Spin-Glass Theory for Pedestrians

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Abstract. In these notes the main theoretical concepts and techniques in the field of mean-field spin-glasses are reviewed in a compact and pedagogical way, for the benefit of the graduate and undergraduate student. One particular spin-glass model is analyzed (the p-spin spherical model) by using three different approaches. Thermodynamics, covering pure states, overlaps, overlap distribution, replica symmetry breaking, and the static transition. Dynamics, covering the generating functional method, generalized Langevin equation, equations for the correlation and the response, the Mode Coupling approximation, and the dynamical transition. And finally complexity, covering the mean-field (TAP) free energy, metastable states, entropy crisis, threshold energy, and saddles. Particular attention has been paid on the mutual consistency of the results obtained from the different methods.

Contents

1. Introduction

The aim of these notes is to provide graduate and undergraduate students in statistical physics with a sort of handbook of the main theoretical concepts in the physics of spin-glasses. It is important to emphasize that this is not an overview of the entire field of disordered systems and spin-glasses: the whole experimental phenomenology is missing; not a word is present on the large amount of numerical investigations and results; only one model is analyzed, compared to the vast number of different models on the spin-glass market; very little is said about the connections between spin-glasses and structural glasses (although *something* is said); and finally, the focus is entirely on mean-field spin-glasses, leaving completely untouched what may be regarded as one of the most challenging open problems of the field, that is whether or not the mean-field picture has some validity also in finite dimensional systems.

The student may thus rightfully ask *what* is contained in these notes. The basic idea is to present the most important theoretical techniques developed in the context of spin-glasses in a coherent, detailed, but at the same time very compact way. For this reason we study just one specific model, which we use as an ideal arena where to discuss, apply and compare different theoretical methods. Although the model we consider has its own relevance in the field, the important point for us is to tell the student a consistent and self-contained story, where each conceptual step has to be logically connected to the previous one.

In order to do this we had to necessarily disregard many important topics in the field, and at the same time to be very brief when introducing new ideas, hoping that their practical implementation would help to grasp their relevance. The perfect example is ergodicity breaking and pure states: an entire chapter, rather than few lines, should be devoted to these tricky, but crucial concepts. In this way, however, the notes would be unbearably long, and the main line of the story would quickly be lost. We opt for a synthetic exposure, leaving the student the freedom to go deeper on certain subjects by a careful use of the extensive list of references.

The concepts and techniques developed in spin-glasses have found in recent years a wide range of applications in statistical physics and beyond, from biology to economics, passing through computer science and optimization theory. Our hope is that these notes may help the student to familiarize with the concepts, to practically learn how to handle them in a non-superficial way, and to eventually apply them to their own field of interest. The basic knowledge required to follow these notes is just a reasonable preparation in standard statistical mechanics.

The three pillars of our discussion are Statics, Dynamics, and Complexity. The test system where all the calculations are done and the consistency of the different results

is analyzed, is the mean-field p-spin spherical model (PSM). This model is particularly apt to our purposes for more than one reason. First, the static (i.e. thermodynamic) analysis of the PSM gives results which are drastically different from the dynamical ones. For example, the two approaches give two different transition temperatures. This naturally leads to the introduction of a third technique, dominated by the concept of complexity, which very nicely reconcile static and dynamic results. Therefore, the PSM is the ideal model where to develop and compare the three approaches. Secondly, the PSM is probably a simpler model than the more famous and extensively studied Sherrington-Kirkpatrick model, which after more than 25 year still puzzles us with its enormous variety of weird, yet very interesting, results. Finally, the PSM has some features which are intriguingly similar to structural glasses, most notably it is described by a set of dynamical equations which are identical to those provided by the Mode Coupling Theory for glasses. Therefore the PSM seems a good model to try and bridge the gap between spin-glasses and structural glasses.

As we have said, the target of these notes are graduate and undergraduate students. For this reason we tried to be as complete as possible when giving the details of the calculations, typically providing more technical steps than it is usual in a technical paper. We hope that in such a way it will always be possible for the student to work out the final result. It is impossible to develop a genuine familiarity with spin-glasses without a serious training in the most technical aspects of the field. We therefore encourage the student to perform and check the calculations in these notes, in order to become as independent as possible when studying similar subjects in her/his future. At the same time, we tried not to lose contact with the broader picture, and to always stick a sense to any calculation we perform. In particular, we stressed as much as possible the mutual consistency of results obtained with different techniques. The theory of spin-glasses is infamous for being crowded with not-too-obvious formal steps, so it is always nice to find the same result with two (or more) different, independent methods.

These notes are the expanded version of the lectures that one of us (AC) delivered in Bangalore, at the Conference and School on Unifying Concepts in Glassy Physics (UCGP III), in June 2004, where also other lectures on different areas in the physics of glassy systems were presented. Wherever we could, we tried to make contact, avoiding overlaps, with the notes of the other participants. In particular, we mention the Mode Coupling approximation in the section on Dynamics, in order to connect with the notes of David Reichmann, and we restricted ourselves to equilibrium dynamics, given that the subject of aging, and off-equilibrium dynamics in general, is extensively treated in the notes of Giulio Biroli. We finally hope that the student will get the similarities between the chapter on the TAP approach and the energy landscape method analyzed by Francesco Sciortino.

We thank the organizers of UCGP III for giving us the opportunity to bring together in a single work what we hope will be a useful collection of ideas and results in such a fascinating field of science.

2. Basic concepts

Before we start studying a specific spin-glass model, we need to introduce a couple of simple concepts and tricks, which we will extensively use all along these notes. Each of them would deserve much more space than we can afford, and therefore we encourage the student to exploit the references. A background in statistical mechanics and in particular in the theory of critical phenomena is very helpful. A nice and compact overview on this subject can be found in references [1] and [2]. We also add here that a very nice and informal introduction to spin glasses can be found in [3], whereas the classic review for spin-glass theory is still reference [4].

2.1. Disorder

There are two main classes of disordered systems. The one spin-glasses belong to is that of *quenched disorder*. In these systems the disorder is explicitly present in the Hamiltonian, typically under the form of random couplings J among the degrees of freedom σ,

$$H = H(\sigma; J) . \tag{1}$$

The disorder J is completely specified by its probability distribution $p(J)\,dJ$ which is the same for each different coupling constant in the system. A famous example is the Edwards-Anderson model [5],

$$H = - \sum_{<ij>} J_{ij}\sigma_i\sigma_j , \tag{2}$$

where the spins $\sigma_i = \pm 1$ are the degrees of freedom, and the couplings J_{ij} are Gaussian random variables. This is a finite dimensional model, since the sum is performed over nearest-neighbor spins. The disorder is *quenched*, meaning that the J are constant on the time scale over which the σ fluctuate. This will have a crucial consequence on the way we will have to perform the averages over J, compared to σ. Spin-glasses are indeed systems with quenched disorder.

Disorder creates frustration: it becomes impossible to satisfy *all* the couplings at the same time, as it would be in a ferromagnetic system. Formally a system is frustrated if there exists a loop on which the product of the couplings is negative. In a frustrated loop, if we fix an initial spin, and starting from it we try to chain-fix the other spins one after the other according to the sign of the couplings, we are bound to return to the initial spin and flip it. The only way to avoid frustration is to consider a lattice where there are no loops, for example a tree. Frustration is the main reason for the proliferation of metastable states in disordered systems.

In some system the disorder is not present in the Hamiltonian, but is in a way self-generated. This is the case of structural glasses, whose Hamiltonian typically takes the form,

$$H = \sum_{ij} V(r_i - r_j) \tag{3}$$

where the degrees of freedom r_i are the positions of the particles, and the function $V(r)$ is a deterministic potential (for example, Lennard-Jones). Even though there is no quenched disorder in the Hamiltonian, *at low temperature*, in a frozen glassy configuration of the system, each particle sees a different, disordered environment around itself. In this sense the disorder is self-generated. The origin of this phenomenon is the large number of non-crystalline local minima of the Hamiltonian.

It may seem odd that systems with quenched and self-generated disorder do have any property in common, given their very different definitions. However, we shall see that *some* spin-glass models do have a phenomenology quite similar to the one of structural glasses.

2.2. Self-averaging quantities

In these notes we deal with spin-glasses, i.e. systems with quenched disorder in the Hamiltonian. Therefore, the first key question is: How do we deal with the disorder? The problem is that, in principle, each observable depends on J, including the free energy of the system,

$$F_N(J) = -\frac{1}{\beta N} \log \int D\sigma e^{-\beta H(\sigma; J)} \tag{4}$$

where N is the size of the system. This is very unpleasant, since it seems to suggest that the physical properties of spin-glasses are different for each different realization of the disorder J, i.e. for each different sample. Were this true, it would be a disaster: we want to build a theory for spin-glasses, and not just for a specific piece of material ! In fact, both common sense and experience tells us that for sufficiently large systems, physical properties *do not* depend on J anymore. Quantities like that are called *self-averaging* [4], and the free energy is one of them,

$$\lim_{N \to \infty} F_N(\beta, J) = F_\infty(\beta) . \tag{5}$$

In this case it is clear that the average over the disorder of a self-averaging quantity is equal to its J-independent value,

$$F = -\lim_{N \to \infty} \frac{1}{\beta N} \overline{\log Z(J)} = F_\infty(\beta) \tag{6}$$

where,

$$\overline{A} = \int dJ \, p(J) \, A(J) . \tag{7}$$

This is good, since it means that analytically we can average over J, and that the result we obtain in this way is in agreement with the physical value of the observable. Self-averageness is basically the same as asking that the distribution of physical quantities is (for N large) sharply peaked around their average value, that is that the variance of

their distribution must go to zero for $N \to \infty$. The free energy is self-averaging, and in particular,

$$\overline{F^2} - \overline{F}^2 = O\left(\frac{1}{N}\right) \tag{8}$$

If a quantity has, for example, a bimodal distribution, it is not self-averaging. Indeed its average is a very poor indicator of the physical values of the quantity itself.

A simple argument to work out equation (8) can be given in finite dimension. We divide our system in a number K of macroscopic sub-systems, with $1 \ll K \ll N$. The total (extensive) free energy will be the sum of the free energies of the sub-systems, plus a contribution coming from the interactions at the interfaces between the sub-systems. Once we compute the free energy *density*, this surface contribution can be neglected in the limit $N \to \infty$. Moreover, the sub-systems free energies are independent random variables and therefore we can apply the central limit theorem to the sum, and get (8).

2.3. Annealed and quenched averages

In order to average the free energy we have to compute the integral,

$$F = -\frac{1}{\beta N} \int dJ \, p(J) \, \log \int D\sigma \, e^{-\beta H(\sigma; J)} \, , \tag{9}$$

which looks pretty bad, since we have to integrate a log over J. We could be tempted to define the following different quantity,

$$F_a = -\frac{1}{\beta N} \log \int dJ \, p(J) \int D\sigma \, e^{-\beta H(\sigma; J)} \, , \tag{10}$$

which is certainly much simpler to compute. Unfortunately, this is not the right solution to our problem. The difference between the two formulas above is in the role played by the disorder J: in (9) we first integrate over the degrees of freedom, then take the log, and finally integrate over the random couplings. In this way, the couplings J are fixed, i.e. quenched, for each integration over the spins. In other words, couplings and spins do not fluctuate together: for each realization of the disorder we compute the free energy, and eventually we average it over J. This kind of average is called *quenched*, and it is precisely what we need to do.

On the other hand, it is clear that in (10) the disorder J and the degrees of freedom σ have been put on the same footing, fluctuating together. This is *not* what we want, since it means that the time scale of variation of J and σ is the same, and therefore the disorder becomes yet another degree of freedom, and it is no longer quenched. This second kind of average is called *annealed*, and, even though it may be correct at high temperatures, where the frustration induced by the disorder is irrelevant, it is normally wrong at low temperatures, where the spins freeze in a state determined by the quenched value of the couplings. A different way to see this point is that in the annealed case we are in fact averaging the partition function Z, rather than the free energy F, over J.

The fact is that F is an extensive quantity, while Z is not (it is *exponential* in N !), and therefore Z is not in general self-averaging.

Therefore, we have to find a way to treat integrals like the one in (9). This is where the replica trick comes into play.

2.4. The replica trick

The replica trick [5] (which becomes in fact a method, when it is explained more deeply than here [4]), stems from the following simple formula,

$$\overline{\log Z} = \lim_{n \to 0} \frac{1}{n} \log \overline{Z^n} \ . \tag{11}$$

If n remains a real number (as it should), there is no advantage at all in computing the r.h.s. compared to the l.h.s., of course. However, if we now promote n to be an *integer*, we can write:

$$\overline{Z^n} = \int D\sigma_1 \dots D\sigma_n \ \overline{e^{-\beta H(\sigma_1, J) \cdots -\beta H(\sigma_n, J)}} \tag{12}$$

which is in fact much simpler to compute. What we do is to replicate the system n times, compute everything as a function of n, and finally cross our finger in taking the limit $n \to 0$. It is crucial to understand that all the Hamiltonians in (12) have the *same* realization of the quenched disorder, and in this sense are replicas one of the other.

A different useful form of the replica trick is the following,

$$\overline{\langle A \rangle} = \overline{\frac{1}{Z} \int D\sigma \ A(\sigma) \ e^{-\beta H(\sigma, J)}} = \lim_{n \to 0} \overline{Z^{n-1} \int D\sigma \ A(\sigma) \ e^{-\beta H(\sigma, J)}} =$$

$$\lim_{n \to 0} \int D\sigma_1 \dots D\sigma_n \ A(\sigma_1) \ \overline{e^{-\beta H(\sigma_1, J) \cdots -\beta H(\sigma_n, J)}} \ . \tag{13}$$

Of course, the label 1 we used for the replica into the observable A is completely arbitrary, and thus we have to be careful that our result *must not* depend on this particular index, otherwise we have a complete nonsense.

To conclude this small section, let us have a look to a case where the replica trick does work. Imagine that we ignore the rule $(x^a)^b = x^{ab}$ with a, b real, but that we know that $x^m = x \cdot \dots \cdot x$, m times. Given $y = x \cdot x$, we want to know what is $y^{1/2}$. We can use the replica trick:

$$y^{1/2} = \lim_{n \to 1/2} y^n = \lim_{n \to 1/2} x \cdot x \cdot \dots \cdot x \cdot x = \lim_{n \to 1/2} x^{2n} = x \ . \tag{14}$$

2.5. Pure states

In the low temperature phase, and in the limit $N \to \infty$ we can have ergodicity breaking: the system at equilibrium explores only a sub-part of the phase space [6, 7, 4]. When this happens the Gibbs measure can be split into sub-components, called *pure states*,

$$\langle \cdot \rangle = \sum_{\alpha} w_\alpha \langle \cdot \rangle_\alpha \tag{15}$$

where α is an index running over all the states, and w_α is the statistical (Gibbs) weight of state α. To better understand this formula, we must assume that it is possible to assign each configuration in the phase space with nonzero thermodynamics weight, to one and only one state. In this case we can write for any observable A,

$$\langle A \rangle = \frac{1}{Z} \int D\sigma \; e^{\beta H(\Sigma)} A(\sigma) \qquad = \frac{1}{Z} \sum_\alpha \int_{\sigma \in \alpha} D\sigma \; e^{\beta H(\Sigma)} A(\sigma) =$$

$$\sum_\alpha \frac{Z_\alpha}{Z} \frac{1}{Z_\alpha} \int_{\sigma \in \alpha} D\sigma \; e^{\beta H(\Sigma)} A(\sigma) = \sum_\alpha w_\alpha \langle A \rangle_\alpha \tag{16}$$

where we have defined,

$$Z_\alpha = \int_{\sigma \in \alpha} D\sigma \; e^{\beta H(\Sigma)} \tag{17}$$

that is the partition function restricted to state α, and

$$w_\alpha = \frac{Z_\alpha}{Z} \tag{18}$$

the statistical weight of state α.

