overlap of the paramagnetic state is zero, meaning that this state is not localized in any special region of the phase space. Actually this is a tricky point, since there are cases where the paramagnetic state coexists with localized states which have self-overlap different from zero. In the case of the ferromagnetic p-spin spherical model, for instance, there is a range of temperature where the ferromagnetic state, strongly localized around the direction $(1, 1, \ldots, 1)$, coexists with the paramagnetic state which is delocalized on the plane orthogonal to that direction. Clearly the self-overlap of the paramagnetic state is still zero, since two random configurations on this plane are orthogonal in average, but the ergodicity is broken, since there is the trapping region of the ferromagnetic state. Besides, the value $q = 0$ can be associated to a very different situation, where there are many localized states which are all mutually orthogonal, even if there is no paramagnetic state at all. From what said we conclude that each times the distribution function $P(q)$ gives $q = 0$ as a possible value in the overlap spectrum of the system, great care has to be taken in the physical interpretation of this fact.

We turn now to the analytical study of this model.

2. The replica method.

When we study the properties of disordered systems obviously we are able to make statements only on quantities averaged over the couplings J. This implies that we are interested in the computation of things which are the same for each sample, i.e. for each given assignment of the couplings J. In other words, if each sample had properties which are completely different from other samples, having nothing to share with them, there would be very little interest in studying disordered system and especially in computing average quantities. Fortunately enough, experience shows that besides some properties which actually depends on the particular sample we are considering, there are quantities which are the same for all the samples, provided that the size N of the system is large enough. Quantities belonging to this second class are called *self-averaging* quantities. For instance, if we break a glass, the shape of the pieces we obtain is surely dependent on that particular glass, while the density or the specific heat of many glasses at the same temperature are the same. Since, by definition, the average over many samples of a self-averaging quantity is equal to the quantity itself, we can compare observed (or simulated) self-averaging quantities with our averaged theoretical values.

The crucial question is then: Which are the self-averaging quantities ? A complete discussion of this problem is far beyond the purpose of this thesis. We limit ourselves to state that extensive quantity are self-averaging [13], so that the free energy of the system is a good quantity to compute. This is not surprising, since all important physical observables, which we hope are self-averaging, are derived from the free energy. This means that our starting point is the computation of the free energy averaged over the disorder:

$$\beta N\overline{F} = -\overline{\log Z} = -\int \mathcal{D}P(J)\ \log \int \mathcal{D}s\ e^{-\beta H(s)}\ . \tag{2.1}$$

We will indicate by F the free energy density. This kind of average is called *quenched*, since the thermal integral over the spins is performed at fixed (quenched) J. On the other hand, by computing $\log \overline{Z}$ we put s and J on the same foot: this is called *annealed* average and in this case is unphysical, since the evolution times of variables s in real systems are much smaller then the ones of J, so that we can consider the J's as fixed during the thermal evolution of the s's. Note that the annealed computation corresponds to taking the average of the partition function, which is not extensive and therefore not self-averaging.

The analytic computation of (2.1) is very difficult, so that we resort to the replica trick [12] to face the problem. We write

$$\overline{\log Z} = \lim_{n\to 0} \frac{1}{n} \log \overline{Z^n} \tag{2.2}$$

which is a much more manageable expression. The replica trick consists in writing

$$Z^n = Z_1 \cdot Z_2 \cdot \ldots \cdot Z_n \tag{2.3}$$

and in considering these Z_a as partition functions of n identical systems with the same realization of the disorder, i.e. *replicas*. This is not trivial at all, since in equation (2.2) n goes to zero, so that we must perform an analytic continuation of many quantities function of an integer variable n when $n \to 0$ [11]. Once introduced the replicated configurations s_a for $a = 1 \ldots n$, expression (2.2) becomes:

$$\overline{\log Z} = \lim_{n\to 0} \frac{1}{n} \log \int \mathcal{D}P(J)\ \int \prod_{a=1}^{n} \mathcal{D}s_a\ e^{-\beta \sum_{a=1}^{n} H(s_a)} \tag{2.4}$$

To perform the average over the disorder we must introduce the overlap matrix [11]

$$Q_{ab} = \frac{1}{N} \sum_i s_{ia} s_{ib} \tag{2.5}$$

among different replicas of the system. The average over J couples replicas, but in so doing the sites of the system are decoupled, so that we can use the saddle point approximation in the limit $N \to \infty$ for the evaluation of (2.4). Once this is done we have:

$$-\beta\overline{F} = \mathop{\mathrm{Ext}}_{Q} \left\{ \lim_{n\to 0} \frac{1}{2n}\left(\frac{\beta^2}{2}\sum_{a,b} Q_{ab}^p + \log\det Q \right) \right\} . \tag{2.6}$$

This expression has to extremized with respect to the overlap matrix Q. It is now necessary to give an ansatz for the overlap matrix Q. Following [3] we take a one step replica symmetry broken form (1RSB) [4],

$$Q_{ab} = (1-q_1)\delta_{ab} + (q_1 - q_0)\epsilon_{ab} + q_0 \ , \tag{2.7}$$

where ϵ_{ab} is equal to one in the diagonal blocks of size x and zero elsewhere. This form of the overlap matrix has to be interpreted in the context of the ultrametric structure of the states [14,11]: q_0 gives the mean overlap between different equilibrium states of the system, while q_1 represents their self-overlap. Therefore with a 1RSB solution we describe a quite simple structure, where all the states are at the same mutual distance q_0 and have the same self-overlap q_1. The parameter x is related to the balance between the thermodynamic weight of the different states (see [4,5,6,11]).

With assumption (2.7) we obtain [3]:

$$-2\beta\overline{F} = \mathop{\mathrm{Ext}}_{q_0,q_1,x} \left\{ \frac{\beta^2}{2}[1+(x-1)q_1^p - xq_0^p] + \log(1-q_1) + \frac{1}{x}\log\left(1 + x\frac{q_1-q_0}{1-q_1}\right) \right\} . \tag{2.8}$$

This expression has to be maximized with respect to the variational parameters (x, q_1, q_0). For zero external magnetic field the saddle point equations give $q_0 = 0$.

It can be shown [3] that there is a temperature T_s called *static transition temperature* above which the solution of the saddle point equations is replica symmetric (RS), so that $q_1 = 0$ and $Q_{ab} = \delta_{ab}$. The free energy and energy densities are given by

$$F_{RS}(\beta) = -\frac{\beta}{4} \quad , \quad E_{RS}(\beta) = -\frac{\beta}{2} \quad , \quad T > T_s \tag{2.9}$$

Below T_s it takes place the 1RSB solution, with

$$0 < q_1 < 1 \quad , \quad x < 1 \quad , \quad T < T_s$$

with a free energy given by equation (2.8). To understand the nature of this transition we analyze the overlap distribution $P(q)$. In the case of a 1RSB solution $P(q)$ has the following form [11]

$$P(q) = x\ \delta(q - q_0) + (1-x)\ \delta(q - q_1) \ . \tag{2.10}$$

For the p-spin spherical model it happens that $x \to 1$ for $T \to T_s^-$, so that we have

$$\begin{aligned} &P(q) = x\ \delta(q) + (1-x)\ \delta(q-q_1) \qquad && T < T_s \\ &P(q) = \delta(q) && T > T_s \end{aligned} \tag{2.11}$$

Therefore we can describe the static transition in the following way: For $T > T_s$ we have just one typical value of the overlap, that is zero. As we have seen in the first section this can mean many things. Yet, given that this is a high temperature region we are leaded to think that this is just the self-overlap of a genuine paramagnetic state, as it happens for the SK model [9]. For $T < T_s$ there are two possible values of the overlap: $q_0 = 0$ which is the typical distance between different states and $q_1 \neq 0$ which is their self-overlap. Therefore at T_s the phase space breaks into localized states and there is a breaking of the ergodicity. These states are all mutually orthogonal and therefore we find the value zero in the spectrum of the overlap.

In this context it is also possible to give a physical interpretation of the parameter x. By definition the free energy density for a given sample is:

$$F = -\lim_{N\to\infty} \frac{1}{N\beta} \log Z \tag{2.12}$$

but we can also write

$$Z = \sum_\alpha Z_\alpha = \sum_\alpha e^{-\beta N f_\alpha} \ . \tag{2.13}$$

This sum is dominated by those states which have the lowest free energy density, which by definition is $f_\alpha = F$. Nevertheless, the free energies of these equilibrium states can differ for quantities of order one, i.e.

$$N f_\alpha = NF + \delta f_\alpha \tag{2.14}$$

with $\delta f_\alpha \sim O(1)$, so that we can write:

$$Z = e^{-\beta NF} \sum_\alpha e^{-\beta\delta f_\alpha} \quad , \quad \lim_{N\to\infty} \frac{1}{N} \log\left(\sum_\alpha e^{-\beta\delta f_\alpha}\right) = 0$$

and for the thermodynamic weight of each state

$$w_\alpha = \frac{e^{-\beta N f_\alpha}}{\sum_{\alpha'} e^{-\beta N f_{\alpha'}}} = \frac{e^{-\beta\delta f_\alpha}}{\sum_{\alpha'} e^{-\beta\delta f_{\alpha'}}} \ . \tag{2.15}$$

If we call $u_\alpha = \exp(-\beta\delta f_\alpha)$ from equations (1.19) and (2.11) we have:

$$(1-x) = \sum_\alpha w_\alpha^2 = \frac{\sum_\alpha u_\alpha^2}{[\sum_\alpha u_\alpha]^2} \ . \tag{2.16}$$

From this equation it is clear that $x = 0$ means that there is just *one* state with free energy density F. In this condition we have only the delta function on the self-overlap of this state and no delta in zero, meaning that there are not other states. On the other hand, when the number of states increases we can roughly conclude from (2.16) that x must increase too, giving contribution to the mutual overlap between the states. Yet, note that the value of x is related to the global balance between the number of states *and* their thermodynamic weight, given by w_α. Nevertheless, the important thing is that, whatever is the value of $x < 1$, the number of states with finite thermodynamic weight in sum (2.16) must be finite. When x reaches the value 1 this is no longer true, since $x = 1$ means that the sums in (2.16) get contribution from an infinite number of terms [15]. Thus in this case the contribution of the self-overlap disappears because the number of states with comparable thermodynamic weight is too large. Since the total weight must be one, we are leaded to the conclusion that for $x = 1$ the weight of the states contributing to the partition function vanishes.

In this context it is very important to take into consideration the behaviour of x and q_1 *at* the transition. From (2.11) we see that $(1-x)$ is the weight of the self-overlap. At T_s, x goes to 1, so that the contribution of the self-overlap disappears. Yet, the important thing is that at T_s the *value* of the self-overlap q_1 is still different from zero [3]:

$$x = 1 \quad , \quad q_1 \neq 0 \quad , \quad T = T_s \ . \tag{2.17}$$

In this sense the transition is discontinuous. It seems that when $T \to T_s^-$ the thermodynamic weight of the states goes to zero, but their self-overlap does not, suggesting that they continue to exist even at higher temperature. To support this hypothesis there is the fact that for $T > T_s$ a 1RSB solution continues to exist, but with a value of x greater then 1, which is not acceptable in the context of the Parisi scheme [11]. Moreover, if we interpret the value $q_0 = 0$ for $T < T_s$ as the mutual overlap of the states, it would be natural to think that this continues to be true also for $T > T_s$, even if these states are hidden by their vanishing weight.

Therefore there are some indications of the fact that for $T > T_s$ the situation could be more complicate then the simple presence of just the paramagnetic state. We will show in the next sections that the real situation is indeed much more complicate then the one stated above.

3. The TAP approach.

A method alternative to the replica one is based on the formulation of mean field equations for the local magnetizations $m_i = \langle s_i \rangle$ at fixed value of the couplings J. These equations has been written in the context of the SK model [9] for the first time in [16] and are called TAP equations. For the p-spin spherical model these equations have been introduced in [8]. We shall see in this section which are the results of this analysis.

Following [8] we introduce a function f_{TAP} which is the mean field free energy density written as a function of the magnetizations m_i at fixed value of the couplings J. The simplest form we can guess for it is

$$f_0(m) = -\frac{1}{N} \sum_{i_1 < \ldots < i_p} J_{i_1 \ldots i_p} m_{i_1} \ldots m_{i_p} - \frac{1}{2\beta} \log[1 - q(m)] \tag{3.1}$$

with

$$q = \frac{1}{N} \sum_i m_i^2 \ . \tag{3.2}$$

To understand expression (3.1) simply note that we have substituted each spin with its mean value and we have written the entropy as the logarithm of the volume of the state which has self-overlap $q \sim \cos\theta$: since θ is the largeness of the state, its volume on the sphere is proportional to $\sin(\theta/2)^{N-1}$ and we obtain (3.1). Yet, this mean field free energy is too simple, since it does not take into consideration the Onsager reaction term [16,11,8]. This can be calculated by means of the cavity method (see [17]) and it is given by:

$$f_{react}(m) = -\frac{\beta}{4}\left[(p-1)q(m)^p - pq(m)^{p-1} + 1\right] \tag{3.3}$$

so that

$$f_{TAP}(m) = f_0(m) + f_{react}(m) \tag{3.4}$$

Once we have introduced this mean field free energy, the TAP solutions are obtained by the minimization of this function with respect to the m_i's. First we note that $m_i = 0 \ \forall \ i$ is always a solution, with $q = 0$ and represents the paramagnetic state, which has

$$F_{para}(\beta) = -\frac{\beta}{4} \quad , \quad E_{para}(\beta) = -\frac{\beta}{2} \tag{3.5}$$

to be compared with (2.9). To better understand the structure of the solutions with $q \neq 0$ we make the change of variables $m_1, \ldots, m_N \to \sigma_1, \ldots, \sigma_N, q$, where

$$\sigma_i = \frac{m_i}{\sqrt{q}} \tag{3.6}$$

so that the *angular* variables σ_i must satisfy the constraint

$$\frac{1}{N}\sum_i \sigma_i^2 = 1 \ . \tag{3.7}$$

We write f_{TAP} as a function of these new variables

$$f_{TAP}(\sigma, q) = -q^{\frac{p}{2}}\frac{1}{N}\sum_{i_1<\ldots<i_p} J_{i_1\ldots i_p}\sigma_{i_1}\ldots\sigma_{i_p} - \frac{1}{2\beta}\log(1-q) - \frac{\beta}{4}\left[(p-1)q^p - pq^{p-1} + 1\right] \ . \tag{3.8}$$

where q has now to be considered as an independent variable. It is very important to note that the dependence on the σ_i's is present only through the function

$$H(\sigma) = -\sum_{i_1<\ldots<i_p} J_{i_1\ldots i_p}\sigma_{i_1}\ldots\sigma_{i_p} \tag{3.9}$$

which is the Hamiltonian of the model valued in the angular variables. The TAP equations can be written as:

$$\begin{aligned} \frac{\partial H(\sigma)}{\partial \sigma_i} &= 0 \quad , \qquad i = 1, \ldots, N \\ \frac{\partial f_{TAP}(H(\sigma), q)}{\partial q} &= 0 \end{aligned} \tag{3.10}$$

together with constraint (3.7). Note that the N equations for the angular variables σ_i do not contains β, so that the solutions of these equations are simply the vectors on the sphere (3.7) which minimize the Hamiltonian $H(\sigma)$. At $T = 0$ the difference between states and configurations vanishes, so that equilibrium or metastable states of the system at zero temperature are just those configurations s (with self-overlap $q = 1$) which minimize the energy $H(s)$ on the sphere. Therefore it is possible to identify the angular variables σ_i's with the configurations of the system at $T=0$, so that $H(\sigma)/N$ in equations (3.10) is the *zero temperature energy density* E and we can write the TAP free energy as

$$f_{TAP}(\sigma,q)=f_{TAP}(E,q) \quad , \quad E=-\frac{1}{N}H(\sigma) \tag{3.11}$$

For what concerns the following of our discussion we are interested in the angular part of the equations. Introducing a Lagrange multiplier λ to implement the constraint, these equations are

$$-pq^{\frac{p}{2}}\sum_{i_2<\ldots<i_p} J_{l,i_2\ldots i_p}\,\sigma_{i_2}\ldots\sigma_{i_p}-\lambda\sigma_l=0 \quad , \quad l=1,\ldots,N\ . \tag{3.12}$$

Multiplying by σ_l, summing over l and using the constraint, we get

$$-p\sum_{i_2<\ldots<i_p} J_{l,i_2\ldots i_p}\,\sigma_{i_2}\ldots\sigma_{i_p}-pE\sigma_l=0 \quad , \quad l=1,\ldots,N \tag{3.13}$$

which contain only the zero temperature energy. Note that we can solve these equations at fixed value of E: by virtue of the constraint the obtained solutions will automatically have zero temperature energy equal to E. These equations contains the disorder J, so that we have to average over J all the interesting quantities coming from their solutions.

We see that the structure of the TAP solutions is very peculiar: We can first solve equations (3.13), independent from β, obtaining a set of $\mathcal{N}$ angular solutions $[\sigma^\alpha]_{\alpha=1,\ldots,\mathcal{N}}$, each one labeled by its zero temperature energy density $E_\alpha=H(\sigma^\alpha)$. Then we introduce E_α in the q-part of equations (3.10), obtaining the corresponding value of $q(E_\alpha,\beta)$. In this way we finally obtain the set of TAP solutions

$$m_i^\alpha(\beta)=\sigma_i^\alpha\cdot\sqrt{q(E_\alpha,\beta)} \tag{3.14}$$

with a finite temperature energy and free energy densities given by

$$\mathcal{E}(E_\alpha,\beta)=q(E_\alpha,\beta)^{\frac{p}{2}}\ E_\alpha \quad , \quad f(E_\alpha,\beta)=f_{TAP}(E_\alpha,q(E_\alpha,\beta)) \tag{3.15}$$

From what above it is clear that the temperature contributes to give the self-overlap, energy and free energy of each particular solution, but the position on the sphere of this solution is always the same at any β. Moreover, all the solutions with the same zero temperature energy density also share the same self-overlap and finite temperature energy and free energy densities. Due to this we can classify TAP solutions by their zero temperature energy density E. Thus in the following of our discussion we shall always use E and not $E(\beta)$ to label different class of TAP equations. Besides, we note from equation (3.15) that the energy ordering among different solutions which hold at $T=0$ holds at any value of T. This means there is no chaoticity nor mixing of the solutions with the temperature: the same structure of the energy landscape at $T=0$ is continuously mapped into an identical free energy landscape at finite T.

Let us now fix a certain value of E and ask: How many solutions of the TAP equations (3.13) are present with this particular zero temperature energy density ? It turns out that this number is given by ([8,18], see chapter IV)

$$\mathcal{N}(E)\sim e^{N\Sigma(E)}\ . \tag{3.16}$$

Therefore the number of TAP solutions into a class characterized by energy E is exponentially large in N. The quantity $\Sigma(E)$ is the *complexity* of that particular class and will play a central role in all our next investigation. The complexity is an increasing function of the energy, so that there is a minimum energy E_0 where $\Sigma = 0$. Thus no solutions with $E < E_0$ are found and we will call these solutions *ground state solutions.*

Moreover, once faced the angular part of the equation, we have to solve the q-equation at temperature T. It is possible to show [8] that this equation has solution as long as (see chapter IV.1)

$$E < E_{th} = -\sqrt{\frac{2(p-1)}{p}} \ . \tag{3.17}$$

E_{th} is called *threshold energy.* Therefore we find TAP solutions only within a strip of zero temperature energy densities $E_0 \leq E \leq E_{th}$. Fixed an energy E in this range, we find that the q-equation has solution as long as the temperature T is lower than a value dependent on that particular energy, $T_{TAP}(E)$: for $T > T_{TAP}(E)$ the solutions in the class labeled by E no longer exist. This temperature is larger the lower is E, so that the last solutions which disappear increasing the temperature are the ground state solutions. Above $T_{TAP}(E_0)$ survives only the paramagnetic solution.

Since the proposal of the TAP approach is to identify solutions of the mean field equations with states of the system, the question is: At a given temperature T which solutions will contribute to the partition function ? In other words, which are the equilibrium states ? To answer this, we write Z as an integral over all the states (TAP solutions) of the system:

$$Z = \sum_\alpha Z_\alpha = \sum_\alpha e^{-\beta N f_\alpha(\beta)} = \int dE \ \mathcal{N}(E) \ e^{-\beta N f(E,\beta)} = \int dE \ e^{-\beta N [f(E,\beta) - T\Sigma(E)]} \tag{3.18}$$

where we used (3.16). Thus in the limit $N \to \infty$ contribute to the partition function only the minima with respect to E of the generalized free energy

$$\phi(E,\beta) = f(E,\beta) - T\Sigma(E) \ . \tag{3.19}$$

In other words, states which dominate the partition function, i.e. equilibrium states, are those which optimize the balance between the free energy and the entropic contribution due to the fact that there is an exponentially high number of states with the same free energy. The minimization of (3.19) with respect to E gives a function E_{eq}^T which is the zero temperature energy density of the TAP states which give equilibrium at temperature T.