As an example we can consider the Ising model below T_c. In the thermodynamic limit the ergodicity is broken, and we have two states, with positive and negative spontaneous magnetization,

$$\langle \cdot \rangle = \frac{1}{2} \langle \cdot \rangle_+ + \frac{1}{2} \langle \cdot \rangle_- \tag{19}$$

that is $w_+ = w_- = 1/2$, in absence of external magnetic field. It is crucial to split the measure, otherwise we would not see any spontaneous magnetization,

$$\langle \sigma \rangle = \frac{1}{2} \langle \sigma \rangle_+ + \frac{1}{2} \langle \sigma \rangle_- = 0 \tag{20}$$

A very important feature of pure states is the *clustering* property. In essence, this property states the very physical concept that the statistical correlation between two different points goes to zero when their distance goes to infinity,

$$\langle \sigma_i \sigma_j \rangle \rightarrow \langle \sigma_i \rangle \langle \sigma_j \rangle \qquad \text{for} \quad |i - j| \rightarrow \infty \; . \tag{21}$$

In other words, a very basic physical requirement is that connected correlation functions decay to zero at large distances [7, 4]. As we have said, this property only holds in pure states. Take, for example, the paramagnetic state in the Ising model below T_c, that is the Gibbs ergodic measure over the full phase space:

$$\langle \sigma_i \sigma_j \rangle = \frac{1}{2} \langle \sigma_i \sigma_j \rangle_+ + \frac{1}{2} \langle \sigma_i \sigma_j \rangle_- \rightarrow \frac{1}{2} \langle \sigma \rangle_+^2 + \frac{1}{2} \langle \sigma \rangle_-^2 = m^2 \neq 0 \; . \tag{22}$$

Therefore, the paramagnetic state is *not* a pure state below the critical temperature.

The example of the Ising model is particularly simple because we know *a priori* what is the structure of pure states below T_c. In particular, we know how to select a state, i.e. how to project the system onto any one of the two states: we simply apply a

magnetic field. In disordered systems the situation is not as simple as that, since *we do not know what is the field projecting the system onto any particular state*. This crucial fact is at the heart of the difficulty in studying disordered systems: we lack the magnetic field as a crucial tool to select states. Of course, given a state, there is a (disordered) magnetic field selecting that state. The problem is that we do not know what this field is !

A final important remark. In finite-dimensional systems, only equilibrium states can break the ergodicity, i.e. states with the lowest free energy *density*. In other words, the system cannot remain trapped for an infinite time in a metastable state, because in finite dimension free energy barriers surrounding metastable states are always *finite*. The extra free energy of a droplet of size r of equilibrium phase in a background metastable phase has a positive interface contribution which grows as r^{d-1}, and a negative volume contribution which grows as r^d,

$$\Delta F = \sigma \, r^{d-1} - \delta f \, r^d \ , \tag{23}$$

where here σ is the surface tension and δf is the bulk free energy difference between the two phases. This function has always a maximum, whose finite height gives the free energy barrier to nucleation of the equilibrium phase (note that at coexistence $\delta f = 0$ and the barrier is infinite).

Therefore, if initially in a metastable states the system will, sooner or later, collapse in the stable state with lower free energy density. For this reason, in finite dimension we cannot decompose the Gibbs measure in metastable components. When this is done, it is always understood that the decomposition is only valid for *finite* times, i.e times much smaller than the time needed for the stable equilibrium state to take over. On the other hand, in mean-field systems (infinite dimension), barriers between metastable states may be infinite in the thermodynamic limit, and it is therefore possible to call 'pure states' also metastable states, and to assign them a Gibbs weight w_α. We will analyze a mean-field spin-glass model, so that we will be allowed to perform the decomposition above even for metastable states.

2.6. Overlap, self-overlap

In non-disordered magnetic systems, a good order parameter is normally the total average magnetization,

$$m = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i \rangle \tag{24}$$

which is zero in the high temperature phase, and different from zero in the low temperature phase, where the $\pm$ symmetry is broken. In disordered systems we may be tempted to use a similar order parameter,

$$m = \frac{1}{N} \sum_{i=1}^{N} \overline{\langle \sigma_i \rangle} \tag{25}$$

However, due to the disorder the local magnetizations in the low temperature phase are all frozen in different directions (if the disorder distribution is unbiased, as we shall assume), and thus the magnetization defined above is zero at all temperatures, even though the $\pm$ symmetry is physically broken for each spin in our sample. A better order parameter is the Edward-Anderson parameter [5],

$$q_{EA} = \frac{1}{N} \sum_{i=1}^{N} \overline{\langle \sigma_i \rangle^2} \tag{26}$$

Such a quantity is nonzero if the local magnetizations m_i are locally nonzero, and thus is a good order parameter. In fact q_{EA} is a particular case of a more general quantity called *overlap*.

In our study of spin glasses we will often need a tool to measure the similarity of two configurations, or two states. To this aim we introduce the overlap. Given two configurations σ and τ, we define their mutual overlap as,

$$q_{\sigma\tau} = \frac{1}{N} \sum_{i=1}^{N} \sigma_i \tau_i \tag{27}$$

With Ising spins $s_i = \pm 1$ we have that,

$$q_{\sigma\tau} = \begin{cases} 1 & \text{if} \quad \sigma \text{ e } \tau \text{ almost coincide} \\ -1 & \text{if} \quad \sigma \text{ e } \tau \text{ are anti-correlated} \\ 0 & \text{if} \quad \sigma \text{ e } \tau \text{ are totally uncorrelated} \end{cases} \tag{28}$$

The overlap is thus a measure of the similarity among different configurations. We can also compute the overlap of a configuration with itself, the *self-overlap*,

$$q_{\sigma\sigma} = \frac{1}{N} \sum_{i=1}^{N} \sigma_i \sigma_i \tag{29}$$

With Ising spins $q_{\sigma\sigma} = 1$. In the following we will always deal with systems where the self-overlap of *configurations* is 1.

The overlap can measure also the similarity between *states*: if the Gibbs measure is split into sub-components α due to ergodicity breaking, we define the overlap between states α and β as,

$$q_{\alpha\beta} = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i \rangle_\alpha \langle \sigma_i \rangle_\beta \tag{30}$$

which can also be written as,

$$q_{\alpha\beta} = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{Z_\alpha} \int_{\sigma \in \alpha} D\sigma \; \sigma_i e^{-\beta H(\sigma)} \frac{1}{Z_\beta} \int_{\tau \in \beta} D\tau \; \tau_i e^{-\beta H(\tau)} =$$

$$\frac{1}{Z_\alpha Z_\beta} \int_{\sigma \in \alpha} \int_{\tau \in \beta} D\sigma \; D\tau \; e^{-\beta H(\sigma)} e^{-\beta H(\tau)} \; q_{\sigma\tau} \tag{31}$$

This expression shows that by measuring the overlap among states, we are in fact measuring the overlaps among configurations belonging to the states, and summing over all pairs of configurations, each one weighted with its own statistical weight.

The self-overlap of a state is simply,

$$q_{\alpha\alpha} = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i \rangle_\alpha^2 \tag{32}$$

The self-overlap will be very important in what follows. It is a measure of the size of the state in the phase space: the larger $q_{\alpha\alpha}$, the smaller the state, i.e. the smaller the number of configurations belonging to the state. On the other hand, a very small self-overlap indicates a very broad state. In particular, the paramagnetic state (unbroken ergodicity) has self-overlap equal to zero.

In the limit $T \to 0$ each states concentrate on its lowest energy configuration. In this case, the self-overlap of *each* state is $q_{\alpha\alpha} = 1$, since it is just the self-overlap of a configuration. When the temperature T grows, more configurations participate to the state and the self-overlap becomes smaller than one.

2.7. Overlap distribution

As we shall see, in mean-field spin-glasses there are many inequivalent pure states at low temperatures. In this case, it is useful to introduce the probability distribution of all the possible values of the overlaps among states. We first compute the overlap distribution by considering two physical systems with the same disorder (also called *real* replicas), and averaging the value of the overlap $q_{\sigma\tau}$ among the two real replicas,

$$P(q) = \frac{1}{Z^2} \int D\sigma D\tau e^{-\beta H(\sigma)} e^{-\beta H(\tau)} \, \delta(q - q_{\sigma\tau}) \, . \tag{33}$$

Using the definitions of the previous sections, we have,

$$P(q) = \sum_{\alpha\beta} w_\alpha w_\beta \frac{1}{Z_\alpha} \int_{\sigma \in \alpha} \frac{1}{Z_\beta} \int_{\tau \in \beta} D\sigma D\tau e^{-\beta H(\sigma)} e^{-\beta H(\tau)} \, \delta(q - q_{\sigma\tau}) \, , \tag{34}$$

and using the clustering property we finally obtain,

$$P(q) = \sum_{\alpha\beta} w_\alpha w_\beta \, \delta(q - q_{\alpha\beta}) \, . \tag{35}$$

In this formula (which can also be taken as a definition of the $P(q)$) the sum is extended over all the possible pairs of states, including pairs of the same state, giving its self-overlap. Once again, the simple Ising model can help us. At low temperature we have

two pure states, so we have in principle four possible overlaps,

$$q_{++} = \frac{1}{N} \sum_i \langle \sigma_i \rangle_+^2 = \frac{1}{N} \sum_i m_i^2 = m^2 \tag{36}$$

$$q_{--} = \frac{1}{N} \sum_i \langle \sigma_i \rangle_-^2 = \frac{1}{N} \sum_i m_i^2 = m^2 \tag{37}$$

$$q_{+-} = q_{-+} = \frac{1}{N} \sum_i \langle \sigma_i \rangle_+ \langle \sigma_i \rangle_- = -\frac{1}{N} \sum_i m_i m_i = -m^2 \ . \tag{38}$$

Therefore the function $P(q)$ has two peaks, at $-m^2$ and $+m^2$, each with weight $1/2$. It is important to stress that the number of peaks of the $P(q)$ is *not* equal to the number of states, but to the number of possible values taken by the overlap. If we had a very large number of states, all with the same self-overlap and mutual overlap, we would still have a bimodal $P(q)$.

   To conclude, we note that the particular structure of states of a given sample depends on the particular realization J of the quenched disorder. For this reason both the pure states weights, and the distribution $P(q)$ depend on the disorder J. In particular, $P(q)$ is not a self-averaging quantity when the structure of states is nontrivial. For the proof and discussion of this crucial statement see [8].

3. Statics

We have now all the tools to start a thermodynamic study of a specific spin-glass. We will use the replica method to compute the free energy of the system, and will discover that replicas have (surprisingly enough) a rather deep physical meaning: they will act as probes exploring the unknown phase space, and sending us important information on the structure of states in it.

   The spin-glass model we will analyze is the *p-spin spherical model* (PSM). Among spin-glasses it is the one which bears more similarities with structural glasses, suggesting that some concepts which are exactly valid for the PSM may be exported to the case of glasses.

3.1. The p-spin spherical model

The Ising version (i.e. with ± 1 spins) of the PSM was introduced in [9], while its spherical, and simpler, counterpart appeared in [10]. The Hamiltonian of the spherical PSM is,

$$H = - \sum_{i_1 > \ldots > i_p = 1}^{N} J_{i_1 \ldots i_p} \sigma_{i_1} \ldots \sigma_{i_p} \qquad p \geq 3 \tag{39}$$

where the spins are now *real* continuous variables. In order to keep the energy finite, we have to put a constraint on the spins,

$$\sum_{i=1}^{N} {\sigma_i}^2 = N \tag{40}$$

this is the *spherical constraint*, from which the model takes its name. With this constraint the self-overlap of each configuration is one. The Hamiltonian is a sum of p-body interactions, and the sum is extended over *all* groups of spins, not only the nearest-neighbor, so the model has no spatial structure, and it is in fact a *mean-field* model. For such models the droplet argument given above does not work (each spin interacts with N other spins, there are no surfaces), and thus the free energy barriers around metastable states may be infinite. For this reason mean-field models are the ideal play-ground to study metastability.

Each random coupling J is a Gaussian variable, with distribution,

$$dp(J) = \exp\left(-\frac{1}{2} J^2 \frac{2N^{p-1}}{p!}\right) dJ \tag{41}$$

where the factors 2 and $p!$ are a matter of convention, whereas the factor N^{p-1} is essential in order to have the Hamiltonian of order N, and thus extensive energy and free energy,

$$\sqrt{\overline{J^2}} \sim \frac{1}{N^{\frac{p-1}{2}}} \quad \Rightarrow \quad H \sim N \tag{42}$$

The relevance of the PSM in the context of glassy physics is due to the great role played by metastable states in such a model. A hint of this fact comes from the ferromagnetic version of the PSM, that is $J_{i_1 \ldots i_p} = 1/N^{p-1}$ for each coupling: unlike its $p = 2$ counterpart, this model has a first order transition between a high T paramagnetic phase and a low T ferromagnetic one (solving the ferromagnetic mean-field PSM is a trivial exercise). In particular, there are two relevant temperatures: a temperature T_d below which a ferromagnetic state develops, but with a free energy higher than the paramagnetic one, and a lower temperature T_s, where the ferromagnetic state becomes stable and the thermodynamic transition takes place. From a dynamical point of view, however, the higher temperature T_d is quite relevant, since for $T < T_d$ the system may remain trapped by the ferromagnetic state, even though metastable, if the initial magnetization is positive and large enough.

The first order transition at T_s in the ferromagnetic PSM is driven by entropy, since the energy of the ferromagnetic states is *always* lower than the paramagnetic one. We can roughly understand this point by noting that the p-body interaction indeed increases very much the entropic contribution of the paramagnet, compared to the canonical $p = 2$ case. Metastability, entropy driven transitions, and purely dynamical transitions will be also key ingredients of the disordered PSM we are about to study.

3.2. First try: the replica symmetric calculation

We start our static study of the PSM by performing an annealed calculation of the free energy. We know it is wrong at low temperatures, but it will be anyway a useful warm-up exercise. In what follows we will often write the indices for the $p = 3$ case, such that $J_{i_1 \ldots i_p}$ becomes J_{ijk}. However, to give formulas that are valid even in the general case, we will write all the factors containing a term p for the generic p case, for example

we will write $N^p/p!$ rather than $N^3/6$. Another short-cut we will use is to disregard all normalizing factors that, once taken the log and divided by N, go to zero in the thermodynamic limit. Finally, we have to remember that all our integrals over σ are restricted to the surface of a sphere by the spherical constraint. The average partition function is given by,

$$\overline{Z} = \int D\sigma \int \prod_{i<j<k} dJ_{ijk} \exp\left[-J_{ijk}^2 \frac{N^p}{p!} + J_{ijk}\beta\sigma_i\sigma_j\sigma_k\right] =$$

$$\int D\sigma \exp\left[\frac{\beta^2}{4N^{p-1}}\left(\sum_i \sigma_i^2\right)^p\right] =$$

$$\exp\left[N\frac{\beta^2}{4}\right]\Omega\ , \tag{43}$$

where Ω is the surface of the sphere. In the equations above we have used the formula,

$$p!\sum_{i<j<k}^{N} = \sum_{ijk}^{N} \tag{44}$$

which is valid in the thermodynamic limit. The annealed free energy is therefore given by,

$$F_a = -\beta/4 - TS_\infty\ , \tag{45}$$

with the infinite temperature entropy, $S_\infty = \log(\Omega)/N$. This is, in fact, the correct free energy at high temperatures, i.e. in the paramagnetic phase. However, it can be proved that at lower temperatures the annealed-paramagnetic solutions has a free energy larger than the free energy found by the quenched computation: as anticipated above the annealed approximation in general only holds at higher temperatures, while at low temperature the quenched computation must be performed. Note that the fact that the annealed entropy becomes negative at low temperatures would not be by itself a sufficient reason to discard it, since the model is continuous, and a negative entropy is thus perfectly legal.

In order to perform the quenched calculation we must compute the average of the replicated partition function. Since now on the indices $i, j, k, \ldots$ will refer to sites, while $a, b, \ldots$ will refer to replicas. We have,

$$\overline{Z^n} = \int D\sigma_i^a \prod_{ijk} \int dJ_{ijk} \exp\left[-J_{ijk}^2 \frac{N^p}{p!} + J_{ijk}\beta\sum_a^n \sigma_i^a\sigma_j^a\sigma_k^a\right] =$$

$$\int D\sigma_i^a \prod_{ijk} \exp\left[\frac{\beta^2 p!}{4N^{p-1}}\sum_{ab}^n \sigma_i^a\sigma_i^b\sigma_j^a\sigma_j^b\sigma_k^a\sigma_k^b\right] =$$

$$\int D\sigma_i^a \exp\left[\frac{\beta^2}{4N^{p-1}}\sum_{ab}^n\left(\sum_i^N \sigma_i^a\sigma_i^b\right)^p\right]\ . \tag{46}$$

We can see here the powerful replica trick at work: we started from a set of coupled sites and uncoupled replicas, and averaging over the disorder we decoupled the sites,

but coupled the replicas (unfortunately in non-mean field models the replica trick is not enough to decouple the sites). In particular, the overlap between two different replicas of the system very naturally appeared in the calculation,

$$Q_{ab} = \frac{1}{N} \sum_i \sigma_i^a \sigma_i^b \tag{47}$$

Note that $Q_{aa} = 1$ due to the spherical constraint. We introduce now a factor 1 in our calculation,

$$1 = \int dQ_{ab} \, \delta \left(N Q_{ab} - \sum_i \sigma_i^a \sigma_i^b \right) , \tag{48}$$

and finally we use an exponential representation for the δ-function, to obtain,

$$\overline{Z^n} = \int DQ_{ab} \, D\lambda_{ab} \, D\sigma_i^a \; \cdot$$

$$\cdot \; \exp \left[\frac{\beta^2 N}{4} \sum_{ab} Q_{ab}^p + N \sum_{ab} \lambda_{ab} Q_{ab} - \sum_i \sum_{ab} \sigma_i^a \lambda_{ab} \sigma_i^b \right] =$$

$$= \int DQ_{ab} \, D\lambda_{ab} \, \exp \left[-N \, S(Q, \lambda) \right] \tag{49}$$

with,

$$S(Q, \lambda) = -\frac{\beta^2}{4} \sum_{ab} Q_{ab}^p - \sum_{ab} \lambda_{ab} Q_{ab} + \frac{1}{2} \log \det(2\lambda_{ab}) \tag{50}$$

In (49) the integration over Q_{ab} is performed over all the matrices with $a \neq b$, while the integration over λ_{ab} includes also $a = b$ to enforce the spherical constraint. The sums in the exponentials are over all the indices, including $a = b$.

The great advantage of this form of the integral is that we can use the saddle point (or Laplace, or steepest-descent) method [11], to solve it in the limit $N \to \infty$. This simplification is the *big* effect of mean-field, and it is the result of the decoupling of the sites operated by the use of the replica trick. The price we had to pay is that we coupled replicas, and this looks somewhat weird at this stage of the computation.

The saddle-point method states that in the limit $N \to \infty$ the integral (49) is concentrated in the minimum of the integrand. However, we have to be careful here, for a twofold reason. First, the free energy is in principle given by,

$$-\beta F = \lim_{N \to \infty} \lim_{n \to 0} \frac{1}{nN} \log \int DQ_{ab} \, D\lambda_{ab} \, \exp \left[-N \, S(Q, \lambda) \right] \tag{51}$$

and thus we should *first* take the limit $n \to 0$, and then $N \to \infty$. Unfortunately, we are unable to do this: S is not an explicit function of n, and moreover we need to send $N \to \infty$ first to solve the integral. As a conclusion, we need to exchange the order of the two limits, solve the integral, find a parametrization of the matrix Q_{ab}, and finally take the $n \to 0$ limit at the end. Of course, this is mathematically risky, to say the least.

The second point we have to pay attention to, is what do we actually mean by "minimum" of S. The problem here is that the number of independent elements of Q_{ab} is $n(n-1)/2$, which becomes negative is the limit $n \to 0$. It is hard to say what is a minimum of a function with a negative number of variables ! There is however a criterion we can use to select the correct saddle point: the corrections to the saddle point result are given by the Gaussian integration around the saddle point itself. This integration gives as a result the square root of the determinant of the second derivative matrix of S, and thus, in order to have a sensible result, we must have all the eigenvalues of this matrix positive. Summarizing, we have to select saddle points with a positive-defined second derivative of S [12].

At this point we can proceed with the saddle point calculation. We first minimize (maximize ?) S with respect to λ_{ab}. By using the general formula,

$$\frac{\partial}{\partial M_{ab}} \log \det M_{ab} = (M^{-1})_{ab} \tag{52}$$

we get,

$$2\lambda_{ab} = (Q^{-1})_{ab} \tag{53}$$

and thus,

$$F = \lim_{n \to 0} -\frac{1}{2\beta n} \left[\frac{\beta^2}{2} \sum_{ab} Q_{ab}^p + \log \det Q_{ab} \right] \tag{54}$$

where Q_{ab} satisfies the saddle point equation,

$$0 = \frac{\partial F}{\partial Q_{ab}} = \frac{\beta^2 p}{2} Q_{ab}^{p-1} + (Q^{-1})_{ab} . \tag{55}$$

Note that $Q_{aa} = 1$ due to the spherical constraint.

What we have obtained is a free energy F, function of an order parameter, Q_{ab}, which is definitely weirder than the simple magnetization $m = \langle \sigma \rangle$ we would have in the ferromagnetic Ising model. This order parameter is the overlap between configuration belonging to different replicas, and its physical meaning will be clearer later on. For now, we limit ourselves to find a solution of the saddle point equation. To do this we have first to find a parametrization of the matrix Q_{ab}, and to write (55) as a function of the elements of Q_{ab} and of its dimension n.

Given that all replicas are equivalent (they just come from a formal trick !), it seems wise to assume a *replica symmetric* form for the matrix Q_{ab}. This is what Sherrington and Kirkpatrick did in their first mean-field spin glass model [13], that is,

$$Q_{ab} = q_0 + (1 - q_0)\delta_{ab} . \tag{56}$$

This means that all the elements of Q_{ab} are equal to q_0, but on the diagonal, where they are 1. The value of q_0 must be found from the saddle point equations. We have,

$$(Q^{-1})_{ab} = \frac{1}{1-q_0}\delta_{ab} - \frac{q_0}{(1-q_0)[1+(n-1)q_0]} \tag{57}$$

and thus (55) becomes, in the limit $n \to 0$,

$$\frac{\beta^2 p}{2} q_0^{p-1} - \frac{q_0}{(1-q_0)^2} = 0 \tag{58}$$

We first see that $q_0 = 0$ is always solution of this equation. This is the paramagnetic solution, and from (54) we get $F = -\beta/4$, which is the same as the annealed result (except for the phase space volume S_∞ we did not include here). Thus, the annealed calculation gives the same result as the quenched calculation when the overlap matrix Q_{ab} is the identity. This is obvious, because when $Q_{ab} = \delta_{ab}$ replicating or not the system is exactly the same.

However, we also have a non-paramagnetic solution $q_0 \neq 0$. Recasting the equation in the following form,

$$q_0^{p-2}(1-q_0)^2 = \frac{2}{p} T^2 \tag{59}$$

we clearly see that at high temperatures there is no nontrivial solution, while by decreasing T we arrive at a critical value $T^\star$ below which a pair of nonzero solutions forms. Of these two solution the only acceptable one is the larger one, which increases with decreasing T (the self overlap must increase if the number of configurations belonging to a state decreases, and this is exactly what we expect when we decrease the temperature). Therefore we seem to have a transition at $T^\star$, and in particular a *discontinuous* transition, since the value of q_0 at the transition is different from zero, i.e. there is a jump of the order parameter at the transition. Moreover, the free energy associated to this new solution is lower than the paramagnetic one, therefore it would seem we have found the new non-paramagnetic state at low temperatures.

All this seems very interesting, but there is a problem: the nontrivial solution we have found is *unstable* [12, 10]. As we have said above, when we select a saddle point, we have to be sure that all the eigenvalues of the second derivative of F around the saddle point are positive. Unfortunately, this is not the case for this solution: both roots of equation (59) have one negative eigenvalue below $T^\star$.

What can we do ? Remember that we did not search the whole space of Q_{ab} to find a solution, but rather assumed a certain parametrization, which looked more or less sensible, and plugged it into the saddle point equation. The fact that the replica symmetric ansatz gave us a nontrivial solution at low T, but which is unstable, clearly means that the low temperature phase of the model must be describe by a *replica symmetry breaking* form of the order parameter Q_{ab}. Before looking for this new solution, it is finally the moment to try and understand what is the physical meaning of the weird order parameter Q_{ab}.

3.3. The key connection between replicas and physics

Let us consider the following quantity,

$$q^{(1)} = \frac{1}{N} \sum_i \overline{\langle \sigma_i \rangle^2} \tag{60}$$

which, as we have seen in the previous chapter, is a quite natural definition of an order parameter, since it is just a generalization of the average magnetization m. By using the technology developed in the first chapter, we can rewrite $q^{(1)}$ in the following way,

$$q^{(1)} = \frac{1}{N} \sum_i \sum_{\alpha\beta} \overline{w_\alpha w_\beta \langle\sigma_i\rangle_\alpha\langle\sigma_i\rangle_\beta} = \sum_{\alpha\beta} \overline{w_\alpha w_\beta \, q_{\alpha\beta}} =$$

$$\int dq \sum_{\alpha\beta} \overline{w_\alpha w_\beta \, \delta(q - q_{\alpha\beta})} \, q = \int dq \, \overline{P(q)} \, q \tag{61}$$

Therefore $q^{(1)}$ is the first moment of the overlap distribution, averaged over the disorder. By using the clustering property, we can easily find a generalization of this formula [4],

$$q^{(k)} = \frac{1}{N^k} \sum_{i_1\ldots i_k} \overline{\langle\sigma_{i_1}\ldots\sigma_{i_k}\rangle^2} = \int dq \, \overline{P(q)} \, q^k \tag{62}$$

The important fact is that we can compute these quantities also using the replica trick. In particular,

$$q^{(1)} = \frac{1}{N} \sum_i \overline{\langle\sigma_i\rangle^2} = \lim_{n\to 0} \overline{\int D\sigma_i^a \, \frac{1}{N} \sum_i \sigma_i^1 \cdot \sigma_i^2 \, e^{-\beta\sum_a H(\sigma^a)}} \tag{63}$$

If we now go on with the calculation along the lines of the previous paragraphs, introducing the overlap matrix Q_{ab}, we get,

$$q^{(1)} = \int DQ_{ab} \, e^{-NS(Q_{ab})} \, Q_{12} = Q_{12}^{\text{SP}} \tag{64}$$

where Q_{ab}^{SP} is the saddle point value of the the overlap matrix (since now on we will drop the suffix SP), and where we have exploited the fact that S is of order n, and therefore does not contribute when $n \to 0$. Of course, there is something wrong about this formula: replicas 1 and 2 cannot be different from the others! If we decided to call them 4 and 7, we would get a different result when Q_{ab} is not replica symmetric: this is nonsense ! What is going on here ? To understand this point we note that if the saddle point overlap matrix is not symmetric, then there must be other saddle point solutions with the same free energy, but corresponding to matrices obtained from Q_{ab} by a permutation of lines and columns [4]. This is a general result: when a saddle point breaks a symmetry corresponding to a given transformation, all the points obtained by applying the transformation to that particular saddle point, are equally valid. This means that we must average over all these saddle points, and this is equivalent to symmetrize equation (64) [14, 15], obtaining,

$$q^{(1)} = \lim_{n\to 0} \frac{2}{n(n-1)} \sum_{a>b} Q_{ab} \tag{65}$$

This result is already telling us that there is a connection between the physical order parameter $q^{(1)}$, and the matrix of the overlap among replicas Q_{ab}. To go further, we can generalize (65), to get,

$$q^{(k)} = \lim_{n\to 0} \frac{2}{n(n-1)} \sum_{a>b} Q_{ab}^k \tag{66}$$

A comparison with equation (62), gives for a generic function $f(q)$ the relation,

$$\int dq \, f(q) \, \overline{P(q)} = \lim_{n \to 0} \frac{2}{n(n-1)} \sum_{a>b} f(Q_{ab}) \tag{67}$$

and in particular choosing $f(q) = \delta(q - q')$, we finally find the crucial equation connecting physics to replicas,

$$\overline{P(q)} = \lim_{n \to 0} \frac{2}{n(n-1)} \sum_{a>b} \delta(q - Q_{ab}) \ . \tag{68}$$

This equation is telling us that the average probability that two pure states of the system have overlap q is equal to the fraction of elements of the overlap matrix Q_{ab} equal to q. In other words, *the elements of the overlap matrix (in the saddle point) are the physical values of the overlap among pure states, and the number of elements of Q_{ab} equal to q is related to the probability of q.*

This is a key connection, and we understand now that Q_{ab} has an enormous physical meaning. As a first application, let us analyze the meaning of the replica symmetric ansatz, $Q_{ab} = q_0$ for each $a \neq b$. From (68) we see that this structure of the overlap matrix implies that the average overlap distribution is given by,

$$\overline{P(q)} = \delta(q - q_0) \ , \tag{69}$$

that is there is one single possible value of the overlap among states. As we have seen, the overlap distribution should also include the self-overlap of the states, and therefore this value q_0 must be the self-overlap of the unique state in the system. The conclusion is that a replica symmetric form of the overlap matrix in the free energy calculation, can only be valid if there is one single equilibrium state. This state will typically be the paramagnetic state, and its self-overlap will be q_0. On the other hand, if at low temperatures there is ergodicity breaking, with the emergence of many inequivalent pure states, then the correct form of Q_{ab} *cannot* be replica symmetric.

Now that we know what is the meaning of the overlap matrix, there is a slight chance to understand how to find a replica symmetry breaking form of it.

3.4. Replica symmetry breaking

Thanks to equation (68) the relations of overlap among states translate into relations of overlaps among replicas. Therefore, in order to give an ansatz on the form of Q_{ab} we have to guess what may be the structure of states in the low temperature phase of a spin-glass model. *Vast programme !* - as someone once said [16].

Our starting point is a fact we already know: if there is ergodicity breaking, that is if there are many states, configurations in the phase space are organized into states. In other words, we can think of states as blobs of configurations in the phase space, with each configuration belonging to just one blob. The self overlap of a state is just the average overlap of the configurations belonging to it, i.e. it is a measure of the largeness

of the blob. On the other hand, the overlap between different states is basically the overlap between configurations belonging to them.

Given this, the simplest possible spectrum of overlaps we can have when there are many states is the following: $q = 1$, if we consider twice the same configuration, $q = q_1 < 1$ if we consider different configurations belonging to the same state, $q = q_0 < q_1$ if we consider configurations belonging to different states. In this way we are assuming that all states have the same self-overlap q_1, and mutual overlap q_0. Moreover, a physical requirement is that $q_1 > q_0$, since configurations belonging to the same state must be closer than those in different states.