At very low temperatures the minimum of ϕ is given by the states with the lowest free energy density available, that is $E_{eq} = E_0$, with $\Sigma(E_0) = 0$. This means that the energy which minimize ϕ lies below the strip of the possible TAP energies.

Yet, increasing the temperature the non-zero complexity of higher states becomes important, so that there is a transition temperature T_c such that for $T > T_c$ we find $E_{eq}^T > E_0$: equilibrium states are no longer those with the lowest free energy. To balance this they have a complexity $\Sigma(E_{eq}^T)$ different from zero. We stress that in this conditions there are states with free energy density both higher and lower than $f(E^T_{eq}, \beta)$ which must be considered as metastable states. The appropriate quantity to fix equilibrium is ϕ, which takes into consideration the contribution of the complexity. We shall return on this rather peculiar situation at the end of this chapter.

Increasing the temperature, E^T_{eq} goes through the whole strip of the solutions, until we arrive at a temperature T_d such that $E^{T_d}_{eq} = E_{th}$: there are no more solutions above E_{th}, thus for $T > T_d$ we cannot continue following E^T_{eq}. T_d is called *dynamical transition temperature* and we will show later why. From what said above it is not clear what should do the system for $T > T_d$. It could stay in the threshold states until their ending temperature $T_{TAP}(E_{th})$ is reached, to pass successively to the paramagnetic state, or something else. We will face this problem in the next section.

4. A comparison between the two methods and a word on the dynamics.

It has came the moment to fix some links between the replica and the TAP approach, since, as they stand, the results coming from these two methods seems quite incompatible.

In the replica approach the low temperature phase is dominated by the 1RSB solution, which leaves place to the RS solution at the static transition temperature T_s. On the other hand we have seen with the TAP approach that the low temperature phase is dominated by the ground state TAP solutions, up to a temperature T_c above which equilibrium is given by a bunch of TAP solution with higher free energy, but finite complexity. Luckily enough, it turns out that

$$F_{RSB}(\beta) = f_{TAP}(E_0, \beta) \quad , \quad q_1^{RSB} = q(E_0, \beta) \ . \tag{4.1}$$

The two methods thus give the same low temperature result: the 1RSB solution of the replica method thus corresponds to the contribution of the ground state TAP solutions. The complexity of these states is zero and they all have the lowest free energy density. As we have seen in the last section, this does not mean that they all have the same free energy: these states have free energy differences of order 1 and the parameter x of the 1RSB solution is the result of the balance between these different free energies, as it happens for the SK model [11]. Moreover, from the $P(q)$ we learn that these ground state TAP solutions are all mutually orthogonal, since $q_0 = 0$.

What is important is that equation (4.1) holds also for $T > T_s$: the ground states TAP solutions correspond to the 1RSB solution even in the domain where this solution is no longer valid ($x > 1$). This demonstrates that what we anticipated in section 2 was correct: these ground states corresponding to the 1RSB solution, survive even at $T > T_s$.

The second important result is that the two transition temperatures are the same

$$T_s = T_c \ . \tag{4.2}$$

In section 2 we stated that for $T > T_s$ the system were dominated by the paramagnetic state, since we found $P(q) = \delta(q)$. Now we must reinterpret this formula. For $T > T_c = T_s$, the TAP approach says that equilibrium is given by a class of states with non-zero self-overlap, each one of them with a high free energy density, counterbalanced by the global complexity of that class. This means that $P(q) = \delta(q)$ indicates that the typical overlap among these states is zero, rather than signalize the self-overlap of the paramagnetic state.

What about the energy of the RS solution ? The first thing we note is that F_{RS} and E_{RS} of (2.9) are really the free energy and energy densities of the paramagnetic state, as is showed in (2.9) and (3.5). Therefore, we could expect this values to be wrong, since we know that for $T > T_s$ equilibrium is not given by the paramagnetic state. Yet, it holds:

$$F_{RS}(\beta) = F_{para}(\beta) = \phi(E_{eq}, \beta) \tag{4.3}$$

where

$$\phi(E_{eq}, \beta) = \operatorname*{Min}_{E} \{f(E, \beta) - T\Sigma(E)\} = f(E_{eq}, \beta) - T\Sigma(E_{eq}) \tag{4.4}$$

That is, the free energy density of equilibrium states for $T > T_s$ minus their complexity is exactly equal to the paramagnetic free energy, that is the same as the RS solution. For the energy we have

$$E_{RS}(\beta) = E_{para}(\beta) = \mathcal{E}(\beta, E_{eq}) \tag{4.5}$$

At present this coincidence is quite mysterious [8,19] and we shall give a possible explanation in section 6. Nevertheless, in this sense the RS solution of the replica method gives the correct result, even if in a rather misleading way: What was naturally interpreted as a single paramagnetic state with self-overlap equal to zero and free energy F_{para}, is actually a bunch of localized states with mutual overlap $q = 0$ and high free energy, but with a collective complexity such that the global free energy is exactly equal to the paramagnetic one.

From equation (4.3) we can also understand what happens at T_d: at this temperature the energy of equilibrium states arrives at the threshold E_{th} and cannot proceed further. Therefore for $T > T_d$ equilibrium must be given by the paramagnetic state, which, by virtue of (4.3), has the correct free energy. It is not clear if in the regime $T_s < T < T_d$ there is a coexistence between the localized equilibrium states and the paramagnetic one, of the same kind as the one we described in section 1, or if there is a problem of double counting of the solutions [19]. We shall return on this point in the last section of this chapter. What we can say is that T_d is the first temperature at which the TAP states have a *global* thermodynamic weight which is comparable with that of the paramagnetic state.

Given this it is easy to imagine that the transition temperature T_d has a crucial role in the dynamics of the system. In [20] it has been studied the Langevin dynamics of this model in the context of equilibrium. Assuming the time translation invariance (TTI) and the validity of the fluctuation-dissipation theorem (FDT), it is possible to derive an equation for the dynamical correlation function $C(t - t') = C(\tau)$: for $T \to T_d^+$ the correlation C as a function of τ develops a plateau whose length goes to infinity at the dynamical transition [20]. In other words, at T_d relaxation times diverge and a freezing of the dynamics occurs. This phenomenon was observed also in [2]. The asymptotic value of C at T_d is equal to the self-overlap of the TAP threshold solutions q_{th}, suggesting that at T_d the system remains trapped by the threshold states.

When the dynamical transition occurs there is a breaking of the ergodicity, so that equilibrium dynamics properties should not be assumed. The off-equilibrium Langevin dynamics of the p-spin spherical model has been studied in [21]. Given a system which at time zero is at high temperature and quenched it below T_d, it happens that in the whole range $T < T_d$ the dynamics asymptotically goes to the threshold states, never visiting the sub-threshold landscape: after a first TTI regime where C goes to q_{th}, suggesting a relaxation into a threshold state, for longer times it appears an aging regime where C goes to zero, showing that there is no *bona fide* relaxation into any specific state [21]. This phenomenon is known as *weak ergodicity breaking.* Nonetheless, the energy goes asymptotically to the threshold energy, never going below it. Therefore the dynamics does not explore the equilibrium states which dominates the partition function: it is trapped by the threshold level, but it is not really trapped into any state. These features indicate that the structure of the threshold landscape must be highly non-trivial.

5. A picture of the situation.

We want now to summarize the results we have collected in this chapter. In its low temperature phase, $T < T_s$, the p-spin spherical model is dominated by a small number of states (zero complexity), which have the lowest free energy density. From the replica method we know that these states are all mutually orthogonal, since the distribution function $P(q)$ shows that their mutual overlap q_0 is zero in absence of external magnetic field. In this phase there is also an exponentially high number of states (non-zero complexity) with higher free energy density. Yet, the temperature is too low to make their complexity play a determinant role, so that all these states are metastable. This situation is quite normal and resemble what happens in the SK model [9,11] below T_c: few equilibrium states with finite thermodynamic weight and many metastable states [22] which do not give any contribution to the partition function. Obviously there is the big difference of the absence of a full replica symmetry breaking in the p-spin spherical model.

At T_s there is an entropic transition: the minimum of the generalized free energy ϕ, which takes into account both the free energy of the states and the complexity of states with the same free energy, is given by states which have free energy higher than the lowest one, but which are so numerous (finite complexity) to overcome this drawback. Once again we stress the difference between the free energy density f of a single state and the global generalized free energy density $\phi = f - T\Sigma$, which is a collective property. In this temperature range, $T_s < T < T_d$, there are also many states with free energy density f both lower and larger than the equilibrium one, which must be considered as metastable, since they do not minimize ϕ. What about the thermodynamic weight of equilibrium states in this phase ? We have

$$Z = e^{-\beta NF} = e^{-\beta N\phi_{eq}} = e^{-\beta Nf_{eq}+N\Sigma_{eq}} \tag{5.1}$$

so that

$$w_{eq} = \frac{e^{-\beta Nf_{eq}}}{Z} = e^{-N\Sigma_{eq}} \to 0 \quad , \quad N \to \infty \tag{5.2}$$

This is a crucial point: each equilibrium state, singularly taken, has a vanishing thermodynamic weight. The complexity contributes to the *global* free energy, but makes each individual state have zero weight.

The thermodynamic weight is obviously zero for all the states, not only of equilibrium, so that in this temperature range there are no states with finite thermodynamic weight. From this point of view there is no substantial difference between equilibrium and metastable states: each one of them *singularly taken* has a vanishing weight. Note how anomalous is this concept of equilibrium. Normally equilibrium states have a finite thermodynamic weight, so that each one of them has a free energy density which is equal to the equilibrium free energy density of the system. This anomalous situation was in part anticipated in section 2. When x goes to one, equilibrium states become too much: the weight of the ground states is normalized by $e^{N\Sigma_{eq}}$ and goes to zero, so that the replica approach *misses* their contribution.

This picture has an important consequence on the possible finite dimensional theory of such a system. Out of mean field all the metastable states must have finite lifetime: the reason is that bubbles of equilibrium into a metastable state are unfavoured by a factor $+L^{D-1}$ (surface interaction), but favoured by a factor $-L^D$ (volume contribution), so that above a given value of their size L there is a collapse into the equilibrium state, which has lower free energy density. If we hypothesize that the finite dimensional version of the p-spin spherical model conserves the structure of the states described above, we see that the situation is quite complicate: When the system is into an equilibrium state it has no idea that there are many other states with a complexity such that its own state is actually an equilibrium one. Bubbles of states with lower individual free energy can be nucleated and the same standard reasoning we stated above can be applied. Yet, these states with lower individual free energy *are not* equilibrium states, since they do not minimize ϕ. Thus it could seem that the system collapsed to the ground states, with lowest energy density, even if they are not the equilibrium states. Nevertheless, we must take into consideration the role of complexity, which is completely disregarded by the standard reasoning: it is true that bubbles with lower free energy can make an equilibrium state unstable, but it is also true that the probability of forming a bubble of a certain state must be proportional to the global thermodynamic weight of the class of that state, which involves the complexity. In this way the most probable thing is that the system continuously 'falls' from an equilibrium state into another equilibrium state: the system is *almost* ergodic, since it is not confined into any part of the phase space, but it takes a very long time to escape from each equilibrium state. We stress that there is at present no finite dimensional theory and there are also many doubts about the possibility of forming bubbles of states in disordered systems, so that the one stated above is only a possibility.

Finally, for $T > T_d$ the statics of the p-spin spherical model is dominated by the paramagnetic state, even if each TAP solution survives until its ending temperature $T_{TAP}(E)$. At T_d a dynamical transition occurs: for $T > T_d$ the system is no longer trapped in the threshold landscape and it relaxes into the paramagnetic state.

We turn now to face the central problem of all our next investigation. From the replica approach we are leaded to conclude that equilibrium states are always mutually orthogonal, both for $T < T_s$ and $T_s < T < T_d$. This follows from the distribution $P(q)$ which always displays a delta function on the value zero of the overlap. Our opinion is that this conclusion is correct for what concerns the phase $T < T_s$, but that it is wrong for $T_s < T < T_d$. The reason is simple:

As we have seen, the number of equilibrium states in the low temperature phase is quite small. This follows either from the replica approach, which gives $x < 1$ for $T < T_s$ and from the TAP approach, where the complexity of the ground states is zero. If we associate to each state a direction in the phase space, we have a non-exponential number of directions which are all mutually orthogonal in a space of dimension N and this is plausible. Moreover, we have no reason to doubt of the replica approach in this temperature range, since we have checked the consistency of its results within the TAP approach.

On the other hand, when $T_s < T < T_d$ the number of equilibrium states grows like $e^{N\Sigma}$, so that we have to imagine an exponentially high number of orthogonal directions in a space of dimension N. Although this is not impossible to realize in a space of dimension N when N goes to infinity, it is in our opinion a very unlikely situation. Our conclusion is that the replica method fails in discriminating the overlap relations among different equilibrium states for the same reason for which it fails to give the contribution of their self-overlap: there are too many states, all of them with vanishing thermodynamic weight and we cannot ask to a method which, after all, compute the equilibrium partition function, to give us any insight into their structure. We can understand this fact in a better way. The replica approach gives the correct free energy of the system, which, as we have seen, is a fully collective quantity in this temperature range. Yet, in order to know the geometrical relations among different states we must necessarily discriminate among them. The replica approach is not able to do this, therefore it gives only the trivial *typical* value of the mutual overlap, that is $q = 0$.

The starting point of our investigation is thus the following: In the temperature range $T_s < T < T_d$ there are too many states to be all mutually orthogonal, so that there must be *many* closer states. The next chapter is dedicated to prove this assertion. If this hypothesis is true we need to investigate in a deep way how these states are geometrically organized in the phase space, since this organization must have some consequences on the behaviour of the system. Yet, we have widely demonstrated that the standard methods are not able to give us any insight into this topic, so that we will follow some new strategies.

6. The nature of the paramagnetic state.

We end this introductive chapter exposing a non-standard scenario on the nature of the paramagnetic state for the p-spin spherical model. With the following discussion we try to formalize some ideas on the nature of the paramagnetic state, which are in part familiar to the community of disordered systems physicists [23], but that in our opinion have never been exposed in a clear way.

We have seen in the previous sections that the role of the paramagnetic state in the temperature range $T_s < T < T_d$ is rather unclear: The replica approach gives a replica symmetric solution with free energy $F_{RS}(\beta)$, which seems to be the paramagnetic one, as $P(q) = \delta(q)$ for $T > T_s$. Yet, we discover within the TAP approach that this $\delta(q)$ refers to the typical mutual overlap of many non-paramagnetic, localized equilibrium states, with high free energy f, but finite complexity Σ. Moreover, we find that the *global* equilibrium free energy of the system $\phi_{eq} = f_{eq} - T\Sigma_{eq}$ is exactly equal to F_{RS}. At this point one could say: Well, this means that the replica approach gives the correct collective free energy, so that there is no paramagnetic state at all !

Yet, actually *there is* the TAP paramagnetic state, since

$$m_i = 0 \quad , \quad \forall\, i \quad , \quad q = \frac{1}{N}\sum_i m_i^2 = 0 \tag{6.1}$$

is always a solution of the TAP equations (3.10) and there is no doubt that it represents the paramagnetic state. For this reason we said in section 4 that the situation is quite mysterious: the bunch of equilibrium states has a global free energy, balance of their individual high free energy and of their collective high complexity, which is exactly equal to that of the paramagnetic state, which, after all, is a rather different object.

Moreover, even if we disregard this coincidence, it is not clear whether the paramagnetic state coexists together with the localized equilibrium states or not. A dynamical study of the system for $T_s < T < T_d$ [19], suggests that this possibility has to be discarded, since when the system starts from an equilibrium configuration it never relaxes into the paramagnetic states, but into one of the localized, trapping equilibrium states. If there were also the paramagnetic state one could expect to find the system into it with a probability $1/2$, since the paramagnetic free energy is equal to the one of the ensemble of equilibrium states. Therefore it seems that the paramagnetic state really does not exist in this temperature range. Yet equation (6.1) seems to say the contrary. Moreover, at T_d we surely need the presence of the paramagnetic state, since for $T > T_d$ the equilibrium dynamics shows that the system is ergodic.

To solve this problem we propose the following scenario. The paramagnetic state is defined by two things: the first is equation (6.1), which gives the value of its magnetizations and self-overlap. The second thing is less quantitative and it is related to the property of ergodicity, since we think at the paramagnetic state as delocalized in the phase space. Our statement is that making a *superposition* of many localized, non-paramagnetic, trapping states we obtain an object which appears exactly as it were the paramagnetic state.

Let us consider the magnetizations of equilibrium states at a given fixed temperature $T \in (T_s, T_d)$

$$\{m_i^\alpha\} \quad , \quad \alpha = 1, \ldots, \mathcal{N} \quad , \quad i = 1, \ldots, N \tag{6.2}$$

where $\mathcal{N} \sim e^{N\Sigma_{eq}}$ is the number of equilibrium states. We introduce now the vector π defined by the following components

$$\pi_i \stackrel{\text{def}}{=} \frac{1}{\mathcal{N}} \sum_{\alpha=1}^{\mathcal{N}} m_i^\alpha \ . \tag{6.3}$$

The self-overlap of this state is

$$\begin{aligned} q_\pi = \frac{1}{N}\sum_{i=1}^{N} \pi_i^2 \;&=\; \frac{1}{N}\sum_{i=1}^{N}\frac{1}{\mathcal{N}^2}\sum_{\alpha,\beta=1}^{\mathcal{N}} m_i^\alpha m_i^\beta \;= \\ &= e^{-2N\Sigma_{eq}} \sum_{\alpha,\beta=1}^{\mathcal{N}} q_{\alpha\beta} \;=\; \sum_{\alpha,\beta=1}^{\mathcal{N}} w_\alpha\, w_\beta\, q_{\alpha\beta} \end{aligned} \tag{6.4}$$

where we have used the thermodynamic weight of equilibrium states given in (5.2). From equation (6.4) we see that the self-overlap of π is equal to the average overlap between the equilibrium states (see (1.16)), which we know to be zero in this temperature range, since $P(q) = \delta(q)$, so that the self-overlap of the solution π is

$$q_\pi = 0 \tag{6.5}$$

and therefore

$$\pi_i = 0 \quad , \quad \forall\, i = 1, \ldots, N \tag{6.6}$$

It is clear that π is a solution of the TAP equations which is not distinguishable from the paramagnetic state. Yet, *it is not* the paramagnetic state, since it is the superposition of many equilibrium TAP solutions: π is actually made by localized trapping states, so that it has nothing to do with a genuine paramagnetic state. We can say more. We write the superposition of two equilibrium states as

$$m_i^{\alpha\oplus\beta} = m_i^\alpha + m_i^\beta = \langle s_i\rangle_\alpha + \langle s_i\rangle_\beta = \frac{1}{Z_\alpha}\sum_{[s^\alpha]} s_i^\alpha\ e^{-\beta H} + \frac{1}{Z_\beta}\sum_{[s^\beta]} s_i^\beta\ e^{-\beta H} \tag{6.7}$$

where s^α, s^β are configurations belonging respectively to states α and β (see section 1). Since both these states are equilibrium states, the two partition functions are both equal to Z_{eq} (this is not the *total* equilibrium partition function, which is given by (5.1), but $Z_{eq} = e^{-\beta N f_{eq}}$). Therefore, we conclude that

$$m_i^{\alpha\oplus\beta} = \frac{1}{Z_{eq}} \sum_{[s\ \in\ \alpha,\beta]} s_i\ e^{-\beta H} \tag{6.8}$$

where $s \in \alpha, \beta$ means that we are now summing over the configurations belonging to both the states. In the same way the value of π_i is obtained by summing over the configurations belonging to *all* the equilibrium states, which are scattered along the phase space. In this sense π is a delocalized state, since configurations belonging to it are mutually very far in the phase space.

Resuming, in the temperature range $T_s < T < T_d$ we have defined a TAP solution π, which is the superposition of all the equilibrium TAP states at temperature T. This *pseudo* state π has a self-overlap $q_\pi = 0$, is delocalized in the phase space and is formally indistinguishable from a paramagnetic state at this level of the discussion. Yet, the dynamics understands that π is not the paramagnetic state, since if the initial configuration is chosen with the equilibrium measure [19], it relaxes (and remains trapped) into one of the many localized equilibrium states composing π.

We conclude that no genuine paramagnetic state in this temperature range exists. The paramagnetic solution $q = 0$ of the TAP equations has to be interpreted as a manifestation of the *pseudo* state π. This solves the problem of having all these localized equilibrium states whose collective free energy ϕ is *exactly* the same as the one of the paramagnetic state: ϕ is the free energy of π, which is nothing else than the collective expression of the equilibrium states.

It is interesting to analyze what happens at T_d: Does it occur the formation of a new genuine paramagnetic state ? In our opinion the answer is no. At T_d the equilibrium energy E_{eq} reaches the threshold, so that π is formed at T_d by the superposition of all the threshold states. We shall show in chapter IV that these states have many peculiar properties, but we anticipate the most important ones: threshold states have some flat directions [21,8,24] and they are continuously connected one to the other along these directions [25]. Therefore at T_d the *pseudo* state π is actually very similar to a genuine paramagnetic state, since states composing it are almost non-trapping.

For $T > T_d$ the situation is even clearer. We will show in chapter IV that for $E > E_{th}$ the greatest part of angular TAP solutions are saddles, while the q-part has no longer solution. In this conditions the TAP components of π are no longer genuine states, since they have many escape directions and they do not trap the system anymore. Therefore their superposition π is now, on the contrary, a true state, that is the paramagnetic state.

III. Looking for closer states

The starting hypothesis of this chapter is that a non-trivial structure of the states is actually present in the p-spin spherical model, i.e. that not all the states are mutually orthogonal. Since this hypothesis seems to contradict the standard results exposed in the last chapter, we must resort to some new tools in order to verify our conjecture. In the context of the real replica method we define and compute a new quantity, the three replica potential, which enable us to show that our hypothesis is correct. Before introducing this potential we give a brief introduction on the real replica method and on its physical motivations.

Contents:

1. An introduction on constrained systems.

If the starting hypothesis of our investigation is correct, i.e. if states with mutual overlap q different from zero are actually present in the phase space of the p-spin spherical model, we have to face the following problem: each times two different states are drawn with a probability equal to their thermodynamic weight, their measured mutual overlap is $q = 0$. This is the result coming from the standard distribution function $P(q)$ in the temperature range $T_s < T < T_d$. Therefore we have to ask: Why we are not able to detect pairs of non-orthogonal states ? From the discussion of the previous chapter we know that the most probable reason is that the probability of drawing a pair of orthogonal states is overwhelming higher then the probability of any other pair with non-zero mutual overlap. This situation can be achieved, for example, if the number of orthogonal pairs is exponentially more numerous then any other pair. We shall return on this point with much more details in the next chapter. For the present we limit ourselves to consider this as a sensible hypothesis. Therefore, if this scenario is true, we must in some sense *force* states to be closer and verify *a posteriori* if this situation is realizable, even if unlikely.

In this context it is naturally to introduce the *real replica method*, first appeared in [26] and successively developed in [8,27,28]. The idea of the method is the following: if there are parts of the phase space which the system does not visit frequently, as metastable states, then one forces the system to stay into these parts by means of some constraints. Once the system is forced in such a way, it tends to minimize its free energy, compatibly with the imposed constraints, i.e. it finds the better place to stay in the phase space portion it is forced to live. In this way it is possible to have new information on the structure of the phase space, since the system is forbidden to thermalize in its normal equilibrium state and it will necessarily explore some unusual regions of the phase space. From a technical point of view one computes the free energy cost to keep the system constrained, as a function of the constraints. This free energy cost is a sort of potential function, whose minima correspond to constrained-equilibrium states of the system.

The name of this method takes place from the fact that the easiest way to make a system stay in a restricted portion of the phase space is to force it to live at a given fixed distance from a second, identical system. In this way we have two (or more) identical physical systems, which are usually called *real replicas*. This name is opposed to the case of the replica trick used to compute averages over the disorder, since in that context the number n of replicas usually goes to zero, thus preventing from considering them as *real* (see chapter II).

The real replica method has two different realizations, a *symmetric* realization and a *hierarchic* one. We explain the difference between them in the case of two replicas. In the symmetric case we impose an overlap q between the two replicas and we compute the total free energy of these two systems as a function of q. It is clear that the two replicas are perfectly equivalent and that no one of them will correspond to an equilibrium system, because of the mutual constraint [8]. On the other hand, in the hierarchic case we let a first system thermalize freely into an equilibrium state and successively we force a second system to thermalize at overlap q with the first one. In this case we compute the free energy of this second constrained system, minus its unconstrained free energy. The quantity we obtain is the free energy cost to keep the second replica at distance q from an equilibrium state. Clearly in this case the role of the two replicas is very different: the first one is simply a reference point in the phase space, while the second one represents the constrained physical system whose free energy is actually computed [27,28]. We will show in the next section how the difference between these two methods is realized from a technical point of view.

The standard replica approach to the p-spin spherical model show that, given an equilibrium state, the closest equilibrium state is at overlap zero with it. Since our task is to contradict this conclusion, it is clear that we are interested in exploring the neighborhood of an equilibrium state, looking for other states close to it. Therefore we see from what said above that the hierarchical real replica method has to be preferred for our investigation: in this way we can fix an equilibrium state and then peruse the free energy landscape around it by means of other systems bound to it.

We end this section with an observation. One could ask: Why we are so interested in the investigation of such unusual situations, given that the system never realizes them by itself ? The answer is that when the structure of the phase space is very complicate, with the presence of many metastable states, standard equilibrium computations give poor results, as we have seen in chapter II, since they completely disregard non-equilibrium situations, which usually play an important role in the dynamics of the system. If the mean lifetime of metastable states is finite but *very* long, we must take them into consideration to have a clear picture of the behaviour of the system.

2. A first result: the two replica potential.

In this section we will expose the results of [27] related to the definition and computation of a two replica potential. As already anticipated the idea is the following: we calculate the free energy of system τ (replica 2) forced to stay at overlap q_{12} with a free system σ (replica 1), which is at equilibrium. In this way we define the potential $V_2(q_{12})$ as the difference between the constrained and the unconstrained free energy densities:

$$-\beta N V_2(q_{12}) = -\beta N \overline{(F_c - F)} =$$

$$\overline{\frac{1}{Z}\int d\sigma \exp(-\beta H(\sigma)) \; \log\left(\int d\tau \exp(-\beta H(\tau)) \; \delta(q_{\sigma\tau} - q_{12})\right)} - \overline{\log Z} \tag{2.1}$$

where the bar indicates the average over the disorder. It is important to note that in this way we compute the constrained free energy density of only the second replica τ, while we operate an average of this free energy over the equilibrium realization of the first replica σ. Indeed, this can be done by virtue of the assumption that the constrained free energy F_c is self-averaging with respect to σ. In formula (2.1) it is clearly legible the hierarchic nature of this potential: the constraint q_{12} is felt only by τ, while σ is let free to thermalize into an equilibrium state. On the other hand, the symmetric case would simply corresponds to having the logarithm outside both the integrals over σ and τ. In this way the two replicas would be exactly equivalent and the free energy density of the whole constrained system formed by σ and τ would be calculated.

To perform the average on the quenched disorder, we use the replica trick:

$$
\begin{aligned}
&-\beta N V_2(q_{12}) = \\
&= \lim_{n,m\to 0} \frac{1}{m} \overline{\log \int d\sigma_a d\tau_b \exp\left[-\beta\left(\sum_{a=1}^{n} H(\sigma_a) + \sum_{b=1}^{m} H(\tau_b)\right)\right] \prod_{b=1}^{m} \delta(q_{\sigma_1\tau_b} - q_{12})} \\
&\qquad - \overline{\log Z} \ .
\end{aligned}
\tag{2.2}
$$

In this formula the different role of σ and τ is less clear, but still present. Indeed, we note that the delta function couples the first one of replicas σ with all replicas τ. Note that τ is replicated because of the logarithm, while σ is replicated for the presence of the partition function at the denominator. This difference is encoded in the normalization by the only factor m.

We introduce the overlap sub-matrices

$$
\begin{aligned}
Q^{\sigma\sigma}_{ab} &= q_{\sigma_a\sigma_b} \qquad a = 1,\ldots,n;\ b = 1,\ldots,n \\
Q^{\sigma\tau}_{ab} &= q_{\sigma_a\tau_b} \qquad a = 1,\ldots,n;\ b = 1,\ldots,m \\
Q^{\tau\tau}_{ab} &= q_{\tau_a\tau_b} \qquad a = 1,\ldots,m;\ b = 1,\ldots,m
\end{aligned}
\tag{2.3}
$$

and the total matrix of the overlap $\mathbf{Q}$, formed by the blocks (2.3). With this definition, equation (2.2) gives (see [28])

$$
-\beta V_2(q_{12}) = \operatorname*{Ext}_{\mathbf{Q}} \left\{ \lim_{n,m\to 0} \frac{1}{2m}\left(\frac{\beta^2}{2}\sum_{a,b} \mathbf{Q}^p_{ab} + \log\det\mathbf{Q}\right)\right\} + \beta F_{free} \ . \tag{2.4}
$$

Before proceeding with the calculation, it is necessary to give sensible ansatz for the overlap sub-matrices. From now on we will consider only temperatures T greater than T_s and zero external magnetic field; therefore, since $Q^{\sigma\sigma}$ is referred to an independent free system, we assume for it the symmetric form

$$
Q^{\sigma\sigma}_{ab} = \delta_{ab} \ . \tag{2.5}
$$

The structure of $Q^{\sigma\tau}$ is in part imposed by the constraint in (2.2), that forces the first row to be equal to q_{12}. The simplest ansatz for the whole matrix is

$$
Q^{\sigma\tau}_{ab} = q_{12}\ \delta_{a,1} \ . \tag{2.6}
$$

This choice is confirmed by the analysis of the potential in the limit[1] $\beta \to 0$; moreover, if we introduce an additional parameter w_{12} for the rest of the matrix, the saddle point equations lead to the solution $w_{12} = 0$. In [27] $Q^{\tau\tau}$ was assumed symmetric, but the successive examination suggested that a more general one step RSB form has to be taken [29,28], with variational parameters (x_r, r_1, r_0):

$$
Q^{\tau\tau}_{ab} = (1 - r_1)\delta_{ab} + (r_1 - r_0)\epsilon_{ab} + r_0 \ , \tag{2.7}
$$

[1] At β=0 the calculation reduces to a purely geometrical problem; indeed, in this case the potential is simply proportional to the volume of the phase space region accessible to the constrained replica. Therefore, the comparison with this limit is crucial to test the ansatz for the overlap matrices.

where ϵ_{ab} is equal to one in the diagonal blocks of size x_r and zero elsewhere. With these assumptions we obtain [28]:

$$
\begin{aligned}
-2\beta V_2(q_{12}) = \operatorname*{Ext}_{r_0,r_1,x_r} \Big\{ & \beta^2 q_{12}^p + \frac{\beta^2}{2}(x_r-1)r_1^p - \frac{\beta^2}{2} x_r r_0^p \\
& + \log(1-r_1) + \frac{1}{x_r}\log\left(1 + x_r \frac{r_1 - r_0}{1-r_1}\right) + \frac{r_0 - q_{12}^2}{1 - r_1 + x_r(r_1 - r_0)} \Big\}
\end{aligned} \tag{2.8}
$$

where, as usual, we have to maximize the free energy with respect to the variational parameters, in this particular case (x_r, r_1, r_0). Once this is done, V_2 remains a function of the only variable q_{12}.

What we expect will be the behaviour of the potential as a function of q_{12} ? First of all, it is clear that V_2 must be zero for $q_{12} = 0$: indeed we already know that the typical overlap between different equilibrium states is zero for $T_s < T < T_d$, therefore putting $q_{12} = 0$ we let the constrained replica τ substantially free to find a normal equilibrium state where thermalize. Yet, as the constraint grows we expect that the price we pay to keep the second replica at overlap q_{12} with the first grows, since this constrained thermalization is the more innatural the more τ is close to σ. This situation is showed in figure 1, where we have plotted the potential $V_2(q_{12})$ in the temperature range $T_s < T < T_d$.

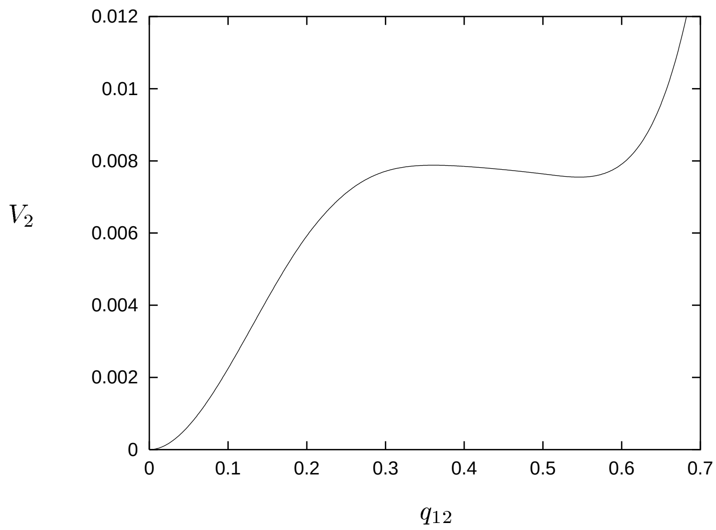

Figure 1: The potential V_2 at β=1.64 and p=3; q_{EA}=0.546.

The potential increases with increasing q_{12} as suggested above, but we see that it develops a secondary minimum M for a high value of the overlap. The important thing is that this value of the overlap is exactly equal to the self-overlap q_{EA} of the equilibrium states at this temperature, coming from the TAP equations. The explanation of this fact is simple: when we increase sufficiently the constraint q_{12} we force the second replica τ to enter in the same equilibrium state as the first free replica σ. Therefore once the two replicas are in the same state, the preferred value of their mutual overlap will be equal to the self-overlap of the state itself. The potential signalizes this situation by the secondary minimum M.

Thus when $q_{12} = q_{EA}$ we are guaranteed that replica τ is into an equilibrium state, so that its energy and free energy densities are the same as those corresponding to this equilibrium state. Nevertheless there is an important difference with a normal equilibrium situation: we have shown in chapter II that in the temperature range $T_s < T < T_d$ the global equilibrium free energy density of the system receives a contribution from the free energy density of the equilibrium states *and* from the entropic contribution due to their complexity, i.e. to the fact that there are many equilibrium states (see eq. (II.4.4)):

$$F = f_{eq} - T\Sigma(f_{eq}) \tag{2.9}$$

where we have written the complexity Σ as a function of the free energy (see chapter II). While the free energy density of replica σ receives both this contributions (σ is a normal equilibrium system), the free energy density of τ does not: τ is forced to stay in the same state of σ, therefore it sees just *one* state and therefore the equivalent complexity for τ is zero. This means that in the secondary minimum we can write:

$$V_2(q_{EA}) = F_c(q_{EA}) - F = f_{eq} - [f_{eq} - T\Sigma(f_{eq})] = T\Sigma(f_{eq}) \ . \tag{2.10}$$

We therefore obtain the important result that the value of the potential in the secondary minimum divided by T gives exactly the complexity of the equilibrium states [27]. This value agrees with the computation of the complexity of [18]. At T_s the complexity of equilibrium states is zero, thus the minimum M reaches the zero at T_s. Result (2.10) is not only an important check for the correctness of this method, but it is symmetrically a check for the computation of [18] based on the TAP approach, since we will show in the next chapter that computing the number of states by computing the solutions of the TAP equations is a procedure which involves many approximations and ambiguities.

When the temperature is higher then the dynamical transition temperature T_d we know from the previous chapter that equilibrium is given by the paramagnetic state. Therefore we do not expect to find a secondary minimum of V_2, since the self-overlap of the paramagnetic state is zero, i.e. there is no localized state of replica 1, where we can force replica 2 to stay. This means that V_2 will develop the secondary minimum at T_d, thus giving an important static way to identify the dynamical transition.

Resuming the results of this section, we can say that the two replica potential is a new static method which permits to obtain results unreachable with the standard replica approach we exposed in chapter II. Indeed, we stress that the minimum M of V_2 is a direct indication of the presence of equilibrium states with self-overlap $q_{EA} \neq 0$ in the temperature range $T_s < T < T_d$ and the value of the potential in this minimum gives the complexity of these states. We had already exposed both these results in the previous chapter, but only in the context of the TAP equations.

From the point of view of the structure of the states we can consider V_2 as a sort of generalized overlap distribution: the absolute minimum in zero is the known contribution of the orthogonal states, while the secondary minimum M is the contribution of the self-overlap. Comparing this result with the standard one, $P(q) = \delta(q)$, we see that we have gained the detection of the self-overlap. Yet, once again, we know nothing about *closer* states. Namely, in the range $0 < q < q_{EA}$ the two replica potential has no minima and therefore gives no information.

Thus the existence of states at overlap $q \neq 0$ and $q \neq q_{EA}$ with a given equilibrium state has not been proved yet.

3. Closer states: the three replica potential.

The potential V_2 gives only two minima: one for $q = 0$ corresponding to typical equilibrium states orthogonal to the reference state of replica 1 and a secondary minimum at $q = q_{EA}$, corresponding to replica 2 in the same state as replica 1. There are no other minima in the intermediate range. Why ? There are two possible explanations: or there are no states at all in the middle or there are *too many* states to be possible for the potential to exhibit other minima. Given our starting hypothesis, we choose this second possibility. The idea is the following: at a given distance $q \neq 0$ from replica 1 *there are* states where replica 2 can thermalize, but this is true also at distance $q \pm dq$, so that there is no preference of replica 2 for staying at overlap q with 1, rather then at smaller or larger overlap, therefore there is no minimum of V_2 at q. Obviously this is no longer true when q is so large that 2 is in proximity of the state of 1, since very close to a state we do not expect to find other states. If this is true, to detect a state at $q \neq 0$ we have to keep fixed into this state the second replica and compute the free energy of a third replica 3 which plays the role of a satellite around 2. Now we expect that this free energy has a minimum when the imposed overlap between 2 and 3 is large enough for these two replicas to be in the same state.

The analytical realization of this idea is the three replica potential introduced in [28]. As in the case of V_2, we take a first independent replica ρ which thermalizes freely at a temperature T. Then we consider a second replica σ constrained to thermalize at a fixed overlap q_{12} with ρ. Finally, we calculate the free energy density of a third replica τ constrained to have overlap q_{13} with ρ and q_{23} with σ. In this way it is possible to define the three replica potential V_3, taking the difference between the constrained free energy of τ and the free energy of the unconstrained system:

$$
\begin{aligned}
&-\beta N V_3(q_{12}, q_{13}, q_{23}) = \\
=&\overline{\frac{1}{Z}\int d\rho \exp(-\beta H(\rho)) \frac{1}{Z(\rho; q_{12})}\int d\sigma \exp(-\beta H(\sigma))\ \delta(q_{\rho\sigma} - q_{12}) \times} \\
&\overline{\times \log \int d\tau \exp(-\beta H(\tau))\ \delta(q_{\rho\tau} - q_{13})\ \delta(q_{\sigma\tau} - q_{23})} - \overline{\log Z}
\end{aligned}
\tag{3.1}
$$

with

$$
Z(\rho; q_{12}) = \int d\sigma \exp(-\beta H(\sigma))\ \delta(q_{\rho\sigma} - q_{12})\ . \tag{3.2}
$$

In our analysis we limit ourselves to the situation in which the temperatures are the same for the three replicas. Our purpose is to study the potential V_3 in the plane (q_{13}, q_{23}) at various fixed values of q_{12}. In this way, replica 1 is fixed into an equilibrium state, while replica 2 is fixed at distance q_{12} from 1 and therefore is not a configuration of equilibrium for the free system. Now we can explore the neighborhood of 2 by means of the position of replica 3.

The computation of V_3 is a bit technical and we will only outline the results. We limit ourselves to the observation that the replica trick needed to perform the average over the disorder leads to the introduction of six overlap matrices Q_{ab}, respectively for the pairs of replicas $\rho\rho, \rho\sigma, \sigma\sigma, \rho\tau, \sigma\tau, \tau\tau$. Each one of these matrices have different variational parameters and we have postulated for them a 1RSB form (see equation (2.7)). The hierarchic structure of V_3 obviously requires that the overlap matrices concerning the first two replicas are independent from the third one and therefore they are identical to the case of V_2. The final expression of V_3 is formally identical to equation (2.8), with the parameter q_{12}^2 substituted by a new parameter y function of q_{12}, q_{13}, q_{23} and of all the variational parameters [28].

Before analyzing the shape of the potential V_3 it is useful to examine under which conditions the case of V_2 is recovered. It turns out that

$$\begin{aligned} V_3(q_{12}=0, q_{13}=0, q_{23}) &= V_2(q_{23}) \\ V_3(q_{12}=0, q_{13}, q_{23}=0) &= V_2(q_{13}) \ . \end{aligned} \tag{3.3}$$

This is just what we expected for the following reason: setting $q_{12}=0$ replica 2 thermalizes as in the free case and so replica 1 and 2 are both equilibrium configurations. In this situation, if we set, for example, $q_{13}=0$, the constraint 1-3 is harmless and the pair 2-3 reproduces the case of V_2; the same is true for $q_{23}=0$.