What is the corresponding structure of Q_{ab} ? What is clear by now is that replicas act as probing configurations of the structure of the states, so we must reproduce for replicas the same clustering procedure we have seen for the configurations: replicas may belong to the same group, having overlap $Q_{ab} = q_1$, or to different groups, with overlap $Q_{ab} = q_0$. Finally, when we select twice the same replica we obtain $Q_{aa} = 1$. To this structure corresponds the matrix [17],

$$
Q_{ab} =
\begin{bmatrix}
1 & q_1 & q_1 & & & & \\
q_1 & 1 & q_1 & & q_0 & & \cdots \\
q_1 & q_1 & 1 & & & & \\
& & & 1 & q_1 & q_1 & \\
& q_0 & & q_1 & 1 & q_1 & \\
& & & q_1 & q_1 & 1 & \\
& \vdots & & & & & \ddots
\end{bmatrix}
\tag{70}
$$

where we have assumed, to make an example, that the number m of replicas in each group is $m = 3$. As we have seen, the parameter m is connected to the probability of having a given value of the overlap, therefore it will become a variational parameter in the saddle point equations, as q_1 and q_0. This structure of Q_{ab} reflects what we have said above. Note that any permutation of lines or column (replica permutation) would also correspond to the same structure, but it would simply be much harder to visualize. This matrix has the important property that $\sum_a Q_{ab}$ does not depend on b, which is an essential requirement, since replicas must be all equivalent [19].

It is clear that the clustering process we have described can be iterated [18]: states can be grouped into clusters, which can be grouped into super-clusters, and so on. The structure of states one obtains in this way is called *ultrametric*, and unfortunately we do not have time to describe it here [8]. The important point is that for the PSM the simple structure described above is sufficient [10]. This kind of replica symmetry breaking (RSB) is called *one step* RSB, or 1RSB.

Let us compute the overlap distribution associated to the 1RSB structure of Q_{ab}. From (68) we get,

$$
\overline{P(q)} = \frac{m-1}{n-1} \delta(q - q_1) + \frac{n-m}{n-1} \delta(q - q_0)
\tag{71}
$$

with,

$$1 \leq m \leq n \tag{72}$$

We clearly see that while the elements q_1, q_0 fix the position of the peaks, the parameter m fixes their height, and therefore the probability of the overlaps. We have now to take the limit $n \to 0$. Here lies possibly the weirdest twist of the replica method. Relation (72) seems to resist strenuously to our will to send n to zero. However, in this limit it is clear that also m must be promoted to be a real number, rather than an integer. To see how to do this we can appeal to physics (for once !), and accept the fact that the *probability* (71) must be positive even in the limit $n \to 0$,

$$\overline{P(q)} = (1 - m)\,\delta(q - q_1) + m\,\delta(q - q_0) \tag{73}$$

For this to be positive we must have $m < 1$ and $m > 0$. Therefore, the correct limit of (72) for $n \to 0$, is,

$$0 \leq m \leq 1 . \tag{74}$$

Summarizing, with the 1-step replica symmetry breaking ansatz we have parametrized the overlap matrix Q_{ab} by means of two values of the overlap,

$$0 \leq q_0 \leq q_1 \leq 1 \tag{75}$$

and one value of the probability parameter m. We have now to fix them via the saddle point equation.

3.5. The 1RSB solution and the static transition

The first thing to do is to compute the free energy as a function of q_1, q_0, m. We had,

$$F = \lim_{n \to 0} -\frac{1}{2\beta n} \left[\frac{\beta^2}{2} \sum_{a,b} Q_{ab}^p + \log \det Q \right] \tag{76}$$

The first piece is easy to compute and gives in the limit $n \to 0$,

$$\frac{1}{n} \sum_{ab} Q_{ab}^p = \sum_a Q_{ab}^p = 1 + (m - 1)q_1^p - m q_0^p \tag{77}$$

The second piece is a bit harder: the 1RSB matrix Q_{ab} has three different eigenvalues and degeneracies (the student should be able to work them out),

$$\lambda_1 = 1 - q \qquad d_1 = n - n/m \tag{78}$$

$$\lambda_2 = m(q_1 - q_0) + (1 - q_1) \qquad d_2 = n/m - 1 \tag{79}$$

$$\lambda_3 = nq_0 + m(q_1 - q_0) + (1 - q) \qquad d_3 = 1 \tag{80}$$

From this, taking *carefully* the limit $n \to 0$, we finally obtain,

$$-2\beta F_{1RSB} = \frac{\beta^2}{2}[1 + (m - 1)q_1^p - m q_0^p] + \frac{m - 1}{m} \log(1 - q_1) +$$

$$+ \frac{1}{m} \log[m(q_1 - q_0) + (1 - q_1)] + \frac{q_0}{m(q_1 - q_0) + (1 - q_1)} \tag{81}$$

to be compared with the replica symmetric (RS) free energy,

$$-2\beta F_{RS} = \frac{\beta^2}{2}[1 - q_0^p] + \log(1 - q_0) + \frac{q_0}{1 - q_0} \tag{82}$$

It is interesting to note that the RS form is obtained either from $q_1 \to q_0$, or $m \to 1$. In the first limit, many states merge to form a single paramagnetic state. This is exactly what happens in the Ising model when $T \to T_c^-$, and it is a consequence of the second order nature of the transition in that model. The $m \to 1$ limit has a different, less trivial, interpretation, as we shall see in a minute.

We have now to study the saddle point equations with respect to q_1, q_0, m. First, the equation $\partial_{q_0} F = 0$ gives as a solution $q_0 = 0$. This solution is correct in absence of external magnetic field: q_0 is the mutual overlap among different states, and it is natural to think that without external field the distribution of states in the phase space is symmetric, and thus all states must be orthogonal to each other.

The two remaining equations $\partial_{q_1} F = 0$ and $\partial_m F = 0$ are,

$$(1 - m)\left(\frac{\beta^2}{2}pq_1^{p-1} - \frac{q_1}{(1 - q_1)[(m - 1)q_1 + 1]}\right) = 0$$

$$\frac{\beta^2}{2}q_1^p + \frac{1}{m^2}\log\left(\frac{1 - q_1}{1 - (1 - m)q_1}\right) + \frac{q_1}{m[1 - (1 - m)q_1]} = 0 \tag{83}$$

These equations can be easily studied on a computer, but most of the physics can be worked out also graphically. At high T the only solution is $q_1 = 0$ and m undetermined: this is the paramagnetic solution, which is equal to the RS one. We want to know whether there is a nontrivial spin-glass solution with $q_1 \neq 0$. The first equation is solved by $m = 1$. So let us plug $m = 1$ into the second equation,

$$\frac{\beta^2}{2}q_1^p + \log(1 - q_1) + q_1 \equiv g(q_1) = 0 \tag{84}$$

The graphical study of this equation for $0 \le q_1 \le 1$ is trivial. The limits are $g(0) = 0$ and $g(1) = -\infty$. At high T the function is monotonous and only the $q_1 = 0$ solution exists. However, by lowering the temperature, $g(q_1)$ develops a maximum, whose height diverges for decreasing T. Therefore, it must exist a temperature T_s, where this maximum touches the axis at $q_1 \equiv q_s \neq 0$. Therefore, at $T = T_s$ a new spin-glass solution appears, with $q_1 = q_s$ and $m = 1$. When $T < T_s$ we have to move m from 1, and one can see that the solution simply shifts, $q_1 > q_s$, $m < 1$ [10]. The important point is that, unlike the RS nontrivial solution, this solution is *stable*. Moreover, its free energy its lower than the paramagnetic one. The temperature T_s where this nontrivial 1RSB solution appears is called *static transition* temperature. It has been proved that the 1RSB solution is *exact* in the PSM [10]. This means that if we take higher order RSB ansatz for Q_{ab}, from the saddle point equations we find that all the extra parameters we introduce have in fact a trivial value, and that the 1RSB solution is recovered.

As we have seen, at T_s the value of the self-overlap is nonzero, $q_1 = q_s$, while $m = 1$. This fact has an interesting physical interpretation. For $T > T_s$ the overlap distribution

is trivial, $P(q) = \delta(q)$. By decreasing the temperature, finally a second peak appears at T_s, for $q = q_s$. This value is nonzero, meaning that at the transition the states are already well formed, that is tight. However, at T_s we have $m = 1$, meaning that the height of this nontrivial peak is in fact zero: the *probability* of these new states is zero at the transition, and it grows below T_s as m becomes smaller than one. In other words, it seems that when the states appear, they are already well formed, but have a zero thermodynamic weight.

This fact has a possible interpretation in terms of metastable states: the calculation we have just performed is a *thermodynamic* one, and therefore by its very nature it is unable to capture the contribution of metastable states. If in this systems there were some metastable states even above T_s, and some of them became stable only below T_s, the behaviour of $P(q)$ would be exactly the one described above. The states are already present in the phase space, even above T_s, with a well defined nonzero self-overlap, but their thermodynamic weight is zero, as long as the temperature does not drop below the static transition. At that point the free energy of these states becomes smaller than the paramagnetic one, therefore their weight is nonzero, and the $P(q)$ develops a secondary peak. For now, this is just a well motivated hypothesis. We will see in the following chapters that it is in fact verified.

Summarizing, in the PSM we find a static transition between a high temperature paramagnetic phase, and a low temperature spin-glass phase below T_s. In this phase many pure states dominate the partition function. The order parameter of this unusual transition is the overlap matrix Q_{ab}, and more precisely, within the 1RSB scheme, the self-overlap q_1 and the probability parameter m. In the paramagnetic phase the overlap matrix has a replica symmetric form, with $q_1 = 0$ and m undetermined, while in the spin-glass phase there is replica symmetry breaking, with nontrivial values of q_1 and m. The nature of this transition is discontinuous if we consider the parameter q_1, but continuous if we consider the whole probability distribution $P(q)$.

4. Equilibrium dynamics

As we have already pointed out, the dynamical behaviour of a system will be very different from its thermodynamic behaviour, if metastable states are present. This is particularly true in mean-field, where metastable states may have infinite lifetime. The results from the previous chapter seem to suggest that something nontrivial is going on in the PSM even for $T > T_s$. It is therefore important that we perform an independent dynamical study of the model, and see whether our guess about the presence of metastable states was right. A nice introduction to the main concepts of dynamics can be found in [20].

4.1. The generating functional formalism

Before focusing on the PSM, we give a brief summary on how to study the dynamics of a degree of freedom $x(t)$, described by an Hamiltonian $H(x)$, which contains some quenched disorder. The starting point of our dynamical study is the Langevin equation [21],

$$\frac{dx}{dt} = -\frac{\partial H}{\partial x} + \eta(t) \tag{85}$$

where $\eta(t)$ is a Gaussian noise, playing the role of the thermal agitation, with

$$\langle \eta(t) \rangle = 0 \tag{86}$$

$$\langle \eta(t)\eta(t') \rangle = 2T \, \delta(t - t') \tag{87}$$

The factor $2T$ is crucial, since it relates the strength of the noise to the friction coefficient in the Langevin equation [20]. In the rest of this chapter we will have to integrate repeatedly over the degrees of freedom $x(t)$, and over the disorder $\eta(t)$, which are both functions of time. Thus, most of the integrals will be *functional integrals*. With the notation Dx we actually mean a measure over all the paths, i.e. $D[x(t)]$ [23]. The probability $P(\eta)$ of the noise can be written as,

$$P(\eta) \sim \exp\left[-\frac{1}{2} \int dt dt' \, \eta(t) D^{-1}(t - t')\eta(t') \right] \tag{88}$$

with

$$D(t - t') = 2T \, \delta(t - t') \tag{89}$$

Every solution $x(t)$ of the Langevin equation depends on the particular realization of the thermal noise $\eta(t)$, and we indicate it as $x_\eta(t)$. From the probability distribution on η we can therefore obtain a distribution on x. To work this out, let us compute the average over the noise of a generic observable A, function of the degree of freedom $x(t)$,

$$\langle A(x) \rangle = \int D\eta \, P(\eta) \, A(x_\eta) = \int D\eta \, P(\eta) \int dx \, \delta(x - x_\eta) \, A(x) =$$

$$= \int dx \left[\int D\eta \, P(\eta) \, \delta(\partial_t x + \partial_x H - \eta) \right] A(x) =$$

$$= \int dx \, P(x) A(x) \tag{90}$$

where we have defined the probability of x as,

$$P(x) = \int D\eta \, P(\eta) \, \delta(\partial_t x + \partial_x H - \eta) \tag{91}$$

Note that in principle we should introduce the Jacobian of the equation in the formula above. However, it can be proved that if we discretize the Langevin equation according to the Ito prescription, this Jacobian is in fact equal to 1, and can therefore be neglected [21, 22].

When the Hamiltonian contains quenched disorder J (as in the case of the PSM) we must find a way to average over J. Clearly, if we simply average the Langevin equation we get a disappointing $0 = 0$. In fact, the correct quantity which has to be averaged over the disorder is the distribution $P(x)$ above, such that to compute the average over J of an observable A we can simply use the formula,

$$\overline{\langle A(x) \rangle} = \int Dx \; \overline{P(x)} \; A(x) \tag{92}$$

Rather than precisely compute $\overline{P(x)}$, we average the integral of $P(x)$, in order to deal with a scalar quantity. This is the generating functional method [24, 25], which has been first applied and studied in the field of spin-glasses in [26, 27, 28]. The starting point of the method is an apparently redundant way to represent the number 1,

$$1 \equiv Z = \int Dx \, P(x) = \int Dx D\eta \, P(\eta) \, \delta(\partial_t x + \partial_x H - \eta) =$$

$$= \int Dx D\hat{x} D\eta \, \exp\left[-\frac{1}{2} \int dt dt' \, \eta(t) D^{-1}(t, t') \eta(t') + \right.$$

$$+ i \int dt \, \hat{x}(t)(\partial_t x + \partial_x H) - i \int dt \, \hat{x}(t)\eta(t) \, \Big]$$

$$= \int Dx D\hat{x} \, \exp\left[-\frac{1}{2} \hat{x} D\hat{x} + i\hat{x}(\partial_t x + \partial_x H) \right]$$

$$\equiv \int Dx D\hat{x} \, \exp\left[S(x, \hat{x}) \right] \tag{93}$$

with $S = -\frac{1}{2}\hat{x}D\hat{x} + i\hat{x}(\partial_t x + \partial_x H)$. We used the integral representation of the delta function and the fact that the functional integral is Gaussian. In our notation we do not indicate explicitly the time contractions: $\hat{x} D\hat{x} = \int dt \, dt' \, x(t) D(t, t') x(t')$, and the same holds for $i\hat{x}(\partial_t x + \partial_x H)$.

The quantity Z is the generating functional. The fact that it is just equal to 1, must not deceive the student. In fact, we can calculate all the interesting dynamical quantities with this functional. Let us see how. When we introduce a time dependent magnetic field in the system, we have an extra term,

$$\int dt \, x(t)h(t) \tag{94}$$

in the Hamiltonian. Thus we have an extra term $h(t)$ in the original Langevin equation, which translate into a term,

$$\int dt \, \hat{x}(t)h(t) \tag{95}$$

in the action S above. Therefore, when we derive the average of any quantity with respect to $h(t)$ we pull down a factor $\hat{x}(t)$ from the exponential, and in particular,

$$\frac{\partial}{\partial h(t)} \langle x(t') \rangle = \langle \hat{x}(t) x(t') \rangle \equiv R(t, t') \tag{96}$$

which is the dynamical response function of the system, i.e. the dynamical equivalent of the susceptibility in thermodynamics. On the other hand, we can couple a field $\hat{h}(t)$ to $x(t)$ in the generating functional, and get,

$$\frac{\partial}{\partial \hat{h}(t)} \langle x(t') \rangle = \langle x(t)x(t') \rangle \equiv C(t,t') \tag{97}$$

that is the time dependent correlation function. Summarizing, once the conjugate fields $h(t)$ and $\hat{h}(t)$ are introduced, we have,

$$R(t,t') = \frac{\partial Z}{\partial \hat{h}(t')\partial h(t)}$$

$$C(t,t') = \frac{\partial Z}{\partial \hat{h}(t')\partial \hat{h}(t)} \tag{98}$$

Let us now consider a system with quenched disorder in the Hamiltonian. We first define,

$$\mathcal{L}(x) \equiv \partial_t x + \frac{\partial H}{\partial x} \tag{99}$$

and then split the Hamiltonian into a part without disorder H_0, and a part with disorder H_J, such that the Langevin equation becomes,

$$\mathcal{L}(x) = \mathcal{L}_0(x) + \mathcal{L}_J(x) = \eta(t) \tag{100}$$

with

$$\mathcal{L}_0 = \partial_t x + \frac{\partial H_0}{\partial x} \qquad \mathcal{L}_J = \frac{\partial H_J}{\partial x} \tag{101}$$

and

$$\langle \eta\eta \rangle = 2T\delta(t - t') \equiv D_0(t - t') \ . \tag{102}$$

The generating functional becomes,

$$Z = \int Dx D\hat{x} \exp\left\{ -\frac{1}{2}\hat{x}D_0\hat{x} + i\hat{x} \ [\mathcal{L}_0(x) + \mathcal{L}_J(x)] \right\} \tag{103}$$

It should be clear by now that Z has, in the dynamical approach, the same role as the partition function in thermodynamic. This may suggest that, when averaging over J, we should consider $\log Z$ rather than Z, in order to reproduce the quenched case. However, this is not the case. In fact, the crucial point is that $Z = 1$, and thus it can be safely averaged over J ! Therefore in the dynamic approach we do not need replicas [27]. This does not mean that the calculation will be simpler. Actually, we will see that *time* plays the same role as *replicas*: by averaging over J we will decouple the sites, but couple different times.

We fact that replicas are not needed in the dynamical case can be understood also in a more direct way. As we have already said, the correct quantity to average over the disorder J is the probability distribution $P_J(x)$ of the degree of freedom x. In the static case we have,

$$P_J^{(s)}(x) = \frac{e^{-\beta H_J(x)}}{\int D\hat{x} \ e^{-\beta H_J(\hat{x})}} \tag{104}$$

In order to be averaged over J this expression must be rewritten in terms of replicas,

$$P_J^{(s)}(x) = \lim_{n \to 0} \int D\hat{x}_{a \neq 1} \ e^{-\beta \sum_a^n H_J(\hat{x}_a)} \ , \tag{105}$$

where $\hat{x}_1 = x$. On the other hand, from (93) we see that the distribution in the dynamic case is given by,

$$P_J^{(d)}(x) = \int D\hat{x}(t) \ e^{\int dt \ S_J[x(t), \hat{x}(t)]} \tag{106}$$

where we have reinstated the dependence on the time t to emphasize the formal similarity between the replicated static case and the unreplicated dynamic one. It is clear that in the latter case we do not need replicas to average over J. However, in the dynamic case the variable t plays a role analogous to the replica index a.

Expression (103) is interesting for two reasons: first, the coefficients of $\hat{x}^2$ and $\hat{x}$ are respectively the correlator of the noise, and the noise-independent part of the original Langevin equation; second, the disorder J is only contained in $\mathcal{L}_J$ at the exponent, and it can be easily integrated out. This average will *renormalize* the coefficients of $\hat{x}^2$ and $\hat{x}$, giving rise to a new effective Langevin equation [29]. More specifically, the average over J gives,

$$\overline{Z} = \int Dx D\hat{x} \exp\left[-\frac{1}{2}\hat{x} D_0 \hat{x} + i\hat{x}\mathcal{L}_0(x)\right] \overline{\exp[i\hat{x}\mathcal{L}_J(x)]} \tag{107}$$

We define the quantity $\Delta(x, \hat{x})$ as

$$\exp[\Delta(x, \hat{x})] \equiv \overline{\exp[i\hat{x}\mathcal{L}_J(x)]} \tag{108}$$

Once the average is done, it is possible in general to isolate various pieces in Δ, and in particular,

$$\Delta(x, \hat{x}) = -\frac{1}{2}\hat{x} D_1(x, \hat{x})\hat{x} + i\hat{x}\mathcal{L}_1(x, \hat{x}) + \ldots \tag{109}$$

where $\mathcal{L}_1$ renormalizes the disorder-independent part of the Langevin equation $\mathcal{L}_0$, and D_1 renormalizes the noise correlator. In the end we have the effective Langevin equation,

$$\mathcal{L}_0(x) + \mathcal{L}_1(x, \hat{x}) = \xi \qquad \text{with} \quad \langle \xi\xi \rangle = D_0 + D_1(x, \hat{x}) \tag{110}$$

In this equation the disorder is no longer present, but we had to pay a price: the original equation gets some nontrivial corrections. The most evident difference is that the variable ξ, the new effective noise, is no longer delta-correlated in time. In other words the integration over J has introduced a sort of memory in the dynamics of the system. This phenomenon is common in statistical physics: whenever starting from a Markovian stochastic process we integrate over some degrees of freedom (the disorder, the fast variables, the momenta, etc.), we end up with a new effective equation which is no longer Markovian, and where modes which were previously uncoupled, are now coupled (a simple example of this phenomenon can be found in [20]).

4.2. Dynamics of p-spin spherical model

In the following section we will apply the technique described above to the PSM [29, 30]. The formalism is trivially generalized to the case of a vectorial degree of freedom σ_k. In the Langevin equation we must add a Lagrange multiplier $\mu(t)$ in order to impose the spherical constraint:

$$\partial_t \sigma_i(t) = -\frac{\partial H}{\partial \sigma_i} - \mu(t)\sigma_i(t) + \eta_i(t) \quad \text{with} \quad \langle \eta(t)\eta(t') \rangle = 2T\delta(t - t') \tag{111}$$

The derivative of the Hamiltonian with respect to σ_i gives,

$$\frac{\partial H}{\partial \sigma_i} = -\frac{p}{p!} \sum_{kl} J_{ikl} \, \sigma_k \sigma_l \tag{112}$$

The generating functional is given by equation (103), with $x \to \sigma_k$, $\hat{x} \to \hat{\sigma}_k$, and,

$$i\hat{\sigma} \cdot \mathcal{L}_0 = \sum_k \int dt \, i\hat{\sigma}_k(t) \, [\partial_t \sigma_k(t) + \mu(t)\sigma_k(t)]$$

$$i\hat{\sigma} \cdot \mathcal{L}_J = -\frac{ip}{p!} \int dt \sum_{ikl} J_{ikl} \, \hat{\sigma}_i(t)\sigma_k(t)\sigma_l(t) \tag{113}$$

If we compare this last expression with the static formulas (see equation 3.2), we can see that in this case the time has the same function as the replica index,

$$\int dt \sum_{ikl} J_{ikl} \, \hat{\sigma}_i(t)\sigma_k(t)\sigma_l(t) \longleftrightarrow \sum_a \sum_{ikl} J_{ikl} \, \sigma_i^a \sigma_k^a \sigma_l^a \tag{114}$$

The following step is to average over the disorder, that is to compute $\overline{\exp(i\hat{\sigma} \cdot \mathcal{L}_J)}$. In the statics this operation gives a coupling among replicas, in this case we will have a coupling among times. A technical remark: before averaging, we need to symmetrize the term $\hat{\sigma}\sigma\sigma$ in (113), since the couplings are completely symmetric. We find,

$$\overline{\exp(i\hat{\sigma} \cdot \mathcal{L}_J)} =$$

$$= \int \prod_{i>k>l} dJ_{ikl} \, \exp\left\{ -\frac{1}{2p!}J_{ikl}^2 2N^{p-1} - J_{ikl}\int dt[i\hat{\sigma}_i\sigma_k\sigma_l + \sigma_i i\hat{\sigma}_k\sigma_l + \sigma_i\sigma_k i\hat{\sigma}_l] \right\} =$$

$$= \exp\left\{ \int \frac{dtdt'}{4N^{p-1}}[p(i\hat{\sigma} \cdot i\hat{\sigma})(\sigma \cdot \sigma)^{p-1} + p(p-1)(i\hat{\sigma} \cdot \sigma)(\sigma \cdot i\hat{\sigma})(\sigma \cdot \sigma)^{p-2}] \right\} \tag{115}$$

where we used the notation,

$$\sigma \cdot \sigma \equiv \sum_{i=1}^{N} \sigma_i(t)\sigma_i(t') \tag{116}$$

As we anticipated, in the calculation appeared a coupling among different times, through the overlap of the configuration at time t and t'. In complete analogy with the static

case, we therefore introduce as an order parameter the *dynamical overlap* [31, 30], and get,

$$\overline{\exp(i\hat{\sigma} \cdot \mathcal{L}_J)} =$$

$$= \int DQ \, \delta\left(NQ_1 - \sum_k i\hat{\sigma}_k(t)i\hat{\sigma}_k(t')\right) \delta\left(NQ_2 - \sum_k \sigma_k(t)\sigma_k(t')\right) \cdot$$

$$\cdot \, \delta\left(NQ_3 - \sum_k i\hat{\sigma}_k(t)\sigma_k(t')\right) \delta\left(NQ_4 - \sum_k \sigma_k(t)i\hat{\sigma}_k(t')\right) \cdot$$

$$\cdot \, \exp\left\{\frac{pN}{4} \int dtdt'[Q_1(t,t')Q_2(t,t')^{p-1} + (p-1)Q_3(t,t')Q_4(t,t')Q_2(t,t')^{p-2}]\right\}$$

It is clear the similarity between the overlap matrix $Q_{ab} = \sum_k \sigma_k^a \sigma_k^b / N$ in the static approach, and $Q_2(t,t') = \sum_k \sigma_k(t)\sigma_k(t')/N$: in the first case we have a static overlap between configurations belonging to different replicas, in the second case we have a dynamic overlap between configurations at different times. It is not only Q_2 that has a physical meaning. From their definitions and from the discussion above, we see that Q_3 and Q_4 are both a response functions, $\langle \sigma \hat{\sigma} \rangle$, with their time arguments exchanged. Finally, it is possible to argue that the (hard to interpret) order parameter $Q_1 = \langle \hat{\sigma}\hat{\sigma} \rangle$ must be zero [31]. Summarizing,

$$\begin{cases} Q_1(t,t') = 0 \\ Q_2(t,t') = C(t,t') \\ Q_3(t,t') = R(t',t) \\ Q_4(t,t') = R(t,t') \end{cases} \tag{117}$$

We now give an exponential representations of the δ-functions. For example,

$$\delta\left(NQ_2(t,t') - \sum_k \sigma_k(t)\sigma_k(t')\right) = \int Dl_2 \exp\left[iN \int dtdt' \, (l_2Q_2 - l_2\sigma \cdot \sigma)\right] \tag{118}$$

and we use the saddle-point method to compute the integral. By setting to zero the derivatives with respect to all the Q's, we get the equations,

$$\begin{cases} il_1 = \frac{p}{4}Q_2^{p-1} \\ il_2 = \frac{p}{4}(p-1)Q_1Q_2^{p-2} + \frac{p}{4}(p-1)(p-2)Q_3Q_4Q_2^{p-3} \equiv 0 \\ il_3 = \frac{p}{4}(p-1)Q_4Q_2^{p-2} \\ il_4 = \frac{p}{4}(p-1)Q_3Q_2^{p-2} \end{cases}$$

The product Q_3Q_4 is zero because of causality: if $t > t'$, then $R(t',t) = 0$ and *vice versa*. In order to write the effective Langevin equation we have to recognize what are the new coefficients of $\hat{\sigma}\hat{\sigma}$ and of $\hat{\sigma}\sigma$. From the definition of the l's we have the following new term in the generating functional,

$$\Delta = \sum_k \int dt \, dt' \left\{-\frac{p}{4}C(t,t')^{p-1}\hat{\sigma}_k(t)\hat{\sigma}_k(t') - \frac{1}{2}p(p-1)R(t,t')C(t,t')^{p-2}i\hat{\sigma}_k(t)\sigma_k(t')\right\} , \tag{119}$$

Note that at this point the sites in the action of the generating functional are all decoupled. Therefore we can write an effective Langevin equation for a scalar degree of freedom σ [29],

$$\partial_t \sigma(t) = -\mu(t)\sigma(t) + \frac{1}{2}p(p-1)\int dt'' R(t,t'')C(t,t'')^{p-2}\sigma(t'') + \xi(t) \qquad (120)$$

with

$$\langle \xi(t)\xi(t') \rangle = 2T\delta(t-t') + \frac{p}{2}C(t,t')^{p-1} \qquad (121)$$

Note that the average over the disorder did not generate terms $\sigma\sigma$, which we would not know how to interpret. The effective Langevin equation does not contain the disorder, and it is uncoupled in the sites. However, it is more complicated than the original one, since the noise is no longer δ-correlated in time, and we have an explicit memory term at the r.h.s., that is a non-local kernel which couples the external time t with all the earlier times $t'' < t$.

4.3. Equations for the correlation and the response

We now want to use the effective Langevin equation to write some self-consistent equations for the correlation and the response function. In order to do this we have to introduce some useful formal relations. The first one is already known,

$$R(t,t') = \frac{\partial \langle x(t) \rangle}{\partial h(t')} = \langle x(t)\hat{x}(t') \rangle \qquad (122)$$

The second relation is the following,

$$\langle \frac{\partial x(t)}{\partial \eta(t')} \rangle =$$
$$\int D\eta \, \exp\left[-\frac{1}{2}\eta D^{-1}\eta\right] \frac{\partial}{\partial \eta(t')} \int DxD\hat{x} \; x(t)\exp[\hat{x}(\partial_t x + \partial_x H) + \hat{x}\eta]$$
$$= \langle x(t)\hat{x}(t') \rangle = R(t,t') \qquad (123)$$

The last relation is a little harder to prove,

$$\langle x(t)\eta(t') \rangle =$$
$$= \int D\eta DxD\hat{x} \; \exp\left[-\frac{1}{2}\eta D^{-1}\eta\right] x(t)\eta(t')\exp[\hat{x}(\partial_t x + \partial_x H) + \hat{x}\eta + j\eta]|_{j=0} =$$
$$= \int D\eta DxD\hat{x} \; \exp\left[\frac{1}{2}\eta D^{-1}\eta\right] x(t)\frac{\partial}{\partial j(t')}\exp[\hat{x}(\partial_t x + \partial_x H) + \hat{x}\eta + j\eta]|_{j=0} =$$
$$= \frac{\partial}{\partial j(t')}\int DxD\hat{x} \; x(t)\exp[-\frac{1}{2}\hat{x}D\hat{x} + \hat{x}(\partial_t x + \partial_x H) + jDj + jD\hat{x} + \hat{x}Dj]|_{j=0}$$
$$= \int DxD\hat{x}x(t)\int dt'' D(t',t'')\hat{x}(t'')\exp[S(x,\hat{x}')]$$
$$= \int dt'' D(t',t'')R(t,t'') \qquad (124)$$

Note that this last equation is only valid for Gaussian noise. We are now ready to write the two equations for the response and the correlation function. To get the equation for the response we differentiate the effective Langevin equation with respect to the effective noise and average,

$$
\frac{\partial R(t_1, t_2)}{\partial t_1} = \frac{\partial}{\partial t_1} \langle \frac{\delta \sigma(t_1)}{\delta \xi(t_2)} \rangle = \langle \frac{\delta \dot{\sigma}(t_1)}{\delta \xi(t_2)} \rangle =
$$

$$
= -\mu(t_1) R(t_1, t_2) + \frac{1}{2} p(p-1) \int_{t_2}^{t_1} dt'' R(t_1, t'') C^{p-2}(t_1, t'') R(t'', t_2) +
$$

$$
+ \delta(t_1, t_2) \tag{125}
$$

The equation for the correlation is obtained by multiplying the effective Langevin equation by σ and averaging,

$$
\frac{\partial C(t_1, t_2)}{\partial t_1} = \frac{\partial}{\partial t_1} \langle \sigma(t_1)\sigma(t_2) \rangle = \langle \dot{\sigma}(t_1)\sigma(t_2) \rangle =
$$

$$
= -\mu(t_1) C(t_1, t_2) + \frac{1}{2} p(p-1) \int_{-\infty}^{t_1} dt'' R(t_1, t'') C^{p-2}(t_1, t'') C(t'', t_2) +
$$

$$
+ \langle \xi(t_1)\sigma(t_2) \rangle \tag{126}
$$

where we can use the third one of the relations above and get,

$$
\langle \xi(t_1)\sigma(t_2) \rangle = \int dt'' D(t_1, t'') R(t_2, t'') = 2T R(t_2, t_1) + \frac{p}{2} \int_{-\infty}^{t_2} dt'' R(t_2, t'') C^{p-1}(t_1, t'')
$$

$$
\tag{127}
$$

Because of causality, the term $2T R(t_2, t_1)$ is zero if $t_2 < t_1$, as we shall assume. Finally we have to get rid of the Lagrange multiplier $\mu(t)$. Differentiating the constant $C(t, t) \equiv 1$, we obtain $[\partial_t C(t, t') + \partial_{t'} C(t, t')]_{t,t'=s} = 0$, giving the equation [30],

$$
\mu(t_1) = \frac{1}{2} p^2 \int_{-\infty}^{t_1} dt'' R(t_1, t'') C^{p-1}(t_1, t'') + T \tag{128}
$$

These are the exact dynamical equations for the PSM. When they were first derived in [29] it was immediately noted that they were formally identical to the approximated equations formulated by Mode Coupling Theory (MCT) for structural glasses [32, 33, 34, 35]. This observation is at the heart of the theory for the glass-transition in structural glasses inspired by p-spin spin-glass models [36]. The physics of the PSM has probably something to do with structural glasses, at least at the dynamical level, and provided that MCT works well. Moreover, it looks like MC theory must also work in the PSM, since it gives the same equations ! Let us analyze this last point more in detail.