The most important information in the study of V_3 comes from the analysis of its minima in the plane (q_{13}, q_{23}) at fixed values of q_{12}, which, as we will show, correspond to metastable or equilibrium states of the system. We must then minimize V_3 with respect of q_{13} and q_{23}. Once this is done we find three different kinds of minima:

M_0 · For any value of q_{12} and for any temperature there is the trivial minimum M_0 with

$$\begin{aligned} q_{13} = q_{23} &= 0 \\ V_3(M_0) &= 0 \ . \end{aligned} \tag{3.4}$$

This is the absolute minimum of the potential in the (q_{13}, q_{23}) plane and corresponds to the situation in which the third replica sees a phase space identical to that of the unconstrained system. This minimum is completely equivalent to the absolute minimum of V_2.

M_1 · For any value of q_{12} and for any temperature in the range (T_c, T_d), we find a minimum M_1 with

$$\begin{aligned} q_{13} &= q_{EA} \\ q_{23} &\sim q_{12} \\ V_3(M_1) = V_2(q_{EA}) &= T\Sigma(f_{eq}) \ . \end{aligned} \tag{3.5}$$

The interpretation of M_1 is very simple: the third replica is in the same pure state as the first one, independently from the value of q_{12}, therefore giving $q_{13}=q_{EA}$. M_1 has exactly the same meaning of the secondary minimum M for the two replica potential. As q_{12} grows, the second replica approaches the state of 1, not changing the potential. For $q_{12}=q_{EA}$ the three replicas are all in the same state and $q_{12}=q_{13}=q_{23}=q_{EA}$. This minimum gives the same degree of information of the two replica potential.

M_2 · More interesting is the presence of a minimum with the third replica close to the second one. For T in the usual range (T_s, T_d) and $0 \leq q_{12} \leq \bar{q}(T)$ we find a minimum M_2 with

$$\begin{aligned} q_{23} &\sim q_{EA} \\ q_{13} &\sim q_{12} \leq q_{EA} \end{aligned} \tag{3.6}$$

and a value of the potential $V_3(M_2)$ which depends in this case on q_{12}. It is important to note that the last value $\bar{q}$ of q_{12} for which M_2 exists is at any temperature less or equal to q_{EA}. Let us fix a reference temperature $T \in (T_s, T_d)$ and examine M_2 at different values of q_{12}. For $q_{12} = 0$ we have $q_{13} = 0$, $q_{23} = q_{EA}$ and $V_3(M_2) = V_2(q_{EA})$; this is trivial because we have seen that in this case V_3 reduces to V_2. When $q_{12} \neq 0$ we force the second replica to thermalize in a restricted portion of the phase space; the fact that we still find the minimum M_2 corresponding to the third replica in equilibrium close to the second one ($q_{23} \sim q_{EA}$), is our first indication of the fact that there are states even at non-zero overlap q_{12} with the state of the first free replica. M_2 disappears at $q_{12} = \bar{q}$, so that $\bar{q}$ is the overlap with the fixed equilibrium states of the states closest to it.

To fully demonstrate our last statement it is crucial to verify if the states corresponding to minima M_2 can be identified with TAP solutions, i.e. if their free energy and self-overlap satisfy the TAP equations. First, at fixed q_{12}, to know which is the self-overlap of the state relative to M_2 we have to look at the overlap matrix $Q_{ab}^{\tau\tau}$, since in this matrix is contained the self-overlap q_{33} of the state visited by replica 3. Secondly, we must compute the free energy of this particular state. To this end we note that

$$V_3(M_2) = F_c - F = (f_3 - T\Sigma_3) - F \ , \tag{3.7}$$

where f_3 is the free energy of the state in which replica 3 thermalizes, and Σ_3 is the logarithm of the number of states accessible to replica 3, compatibly with the constraints. Obviously, since replica 3 is in the same state of replica 2, which is fixed, we have $\Sigma_3 = 0$ (cfr. equation (2.10)) and therefore

$$f_3 = V_3(M_2) + F \ . \tag{3.8}$$

It turns out that the relation holding between f_3 and q_{33} in M_2 is always the same of the TAP approach. In other words, the state corresponding to M_2 coincides with that particular TAP solution specified by the following values of the free energy density and self-overlap:

$$\begin{aligned} f_{TAP} &= f_3 \\ q_{TAP} &= q_{33} \ . \end{aligned} \tag{3.9}$$

Since in M_2 replica 2 and replica 3 are in the same state, one can expect that not only q_{33} but also q_{23} is equal to the self-overlap q_{TAP} of the corresponding TAP solution. Actually, this is not true: q_{23} is very near to $q_{33} = q_{TAP}$, but not exactly the same (the difference being of order 10^{-3}). The physical reason of this lies in the different role of the two replicas, how we have already stressed: replica 2 is quenched in the state corresponding to M_2 with a non equilibrium distribution, it is not in general a typical configuration of this state and then q_{23} is not a good measure of the self-overlap. On the other hand, replica 3 truly thermalizes into this state and thus q_{33} identifies the correct self-overlap.

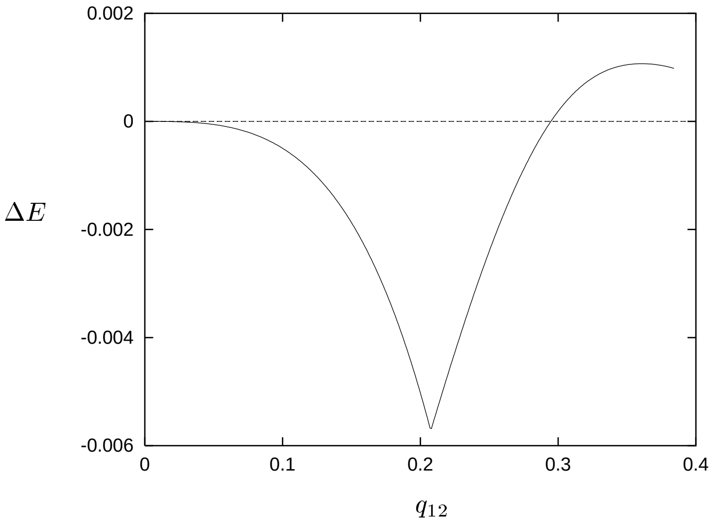

Figure 2: The energy density difference ΔE in M_2 as a function of q_{12} at β=1.64; $q^\star$=0.295, $\bar{q}$=0.385 The behaviour of V_3 in M_2 is qualitatively the same.

Let us now consider the behaviour in M_2 of the energy difference $\Delta E = E_c - E$, between the constrained and the unconstrained energy densities. This is shown in figure 2. We note that there is a value $q_{12} = q^\star$ for which

$$\Delta E(q^\star) = \ 0 \ . \tag{3.10}$$

The fact that in this minimum the energy is equal to the one of the unconstrained system means that replicas 2 and 3 are in a state of the same kind of the one chosen by the unconstrained system, that is an equilibrium state. Indeed, we have

$$q_{33}|_{q_{12}=q^\star} = q_{EA} \tag{3.11}$$

(the same happens in the minimum M of V_2). For this reason we expect that

$$V_3(M_2)|_{q_{12}=q^\star} = V_2(q_{EA}) = T\Sigma(f_{eq}) \tag{3.12}$$

that is what we find [28].

At this point we have fully demonstrated that our starting hypothesis was correct: given an equilibrium state, *there are* states, both of equilibrium and metastable, at overlap different from zero with it. By means of the three replica potential we are able not only to detect the presence of these state, but also to know their energy and free energy density.

We end this section with an important technical remark. As we have said we postulated a 1RSB form for all the overlap matrices. Depending on the solutions of the saddle point equations the replica symmetry can be *actually* broken or not. The physical meaning of breaking or not the replica symmetry is the one we stated in chapter II, adapted to this context. An RS form of the overlap matrix can be associated to two very different situations: the first one corresponds to a system which finds an exponentially high number of states (as in the p-spin spherical model for $T_s < T < T_d$), while in the second one the phase space consists of just one state (as in the paramagnetic case, $T > T_d$). On the other hand, an 1RSB form means that the phase space is dominated by a number of order N of states (as in the p-spin spherical model for $T < T_s$). It turns out that the overlap matrix $Q_{ab}^{\tau\tau}$ of replica 3 evaluated in the minimum M_2 is always replica symmetric. The reason is simply that in M_2 the phase space of replica 3 reduces to one single state, the same as replica 2, so that $Q_{ab}^{\tau\tau} = q_{33}$ is the self-overlap of this state. On the other hand, the overlap matrix $Q_{ab}^{\sigma\sigma}$ of replica 2 has two regime: it is replica symmetric as long as $q_{12} < q_{rsb}$ and it is 1RSB for $q_{12} > q_{rsb}$. This value q_{rsb} corresponds to the cusp of figure 2. At this level of our discussion it is not clear why this happens, but we can make the following conjecture: for $q_{12} < q_{rsb}$ the portion of the phase space accessible to replica 2 is so large that it finds an exponentially high number of states, while for $q_{12} > q_{rsb}$ the number of states found is of order N. This remains an hypothesis in the context of the real replica method, but we will prove in the next chapter that this conjecture is correct.

4. Open problems.

We shall now briefly summarize the results coming from the three replica potential and we shall show which are the limits of this method.

We know from the TAP approach (see chapter II) that in the temperature range $T_s < T < T_d$ equilibrium is given by a superposition of states, all of them with a high free energy density, counterbalanced by an entropic contribution due to their complexity. In this context, we fix a first replica 1 into one of these equilibrium states and we force a second replica 2 to thermalize at distance q_{12} from 1. As a consequence replica 2 thermalizes into one of the states it finds at distance q_{12} with 1, state which in general will not be of equilibrium. At this point we calculate the free energy density V_3 of a third replica 3 as a function of its distances from 1 and 2. If replica 2 is really thermalized into a state, we must find a minimum of V_3 corresponding to replica 2 and 3 very close one to each other and both at the same distance from 1. This is exactly what happens: we find this minimum up to a value $\bar{q}$ of the overlap which represents the distance from the reference equilibrium state of the states nearest to it (see figure 2). We can conclude that our starting hypothesis was correct: given an equilibrium state there are states at any value of the overlap with it. Therefore the structure of the state is highly non-trivial and worth of further investigation. As we have seen in chapter II, the standard methods, both the replica method and the TAP method, are not able to give any insight into this structure, therefore we say that the structure of the states of the p-spin spherical model is *hidden*.

Unfortunately, the three replica potential cannot be pushed further in the investigation of this hidden structure of the states. Indeed, given the reference equilibrium state, we were able to detect the presence of at least one state at overlap $q \neq 0$. Yet, we do not expect that this detected state is the only one existing at distance q. Therefore it is not clear why replica 2 thermalizes into this particular state and, as a consequence, we are not able to explain the peculiar shape of the energy spectrum of figure 2: neither the maximum nor the cusp of this curve have an explanation in the context of our discussion. We have only stated that the cusp occurs in correspondence with the replica symmetry breaking of the overlap matrix of replica 2.

Moreover, even if we understood which is the process of selection of the states operated by replica 2, it is clear that we would have no control on this process, in the sense that we would know nothing about the unselected states. In other words, by means of the three replica potential we have not the opportunity of investigate with the greatest freedom the *whole* structure of the states, since we are allowed to examine only the states chosen by replica 2. Indeed, we expect that a tool which enable us to understand the energy spectrum coming from the three replica potential and explains what is the criterium for equilibrization at distance q, would be very useful for the whole investigation.

With this in mind we turn now to the definition of a new tool, which will lead us to the disclosure of the hidden structure of the states.

IV. The hidden structure of the states

In this chapter are exposed the main results of the thesis. In the preliminary sections it is shown which is the general method used to compute the complexity, a crucial quantity for the p-spin spherical model, since, as we have seen, it gives a finite entropic contribution to the global free energy of the system. The method consists in the computation of the number of solutions of the TAP equations, computation which is not trivial, since it contains heavy ambiguities related to the presence of many kinds of stationary points of the TAP free energy, while only minima can be identified with genuine states of the system. We clarify these ambiguities, introducing a new method able to discriminate among minima and saddles. In doing this we discover the interesting organization of the stationary points of the TAP free energy. Once developed the general formalism, we introduce and compute the constrained complexity, which is the main result of our research, since it gives us the complete overlap distribution of the states. This distribution is analyzed in detail, since it shows a structure of the states which is highly non-trivial. Once showed which is the typical behaviour of the constrained complexity, we use this quantity to explain the results obtained with the real replica method and, more important, we investigate the structure of the threshold landscape, which plays a fundamental role in this model.

Contents:

1. The complexity.

We have shown in chapter II.3 that in the temperature range between the static and the dynamical transition, the p-spin spherical model has an exponentially high number of states (TAP solutions), with free energy densities in a finite range $[f_0, f_{th}]$. What happens is that *equilibrium* states at temperature T are not the lowest ones corresponding to f_0, but rather those which optimize the balance between the free energy and the entropic contribution due to the presence of a great number of states with the same free energy. This entropic contribution is called *complexity*, $\Sigma(f)$ and it is simply the logarithm of the number of states with free energy density f, divided by N. Thus equilibrium states are those which minimize the collective free energy density $\phi(f) = f - T\Sigma(f)$. Note that we have used here the free energy f to label the classes of TAP solutions, instead of the zero temperature energy density E. As we have shown in chapter II these two labeling are completely equivalent, since once given the energy E of a class, its free energy f at temperature T is unambiguously fixed.

The states with free energy density f either lower or larger then the value which minimizes ϕ must be considered as metastable. On the other hand, *all* these states, the equilibrium as well as the metastable ones, singularly taken have a vanishing weight in the thermodynamic limit. In this sense, an equilibrium state is not different from a metastable state, since the equilibrium condition is a fully collective effect [8,18].

It is clear that in this context the knowledge of the complexity is crucial, since it gives a finite entropic contribution to the global free energy density of the system. It is therefore particularly important to have a well definite method to compute the number of the states of the system.

As we have seen in chapter II, it is possible to split the TAP equations for the p-spin spherical model into a single equation involving the temperature T and the self-overlap q and a different set of equations involving the angular part σ_i of the magnetizations m_i

$$m_i = \sqrt{q}\,\sigma_i \quad ; \qquad \sigma \cdot \sigma = \sum_i \sigma_i^2 = N \ . \tag{1.1}$$

The TAP equations for σ read [8] (see II.3.13)

$$0 = -p \sum_{i_2 < \ldots < i_p} J_{l,i_2\ldots i_p}\,\sigma_{i_2}\ldots\sigma_{i_p} - pE\sigma_l \stackrel{\text{def}}{=} \mathcal{T}_l(\sigma; E) \quad , \quad l = 1, \ldots, N \tag{1.2}$$

where E is the zero temperature energy density

$$E = -\frac{1}{N} \sum_{i_1 < \ldots < i_p} J_{i_1\ldots i_p}\sigma_{i_1}\ldots\sigma_{i_p} \ . \tag{1.3}$$

The multiplicity of different solutions of the TAP equations entirely comes from the set of equations (1.2). As we have said many times in our discussion, the striking feature of the p-spin spherical model is that these equations admit an exponentially large number of solutions as long as the zero temperature energy density E is lower then the threshold energy E_{th}. The complexity $\Sigma(E)$ is defined by the equation

$$\mathcal{N}(E) \sim e^{N\Sigma(E)} \tag{1.4}$$

or, more precisely

$$\Sigma(E) \stackrel{\rm def}{=} \lim_{N\to\infty} \frac{1}{N} \overline{\log \mathcal{N}(E)} \tag{1.5}$$

where $\mathcal{N}(E)$ is the number of angular solutions of equations (1.2) with zero temperature energy density E. In this first section we shall perform the computation of $\Sigma(E)$ and analyze all the different approximations involved in this computation.

Before proceeding it is important to make some observations. We have seen in the previous chapter that it is possible to identify TAP solutions with genuine states of the system, i.e. with local or global *minima* of the true free energy. More precisely, we found that each time we were able to recognize a state by means of the real replica method, its energy and self-overlap fulfilled the TAP equations. In particular this is true for minimum M_2 of the three replica potential V_3, which, depending on the value of the constraint, identifies many different metastable and equilibrium states of the system (see chapter III). Nevertheless, we surely do not expect that *all* the solutions of the set of equations (1.2) are minima. There will be saddles of any order and maxima, at various values of the energy. Therefore not all the TAP solutions will correspond to states of the system, intended as local or global minima of the free energy. In this context it is not clear why the quantity $\Sigma(E)$ should only represent the complexity of the minima (which is the quantity we want), neither if there is a sensible way to extract the contribution of the minima from the whole number of stationary points. Yet, we have seen in chapter III that by means of the two replica potential it is possible to compute the complexity of the equilibrium states in an unambiguous way and that this quantity coincides with the standard complexity computed in [18] with a method which disregard completely the problem we are talking about. Thus it seems that is some way *it is* possible to extract the contribution of the only minima, even if it is not clear how.

From what said above we see that in the computation of $\Sigma(E)$ great care has to be used in what we are actually computing: as we will show, depending on which method it is used and on which solution of the saddle point equations is taken, different complexities $\Sigma_0, \Sigma_1, \ldots$ are obtained from the same set of equations (1.2). Given this, it is even less clear which should be the right complexity, the one related to minima. The main goal of this first part of the chapter is to clarify all the ambiguities exposed above. This is crucial for our following discussion, since the quantity we will introduce in section 4, the constrained complexity, is deeply grounded on the capacity of recognize those TAP solutions which are genuine states of the system.

In equation (1.5) we average the logarithm of $\mathcal{N}$, since we expect that this is the extensive quantity. To perform this average it is necessary to introduce replicas already at this level of the calculation and in this way the calculation turns out to be very complicate. Therefore our first approximation is to average directly the number $\mathcal{N}$ of the solutions, i.e. to perform an annealed computations. At this point of the discussion there is no real justification of this approximation. We shall verify that the correct solutions of the saddle point equations are compatible with this approximation. Thus in terms of the angular parts (1.1) we can write

$$\Sigma(E) = \lim_{N\to\infty} \frac{1}{N} \log \overline{\int \mathcal{D}\sigma \ \delta(\sigma\cdot\sigma - N) \prod_{l=1}^{N} \delta(\mathcal{T}_l(\sigma;E)) \ \ |\det \mathcal{H}(\sigma;E)|} \tag{1.6}$$

where $\mathcal{H}(\sigma;E)$ is the Hessian of the TAP equations evaluated in the solution σ of energy density E. It is given by

$$\mathcal{H}_{r,l}(\sigma;E) = \frac{\partial \mathcal{T}_r(\sigma;E)}{\partial \sigma_l} = -p(p-1) \sum_{i_3<\ldots<i_p} J_{r,l,i_3\ldots i_p}\, \sigma_{i_3}\ldots\sigma_{i_p} - pE\delta_{r,l}\ . \tag{1.7}$$

Equation (1.6) is the standard formula to compute the number of solutions of a set of equations: we integrate over all the variables σ_i a delta function which implements the equations, $\delta(\mathcal{T})$, together with the Jacobian of the equations themselves, $|\det \mathcal{H}|$. Furthermore, to the set of equations (1.2) we have to add the spherical constraint of (1.1). In this context, the energy density E can be simply viewed as a fixed parameter: in other words, if we find a solution of the system of $N+1$ equations (1.1)(1.2) we are sure that this solution will verify equation (1.3) too, as can be easily seen multiplying (1.2) by $\sum_l \sigma_l$. Therefore the spherical constraint in formula (1.6) is equivalent to the requirement that the solutions have energy E.

Nevertheless there is a way to read formula (1.6) which is more adapted for our discussion. Indeed, solution of equations (1.2) are nothing else that extrema of the TAP free energy, with a given energy density E. In this context the modulus of the TAP Hessian (Jacobian of the equations) in (1.6) has a crucial role to avoid a trivial result [30]: if one tries to count the number of stationary points of a function *without* this modulus, each stationary point is weighted with the sign of the Hessian and one obtains a simple topological constant, by virtue of the Morse theorem [31]. Nonetheless, in the standard approach this modulus is always disregarded to simplify the computation [18,22] and, from what said above, this seems really a brutal approximation. However, we stress that by means of formula (1.6) we are counting only the solutions with a *given* energy density E. This is a crucial point: the principal effort of our discussion will be to show that, as long as $E < E_{th}$, if we keep the energy fixed, the modulus in (1.6) can be dropped without affecting the result in the limit $N \to \infty$. We shall return on this point with much more details at the end of our discussion. We therefore perform the calculation without the modulus, showing *a posteriori* which are the justifications of this procedure.

Let us introduce a Bosonic representation both for the determinant and the delta functions that implement the TAP equations:

$$\begin{aligned} \det \mathcal{H} = \lim_{n\to -2} \{\det \mathcal{H}\}^{-\frac{n}{2}} &= \lim_{n\to -2} \int \mathcal{D}\phi^a \exp\left(-\frac{1}{2}\sum_{a=1}^{n}(\phi^a \mathcal{H}\phi^a)\right) \\ \prod_{l=1}^{N} \delta(\mathcal{T}_l(\sigma;E)) &= \int \mathcal{D}\mu \exp(i\mu\mathcal{T}) \end{aligned} \tag{1.8}$$

where sums over repeated site indices are understood, since both ϕ^a and μ carry an index $i=1,\ldots,N$. The average over the disorder generates couplings between the fields ϕ, σ and μ. A crucial approximation is to set equal to zero the couplings $\phi^a\cdot\sigma$ and $\phi^a\cdot\mu$ which depend on one replica index and which break the rotational invariance in the space of the replicas. We will see that this approximation is consistent with all the solutions we shall consider for the saddle point equations. Thus we retain only the terms $\phi_a\cdot\phi_b$, $\mu\cdot\mu$ and $\mu\cdot\sigma$. It is easy to see that this approximation is equivalent to write

$$\Sigma(E) = \lim_{N\to\infty} \frac{1}{N} \log \int \mathcal{D}\sigma\ \delta(\sigma\cdot\sigma - N)\ \overline{\prod_{l=1}^{N} \delta(\mathcal{T}_l(\sigma;E))\ \times\ \det\mathcal{H}(\sigma;E)}\ . \tag{1.9}$$

Once averaged over the disorder, because of the spherical constraint the part of the determinant does not depend on σ any more. Therefore we have

$$\Sigma(E) = A(E) \ + \ B(E) \tag{1.10}$$

$$\begin{aligned} A(E) &= \lim_{N\to\infty} \frac{1}{N} \log \int \mathcal{D}\sigma \ \delta(\sigma\cdot\sigma - N) \ \ \overline{\int \mathcal{D}\mu \exp(i\mu\mathcal{T})} \\ B(E) &= \lim_{N\to\infty} \frac{1}{N} \log \int \mathcal{D}\sigma \ \delta(\sigma\cdot\sigma - N) \ \ \overline{\lim_{n\to -2} \int \mathcal{D}\phi^a \exp\left(-\frac{1}{2}\sum_{a=1}^{n}(\phi^a \mathcal{H}\phi^a)\right)} \ . \end{aligned} \tag{1.11}$$

The first integral does not involve replicas and gives the following contribution

$$A(E) = \frac{1}{2} - \frac{1}{2}\log\frac{p}{2} - E^2 \ . \tag{1.12}$$

The second integral is more subtle to solve because it contains replicas and an appropriate ansatz has to be chosen to solve the saddle point equations. Moreover this integral is related to the Hessian of the TAP solutions and thus it contains information on the nature of the solutions (minima, saddles or maxima) that we are counting. Once averaged over the disorder and introduced the overlap matrix $Q_{ab} = -p(p-1)(\phi^a\cdot\phi^b)/2N$, we obtain

$$B(E) = \lim_{N\to\infty} \frac{1}{N} \log \ \lim_{n\to -2} \int \mathcal{D}Q_{ab} \exp\left\{-N \ \left(\frac{\mathrm{Tr}\ Q^2}{2p(p-1)} + \frac{1}{2}\log\det(-pE+Q)\right)\right\} \ . \tag{1.13}$$

As an ansatz for the matrix Q we take $Q_{ab} = q_a \ \delta_{ab}$. In this way the exponent of (1.13) splits into n independent parts, each one giving the same saddle point equation for q_a, whose possible solutions are

$$q_a = q_\pm = \frac{p}{2}\left(E \pm \sqrt{E^2 - E_{th}^2}\right) \quad , \quad E_{th} = -\sqrt{\frac{2(p-1)}{p}} \ . \tag{1.14}$$

We restrict our discussion to $E < E_{th}$, so that $q_\pm$ are real. We understand now which is the origin of the threshold energy E_{th}. Since each q_a can assume one of these two values, we have a multiplicity of different solutions. The analysis of the fluctuations shows that there is a stable solution $\mathcal{S}_0$, given by

$$\mathcal{S}_0 : \qquad q_a = q_+ \quad , \quad a = 1, \ldots, n \tag{1.15}$$

This solution is invariant under rotations in the replica space and thus the approximation we made setting to zero the terms depending on one replica index turns out to be consistent. The solution $\mathcal{S}_0$ gives the complexity

$$\Sigma_0(E) = \frac{q_+^2}{p(p-1)} + \log(-pE + q_+) + A(E) \tag{1.16}$$

with A given by equation (1.12). This is the standard result for the complexity of [18]. The important thing is that this result is in agreement with the one coming from the two replica potential V_2 of [27], as we have shown in chapter III. Therefore Σ_0 is actually equal to the logarithm of the number of genuine states of the system. Thus it is the complexity of the *minima* of the TAP free energy and not of the whole number of solutions. This means that *in some way* we succeeded in extracting just the contribution of the minima, although it is not clear *how* we did it. Looking back at our derivation of Σ_0 we see that the unique point where a big arbitrary is present is in the choice of a certain sequence of roots $q_\pm$ for the diagonal of Q_{ab}, to give a global solution of the saddle point equations. To obtain $\mathcal{S}_0$ we have taken all the $q_a = q_+$, since this solution is stable. Nevertheless we can hypothesize that in this arbitrariness is hidden all the variety of different stationary points of the TAP free energy. Indeed there are many other solutions of the saddle point equations, involving both the values $q_\pm$. In particular we are interested in the solution $\mathcal{S}_1$ with the lowest degree of instability, that is

$$\mathcal{S}_1 : \qquad q_1 = q_- \quad , \quad q_a = q_+ \quad , \quad a = 2, \ldots, n \tag{1.17}$$

(and permutations). This solution presents a one step breaking of the rotational invariance in the replica space. Therefore one can concern about the fact that we have disregarded terms breaking this invariance. To check this point, we have performed the whole computation retaining the terms $\phi^a \cdot \sigma$, $\phi^a \cdot \mu$ and we have looked for a solution breaking the rotational invariance in the replica space. We found analytically that the saddle point equations give as a unique solution $\phi^a \cdot \sigma = 0$ and $\phi^a \cdot \mu = 0$ and thus that solution $\mathcal{S}_1$ is recovered. The complexity Σ_1 arising from $\mathcal{S}_1$ is

$$\Sigma_1(E) = \frac{3}{2}\,\frac{q_+^2}{p(p-1)} - \frac{1}{2}\,\frac{q_-^2}{p(p-1)} + \frac{3}{2}\log(-pE + q_+) - \frac{1}{2}\log(-pE + q_-) + A(E) \tag{1.18}$$

which is *lower* than Σ_0, since $|q_-| \geq |q_+|$. In this context it is not clear which is the physical meaning of the complexity Σ_1, neither if there is one. Moreover, apart from the fact that the complexity Σ_0 is confirmed by a different method to be related to the number of minima, we have given no justification of dropping the modulus in the original formula. We shall see in the next sections that the analysis of the average spectrum of the TAP Hessian gives an answer to both these questions, supporting our hypothesis that in the variety of solutions of the saddle point equations is encoded the variety of different stationary points of the TAP free energy.

2. The Hessian spectrum.

In the previous section we made the approximation of setting to zero the couplings $\phi^a \cdot \sigma$ and $\phi^a \cdot \mu$. We stress that this approximation is consistent when considering the solutions $\mathcal{S}_0$ and $\mathcal{S}_1$. As a consequence of this approximation, what appears in expression (1.9) is the Hessian function evaluated in a *generic* vector σ, and not in a TAP solution. This means that, in the context on this approximation, the properties of the TAP Hessian that are relevant in determining the behaviour of Σ, are well encoded in the matrix $\mathcal{H}(\sigma; E)$ which has the same functional form of the TAP Hessian, but requires σ only to satisfy the spherical constraint. The average spectrum is then defined in the following way

$$\rho(\lambda; E) = \lim_{N\to\infty} \overline{\int \mathcal{D}\sigma \;\delta(\sigma\cdot\sigma - N)\; \rho_J(\lambda; \sigma)} \tag{2.1}$$

where $\rho_J(\lambda;\sigma)$ is the spectrum for a given realization of the disorder, whose standard expression is [32]:

$$\rho_J(\lambda;\sigma) = -\frac{1}{N\pi} \,\mathrm{Im}\ \mathrm{Tr}(\mathcal{H} - \lambda + i\epsilon)^{-1} \ . \tag{2.2}$$

We can write the trace in the following way:

$$\begin{aligned} \mathrm{Tr}(\mathcal{H} - \lambda + i\epsilon)^{-1} &= \sum_{l=1}^{N} [(\mathcal{H} - \lambda + i\epsilon)^{-1}]_{ll} = \\ = \lim_{n\to 0} \int \mathcal{D}\phi^a \ \phi^1 \cdot \phi^1 \ \exp &\left\{ -\frac{1}{2} \sum_{a=1}^{n} \phi^a (\mathcal{H} - \lambda + i\epsilon)\phi^a \right\} \ . \end{aligned} \tag{2.3}$$

Once averaged over the disorder J and exploited the spherical constraint on σ, this computation becomes analogous to the one of the average spectrum of a Gaussian ensemble of symmetric random matrices [32]. If we introduce the overlap matrix $Q_{ab} = -p(p-1)(\phi_a \cdot \phi_b)/2N$ we finally get

$$\begin{aligned} \rho(\lambda;E) = \lim_{N\to\infty} -\frac{1}{N\pi}\ \mathrm{Im}\ \lim_{n\to 0} \int \mathcal{D}Q_{ab} \ (-pE - \lambda + Q)^{-1}_{11} \ \times \\ \times \ \exp\left\{ -N \ \left(\frac{\mathrm{Tr}\ Q^2}{2p(p-1)} + \frac{1}{2}\log\det(-pE - \lambda + Q) \right) \right\} \end{aligned} \tag{2.4}$$

It is important to note the great similarity between equations (2.4) and (1.13). If we choose once again a diagonal ansatz $Q_{ab} = w_a \delta_{ab}$, we get the following solutions of the saddle point equations

$$w_a = w_\pm(\lambda) = \frac{p}{2}\left(\frac{\lambda}{p} + E \pm \sqrt{\left(\frac{\lambda}{p} + E\right)^2 - E_{th}^2} \right) \tag{2.5}$$

where E_{th} is the same as in equation (1.14). For $\lambda = 0$ the integrand in (2.4) is identical to the one of (1.13) and $w_\pm(0) = q_\pm$. As in the case of the complexity we have a multiplicity of different solutions. To get a finite contribution to ρ it is necessary that the argument of the exponential in (2.4) is zero. Since $n \to 0$, this can be achieved taking the same value for each w_a, since in this way we gain a factor n which brings to zero the exponent. Moreover, the condition $\rho \geq 0$ shows that we must take the solution

$$\mathcal{S}_0 : \qquad w_a = w_+(\lambda) \ \ , \ \ a = 1, \ldots, n \tag{2.6}$$

that is exactly the same kind of solution that leaded to Σ_0 (cfr. eq. (1.15)). If we look at (2.5) we can see that the non-zero contribution to ρ comes from the region $-pE + pE_{th} < \lambda < -pE - pE_{th}$, where w_+ develops an imaginary part. Thus

$$\rho_0(\lambda;E) = \frac{1}{\pi p(p-1)} \sqrt{p^2 E_{th}^2 - (\lambda + pE)^2} \ . \tag{2.7}$$

We stress that the solution $\mathcal{S}_0$ is the only one that gives a finite positive contribution ρ_0 to ρ. Formula (2.7) is the well known Wigner semicircle law [33], that can be obtained for symmetric Gaussian random matrices also without using replicas [32]. This result tells us that for $E < E_{th}$ the averaged spectrum has a strictly positive support and thus the typical determinant of the Hessian is positive, i.e. that the dominant part of TAP solutions with energy density $E < E_{th}$ are *minima*. On the other hand, when E approaches E_{th} the lowest eigenvalue $\lambda = p(E_{th} - E)$ goes to zero. Therefore the typical solutions with $E = E_{th}$ have some flat directions [21].

We understand now the reason why the complexity of (1.16) is related to the number of minima: solution $\mathcal{S}_0$ of the saddle point equations leading to Σ_0 is exactly the same as the one leading to the eigenvalue distribution ρ_0, which has positive support: in this way, by this solution we are automatically counting stationary points with all the eigenvalues greater than zero, i.e. minima.

The important thing is that in this context it is possible to give a precise physical interpretation of solution $\mathcal{S}_1$ of (1.17): as we are going to show in the next section, $\mathcal{S}_1$ is related to the exponentially small corrections to the distribution ρ_0 and therefore gives informations on those TAP solutions which are not minima.

3. Exponential tails and complexity of the saddles.

For an ensemble of symmetric random matrices with a Gaussian distribution it is possible to compute corrections to the semicircle law, when N is large but finite. In particular, it is possible to compute the correction to the averaged spectrum related to the probability of having a single eigenvalue outside the semicircle support.

In the context of our calculation this can be achieved by considering solutions of the saddle point equations for ρ different from $\mathcal{S}_0$. In particular, we are interested in corrections to ρ_0 in the eigenvalue region on the left of the semicircle region, i.e. for $\lambda < -pE + pE_{th}$, since this tail contains the contribution of the negative eigenvalues. In this region we consider the solution $\mathcal{S}_1$

$$\mathcal{S}_1 : \qquad w_1 = w_-(\lambda) \quad , \quad w_a = w_+(\lambda) \quad , \quad a = 2, \dots, n \tag{3.1}$$

(and permutations), to be compared with (1.17). From equation (2.4) we get

$$\rho_1(\lambda, E) = r(\lambda, E)\; e^{-N\Delta(\lambda,E)} \tag{3.2}$$

with

$$\Delta(\lambda, E) = \frac{w_-^2}{2p(p-1)} - \frac{w_+^2}{2p(p-1)} + \frac{1}{2}\log\left(\frac{-\lambda - pE + w_-}{-\lambda - pE + w_+}\right) \tag{3.3}$$

and

$$\Delta(\lambda, E) > 0 \quad \text{for} \quad \lambda < -pE + pE_{th} \;. \tag{3.4}$$

We note that ρ_1 goes exponentially to zero as $N \to \infty$. In the computation of ρ_1 a crucial role is played by the fluctuations around the saddle point solution $\mathcal{S}_1$, since the fluctuations matrix has an instable direction which provides the imaginary part necessary for ρ_1 to be non-zero outside the semi-circle. The expression of $r(\lambda, E)$ is irrelevant for our discussion, but one can easily check that both $r(\lambda, E)$ and $\Delta(\lambda, E)$ coincide with the expressions obtained for the Gaussian random matrices with other methods [32]. This is therefore a correct result.

Solution $\mathcal{S}_1$ then gives the exponentially vanishing left tail, due to the probability of having one eigenvalue outside the semicircle. Since this tail is different from zero also in the negative semi-axis, we can calculate the probability of having a negative eigenvalue, i.e. the exponentially small probability of finding a TAP solution which is a saddle with one negative eigenvalue and has energy density E. This probability is

$$P_{(-)} = \int_{-\infty}^{0} d\lambda \; \rho_1(\lambda, E) \sim \; e^{-N\Delta(0,E)} \qquad , \qquad N \to \infty \tag{3.5}$$

In this context solution $\mathcal{S}_1$ has a clear physical interpretation: it is related to the contribution of TAP saddles with one negative eigenvalue, in the energy range $E < E_{th}$. Given this, we can try to push further this interpretation. As we have seen in section 1, the same solution $\mathcal{S}_1$ gives rise to a complexity Σ_1 smaller than Σ_0, whose meaning was not clear. Now we can make the hypothesis that Σ_1 is the complexity of the saddles with one negative eigenvalue. To prove this statement we note that once we have the number $\mathcal{N}_1(E) \sim \exp(N\Sigma_1(E))$ of saddles with one negative eigenvalue and energy density E, we can easily compute the probability $P_{(-)}$ of having one of these saddles in the following way:

$$P_{(-)} = \frac{\mathcal{N}_1(E)}{\mathcal{N}_{total}(E)} = \frac{e^{N\Sigma_1(E)}}{e^{N\Sigma_0(E)} + e^{N\Sigma_1(E)}} \sim e^{-N[\Sigma_0(E)-\Sigma_1(E)]} \tag{3.6}$$

where we used the relation $\Sigma_0(E) > \Sigma_1(E)$. From a comparison between (3.6) and (3.5) we see that it must hold

$$\Delta(0,E) = \Sigma_0(E) - \Sigma_1(E) \tag{3.7}$$

It is not difficult to see from equations (1.16), (1.18) and (3.3) that this equation is fulfilled. Our hypothesis is therefore correct and we can then write:

$$\Sigma_1(E) = \lim_{N\to\infty} \frac{1}{N} \log \overline{\mathcal{N}_1(E)} \tag{3.8}$$

where, as already said, $\mathcal{N}_1(E)$ is the number of TAP solutions of energy density E, which are saddles with one negative eigenvalue. This result can be generalized. If we consider the following solution $\mathcal{S}_k$ of the saddle point equations for Σ

$$\mathcal{S}_k : \quad q_a = q_- \;,\; a = 1, \ldots, k \quad , \quad q_a = q_+ \;,\; a = k+1, \ldots, n \tag{3.9}$$

(and permutations), we obtain from (1.13) the complexity

$$\Sigma_k(E) = \frac{k+2}{2} \, \frac{q_+^2}{p(p-1)} - \frac{k}{2} \, \frac{q_-^2}{p(p-1)} + \frac{k+2}{2} \log(-pE + q_+) - \frac{k}{2} \log(-pE + q_-) + A(E) \; . \tag{3.10}$$

It is not a surprise the fact that Σ_k is related to the number of TAP solutions which are saddles with k negative eigenvalues. Indeed the probability of finding such a solution is

$$P_{(k,-)} = \left[P_{(-)}\right]^k \sim e^{-Nk\Delta(0,E)} \tag{3.11}$$

so that to prove our assertion it is sufficient to verify that it holds the relation

$$k \; \Delta(0,E) = \Sigma_0(E) - \Sigma_k(E) \tag{3.12}$$

as it does. In writing equation (3.11) we can disregard the correlations between different negative eigenvalues, as long as k is much smaller than N. We conclude that, as a general result, $\Sigma_k(E)$ is the complexity of TAP saddles with k negative eigenvalues and energy density E. This is an original result [24].

Since $|q_-| \geq |q_+|$ we have that $\Sigma_0(E) \geq \Sigma_1(E) \geq \ldots \geq \Sigma_k(E) \geq \Sigma_{k+1}(E) \ldots$. Thus all the TAP solutions, also those with some negative eigenvalues, are exponentially numerous in N. Nevertheless, the number of minima is exponentially higher than the number of saddles with one negative eigenvalue, which is exponentially higher than the number of saddles with two negative eigenvalues, and so on. This is the very reason why, as long as $E < E_{th}$, the approximation of dropping the modulus in (1.6) is justified. In Figure 1 we have plotted Σ_0, Σ_1 and Σ_2 as a function of E.

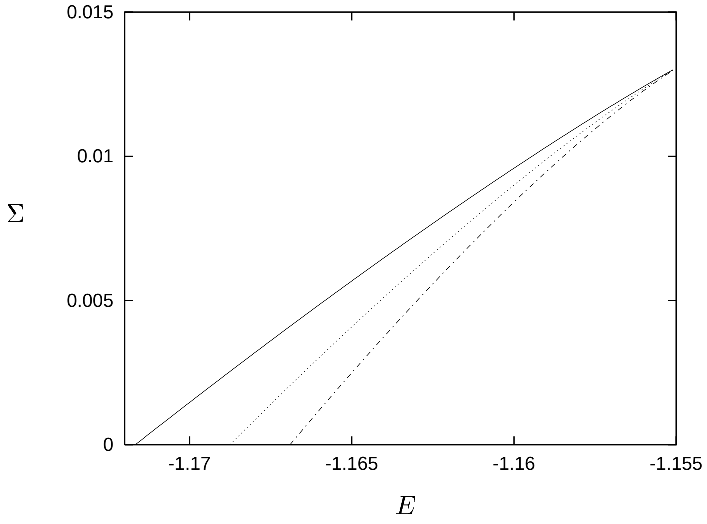

Figure 1: The complexity Σ_0 of the TAP minima (solid line) and the complexities Σ_1 and Σ_2 of the TAP saddles with one and two negative eigenvalues (respectively dotted and chain line), as a function of the zero temperature energy density E. The threshold energy is E_{th}=-1.1547 for p=3. The minimum saddles energy, defined by $\Sigma_1(E_0)$=0 is E_0=-1.1688.