4.4. Diagrammatic technique and Mode Coupling approximation

The dynamical equations (125) and (126) can indeed be obtained within the Mode Coupling approximation. Within this approach we consider the perturbative expansion of the Langevin equation and write all the physical quantities using a diagrammatic
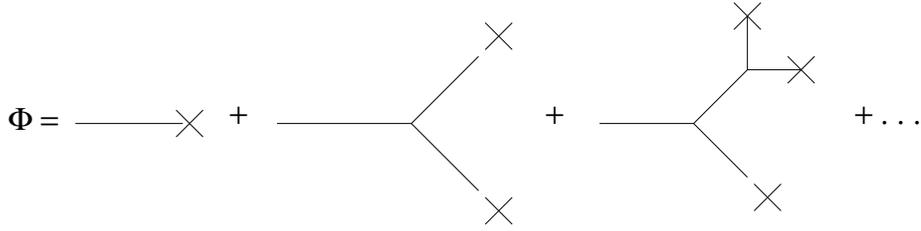
Figure 1. Diagrammatic representation of the perturbative solution to equation 130. The various terms of the equation for $\phi(t)$ are represented: a line stands for the bare propagatore R_0, a cross indicates the noise. As usual in Feynman diagrams, a vertex stands for a time convolution.

representations. For the rest of this section see [38, 39]. For the sake of simplicity, we consider the case of a single scalar degree of freedom ϕ, with an energy

$$H = \frac{\mu(t)}{2}\phi^2 + \frac{g}{p!}\phi^p \tag{129}$$

and we assume that the dynamics of ϕ is described by the Langevin equation

$$\frac{\partial \phi}{\partial t} = -\mu(t)\phi - \frac{g}{(p-1)!}\phi^{p-1} + \eta \tag{130}$$

with the initial condition $\phi(0) = 0$. Note that this Hamiltonian is a scalar version, without disorder, of the p-spin one. The thermal noise η is defined as in the previous case.

We consider the inverse operator $R_0 = [\mu(t) + \frac{\partial}{\partial t}]^{-1}$, which we use to write the perturbative expansion of $\phi(t)$. In figure 1 we can see the diagrammatic representation of this expansion in the case $p = 3$. In this case we can write the following equation:

$$\phi(t) = R_0 \otimes \eta - \frac{g}{2!}R_0 \otimes \{R_0 \otimes \eta \cdot R_0 \otimes \eta\} + \dots \tag{131}$$

where $\otimes$ stands for time convolution: $(R_0 \otimes f)(t) = \int_0^t dt' R_0(t,t')f(t')$. The explicit expression of R_0 is

$$R_0(t,t') = \exp\left[-\int_{t'}^t du\, \mu(u)\right] \tag{132}$$

as we can easily see by differentiating $\phi(t)$. The correlation and response function can be written as,

$$C(t,t') = \langle \phi(t)\phi(t') \rangle \tag{133}$$

$$R(t,t') = \langle \frac{\partial \phi(t)}{\partial \eta(t')} \rangle = \frac{1}{2T}\langle \phi(t)\eta(t') \rangle \tag{134}$$

These functions can be diagrammatically represented, in figure 2 we show the case $p = 3$. In what follows we shall assume that all tadpoles (like the second diagram in figure 2) are
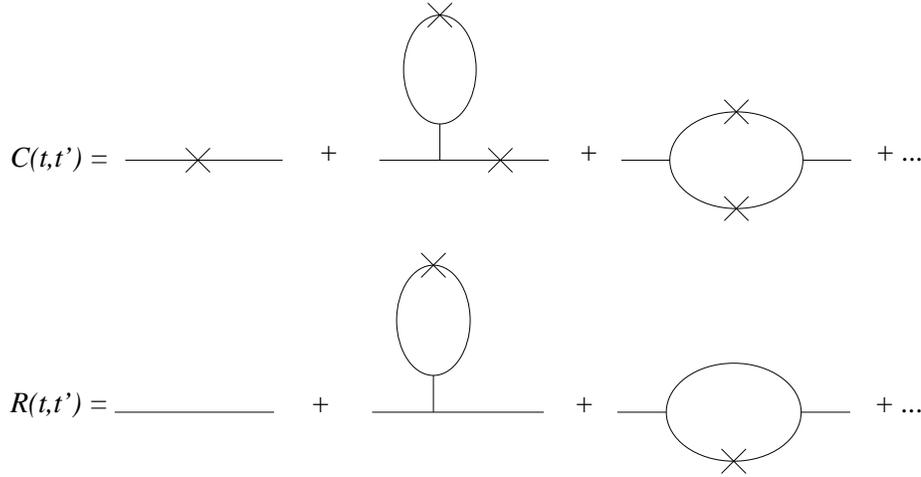
Figure 2. Diagrammatic representations of the perturbative expansions of the correlation and response function. These diagrams are obtained combining all the different terms of the diagrams for the perturbative solution.

already resummed. The contribution of these diagrams to the self-energy Σ that we are going to write is in fact simply a constant: disregarding tadpoles is equivalent to operate mass renormalization in a usual field theory [2, 39]. The diagrammatic expansion of C and R can be self-consistently resummed, given the following Dyson equations (fig. 3, upper panel),

$$R(t,t') = R_0(t,t') + \int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 R_0(t,t_1)\Sigma(t_1,t_2)R(t_2,t') \tag{135}$$

$$C(t,t') = \int_{0}^{t} dt_1 \int_{0}^{t'} dt_2 R(t,t_1)D(t_1,t_2)R(t',t_2) \tag{136}$$

where the self-energies (or kernels) $\Sigma(t,t')$ and $D(t,t')$ are, as usual, the sum of all the amputated connected diagrams. If we multiply by R_0^{-1} we can write the equations in the following way:

$$R_0^{-1} \otimes R = I + \Sigma \otimes R \tag{137}$$

$$R_0^{-1} \otimes C = D \otimes R + \Sigma \otimes C \tag{138}$$

where I is the identity operator. Explicitly we have

$$\frac{\partial R(t,t')}{\partial t} = -\mu(t)R(t,t') + \delta(t-t') + \int_{t'}^{t} du\Sigma(t,u)R(u,t') \tag{139}$$

$$\frac{\partial C(t,t')}{\partial t} = -\mu(t)C(t,t') + \int_{0}^{t'} duD(t,u)R(t',u) + \int_{0}^{t} du\Sigma(t,u)C(u,t')$$

Up to know this was very general, and most importantly exact. The mode coupling approximation (MCA) consists in approximating the kernels $\Sigma(t,t')$ and $D(t,t')$: we neglect all the vertex corrections and keep only line corrections, that is we take the values of Σ and G at order g^2 and substitute in them the bare response and correlation
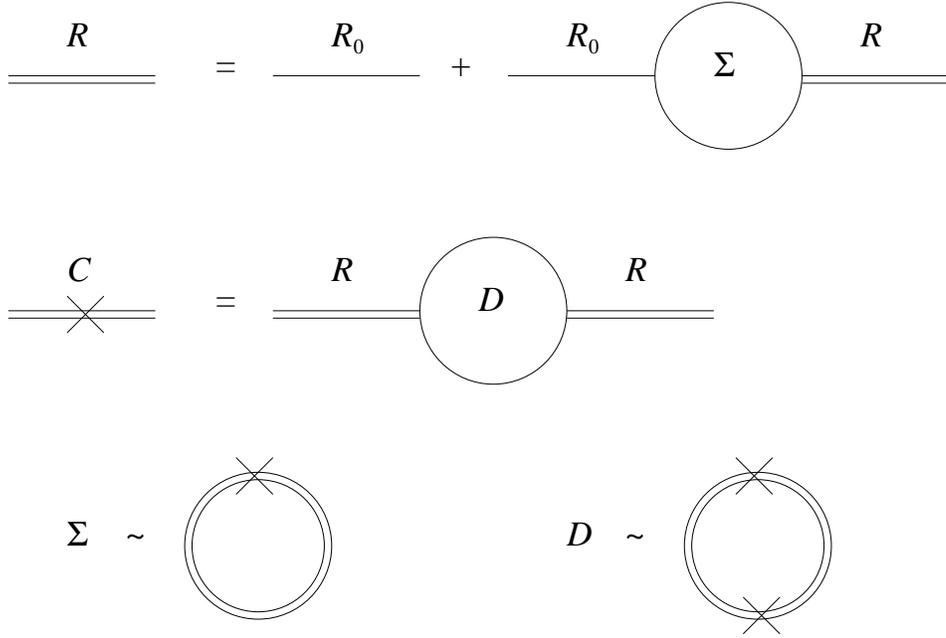
Figure 3. The first two lines are the exact Dyson equations for the correlation and the response. The third line gives the value of the kernels Σ and D within the Mode Coupling Approximation.

by their renormalized values, $R_0 \to R$, $C_0 \to C$. In this way we get the following equations:

$$\Sigma(t, t') = \frac{g^2}{2} C^{p-1}(t, t') R(t, t')$$

$$D(t, t') = 2T\delta(t - t') + \frac{g^2}{6}[C(t, t')]^p \tag{140}$$

If we now plug this MCA form of Σ and D into equations (139), it is easy to see that they become identical to the equations we wrote for the p-spin model in the previous section within the generating functional method (we have considered a scalar field, but the same equations can be obtained for a vectorial field). This raises an interesting question: how is that the equations obtained with the Mode Coupling *approximation* are identical to those obtained with the *exact* generating functional method ? The answer is that in a mean-field disordered system, thanks to the scaling with N of the couplings J, vertex corrections are sub-leading, and vanish when $N \to \infty$, while line corrections remain finite in the thermodynamic limit. In other words MCA is in fact exact for mean field systems !

To understand this fact, we can write the Hamiltonian with a vector σ_i (where $i = 1, \ldots, N$). The interaction term for $p = 3$ is $g \sum_{i<j<k} J_{ijk} \sigma_j \sigma_j \sigma_k$. In this case the average value of J^2 is $1/N^{p-1}$. When averaging over the disorder, the behavior in the limit $N \to \infty$ is different for vertex and line corrections. In the first case we have (for $p = 3$) that in the term $J_{ijk} J_{jlm} J_{mni} J_{kln}$ the average over the noise causes the indices to couple two by two, e.g. $i = l$ and $k = m$. We obtain a factor $(1/N^2)^2$, which we must

multiply by N^4 having in the best case four free indices over which we have to sum. This factor is then of order 1 and vanishes once we normalize the correlation by N. Instead in the line correction the average over the noise causes only two indices to coincide in the best case, giving a N factor that remains finite also after the normalization [39].

Although a bit boring, this last section proved an important point: the exact dynamical equations of the PSM are identical to the MC equations, and in particular to the (approximated) equations that MC theory writes for deeply supercooled liquids close to the glass transition. This is one of the main evidences supporting the idea that the PSM is a sort of mean-field model for structural glasses, and that some of the main physical concepts valid in the PSM, should be valid in real glasses as well. As long as one believes that MC theory describes reasonably well fragile glasses [40, 41], one has to accept that the physics of these systems caught by MC must have something to do with the physics of the PSM.

4.5. The dynamical transition

It is now time to solve the dynamical equations of the PSM. In order to do this we must make some simplifications on the correlation and response functions. First, we shall assume that Time Translation Invariance (TTI) holds: correlation and response no longer depend independently on the two times, but only on their difference. This is true only at *equilibrium*, and therefore we are restricting ourselves to equilibrium dynamics. The second simplification is in fact a consequence of TTI, and is the validity of the Fluctuation-Dissipation Theorem (FDT). These two properties can be written as,

$$\text{TTI:} \begin{cases} C(t_1, t_2) = C(t_1 - t_2) \equiv C(\tau) \\ R(t_1, t_2) = R(t_1 - t_2) \equiv R(\tau) \end{cases} \quad (\tau \equiv t_1 - t_2) \tag{141}$$

$$\text{FDT:} \quad R(\tau) = -\frac{1}{T}\frac{dC(\tau)}{d\tau} \tag{142}$$

Using these formulas, and a bit of algebra, we can reduce the two coupled equations (125) and (126) to a single equations for $C(\tau)$, namely [30],

$$\dot{C}(\tau) = -TC(\tau) - \frac{p}{2T}\int_0^\tau du\ C^{p-1}(\tau - u)\dot{C}(u) \tag{143}$$

A crucial point: in order to perform the integrals we have supposed $C(\infty) = 0$, that is we assumed that *there is no ergodicity breaking*: after a sufficiently long time the dynamic configuration must be allowed to go as far as possible from the initial time configuration. In terms of overlap, this means that the overlap between $\sigma(\tau = 0)$ and $\sigma(\tau = \infty)$ must be zero. Recall that we have,

$$C(\tau) = \frac{1}{N}\sum_k \langle \sigma_k(\tau)\sigma_k(0)\rangle \tag{144}$$

so that the dynamical correlation function is exactly the average overlap between the two configurations at times 0 and τ. Therefore assuming unbroken ergodicity is equivalent

to assume that $C(\infty) = 0$. Ergodicity will be verified self-consistently at the end of the calculation.

The first term on the r.h.s. of equation (143) comes from the J-independent part of the original Langevin equation, i.e. from the spherical constraint. The second term, that comes from the integration over J, is clearly a memory term, for it causes the properties of the system at time t to depend on all times between 0 and t.