From equation (3.10) and from figure 1 we note that $\Sigma_k(E_{th}) = \Sigma_0(E_{th})$, for each k, since $q_+ = q_-$ at the threshold energy. This equality is very important. If we try to count the *total* number of solutions neglecting the modulus in equation (1.6), a trivial result must be obtained [30], since we are weighting each stationary point with the sign of the determinant (this is the Morse theorem). This is the reason why we considered solutions with a *given* fixed energy E. Yet, for what said above, if we integrate our result over all the energies E, we must recover the result predicted by the Morse theorem. Remembering that the q part of the TAP equations admits solutions only for $E < E_{th}$, we have from our calculations:

$$\begin{aligned} \int^{E_{th}} dE \ \overline{\int \mathcal{D}\sigma \ \delta(\sigma\cdot\sigma - N) \prod_{l=1}^{N} \ \delta(\mathcal{T}_l(\sigma;E)) \ \det\mathcal{H}(\sigma;E)} = \\ = \ a_0 \ e^{N\Sigma_0(E_{th})} + a_1 \ e^{N\Sigma_1(E_{th})} + a_2 \ e^{N\Sigma_2(E_{th})} + \ldots \end{aligned} \tag{3.13}$$

In this formula we must introduce all the Σ_k's coming from all the solutions of the saddle point equations for Σ, which refer to stationary points of any nature. One can easily see that all the Σ_k's are monotonously increasing functions of E which reach their maximum value at E_{th}, so that we can substitute the integral in (3.13) with the maximum of the integrand. The prefactors $a_0, a_1, \ldots$ come from the fluctuations around each saddle point solution and contain the sign of the determinant. It is exactly the combination of these signs that gives rise to the Morse theorem. From equation (3.13) is then clear that a necessary condition to get a trivial topological constant is that $\Sigma_0(E_{th}) = \Sigma_1(E_{th}) = \Sigma_2(E_{th}) = \ldots$, so that we can sum *all* the terms on the same foot, to give a finite result. As said above, this necessary condition is fulfilled by our calculation.

Besides, from equation (3.13) it is finally clear what is the role of the modulus in the calculation: taking $|\det \mathcal{H}|$ is equivalent to take the absolute value of the prefactors a_k, thus preventing from obtaining a trivial result. Yet, at fixed energy $E < E_{th}$, one of the terms $\exp(N\Sigma_k(E))$ is always bigger than all the others and therefore in the limit $N \to \infty$ the signs of the prefactors a_k have no influence on the final result. As we have said, this dominant term turns out to be the one with $k = 0$, which gives exactly the contribution of the minima.

We have now the possibility of fully clarify all the ambiguities related to the computation of the complexity Σ. The global number of TAP solutions with a given energy density E is a sum of exponential terms, each one related to extrema of different nature, minima, saddles, etc. When the energy E is lower than E_{th} just one of this terms dominates over all the others, the term related to the number of minima. Thus with exponential precision we can say that the total number of solution coincides with the total number of minima in this energy range. This is not a contradiction, but a simple consequence of adding exponentials with different growing rates, when N tends to infinity. For this reason every naive approach to the calculation gives the correct number of minima. On the other hand, we have shown that it possible to extract the sub-dominant contributions to the total number of TAP solutions, just by taking different solutions of the saddle point equations and we have obtained in this way the complexity of the TAP saddles with k negative eigenvalues.

We note that it should be possible to show that Σ_k is related to the number of the saddles with k negative eigenvalue directly from (1.13). If we keep n finite this integral is equivalent to $\overline{(\det \mathcal{H})^n}$. Taking the saddle point solution $\mathcal{S}_k$ and appropriately computing the Gaussian fluctuations around it, it should be possible to single out a factor $(-1)^{kn}$ related to the sign of the determinant. Unfortunately, we did not succeed in performing this quite complex computation.

From figure 1 we see that there is a minimum energy density E_0, defined by $\Sigma_1(E_0) = 0$ below which no saddles with finite complexity are found. Therefore when considering a state with energy density $E < E_0$, the value $\Delta E = E_0 - E$ is a lower bound for the energy density barrier between this state and any other state of the system. In the context of the three replica potential introduced in chapter III it is possible to give an estimate for the barriers separating two states [34]. It turns out that this estimate is fully consistent with the result of the present discussion.

We end this section with an interesting remark. From equation (2.7) we see that for $E > E_{th}$ the semicircle invades the negative semi-axis. This means that the dominant part of the stationary point at this energy has a number of negative eigenvalue which is of order N, for $N \to \infty$, that is above the threshold energy the greatest part of the angular TAP solutions are *saddles*. Therefore we expect to see this phenomenon also in the context of section 2, where by means of equation (1.13) we computed the determinant of the Hessian, since we want this quantity to contain the sign of these saddles. For $E > E_{th}$ both the roots $q_\pm$ develop an imaginary part different from zero, which inserted in equation (1.13) gives exactly the oscillating contribute we expect the determinant to have. Furthermore, we see from equation (1.14) that the real part of $q_\pm$ is equal for the two roots, so that the real contribution to the complexity, which gives the actual number of saddles, does not depend any more on the number k of roots equal to q_- we put in the saddle point solution. This is correct, since in a situation where the number of saddles is already exponentially dominant, we do not expect to have any correction to the number of negative eigenvalues from the exponential tail in the negative semi-axis, since the mean number of negative eigenvalue is already of order N.

We are now in the position of define and compute a more complicate quantity, the constrained complexity, without any ambiguity.

4. The constrained complexity.

We turn now to face the main task of this research, that is to find the overlap distribution of the states for the p-spin spherical model.

To clarify what we intend with distribution of the states it is useful to think about the Sherrington-Kirkpatrick (SK) model [9]. In this case, in the context of the replica method, the solution given in [4,5,6] has permitted to define and calculate the overlap distribution $P(q)$ of the pure states: as we have shown in chapter II, $P(q)$ is defined as the probability that, drawn two states, their mutual overlap is equal to q. Therefore, in the distribution $P(q)$ two different contributions are present: the existence of states having mutual overlap q and their individual statistical weights. The function $P(q)$ gives for the SK model an important structural information on the distribution of the states in term of the overlap [11]: there is a continuous spectrum of states, going from zero up to the self-overlap q_{EA}, consequence of the full RSB of the saddle point overlap matrix. This continuous spectrum indicates that, given a state, we can find other states at *any* value of the overlap with it, with a probability different from zero.

For the p-spin spherical model we would like to have a structural information of the same kind as the one given by the distribution $P(q)$ for the SK model.

Unfortunately, as we have seen in chapter II, applying the standard replica method to the p-spin spherical model a trivial result is obtained [3]: in the intermediate temperature phase that we are considering $T_s < T < T_d$ the model is solved by a replica symmetric solution, corresponding to a trivial distribution function $P(q) = \delta(q)$. This delta function simply means that the *typical* overlap between two states is zero. On the other hand, let us consider why this distribution does not get any contribution from the self-overlap of the equilibrium states, which is different from zero. The answer is that all these states singularly have a weight so low that the contribution of their self-overlap is not present in the distribution $P(q)$. In other words, it is highly unlikely to draw the same state twice and measure its self overlap, if this is either an equilibrium state or a metastable one. We have seen in chapter III that by means of the potential V_2 we have indeed detected the self-overlap of the states, but only by forcing two systems to stay unnaturally in the same state.

For the same reason it is possible that the distribution $P(q)$ does not catch a contribution from *all* the other possible values of the overlap q, simply because drawing two states with overlap different from zero has a vanishing probability in the thermodynamic limit. This would mean that the trivial form of $P(q)$ is not a consequence of the absence of states with mutual overlap different from zero, but rather of the difficulty of finding them. On the contrary, there is the possibility that indeed *all* the states of this model have mutual overlap of zero, i.e. that states with an overlap different from zero do not exist at all. In this last case it is clear that there would be only a trivial structure of the states, exactly reproduced by a trivial $P(q)$. The standard static approaches cannot distinguish between these two pictures, and more than this, in the case in which a non trivial hidden structure were present, they are not able to give us any insight into the problem. In our opinion it seemed very strange to have this huge number of states without any interesting geometrical structure and therefore we have tried to develop some non standard methods which could provide some information on this topic.

The first question to answer was then: Does a non trivial structure of the states exist ? This question has been fully answered in chapter III, by the definition of the three replica potential [28]. Within this method we demonstrated that, given an equilibrium state, there are other states, both metastable and equilibrium, at *any* value of the overlap q with it, until a certain maximum value. This shows clearly that a non trivial structure of the states for this model is present, and that the second picture we stated above has to be discarded. Furthermore we hypothesized in chapter III that the number of non orthogonal states was very high, presumably exponentially large in N. On the other hand, as we have seen, the energy spectrum of the states found with V_3 was not completely understood and there was no control on the choosing procedure of the detected states.

Therefore it is necessary to define a new tool by which the hidden structure of the states for the p-spin spherical model can be analyzed in a deep way. Yet, as we have seen, there is the problem of the vanishing weight of these states, that leads to the trivial form of the standard distribution function $P(q)$. Bearing this in mind, the most natural thing to do is to perform a purely *entropic* computation, disregarding the thermodynamic weight of the states. Thus, what we are going to do is to fix a reference state in the phase space and simply *count* how many states of a given kind are present at overlap q with it. More precisely, what we have actually computed is the number of TAP solutions having a given overlap q with a single fixed solution. The resulting quantity is what we have called the *constrained complexity* Σ_c.

It is important to note that the identification of TAP solutions with true thermodynamic states of the system is not trivial, but it has been demonstrated many times in the previous discussion. In particular, by virtue of our results on the complexity of the saddles of the previous sections we now have the technical means to exactly control the nature of the stationary points of the TAP free energy. This fully justify the use of the TAP approach for an investigation of the structure of the states.

We can now introduce the constrained complexity

$$\Sigma_c(E_2, q|E_1) \stackrel{\text{def}}{=} \lim_{N\to\infty} \frac{1}{N} \overline{\log \mathcal{N}(E_2, q|E_1)} \; . \tag{4.1}$$

In this definition $\mathcal{N}(E_2|q, E_1)$ is the number of TAP solutions with energy density E_2 having overlap q

with a single fixed solution of energy density E_1. The bar indicates the average over the disorder. What we are doing here is to fix a single state of energy E_1 and simply count how many states of energy E_2 are found at overlap (distance) q with it. We remark that q is the overlap between these TAP solutions at finite temperature, while, as usual, E_1 and E_2 are their zero temperature energy densities.

In definition (4.1) we have averaged the logarithm of $\mathcal{N}$, since this is the extensive quantity. However, we have seen in the previous sections that in the unconstrained case [18], the correct ansatz for the overlap matrix is symmetric and diagonal and this is equivalent to average directly the number $\mathcal{N}$ of the solutions. In our case the same prescription leads to the formula

$$\Sigma_c(E_2,q|E_1) = \lim_{N\to\infty} \frac{1}{N} \log \overline{\mathcal{N}(E_2,q|E_1)} \tag{4.2}$$

and this is the quantity we shall compute. It is surely possible that the introduction of the constraint q requires a breaking of the replica symmetry and therefore definition (4.2) has to be considered as a first approximation. Yet, as we shall show, the results obtained with formula (4.2) suggest that this is a good approximation.

The complexity Σ_c can be obtained by counting all pairs of solutions with energies (E_1,E_2) at mutual overlap q and dividing it by the number of solutions with energy E_1, i.e.

$$\Sigma_c(E_2,q|E_1) = \lim_{N\to\infty} \left\{ \frac{1}{N} \log \overline{\mathcal{N}(E_1,E_2,q)} - \frac{1}{N} \log \overline{\mathcal{N}(E_1)} \right\} \stackrel{\rm def}{=} \Gamma(E_1,E_2,q) - \Sigma_0(E_1) \tag{4.3}$$

where $\Sigma_0(E_1)$ is the usual unconstrained complexity computed in [18] and in section 1. We note that the quantity Γ, which is the pairs complexity, is symmetric in (E_1,E_2) while Σ_c is not. Moreover, $\Gamma(E_1,E_2,0) = \Sigma_0(E_1) + \Sigma_0(E_2)$, since *almost* all TAP solutions are mutually orthogonal. For this same reason we had in chapter III $V_3(q_{12}=0) = V_2(q_{12}=0) = 0$. Therefore it must hold

$$\Sigma_c(E_2,0|E_1) = \Sigma_0(E_2)\ . \tag{4.4}$$

This is the first check we have to face in our calculation.

Let $m_i^{(1)}$ and $m_i^{(2)}$ be two TAP solutions with self-overlaps q_1 and q_2, and mutual overlap q; using the notation $m\cdot m' = \sum_i m_i m_i'$, we have

$$m^{(1)}\cdot m^{(1)} = Nq_1 \quad ; \quad m^{(2)}\cdot m^{(2)} = Nq_2 \quad ; \quad m^{(1)}\cdot m^{(2)} = Nq \tag{4.5}$$

As usual we write TAP equations in terms of the angular part of the magnetizations σ_i, τ_i:

$$m_i^{(1)} = \sqrt{q_1}\,\sigma_i \quad ; \quad m_i^{(2)} = \sqrt{q_2}\,\tau_i \tag{4.6}$$

for which it holds

$$\sigma\cdot\sigma = N \quad ; \quad \tau\cdot\tau = N \quad ; \quad \sigma\cdot\tau = N\frac{q}{\sqrt{q_1 q_2}} \stackrel{\rm def}{=} Nq_0\ . \tag{4.7}$$

Let us recall that in terms of the angular variables σ and τ, the TAP equations read

$$0 = -p\sum_{i_2<\ldots<i_p} J_{i,i_2\ldots i_p}\,\sigma_{i_2}\ldots\sigma_{i_p} - pE_1\sigma_i \stackrel{\rm def}{=} \mathcal{T}_i(\sigma;E_1) \quad , \quad i=1,\ldots,N \tag{4.8}$$

where E_1 is the zero temperature energy density

$$E_1 = -\frac{1}{N} \sum_{i_1 < \ldots < i_p} J_{i_1 \ldots i_p} \sigma_{i_1} \ldots \sigma_{i_p} \ . \tag{4.9}$$

Relations of the same kind of (4.8) and (4.9) hold for τ and E_2. It is now possible to write Γ with the standard method of section 1 in the following way:

$$\begin{aligned} &\Gamma(E_1, E_2, q) = \\ &= \frac{1}{N} \log \int \mathcal{D}P(J) \int \mathcal{D}\sigma \mathcal{D}\tau \prod_i \ \delta(\mathcal{T}_i(\sigma; E_1)) \ \delta(\mathcal{T}_i(\tau; E_2)) \ \left| \det \left(\frac{\partial \mathcal{T}(\sigma; E_1)}{\partial \sigma} \right) \right| \ \left| \det \left(\frac{\partial \mathcal{T}(\tau; E_2)}{\partial \tau} \right) \right| \times \\ &\times \delta(\sigma \cdot \sigma - N) \ \delta(\tau \cdot \tau - N) \ \delta(\sigma \cdot \tau - N q_0) \end{aligned} \tag{4.10}$$

with

$$\mathcal{D}P(J) = \prod_{i_1 < \ldots < i_p} \sqrt{\frac{N^{p-1}}{\pi p!}} \exp(-J^2_{i_1 \ldots i_p} N^{p-1}/p!) \ dJ_{i_1 \ldots i_p} \ . \tag{4.11}$$

We note that the dependence on the temperature is entirely contained in q_0 through q_1 and q_2, functions respectively of E_1, E_2 and β [8].

In formula (4.10) we can drop the two modulus since we have shown in sections 1-3 that this is equivalent to disregard the sign of terms exponentially vanishing in the thermodynamic limit. We recall that a necessary condition for this to be true is that we keep fixed the energy of the solutions we are counting, as done in formula (4.10). In this way we are sure that the TAP solutions we are taking into considerations are actually minima.

In order to perform the calculation we follow the same line of reasoning of section 1: we introduce a Bosonic representation both for the delta functions and the determinant and we disregard terms which break the rotational symmetry in the replica space. This simplifies a lot the calculation, since it turns out that the determinant part has exactly the same form as in the unconstrained case, while, due to the constraint q_0 this is no longer true for the part concerning the delta functions. In section 1 we have written the unconstrained complexity as

$$\Sigma_0(E) = A(E) + B(E) \tag{4.12}$$

with

$$A(E) = \frac{1}{2} - \frac{1}{2} \log \frac{p}{2} - E^2 \qquad B(E) = \frac{q_+^2}{p(p-1)} + \log(-pE + q_+) \tag{4.13}$$

$$q_+ = \frac{p}{2} \left(E \pm \sqrt{E^2 - E_{th}^2} \right) \quad , \quad E_{th} = -\sqrt{\frac{2(p-1)}{p}} \tag{4.14}$$

Similarly, for what said above, we can write

$$\Gamma(E_1, E_2, q) = \Delta(E_1, E_2, q) + B(E_1) + B(E_2) \tag{4.15}$$

where Δ is the contribution to (4.10) due to the delta functions. In this way Σ_c has the form

$$\Sigma_c(E_2, q|E_1) = \Delta(E_1, E_2, q) - A(E_1) + B(E_2) \ . \tag{4.16}$$

Besides the variables σ and τ there are the two Bosonic fields coming from the integral representation of the delta functions, respectively μ and λ. All these Bosons couple because of the average over the disorder J. To perform the saddle point approximation we introduce the following set of variational parameters:

$$\begin{aligned} Nx_1 = \mu \cdot \mu \quad ; \quad Nx_2 = \lambda \cdot \lambda \quad ; \quad Nx_3 = \mu \cdot \lambda \\ Ny_1 = \sigma \cdot \mu \quad ; \quad Ny_2 = \tau \cdot \lambda \quad ; \quad Ny_3 = \sigma \cdot \lambda \quad ; \quad Ny_4 = \tau \cdot \mu \quad . \end{aligned} \tag{4.17}$$

We remind that $\sigma \cdot \tau = Nq_0$, while $\sigma \cdot \sigma = \tau \cdot \tau = N$. The explicit calculation gives

$$\begin{aligned} \Delta(E_1, E_2, q) = \\ = \operatorname*{Ext}_{x,y} \Big\{ & ipE_1 y_1 + ipE_2 y_2 - \frac{p(p-1)}{2} q_0^{p-2} y_3 y_4 - \frac{p}{4}(x_1 + x_2) - \frac{p}{2} q_0^{p-1} x_3 \\ & - \frac{p(p-1)}{4}(y_1^2 + y_2^2) + \frac{1}{2} \log\left(\frac{\Lambda}{1-q_0^2}\right) + 2 \Big\} \end{aligned} \tag{4.18}$$

with

$$\Lambda = [x_1(1-q_0^2) - k_1][x_2(1-q_0^2) - k_2] - [x_3(1-q_0^2) - k_3]^2 \tag{4.19}$$

$$k_1 = y_1^2 - 2q_0 y_1 y_4 + y_4^2 \quad ; \quad k_2 = y_2^2 - 2q_0 y_2 y_3 + y_3^2 \quad ; \quad k_3 = y_1 y_3 - q_0(y_1 y_2 + y_3 y_4) + y_2 y_4 \tag{4.20}$$

and we remind that $q_0 = q/\sqrt{q_1 q_2}$. The saddle point equations are easily solved numerically, while it is possible to check analytically that for $q_0 = 0$ we have $\Delta(E_1, E_2, 0) = A(E_1) + A(E_2)$, so that equation (4.4) is fulfilled.

Before proceeding we note that we have used here the notation of [24], that is the same of the previous sections. In the original paper where the constrained complexity has been introduced [25] a Fermionic representation for the determinants was used and thus the notation was different: functions Ξ and Ω were introduced instead of A and B. This is the reason why it appears a factor 2 in formula (4.18) absent in the same formula of [25].

5. Normal and anomalous regimes.

In this section we analyze the dependence of the constrained complexity Σ_c on E_2 and q, at a fixed value of E_1. In particular, we are interested in the dependence of Σ_c on the overlap q, i.e. in the overlap spectrum of the system, since this can give us insight into the geometrical distribution of the states in the phase space. In what follows it is always assumed $T \in [T_s, T_d]$, where T_s and T_d are respectively the static and the dynamical transition temperatures.

As a value for the reference energy E_1 we choose $E_1 = E_{eq}^T$, where E_{eq}^T is the zero temperature energy density of those TAP solutions that dominate at temperature T (see chapter II.3). In this way, we are fixing an equilibrium state and counting how many states of energy density E_2 are present at distance q from it. We stress however that we could choose any other value for the reference energy E_1, obtaining qualitatively the same results.