By imposing the physical condition $\dot{C}(\tau) \leq 0$ (the average correlation cannot increase with time), we obtain from (143) the following relation [37],

$$\underbrace{C^{p-2}(\tau)[1 - C(\tau)]}_{\equiv g(C)} \leq \frac{2T^2}{p} \ . \tag{145}$$

This inequality can be easily studied graphically: for $\tau = 0$ we have $C = 1$ and $g(1) = 0$, and for $\tau = \infty$ we have $C = 0$ and $g(0) = 0$. The function $g(C)$ has thus a maximum between zero and one: let us call q_d the position of this maximum, given by,

$$q_d = \frac{p - 2}{p - 1} \tag{146}$$

The r.h.s. of the inequality is a constant larger the larger the temperature. At very high temperatures the inequality is always satisfied, since $g(q_d) \ll 2T^2/p$. This is the paramagnetic phase, which is indeed ergodic. When we lower the temperature, the difference between $2T^2/p$ and $g(C)$ gets smaller. From equation (143) we see that this difference is proportional the time-derivative of C: it is large when $C \sim 1$, that is for short times, it becomes smaller when $C \sim q_d$, and again large for $C \sim 0$, i.e. for very long times. In other words, when we lower the temperature, we observe the formation of a *plateau* of the correlation function, with $C(\tau) \sim q_d$.

If we lower further the temperature, we arrive at a point where the r.h.s. of the inequality touches the curve, i.e. there is a temperature T_d such that $2T_d^2/p = g(q_d)$. Using (146) and the definition of $g(C)$, we have,

$$T_d = \sqrt{\frac{p(p - 2)^{p-2}}{2(p - 1)^{p-1}}} \tag{147}$$

At this temperature the correlation function remains stuck at a plateau $C = q_d$, since $\dot{C} = 0$. Ergodicity is therefore broken. We cannot go below T_d, since all our assumptions are violated in this phase, and in particular $C(\infty) \neq 0$. What we have just proved is that there is a *dynamical transition* at T_d: the system passes from the paramagnetic state, to a phase where ergodicity is broken. Let us give a physical interpretation of what we have found, in terms of overlap of the configuration at time t with the configuration at time 0.

T $\gg$ T$_\mathbf{d}$: The dynamical overlap (i.e. the correlation function) rapidly decays to zero, such that the configuration goes as far as it wants in the phase space from its initial position. This is the fast equilibrium dynamics in the paramagnetic state. In this phase relaxation is exponential, and nothing particularly exciting happens.

T $\overset{>}{\sim}$ T$_\mathbf{d}$: In this phase the dynamics is still ergodic, but something strange happens: for a long time (longer the closer to T_d we are) the configuration stays close to its initial value, since $C(\tau)$ has a plateau. More precisely, the dynamics explores a "spot" of phase space around the initial configuration, of largeness roughly equal to q_d, which is the value of C at the plateau. This "spot" cannot be a true state: if it were, the system would stay trapped there forever, while in this case, after a long while, the system drifts away. Eventually the overlap goes to zero, consistently with the paramagnetic state. So what is going on ? Why the system is *almost trapped* close to the dynamical transition ? We shall answer these key questions in the next chapter.

T $\to$ T$_\mathbf{d}^+$: The plateau becomes infinite, the correlation function does not decay anymore, so that the system takes an infinite time to equilibrate. The configuration remains close to its initial position for an infinite time, and it is clearly trapped by a state of self-overlap q_d. Ergodicity is broken and our dynamical equations break down.

The behaviour of the correlation function we have just described is not a peculiarity of the PSM. In fact, it is the typical phenomenology of glassy systems, and in particular of structural glasses. The core aim of Mode Coupling Theory is indeed to explain this phenomenology in fragile glasses. The interpretation of the plateau in finite dimensional glasses is usually given in terms of *cage effect*: at low enough temperature, each particle is surrounded by a cage of nearest-neighbor particles, and it takes a long time (longer the lower the temperature) to the particle to break this cage and achieve asymptotic relaxation. This interpretation is very nice for structural glasses, but of course it cannot be applied to the mean-field PSM, where there is no space structure, nor cage. However the behaviour of the correlation function is indeed the same. This suggests that the cage effect must have a deeper interpretation, which must be valid both in finite-dimensional and mean-field systems. We will propose such an interpolation in the next chapter.

Let us make a brief summary of the dynamical results. Using the generating functional method we obtained two exact equations for the correlation and the response, which are formally identical to those obtained with the MC approximation. In fact MC is exact for the mean-field PSM. We studied the equations assuming that the system is at equilibrium and that ergodicity is not broken, in other words we studied the properties of the (ergodic) paramagnetic state. The correlation function decays to zero, but it develops a plateau as the temperature lowers. In particular, as $T \to T_d^+$ the plateau diverges and ergodicity is broken in this limit. Thus, this must be the limit of existence of the paramagnetic phase, and therefore T_d marks a dynamical transition in the system. The relaxation time (roughly, the time the correlation takes to decay to zero) diverges at T_d.

A natural question is whether this dynamical transition at T_d coincides with the static one at T_s. The answer is *no*. One can easily check that $T_d > T_s$: dynamically, the ergodicity is broken at a temperature higher than the thermodynamic

singularity. Clearly, metastability, combined with the peculiar features of mean-field, must be responsible for this: metastable states trap the dynamics at T_d, while the thermodynamics cannot detect these states. This is what we suspected when we studied the statics: at T_s the equilibrium spin-glass states appeared as a secondary peak in the $P(q)$. This peak had zero weight, but nonzero overlap q_s, suggesting that even *above* T_s some metastable states existed. From the dynamics we have a clear evidence that metastable states exist from the simple fact that $T_d > T_s$. The mean-field nature of the PSM makes the barrier around these states infinite, so that the equilibrium states are never reached.

A last important comment: we assumed ergodicity, so we can see ergodicity breaking at T_d as the limit of validity of our calculation. In fact, what we should do for $T \leq T_d$ is to give up the assumption of TTI and FDT, and solve the full equations. This is hard, but can be done (with some suitable approximation) [42, 43]. What is found in this way is that if the system starts from a high temperature (random) configuration, it never reaches the static equilibrium energy, and in this sense dynamics and statics strongly differ. However, the correlation function behaves differently from what one may think. The plateau is not infinite below T_d, but rather has a length that increases as the earlier of the two times in $C(t, t')$ increases. This phenomenon is known as *aging*, and its description is beyond the scope of these notes [44]. What happens is the following: if we constrain the system to be at *equilibrium*, then for $T \rightarrow T_d$ we have divergence of the relaxation time, and thus ergodicity breaking. Therefore we cannot study the equilibrium properties of the system for $T \leq T_d$, and we have to give up equilibrium. When this is done, what we find is a *weak* ergodicity breaking below T_d, which is an intrinsically off-equilibrium phenomenon [42].

Even though we have an explanation in terms of metastable states of why the two sets of results from statics and dynamics differ, it would be nice to have a way to unify the two pictures, and obtain *both* results. This will be achieved in the next chapter.

5. Complexity

We have seen that in the PSM different results are obtained from the static and dynamic approaches. Are we able to find a unifying approach, within which it is possible to give an interpretation of all the results collected until now ? The answer is yes. By now we have understood that the discrepancy between statics and dynamics is due to the presence of many metastable states. It is time to directly study these states.

5.1. What is the TAP free energy ?

Up to know we have seen the effect of the existence of many pure states only in a indirect way. In the statics, we had to break the replica symmetry because of ergodicity breaking, but the free energy we computed was not the individual free energy of the states, but rather the average free energy over all the thermodynamically relevant states. On the

other hand, we have seen that dynamically the ergodicity is broken at a temperature $T_d > T_s$ because of the presence of metastable states. However, even in that case we could not put our finger on the individual states trapping the dynamics. To do this we need to introduce the TAP free energy.

Pure states are objects living in an N dimensional phase space: in each state α the local magnetizations have a well defined value depending on the site, $m_i^\alpha = \langle \sigma_i \rangle_\alpha$, and a state is identified by the vector of its magnetizations. Therefore, what we need is a function defined on this space, i.e. a function of the local magnetizations m_i, whose local minima coincide with the pure states of the system. The minimization of such a function must provide a set of equations for the vector m_i, equivalent to the mean field equation for m in the Ising model, $m = \tanh(\beta m)$. This function is the *mean-field free energy*, which is known in the context of spin-glasses as Thouless-Anderson-Palmer (TAP) free energy, $f_{\text{TAP}}(m_1 \dots m_N)$ [45].

It is important to stress that the mean-field, or TAP, free energy is a function of the magnetizations m_i and *not* of the microscopic degrees of freedom σ_i. In particular its minima do not necessarily coincide with the energy minima, that is the minima of the Hamiltonian $H(\sigma_i)$. In fact, pure states *cannot* in general be simply identified with minima of the energy. The problem is that different energy minima may be separated by energy barriers which at high temperature are small compared with $k_B T$, and thus belong to the *same* pure state. Even though for $T \to 0$ a state essentially collapses onto its lowest energy configuration, it is important to keep the two concepts distinct. A pure state α, identified by the vector $m_1^\alpha \dots m_N^\alpha$, is fundamentally a subcomponent of the Gibbs measure, $\langle \cdot \rangle_\alpha$. As we have stressed in the first chapter, a pure state enjoys the crucial clustering property, property that is meaningless when referred to a simple configuration $\sigma_1 \dots \sigma_N$.

The TAP free energy density for the PSM is the following [46, 47, 48],

$$f_{TAP} = -\frac{1}{Np!} \sum_{ikl} J_{ikl} m_i m_k m_l - \frac{1}{2\beta} \log(1 - q) - \frac{\beta}{4}[(p-1)q^p - pq^{p-1} + 1] \quad (148)$$

with,

$$q = \frac{1}{N} \sum_i m_i^2 \qquad ; \qquad m_i = \langle \sigma_i \rangle \quad (149)$$

The first term is the energy, the second term is minus the entropy multiplied by the temperature, and the third one is the so-called reaction term [49]. By setting $m_i = 0$ for each i, we get $f_{TAP} = -\beta/4$, the correct result for the paramagnetic state we already met in the statics. The mean-field equations are obtained by finding the minima of the TAP free energy, $\partial_{m_i} f_{TAP} = 0$ for $i = 1 \dots N$. However, in order to study these equations, it is convenient to change variables [47]. Let us introduce the new set of variables $\{\sigma_1 \dots \sigma_N; q\}$, defined in the following way,

$$m_i = \sqrt{q}\, \sigma_i \qquad \sum_i \sigma_i^2 = N \quad (150)$$

These variables σ_i (sometimes called angular variable) are formally different from the original spin degrees of freedom, even though they play a very similar role, and are subject to the same spherical constraint. In terms of the new variables the TAP free energy becomes,

$$f_{TAP}(\sigma_i, q) = \frac{1}{N} \, q^{p/2} \, H(\sigma) + R(q, \beta) \tag{151}$$

where H is formally the original Hamiltonian (this clarifies why we called σ_i the new variables), and R is the q dependent part in (148). Now we must minimize this free energy with respect to the angular variables σ_i and the self-overlap q, taking into account the spherical constraint. We have,

$$\begin{cases} \dfrac{\partial f_{TAP}}{\partial \sigma_i} = 0 \;\; \rightarrow \;\; \begin{cases} \dfrac{\partial H(\sigma)}{\partial \sigma_i} = 0 & i = 1 \dots N \\ \sum_i \sigma_i{}^2 = N \end{cases} \\ \dfrac{\partial f_{TAP}}{\partial q} = 0 \;\; \rightarrow \;\; \dfrac{1}{N}\dfrac{p}{2}q^{\frac{p}{2}-1}H(\sigma) + \dfrac{\partial R}{\partial q} = 0 \end{cases} \tag{152}$$

The first N equations, at fixed values of the random couplings J, contain all the complexity of the problem: if there are many states, i.e. many solutions of the mean-field equations, it is because of these N equations. What is surprising is that in the PSM these equations *do not* depend on the temperature ! Moreover, they formally coincide with the minimization equations of the Hamiltonian of the model. Once we have a solution of these first N equations, call it σ_i^α, we can compute its zero temperature energy $E_\alpha = H(\sigma^\alpha)$, and plug it into the equation for q. This equation *does* depend on β, so that the self-overlap of a state depends on its zero temperature energy and on the temperature.

This result is surprising. We said above that in general the minima of the mean-field free energy do not coincide with the minima of the Hamiltonian, but we seem to have right here an exception to this rule: in the PSM minima of the TAP free energy are basically minima of the Hamiltonian. Their positions in the phase space does not depend on the temperature, while their self-overlap does. In other words, in the PSM there is a one-to-one mapping between minima of the Hamiltonian (the energy) and states, i.e. minima of the free energy. At $T = 0$ a state (stable or metastable) is just a minimum (absolute or local) of the energy. When T grows energy minima get dressed up by thermal fluctuations, and become states. So the structure of states of the PSM is just the structure of minima of the Hamiltonian.

It is *very* important to understand that this is a peculiar feature of the PSM, due to its homogeneous nature, and that in general it is not like that. However, in the PSM such a simplification holds. If one wants to extend such a simplification to more realistic, finite-dimensional systems (as structural glasses), it is crucial that *the temperature is small enough and times are short*. Nevertheless, in realistic systems barriers are finite, so that identifying minima of H with states is in fact conceptually very risky.

In the PSM, thus, the zero temperature energy density, or *bare energy density* $E = H(\sigma)$ of the minima of the Hamiltonian, is the only relevant quantity to label

states. The self-overlap q, the free energy density f, and the finite temperature energy $\mathcal{E}$ thus depend on the bare energy and on the temperature,

$$q = q(E, \beta)$$

$$f = f(E, \beta) \tag{153}$$

$$\mathcal{E} = \mathcal{E}(E, \beta) = \frac{\partial(\beta f)}{\partial \beta} \tag{154}$$

Where, of course, $\mathcal{E}(E, \infty) = E$: the zero-temperature average energy of a state is equal to its bare energy.

5.2. Definition of complexity (and a problem with the modulus).

The states of the systems, i.e. the minima of the TAP free energy, have the same structure as the minima of the Hamiltonian. Therefore, we want to study the structure of minima of H, and in particular their number. The number of minima $\mathcal{N}$ grows exponentially with the size of the system,

$$\mathcal{N} \sim e^{N\Sigma} \tag{155}$$

The quantity Σ is called *complexity* in the spin-glass community, and *configurational entropy* in the glass community, where minima of the potential energy are considered. In order to compute $\mathcal{N}$ (and thus Σ), we have to compute the number of solutions of the equations,

$$\frac{\partial H}{\partial \sigma_i} = 0 \qquad i = 1 \ldots N \tag{156}$$

By calling σ_α a solution of these equations, we have,

$$\mathcal{N} = \int D\sigma \sum_{\alpha=1}^{N} \delta(\sigma - \sigma_\alpha) \tag{157}$$

By using the standard formula,

$$\delta(\partial H) = \sum_\alpha \frac{\delta(\sigma - \sigma_\alpha)}{|\partial\partial H|} \tag{158}$$

we have [50],

$$\mathcal{N} = \int D\sigma \, \delta(\partial H) \, |\partial\partial H| \tag{159}$$

where $\partial\partial H$ is a short-cut for the determinant of the second derivative matrix of H (the Hessian). Here we have two problems: first, having the modulus in such an equation is algebraically very unpleasant; second, in this way we are counting *all* stationary points of H, not simply minima, but also unstable saddles, which can hardly be associated to pure states of the system. To solve the first problem we are tempted to disregard the modulus, and define,

$$\hat{\mathcal{N}} = \int D\sigma \, \delta(\partial H) \, \partial\partial H \tag{160}$$

However, now we have a very severe problem: this quantity is a topological invariant (the Morse constant), which has no connections whatsoever with the number of minima [51]. By disregarding the modulus we are weighting each stationary point with the sign of its Hessian, such that,

$$\hat{\mathcal{N}} = \int D\sigma \sum_\alpha \delta(\sigma - \sigma_\alpha) \operatorname{sign}(\partial\partial H) = +1 - 1 + 1 - 1 + 1 \ldots \tag{161}$$

The situation seems to be going from bad to worse. However, if we restrict our counting to a *fixed* energy density level E, things improve a lot. What we want to do is to count minima of H which have energy E. To do this we can use the formula,

$$\mathcal{N}(E) = \int D\sigma \, \delta(\partial H) \, \partial\partial H \, \delta(H - E) \tag{162}$$

By restricting ourselves to the level E and by *keeping E low enough* we can hope that we are in a region of the phase space where minima dominate, and thus where the Hessian is positive and the modulus can in fact be disregarded [52]. This is certainly true close to the ground state E_0. Moreover, the quantity defined in (162) has a further advantage in its very limitation: if we push E high enough to arrive in a region which is no longer dominated by minima, but by *saddles*, we expect to have some instability in the calculation due to the change in the sign of the Hessian. Thus, we expect that an instability in our calculation will be telling us something relevant about the nature of the stationary points we are counting.