It is useful to distinguish two different regimes: a *normal* regime, corresponding to values of E_2 well below the threshold, in which geometrical considerations at least qualitatively apply, and an *anomalous* regime, characterized by values of E_2 just below the threshold, which shows a rather peculiar behaviour of Σ_c.

- *The normal regime:*

The normal regime is defined by values of the energy E_2 of the states we are counting well below the threshold energy E_{th}. Intuitively, we expect that Σ_c decreases with increasing q, since larger values of q correspond to smaller portions of the phase space. This is indeed what happens in the normal regime, as shown in figure 2, where we have plotted Σ_c as a function of q.

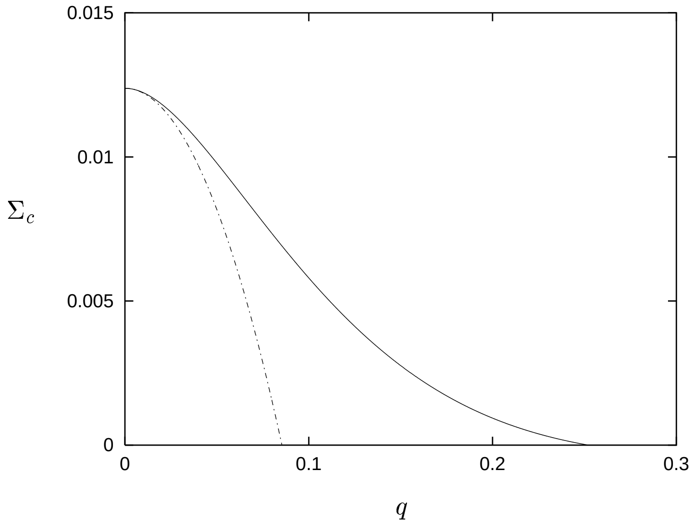

Figure 2: The constrained complexity Σ_c as a function of the overlap q (full line), with $E_1{=}E_2{=}E_{eq}{=}-1.156$, for $\beta{=}1.64$ and $p{=}3$. The self overlap of the two states is $q_1{=}q_2{=}0.55$, while $\Sigma_c{=}0$ at $q_{last}{=}0.25$. The dashed-dotted line is the curve predicted by a random distribution of the states (see the text). For $q{=}0$ both the curves coincide with the unconstrained complexity $\Sigma_0(E_2)$.

This curve provides us some important information: First of all this is a *continuous* curve, meaning that there is a continuous spectrum of states with energy E_2 around the fixed reference state of energy E_1. In particular in figure 2 we have set $E_2 = E_{eq}^T$. This means that there is an exponentially high number of states at any value of q, until a value q_{last} for which $\Sigma_c = 0$. Thus q_{last} gives the overlap of the nearest states with energy E_2.

Note the difference with the results coming from the three replica potential (III.3): there at each different value of the overlap we found states with different energies, while here we have the possibility to keep fixed the energy of the detected states. In figure 2 we see that, given an equilibrium state, we find other equilibrium states at any value of the overlap q, up to q_{last}.

It is important that, as long as E_1 and E_2 are different from E_{th}, the value of q_{last} is *smaller* than the self overlap of the considered states. This gap between the last value of the overlap in the spectrum and the self overlaps q_1, q_2 simply means that these states are well separated one with respect to the other: according to the definition given in chapter II, when the distance between two different states is equal to their largeness, it means that these two states are coincident in the thermodynamic limit. In this case states are well separated and formally this can be written as:

$$\frac{q_{last}}{\sqrt{q_1 q_2}} < 1 \ . \tag{5.1}$$

This has to be compared with the case of the Sherrington-Kirkpatrick model [9] in which as well as in this case there is a continuous distribution of states, but with mutual overlap going from $q = 0$ up to the self overlap $q = q_{EA}$ [11,14]. We stress that the coincidence of two states having mutual overlap equal to their self-overlap has to be understood in the limit $N \to \infty$, as already explained in chapter II.

The second important feature of figure 2 can be caught if we compare Σ_c with the corresponding quantity that would be obtained in the case of a *random* distribution of the states. The simplest hypothesis we can formulate on the geometrical structure of the states is that they are randomly distributed in the phase space, as they were drops of rain on the sphere. In this case, the number of states at distance q from a given fixed point in the phase space would be simply given by the total number of states multiplied by the volume of the manifold defined by fixing q. The value of this volume is

$$V \sim (\sin\theta)^{N-2} \tag{5.2}$$

where θ is the average angle between the fixed state and states at overlap q with it, i.e.

$$\cos\,\theta = \frac{q}{\sqrt{q_1 q_2}} \tag{5.3}$$

and q_1, q_2 are the self overlaps of the two states. To understand equation (5.3) simply note, once again, that we want two states to be coincident ($\theta = 0$) when their largeness q_1 is equal to their distance q. The number of states found at distance q is then

$$\mathcal{N}_{random}(q,E) = \mathcal{N}_{tot}(E)\left(1 - \frac{q^2}{q_1 q_2}\right)^{\frac{N-2}{2}} \tag{5.4}$$

Taking the logarithm and dividing by N we obtain

$$\Sigma_{random}(q,E) = \Sigma_0(E_2) + \frac{1}{2}\log\left(1 - \frac{q^2}{q_1 q_2}\right) \tag{5.5}$$

where $\Sigma_0(E_2)$ is the unconstrained complexity. If we plot this quantity as a function of q and compare it with $\Sigma_c(q)$ (figure 2), it can be seen that there is a violation of the random distribution and that this violation goes in the direction of having a higher number of states when looking at small distances.

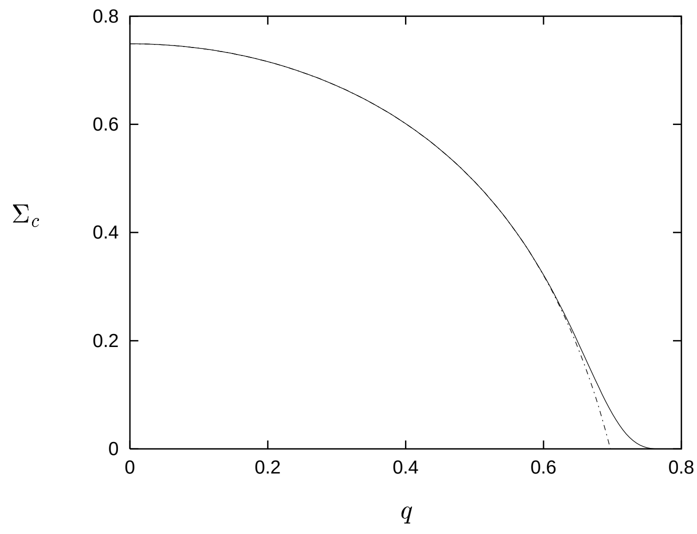

Figure 3: The constrained complexity Σ_c (full line), compared with the random distribution (5.5) (dashed-dotted line) for p=30. All other parameters are the same as in Figure 2.

The comparison with the random distribution of the states suggests an interesting check. It is known that the p-spin model in the limit $p \to \infty$ coincides with the Random Energy Model of [35]. This model is characterized by a complete decorrelation of the energy levels of the system: one simply draw M levels (states) following a given probability distribution of the energy, so that all these levels are uncorrelated random variables. Therefore we expect that increasing the value of p, the constrained complexity Σ_c becomes more and more similar to the random distribution (5.5). This is shown in figure 3, where we see that for $p = 30$ it remains only a little tail for large q where the two distributions are different. For $p \to \infty$ they coincide. We note that in the Random Energy Model there is no geometrical structure at all. Therefore what we have shown here is that a complete *energetic* decorrelation between different states corresponds to a complete *geometrical* decorrelation of the states in the phase space.

Finally we consider the dependence of Σ_c on the energy E_2 of the states that we are counting. In figure 4 we have plotted $\Sigma_c(E_2)$ at various values of q. The curve on the top corresponds to $q = 0$ and then reproduces the unconstrained complexity $\Sigma_0(E_2)$ (see equation (4.4)). We note that, even at fixed $q \neq 0$, $\Sigma_c(E_2)$ increases with increasing E_2, as in the unconstrained case. Furthermore, as expected, the whole curve $\Sigma_c(E_2, q)$ decreases with increasing q.

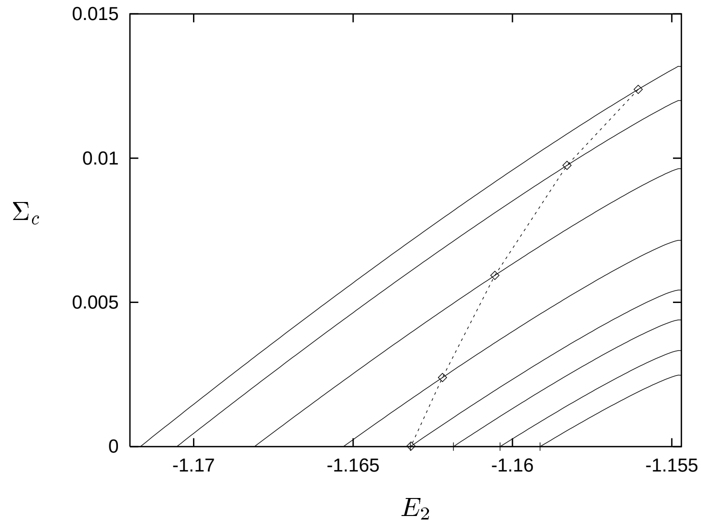

Figure 4: The constrained complexity Σ_c as a function of the energy E_2, at various values of the overlap q and $E_1 = E_{eq} = -1.156$, for $\beta = 1.64$ and $p = 3$. The first curve on the top has $q = 0$ and thus corresponds to the unconstrained complexity $\Sigma_0(E_2)$. The threshold energy is $E_{th} = -1.1547$. The squares indicate the minimum of the function ϕ_c (see Section 4), which reaches the axis $\Sigma_c(E_2) = 0$ at $q_{low} = 0.113$.

• *The anomalous regime:*

We turn now to examine the anomalous regime. If we plot Σ_c as a function of E_2 exactly as in figure 4, but now expanding a narrow range of energies E_2 just below the threshold ($E \in [E_{th} - 5 \times 10^{-4}, E_{th}]$), we obtain the behaviour shown in figure 5.

The curves get lower and lower with increasing q, until for a value of q that we call q_{max} they begin to reverse, folding upwards. In figure 5, q_{max} corresponds to the curve whose intersection with the $\Sigma_c(E_2) = 0$ axis begins going backward. If now we make a section of these curves at a fixed value of E_2 in this range, plotting Σ_c as a function of q, we find the anomalous behaviour of Figure 6: there is an interval of q where Σ_c *increases* with increasing q.

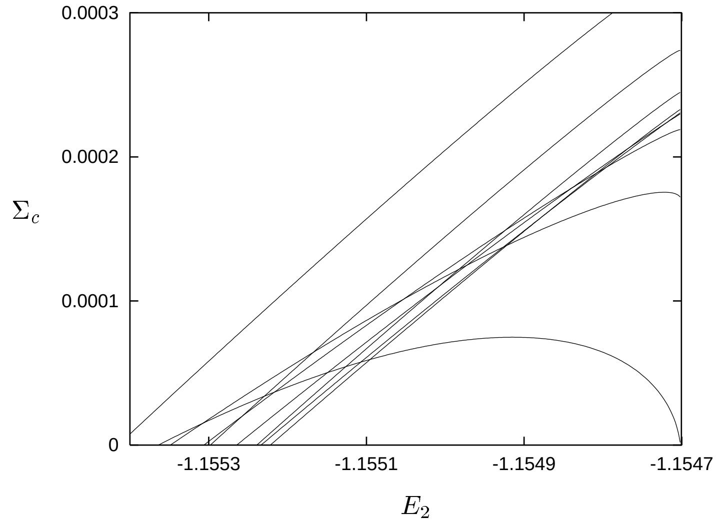

Figure 5: The constrained complexity Σ_c as a function of the energy E_2 just below the threshold, at various values of q. The value q_{max} corresponds to the curve whose intersection with the axis $\Sigma_c(E_2)$=0 begins to reverse.

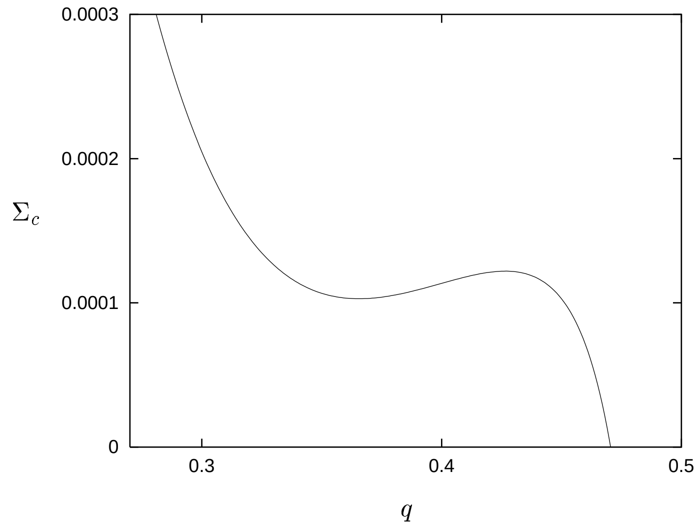

Figure 6: The constrained complexity Σ_c as a function of the overlap q in the anomalous regime. E_1=E_{eq} and E_2=-1.1550.

The reversed behaviour of $\Sigma_c(q)$ clearly has no geometrical origin and for this reason we talk of an anomalous regime. What it seems is that, given a state (in this case an equilibrium state), there is a sort of clustering of states with high energy at small distances (large overlap) from it, thus giving the distribution of figure 6. We can interpret this fact in the following way: starting far away and approaching to the reference state we find always less states the more we get closer, since the available portion of the phase space continuously reduces, according to (5.2). At a given moment we reach a minimum of the number of detected states, just before entering into a sort of correlated structure of states, localized around the fixed reference state. Here the number of states starts increasing, the more the more we enter in the local cluster, until, as usual, we are too close to the reference state and we do not find any other state, so that Σ_c abruptly falls to zero.

Moreover, from figure 5 we note that for high enough values of q, Σ_c is no longer monotonic with respect to E_2, and it develops a maximum. Therefore, in this range of q threshold solutions are not the most numerous states around the fixed equilibrium state.

To conclude, we note that the amplitude of the anomalous regime depends on the reference energy E_1: the range of energies E_2 into which this anomalous behaviour occurs is larger for low values of E_1 and shrinks to zero as E_1 approaches E_{th}.

6. The spectrum of the dominant states.

At a first sight the increasing of Σ_c with q, together with the role of q_{max} in the anomalous regime could seem an artifact of the calculation. Nevertheless, how we are going to show, this behaviour is able to explain the energy spectrum obtained with the three replica potential we introduced in chapter III, where a completely different kind of computation was performed [28]. This is a very important check for both the new methods we introduced.

We ask: Which are the *dominant* state at overlap q with a given fixed state ? We have seen many times that in the unconstrained case equilibrium states of the system are defined as those TAP solutions that minimize the generalized free energy density $\phi(f) = f - T\Sigma(f)$. Similarly, we can wonder which solutions dominate at distance q from a given equilibrium state. To this end we look for the minimum of the function $\phi_c(f,q) = f - T\Sigma_c(f,q)$, with $E_1 = E_{eq}^T$ and Σ_c expressed as a function of the free energy density f of the states found at distance q. In Figure 4, for each given value of q, we have signed on the corresponding curve the point that minimizes ϕ_c. As it is easily seen, there is a value of q for which the minimum of ϕ_c reaches the axis $\Sigma_c(E_2) = 0$. We call this value q_{low}. If we look for a minimum of ϕ_c when $q > q_{low}$ we would be brought to a negative value of Σ_c, that is to non existing solutions (in the limit $N \to \infty$). In this situation, the dominant solutions are those with the lowest energy density and a non negative value of the complexity, i.e. with $\Sigma_c(E_2) = 0$. Due to this, at q_{low} there is a sharp change in the energy behaviour of the dominant solutions: this energy decreases following the minimum of ϕ_c until $q = q_{low}$, then, for higher values of q, it increases following the intersection of the curves $\Sigma_c(E_2)$ with the axis $\Sigma_c(E_2) = 0$. Yet, from figure 5 we see that when q reaches q_{max}, due to the anomalous behaviour of $\Sigma_c(E_2)$ this intersection point inverts its direction, so that the energy of the dominant solutions starts to decrease.

We conclude that the energy density of the solutions dominating at distance q from a fixed equilibrium state has a cusp for $q = q_{low}$ and reaches a maximum at $q = q_{max}$. What said above is shown in figure 7.

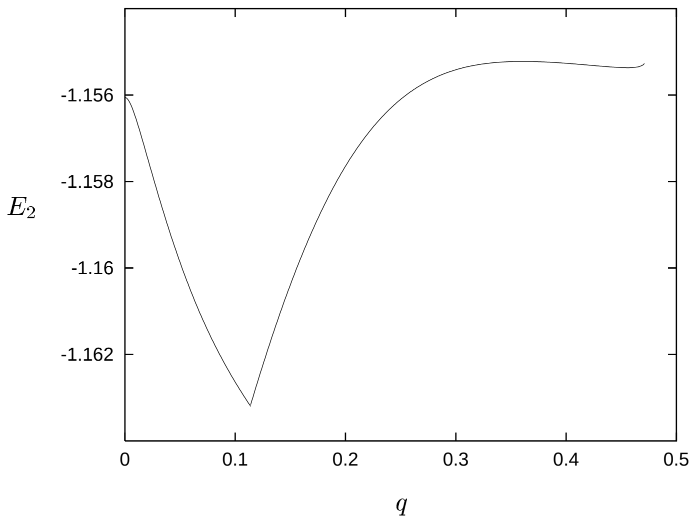

Figure 7: The energy density E_2 of the solutions dominating at distance q from the fixed equilibrium solution. The cusp is at q_{low}=0.113 and the maximum is at q_{max}=0.360. The last point of the curve represents the distance of the nearest solutions.

It is clear to the reader that this mechanism finally explains the energy spectrum found with the potential V_3 (see figure 8). In that case a first replica is quenched into an equilibrium state, while a second replica is forced to thermalize at distance q from it. It is then natural to think that the second replica thermalizes into one of the states that dominate at distance q in the sense described above, so that the spectrum of the states visited by this second replica should be of the same kind as the spectrum of figure 7. This is indeed what happens, as we will show with more details in the next section: the spectrum found with the potential V_3 presents a cusp and has a maximum exactly at $q = q_{max}$, thus providing a confirmation of the existence of the anomalous regime.

In analyzing figure 7 it is important to note that the number of dominant states is exponentially high in N as long as $q < q_{low}$, while it is of order N for $q > q_{low}$. As we have seen in chapter III and as we are going to explain in detail in the next section, the three replica potential signalizes this phenomenon by the breaking of the replica symmetry in the overlap matrix and this is another confirmation of the consistency of these two different methods [28,36].

The ending point of this curve corresponds to that value of the overlap above which no states of any energy are found with $\Sigma_c \geq 0$. Thus it indicates which is the overlap with the fixed state of energy $E_1 = E_{eq}^T$ of the states nearest to it. It turns out that these nearest states have an energy density *greater* than the energy E_{eq}^T of the fixed reference state, even if in general they are not threshold states. What is important is that this is not a special feature of the equilibrium states: indeed, given a state of *any* energy E_1, the states nearest to it *always* have an energy density greater than E_1.

This behaviour is not a trivial consequence of the fact that states with higher energy are in general more numerous, since following this reasoning the nearest states would always be the threshold ones (which have the greatest unconstrained complexity), while we know that this is not true. Actually, as mentioned in section 5, at large values of the overlap q, i.e in the anomalous regime, threshold states are no longer the most numerous around a given fixed state. In other words, once the curve of the dominant states of figure 7 develops a maximum at q_{max}, it is not obvious which should be the energy of the states corresponding to the ending point of this curve.

7. A comparison with the three replica potential.

As we have seen, the real replica method [8,27,28,26] consists in studying the static properties of a certain number of real replicas of the system, as a function of the overlaps imposed among them. In chapter III we introduced the three replica potential V_3 by which we analyzed the structure of equilibrium and metastable states of the p-spin spherical model: the first replica is fixed into an equilibrium state, while the second replica is forced to equilibrate at overlap q_{12} with the first one. Clearly, the way in which replica 2 chooses its constrained equilibrium state is heavily conditioned by the complexity Σ_c of the states at that distance. Once fixed replicas 1 and 2, the potential V_3 is defined as the free energy density of a third replica 3 as a function of its distances q_{13} and q_{23} from the first two. The most important minimum of V_3 corresponds to replica 3 in local equilibrium into the state chosen by replica 2. In this minimum, that we called M_2, the energy and the self overlap of replica 3 satisfy TAP equations, meaning that replicas 2 and 3 have found a state of the unconstrained system at distance q_{12} from the equilibrium state of replica 1.

Before proceeding further it is crucial to clarify the different roles of the three replicas, beginning from the way in which replica 2 chooses the state at distance q_{12} from 1. If the TAP free energy is minimized *on* the manifold defined by fixing q_{12}, the number of minima found is clearly greater than the number of *genuine* TAP solutions at that distance and for the most part consists of projections on the manifold of nearby true TAP solutions. These projections are what replica 2 sees as states. Therefore, we can say that replica 2 thermalizes in the vicinity of a TAP solution, but this solution is in general at distance $q \neq q_{12}$ from replica 1. On the other hand, this TAP solution is that into which replica 3 thermalizes giving the minimum M_2, and this is why replica 3 gives the right TAP energy of this state and its right distance from replica 1, while replica 2 does not. To understand the energy spectrum of the states visited by replica 3, we must then investigate how replica 2 chooses these states.

As usual, replica 2 tries to optimize the balance between the free energy and the complexity of the solutions it finds on the manifold, minimizing a function $\phi_2 = f_2 - T\Sigma_2(f_2, q_{12})$. It is important to note that Σ_2 is *not* the same function as Σ_c: There are *many* genuine TAP solutions with different TAP free energies f and at slightly different distances q, either higher or lower than q_{12}, whose projections on the manifold of replica 2 all have the same free energy f_2. Of these TAP solutions the relevant ones are those with the maximum complexity $\Sigma_c(f, q)$. This maximum value will then give $\Sigma_2(f_2, q_{12})$. Summarizing, $\Sigma_2(f_2, q_{12})$ is equal to the complexity Σ_c of the most numerous TAP solutions whose projections on the manifold fixed by q_{12} have free energy f_2 (the computation of Σ_2 is explicitly performed in [36]).

The minimization of ϕ_2 with respect to f_2 then selects a particular class of TAP solutions. Replica 2 is quenched into one of these solutions in the distorted way explained above, while replica 3 truly thermalizes into it. For this reason, the dependence on q_{12} of the energy of replica 3 in the minimum M_2 is a mere manifestation of the process of equilibration of replica 2 above described.

Summarizing, the states visited by replica 3 are chosen minimizing ϕ_2, which does not coincide with the function ϕ_c of section 6 as well as Σ_2 is not the same function as Σ_c. Nevertheless, it is clear that the spectrum given by the minimization of ϕ_2 must be similar to the one given by ϕ_c in section 6.

To make then a comparison with figure 7, it is convenient to plot the zero temperature energy of replica 3 in the minimum M_2 as a function of the overlap q_{13}, instead of q_{12}, since, as stated above, q_{13} better represents the real overlap between the two states. This parameterization is possible because in the minimum M_2 the values of q_{13} is uniquely determined by q_{12} (see chapter III.3).

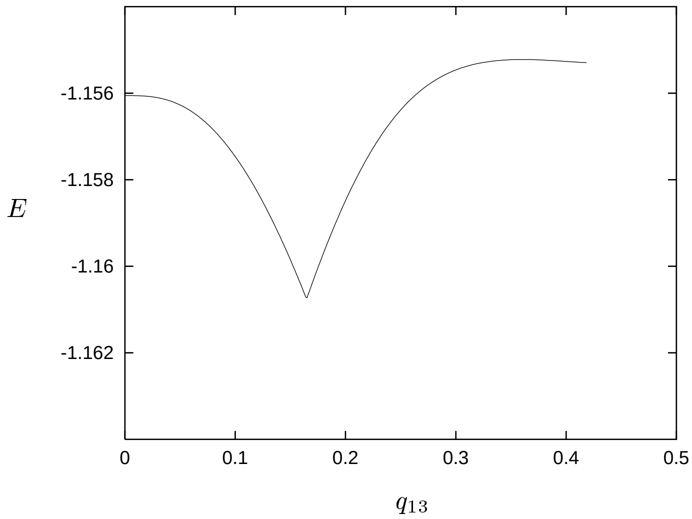

Figure 8: The energy density E of replica 3 in the minimum M_2 of the three replica potential, as a function of the overlap q_{13}, for β=1.64 and p=3. Here, as in Figure 8, q_{max}=0.360.

It can be seen from a comparison between figure 7 and figure 8 that, as we expected, the processes of minimization of ϕ_c and ϕ_2 are qualitatively the same:

Firstly, we note from Figure 8 that there is a value of q_{13} for which the curve has a cusp. In III.3 we called the corresponding value of q_{12} in the minimum M_2 for which this cusp occurs, q_{rsb}. Indeed, following the same line of reasoning of Section 6, we argue that this cusp must correspond to the point where Σ_2 becomes zero. In chapter III we specified that for value of q_{12} greater than q_{rsb} the overlap matrix $Q^{\sigma\sigma}$ of replica 2 breaks the replica symmetry. Physically, an RS form of the overlap matrix means either that the systems finds an exponentially high number of states or that the phase space consists in just one state. On the other hand, an RSB form means that the phase space is dominated by a number of order N of states (as in the p-spin model for $T < T_c$). Therefore, the breaking of the replica symmetry of $Q^{\sigma\sigma}$ for $q_{12} = q_{rsb}$ is a strong indication that here replica 2 ceases to see an exponentially high number of dominant states and confirms that in this point Σ_2 becomes zero, as we argued above. As already stressed, the functions ϕ_2 and ϕ_c, even though they have a very similar physical meaning, are actually different and this is why the corresponding minimization curves (first branches in Figures 7 and 8) are different.

Secondly, in Figure 8 we note a maximum for $q_{13} = q_{max}$, i.e. exactly in the same point as in Figure 7. This is a consequence of the reversing in the behaviour of Σ_c that occurs in the anomalous regime. This behaviour is directly inherited by Σ_2: loosely speaking, if there are TAP solutions whose number starts to increase getting closer to the state of replica 1, the corresponding projections on a fixed manifold will increase too. This is an important confirmation of the role of the quantity q_{max} and, as a consequence, it is a confirmation of the existence of the anomalous regime we described in section 5.

Finally, it is worth to observe that the ending point of the two curves is different, i.e. the potential V_3 ceases to see states around replica 1 at a distance that is *greater* than the one corresponding to the nearest TAP solutions given by Σ_c. At the present moment this is an open question.

Summarizing the considerations of this section we can say that the energy spectrum given by the real replica method is well explained by the behaviour of the constrained complexity. This mutually confirms the results found with the two methods.

8. The threshold landscape.

We turn now to examine the structure of the threshold states. We remind that threshold states are those solutions of the TAP equations with the highest energy density E_{th}. These states have a great importance under several aspects.

From a static point of view, we have seen in Section 2 that threshold states are *marginal*: the typical spectrum of the free energy Hessian evaluated in a TAP solution of energy E is a semicircle with support in the positive semi-axis and its lowest eigenvalue λ_{min} goes to zero as E goes to E_{th}. In this sense threshold states develop some flat directions.

On the other hand, in the temperature range $T < T_d$, threshold states play a fundamental role in the off-equilibrium dynamics of this model. We have seen in chapter II that solving analytically the dynamical equations with random initial conditions (i.e. high energy initial conditions), one finds that the asymptotic limit of the energy $\mathcal{E}_\infty$ coincides with the threshold energy E_{th}. In other words, the asymptotic dynamics takes place at the threshold level, never visiting the sub-threshold landscape. Moreover, the dynamical evolution of the system presents a first equilibrium regime in which the correlation function goes to the value of the self-overlap of the threshold states q_{th}, followed by an off-equilibrium aging regime in which the correlation function goes to zero, this meaning that the system never truly thermalizes into any of the threshold states, but that rather it continuously drifts away [21].

Therefore it is intriguing to investigate the eventual relations between the peculiar dynamical behaviour that occurs at the threshold level and the geometrical structure of the threshold states.

To perform an analysis of this kind we set $E_1 = E_2 = E_{th}$, and we study the constrained complexity Σ_c as a function of q, i.e. we fix a threshold solution and count how many other threshold solutions are present at distance q from it. The corresponding curve is shown in figure 9.

The important result is that

$$\Sigma_c(q) \to 0 \quad \text{for} \quad q \to q_{th}(\beta) \tag{8.1}$$

where $q_{th}(\beta)$ is the self-overlap of the threshold states at the temperature β we are considering. More precisely we find

$$\Sigma_c(q) \sim (q_{th} - q)^5 \quad \text{for} \quad q \sim q_{th} \ . \tag{8.2}$$

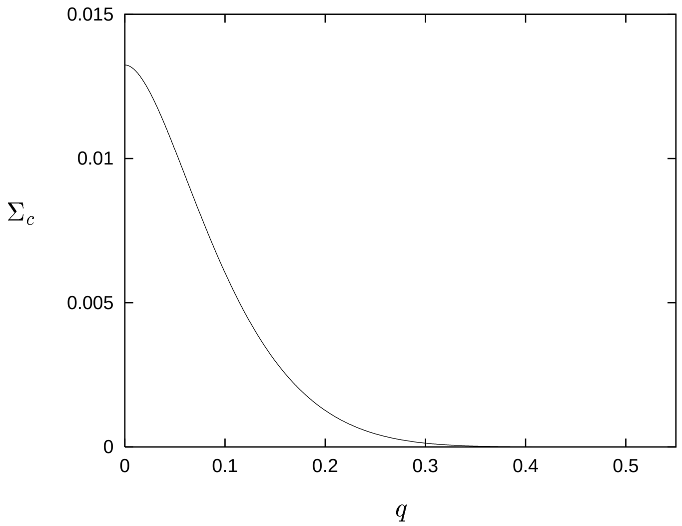

Figure 9: The constrained complexity Σ_c as a function of q with E_1=E_2=E_{th}, for β=1.64 and p=3. For q>0.35 the curve is indistinguishable from the axis and it reaches zero for q=q_{th}=0.504.

When the overlap between two states of the same kind is equal to their self overlap, it means that these two states are coincident in the thermodynamic limit. Thus, thinking of well separated states, one expects that Σ_c goes to zero at a value of q which is lower than the self overlap: indeed this is what happens for all the states below the threshold (see figure 1 and equation (5.1)).

On the other hand, from (8.1) we see that, fixed a threshold state, other threshold states with vanishing complexity are found until a distance zero from the fixed one.

Therefore we can say that there is no sharp separation among threshold states, but that they rather form a structure of coalescent states. This means that these states are separated by free energy *density* barriers which are vanishing in the limit $N \to \infty$, i.e. that the free energy barriers grow as N^α with $\alpha < 1$ [37].

As previously said, these states are minima of the TAP free energy with some flat directions. We can then argue that they are connected along these flat directions, forming a unique channel of states which develops along these directions, while we expect that along the directions with a non-zero curvature the free energy grows like N. Into this frame the dynamical drifting of the system (i.e. the decreasing to zero of the correlation function in the off-equilibrium regime) can be viewed as a wandering of the system along this channel of threshold states, in agreement with the ideas outlined in [21].

Finally, we note that, due to equation (8.1), the distribution of threshold states has no gap between the last value of the overlap in the spectrum and the self overlap, unlike all other sub-threshold states.

This feature is reminiscent of the overlap distribution in the Sherrington-Kirkpatrick model [11]. Besides, we remind that in the SK model all the states are marginal, as it happens for the threshold states in the p-spin spherical model. From this point of view, we can say that threshold states are the most SK like. Yet, it is interesting to note that from an energetic point of view the two situations are somehow opposite: the marginal equilibrium states of the SK model are those with the *lowest* free energy density, while the threshold states in the p-spin spherical model are the ones with the *highest* free energy density. Moreover, we have seen in chapter II that the states which from a thermodynamic point of view are most similar to the SK states are the ground TAP solutions, for $T < T_s$, since they have finite thermodynamic weight and their number is small. We conclude that the *geometrical* features of the SK states are typical of the p-spin threshold landscape, while their *energetic* features are typical of the p-spin ground states.

We can now return on the considerations done in chapter I.6 on the nature of the paramagnetic state. We have made there the hypothesis that the paramagnetic state has to be identified with an *actual* superposition π of equilibrium states at temperature T, in the sense that the ensemble of configurations belonging to it is the union of all the configurations belonging to these states. At T_d equilibrium states composing π are the threshold states. Therefore, according to what said above on the structure of the threshold landscape, we conclude that the *pseudo* state π at T_d is exactly the channel of threshold states described above, where the free energy density barriers among states are vanishing.

Moreover, we have explicitly seen in section 3 that for $E > E_{th}$ the number of saddles, solutions of the angular part of TAP equations, is exponentially dominant over the number of minima. For this same reason the q-equation has no solution above E_{th}: the self-overlap q is a measure of the largeness of a state, that is a measure of its basin of attraction in the phase space. Thus there is no sensible value of q which a saddle could have, as there is no sensible value of its free energy, which indeed is related by the TAP equations to q. We can understand this fact also saying that for $E > E_{th}$, angular TAP saddles are no longer stationary in the q direction. In these conditions, the very concept of local magnetization *in* the state α intended as

$$m_i^\alpha = \langle s_i \rangle_\alpha \tag{8.3}$$

has no longer meaning, since the average $\langle \cdot \rangle_\alpha$ cannot be interpreted as a component of the Boltzmann measure. We conclude that there is no way to define a collective free energy ϕ above the threshold.

Nonetheless, we remind that the angular variables of the TAP approach can be identified with configurations of the system at temperature $T = 0$. This means that at zero temperature, the angular saddles above the threshold energy can be interpreted as real saddles of the Hamiltonian in the phase space. Due to the non-chaoticity of TAP stationary points showed in chapter II.3, we can imagine to *continue* these saddles even at finite temperature. In this context the partition function for $T > T_d$ will be dominated by a bunch of such a kind of saddles, exactly as for $T < T_d$ is dominated by a bunch of minima. Thus for $T > T_d$ the *pseudo* state π is composed by many saddles which do not trap the system anymore, so that π can be correctly interpreted as a genuine paramagnetic state.

V. Conclusions

The results obtained by means of the constrained complexity, together with the indications coming from the real replica method, enable us to give a much clearer picture of the structure of the states for the p-spin spherical model.

First of all we want to answer our old question: If many states are present at *any* value of the mutual overlap q, why the standard methods are not able to detect them ? The answer is simply that there are *too many states*.

We can explain this fact in the following way: let us imagine the simplest situation we can think about, where all the states of the system have the same thermodynamic weight, so that they are just like spots on the phase space sphere, with a geometric distribution given by the constrained complexity $\Sigma_c(q)$. Now we begin drawing pair of states and measuring their mutual overlap. We know that the spectrum of the possible values of the overlap is continuous, so that we could expect that measuring the overlap of the pairs we obtain just this spectrum. But this is not true: Drawing a very large number of pairs we will obtain an *exponentially dominant* number of pairs with mutual overlap equal to zero. The reason of this is simply that the probability of having a pair of states with overlap $q \neq 0$ is proportional to the number of such pairs divided by the total number of pairs, that is

$$P(q) \sim \frac{e^{N\Gamma(q)}}{e^{N2\Sigma}}$$

where $\Gamma(q)$ is the complexity of the pairs at distance q introduced chapter IV.4 and we have indicated the unconstrained complexity simply with Σ. Since we can write

$$\Sigma_c(q) = \Gamma(q) - \Sigma \quad , \quad \Sigma = \Sigma_c(0)$$

we have

$$P(q) \sim e^{-N[\Sigma_c(0)-\Sigma_c(q)]} \to 0 \quad , \quad N \to \infty$$

because the maximum of the constrained complexity $\Sigma_c(q)$ is always at $q = 0$. This is what we meant when we said that *almost all* the states are mutually orthogonal. We stress that this would be true also in the case of a trivial random distribution as the one described in IV.5. In other words, the whole problem of the missed detection of close states is due to a *very* trivial entropic reason: e^{aN}/e^{bN} is zero if N is large and $a < b$. We encountered a similar situation when talking about the complexity of the saddles in IV.3: there are many saddles and many minima, but again $e^{N\Sigma_0} + e^{N\Sigma_1} = e^{N\Sigma_0}$ if N is large and $\Sigma_1 < \Sigma_0$, so that the contribution of the saddles Σ_1 is hidden by the complexity of the minima. It is quite amusing that the whole structure of the states in the p-spin spherical model is hidden for this trivial reason, reason which, at the end, can be visualized just by saying that, on a sphere, the largest parallel is the equator.

If we consider the overlap distribution of equilibrium states in the temperature range $T_s < T < T_d$, the above scenario can be stated more exactly, since all these states have the same vanishing thermodynamic weight. In particular, if we are interested in the contribution of the self-overlap, we get:

$$P(q_{EA}) = \sum_\alpha w_\alpha^2 \ \ \delta(q - q_{EA}) =$$

$$e^{N\Sigma_{eq}} \ \frac{e^{-2\beta N f_{eq}}}{e^{-2\beta N[f_{eq} - T\Sigma_{eq}]}} \ \ \delta(q - q_{EA}) = e^{-N\Sigma_{eq}} \ \ \delta(q - q_{EA}) \ .$$

If we compare this equation with the result coming from the two replica potential of chapter III.2

$$V_2(q_{EA}) = T\Sigma_{eq}$$

we understand in which sense the two replica potential is a generalized overlap distribution of the states: V_2 is roughly the logarithm of the overlap distribution function, divided by N, so that it is non-zero in the thermodynamic limit, while the standard distribution assumes its trivial form $P(q) = \delta(q)$. This is also the reason why, by computing the constrained complexity, which is the logarithm of the number of states divided by N, we obtain a non-trivial quantity, able to investigate the whole structure. We conclude that from a *thermodynamic* point of view, the structure of the states is now quite well understood.

Fortunately enough for our research, we did not only succeeded in answering the above question.

By means of the constrained complexity Σ_c we obtained the complete overlap spectrum of the states and first verified that this distribution is geometrically non-trivial, in the sense that it is very different from the one obtained supposing a random distribution of the states: the real distribution exhibit a major crowding the of states at small distances from the fixed reference state. This shows that geometrical correlations between different states are present and that these correlations are strong at small distances. On the other hand, the distribution given by Σ_c coincides, as it should, with the random one in the limit $p \to \infty$, when the case of the Random Energy Model is recovered.

The overlap distribution $\Sigma_c(q)$ show that for sub-threshold states there is a gap between the last value of the overlap, corresponding to the closest states, and the value of the self-overlap, meaning that these are well separated states, i.e. that the barriers in free energy grow at least as N in the thermodynamic limit. On the other hand, the analysis of the threshold landscape has given some interesting results: these marginal states have an overlap distribution which goes continuously to zero at a value of q equal to their self-overlap q_{th}. This means that these states are *not* well separated, but probably they are connected along their flat directions, forming a sort of channel that winds along the phase space. This feature may have a role in the asymptotic dynamics of the system, which occurs at the level of the threshold landscape.

The most unexpected result given by Σ_c concerns the presence of an anomalous regime: this result shows that the correlation among the states can be so high to invert the natural geometrical behaviour of the constrained complexity. The fact that $\Sigma_c(q)$ increases with q at very high value of the overlap indicates the presence of some local structures around the states, which are surely worth of further investigation. Moreover, this anomalous regime perfectly explains the results achieved with the three replica potential of chapter III. Indeed, by means of the constrained complexity we have obtained the spectrum of the dominant states at distance q from a given fixed state. This spectrum shows that below a certain value of the overlap, the number of the dominating states is exponentially large in N, while above this value (close states) this number is of order N. Besides, we have seen that the states nearest to any given state have always higher energy and free energy density.

To comment the continuous distribution of the overlap and in particular the coalescent structure of the threshold states, we have sometimes referred to the SK model, where a continuous structure with respect to the overlap q is directly given by the standard distribution function $P(q)$. However, in doing this comparison it is necessary to make some specifications. In the ultrametric structure of the states of the SK model [14], the main role is played by the equilibrium states, which have the lowest free energy density, finite weight and whose number remains small in the limit $N \to \infty$. This means that one can disregard the exponentially high number of states with higher free energy densities and vanishing weight. This can be done by introducing a cut-off on the branches size of the ultrametric tree [38]. The situation for the p-spin spherical model is somehow the opposite: here the states, both of equilibrium and metastable, *all* have vanishing weight and are in exponentially high number. Therefore none of these states, whatever energy it has, can be disregarded. In this sense the investigation of the structure of the states for this model is complicated by the existence of a new relevant variable, that is the energy. Moreover, we stress that there is at the present moment no evidence of an ultrametric organization of the states in the p-spin spherical model. The only fair indication of a clustering structure of the states comes, as we have seen, from the existence of the anomalous regime, into which the constrained complexity grows with the overlap.

To conclude, the main open issue on this topic is the pursuit of a unifying frame into which inserting all the results obtained with our methods, in order to describe in a synthetic way the rich and complex structure of states of the p-spin spherical model.

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