5.3. The calculation of the complexity.

To find the stationary points of H with the spherical constraint we can use the Lagrange method. In this way we obtain [53],

$$-\frac{p}{p!} \sum_{kl} J_{ikl}\sigma_k\sigma_l - p\frac{1}{N}H(\sigma)\sigma_i = 0 \tag{163}$$

Given that we want to fix the energy density $H(\sigma)/N = E$, the equations become,

$$-\frac{p}{p!} \sum_{kl} J_{ikl}\sigma_k\sigma_l - pE\sigma_i = 0 \tag{164}$$

and thus we have,

$$\mathcal{N}(E) = \int D\sigma \, \prod_i \delta\left(-\frac{p}{p!} \sum_{kl} J_{ikl}\sigma_k\sigma_l - pE\sigma_i\right) \, \det\left(-\frac{p(p-1)}{p!} \sum_{kl} J_{ikl}\sigma_l - pE\delta_{ik}\right) \tag{165}$$

with the complexity given by,

$$\Sigma(E) = \lim_{N\to\infty} \frac{1}{N} \log \mathcal{N}(E) \tag{166}$$

In order to average over J we have to understand whether the self-averaging quantity is $\mathcal{N}$ or Σ. In general it is the complexity, since extensive quantities are self-averaging, while exponentials are not (in the statics we had to average F rather than Z). However, in the PSM we have a further simplification: in absence of external magnetic field we have that

$$\overline{\log \mathcal{N}} = \log \overline{\mathcal{N}} \tag{167}$$

and thus we can simply average the number, which is much simpler than averaging the logarithm of it. Equation (167) holds because the PSM is a 1RSB system at the static level. It can be proved [54] that if the static overlap matrix of *configurations* is kRSB, the corresponding overlap matrix of *magnetizations* is $(k-1)$RSB. For the PSM this implies that the complexity calculation is 0RSB and can therefore be performed at an annealed level. We give the usual exponential representation of the δ-function,

$$\prod_i \delta(X_i) = \int \frac{D\mu}{(2\pi)^N} \, \exp\left(i \sum_{i=1}^N \mu_i X_i \right) \tag{168}$$

On the other hand, for the determinant we can use an integral representation in terms of Grassmann variables (fermions) [23],

$$\det A_{ik} = \int D\bar{\psi} \, D\psi \, \exp\left(\sum_{ik=1}^N \bar{\psi}_i A_{ik} \psi_k \right) \tag{169}$$

where $\bar{\psi}$ and ψ are anti-commuting N-dimensional Grassmann vectors,

$$\{\bar{\psi}_i, \psi_i\} = 0 \tag{170}$$

Note that we could have used commuting variables to write the determinant, but at the price of introducing replicas [50]. So, putting all together, we have,

$$\Sigma(E) = \frac{1}{N} \log \overline{\mathcal{N}(E)} = \frac{1}{N} \log \int D\sigma \frac{D\mu}{(2\pi)^N} D\bar{\psi} D\psi \, \overline{\exp[S(\sigma, \mu, \bar{\psi}, \psi)]} \tag{171}$$

where the action S is given by,

$$S(\sigma, \mu, \bar{\psi}, \psi) = -ipE \sum_i \mu_i \sigma_i - i\frac{p}{p!} \sum_{ikl} J_{ikl} \mu_i \sigma_k \sigma_l - pE \sum_i \bar{\psi}_i \psi_i - \frac{p(p-1)}{p!} \sum_{ikl} J_{ikl} \bar{\psi}_i \psi_k \sigma_l \tag{172}$$

Part of this action depend on the disorder and it therefore must be averaged over the couplings J_{ikl}. This is not difficult to do, since these are Gaussian integral of the form,

$$\overline{\exp[S_J]} = \prod_{ikl} \int dJ_{ikl} \exp\left[-\frac{1}{2} J_{ikl}^2 \frac{2N^{p-1}}{p!} - J_{ikl}(\dots) \right] \tag{173}$$

we only have to be careful about a few technical details: first, the terms $\mu\sigma\sigma$ and $\bar{\psi}\psi\sigma$ must be symmetrized before averaging; second, it can be proved that the mixed

commuting-anticommuting terms obtained from the integrals are zero [52], so that we can effectively treat separately the commuting and anticommuting parts; third, we have to remember that we are integrating on the surface of a sphere of radius $\sqrt{N}$, due to the spherical constraint. The integral of the commuting part can be performed exactly, while for the anticommuting part we will have to work a bit more. Once the J integral is performed, we obtain,

$$\Sigma(E) = \left[-\frac{1}{2} \log(p/2) + \frac{1}{2} - E^2 \right] + \frac{1}{N} \log I \tag{174}$$

The term in square bracket comes from the J integral of the commuting part, while I comes from the fermionic part,

$$I = \int D\bar\psi D\psi \exp\left[-\frac{1}{4N} p(p-1) \left(\sum_i \bar\psi_i\psi_i \right)^2 - pE \sum_i \bar\psi_i\psi_i \right] \tag{175}$$

To treat this integral we use an inverse Gaussian integration (Hubbard-Stratonovich transformation), and write,

$$I = \int D\bar\psi D\psi \int d\omega \ \exp\left[-\frac{N\omega^2}{p(p-1)} + (i\omega - pE) \sum_i \bar\psi_i\psi_i \right] =$$
$$\int d\omega \ \exp\left[N \left(-\frac{N\omega^2}{p(p-1)} + \log(i\omega - pE) \right) \right]$$
$$\int d\omega \ \exp\left[NG(\omega) \right] \tag{176}$$

where we have performed the (diagonal) fermionic integral. The crucial feature of this formula is the factor N in the exponential: for $N \to \infty$ we can use the saddle-point method and write,

$$I = \exp[NG(\hat\omega)] \tag{177}$$

where $\hat\omega$ satisfies the saddle-point equation,

$$\left. \frac{\partial G(\omega)}{\partial \omega} \right|_{\hat\omega} = 0 \tag{178}$$

It is easy to check that the saddle-point solution $\hat\omega$ lies on the imaginary axis, and thus it is convenient to define,

$$\omega = iz \tag{179}$$

such that,

$$G(z) = \frac{Nz^2}{p(p-1)} + \log(z - pE) \tag{180}$$

Finally we can write the complexity of the PSM as,

$$\Sigma(E) = -\frac{1}{2} \log(p/2) + \frac{1}{2} - E^2 + \frac{N\hat z^2}{p(p-1)} + \log(\hat z - pE) \tag{181}$$

where the solution $\hat{z}$ of the saddle point equation $\partial_z G(\hat{z}) = 0$ is,

$$\hat{z} = \frac{p}{2}\left(E + \sqrt{E^2 - \frac{2(p-1)}{p}}\right) \tag{182}$$

The second root gives a sub-leading contribution in the thermodynamic limit [53].

5.4. Threshold energy and saddles.

From the form of $\hat{z}$ we clearly see that something weird happens when the absolute value of the energy E becomes too small. In fact, for the complexity to be a well defined physical quantity we must have $\hat{z}$ real. If we define the *threshold energy* as [47, 42],

$$E_{th} = -\sqrt{\frac{2(p-1)}{p}} \tag{183}$$

we can write,

$$\hat{z} = \frac{p}{2}\left(E + \sqrt{E^2 - E_{th}^2}\right) \tag{184}$$

We see that $\hat{z}$ is real, and thus the complexity physically defined, only for,

$$E \leq E_{th} \tag{185}$$

What have we obtained ? If we plot the complexity, we see that it is an increasing function of E, with negative second derivative. The complexity is zero at an energy E_0: below this energy the complexity is negative, and thus the number of states is exponentially small in the thermodynamic limit. The energy E_0 corresponds thus to the *ground state* of the system, the lowest part in our landscape. On the other hand, the complexity grows up to $E = E_{th}$ beyond which it is no longer defined, since $\hat{z}$ takes an imaginary part. Therefore, the interval $[E_0 : E_{th}]$ is the physical band of states of the PSM, and all the states with $E > E_0$ are *metastable*.

A natural question at this point is: what happens above the threshold energy ? Why is the complexity no longer defined in that regime ? In order to answer these questions, we have to remember that we disregarded the modulus of the determinant of the Hessian, and that we therefore expected to have some problems if minima were no longer dominant in the energy regime under consideration. This is exactly what is going on here: above E_{th} minima are not dominant anymore, but unstable saddles are, so the Hessian gets the contribution of the negative eigenvalues of saddles. To see this we have to recall that the anticommuting (fermionic) part of our total integral was basically nothing else that the *average determinant of the Hessian*,

$$\Delta = \overline{\det\left(\frac{\partial H}{\partial\sigma_i\partial\sigma_k}\right)} \tag{186}$$

What we have obtained above can thus be rewritten as,

$$\Delta = \exp\left(\frac{N\hat{z}^2}{p(p-1)}\right) \, (\hat{z} - pE)^N \tag{187}$$

We see that as long as $E \leq E_{th}$, and thus $\hat{z}$ is real, Δ is positive (it is easy to see that the term $\hat{z} - pE$ is positive). This means that below the threshold the Hessian is *on average* positive-defined, and this is the same as saying that *on average* minima dominate in this energy regime. On the other hand, for $E > E_{th}$, we have $\hat{z} = a + ib$, and if we plug this into Δ we obtain [55],

$$\Delta(E) = (-1)^{k(E)N} \, \exp[Ng(E)] \tag{188}$$

where $k(E)$ and $g(E)$ are two not-too-complicated functions of E. In this energy regime, thus, the sign of the determinant oscillates when N goes to infinity. This is exactly what we would expect from the determinant of a matrix with $k(E)N$ *negative eigenvalues*. In fact, it is possible to calculate the eigenvalue spectrum of the Hessian and prove that $k(E)$ is exactly the fraction of negative eigenvalues of the Hessian [55].

The physical picture is therefore the following: below the threshold the energy landscape is dominated by minima, and the Hessian is positive on average. In this phase disregarding the modulus is harmless, and the complexity we find in this way is well defined. On the other hand, above the threshold the landscape is dominated by unstable saddles, and the average determinant gets an oscillating part. Having disregarded the modulus, we detect this transition as the point where the complexity develops an imaginary contribution. However, if we are not too picky, we can define a new physical complexity in this phase, by isolating the factor $(-1)^{kN}$ and taking the logarithm of the real part $\exp[Ng]$. By doing this we are in fact computing the complexity of saddles dominating at energy $E > E_{th}$ [56].

5.5. The equation for the self-overlap

What we have said above about the threshold and saddles may seem a bit exotic. In order to check all that, it is sound to consider the remaining equation for the self-overlap q. Once we specify the bare energy E of a minimum, we can work out the self-overlap of the associated finite T state. We expect that a *bona fide* pure state, i.e. a minimum of the TAP free energy, must have a well defined self-overlap, indicating roughly the size of the state in the phase space. On the other hand, we definitely do not expect saddles to have a well defined self-overlap, since saddles are not trapping stationary points, and it is hard (although perhaps not impossible [57]) to define their size.

Given a solution with bare energy E of the first N equations, the corresponding equation for q reads,

$$-\frac{p}{2}q^{\frac{p}{2}-1} \, E + \frac{1}{2\beta(1-q)} - \frac{\beta}{4}\left[p(p-1)q^{p-1} - p(p-1)q^{p-2}\right] = 0 \tag{189}$$

By introducing the auxiliary variable,

$$y = \frac{1}{T} q^{\frac{p-2}{2}}(1-q) \tag{190}$$

we can rewrite the equation as,

$$p(p-1)y^2 + 2pEy + 2 = 0 \quad \text{giving} \quad y = \frac{-E \pm \sqrt{E^2 - E_{th}^2}}{p-1} \tag{191}$$

where E_{th} is the *same* threshold energy as we have introduced in the calculation of the complexity. Given that the self-overlap $q = \sum_i m_i^2/N$ must definitely be real, equation (189) does not admit solutions for $E > E_{th}$ and the self-overlap is not physically defined above the threshold. This is indeed what we expected: it is natural to associate a state to a minimum of the energy when we turn on the temperature, but it is not natural at all to do the same with a *saddle*.

What is the self-overlap at the threshold energy ? For $E = E_{th}$ we have $y^2 = E_{th}^2/(p-1)^2$ and thus from (190),

$$q_{th}^{p-2}(1 - q_{th})^2 = T^2 \frac{2}{p(p-1)} \tag{192}$$

This equation gives the self-overlap of the threshold states as a function of the temperature. We know that the PSM has a purely dynamic transition at T_d, where the correlation function, instead of decaying to zero, remains trapped for an infinite time at a plateau, $C(\tau) \to q_d$, for $\tau \to \infty$. Our interpretation of this phenomenon was that the dynamic configuration remains trapped in a region of the phase space of size (self-overlap) q_d. It is tempting to compare this value q_d with the self-overlap of the threshold states at T_d: indeed these are the *highest* metastable states, so it is reasonable to expect they are responsible for trapping the dynamics at T_d. Recalling the definition of T_d, we have,

$$T_d^2 = \frac{p(p-2)^{p-2}}{2(p-1)^{p-1}} \quad \Longrightarrow \quad q_{th}^2(1 - q_{th})^2 = \frac{(p-2)^{p-2}}{(p-1)^p} \tag{193}$$

This equation could easily be solved on a computer. However, we have a good guess for the solution: if we plug into it $q_d = \frac{p-2}{p-1}$, we see that it is identically satisfied. The important conclusion is that,

$$q_{th}(T_d) = q_d \tag{194}$$

This result confirms all our expectations: the dynamical overlap at the transition T_d has an asymptotic limit equal to the self-overlap of the threshold states. These states therefore are the ones trapping the dynamics, and forbidding it to relax to the equilibrium values.

Another way for the q equation to stop having solution, is by increasing the temperature, $T > T^\star(E)$, at fixed bare energy E. This means that, even though minima of the energy do not depend on the temperature, states, i.e. minima of the free energy,

do. When the temperature becomes too large, the paramagnetic states becomes the only pure ergodic states, even though the energy landscape is broken up in many basins of the energy minima. This is just one particularly evident demonstration of the fundamental different between pure states and energy minima.

5.6. Life with many metastable states

We have computed the complexity $\Sigma(E)$, a function of the bare energy E of the minima, which does not depend on the temperature. All these minima become states when $T \neq 0$. As we have seen, the bare energy E and the temperature T are the only variables we need in order to compute the other properties at finite temperature. In particular the free energy density of the states is a function $f = f(E, T)$.

We now ask what is the role (if any) of the complexity when computing the equilibrium properties of the system. A first intuitive answer is that there must be no role at all: after all, the complexity is zero for ground (stable) states, which rule the equilibrium properties of the system, and it is only different from zero for metastable states, which we expect to have no influence on equilibrium. In fact, it is not like that. We must remember that the PSM is a mean-field model, where even metastable states have an infinite lifetime, and contribute as stable states in partitioning the phase space in ergodic sub-components. So, metastable states do play a role also in determining equilibrium properties. We could expect, thus, that what follows is valid only for mean-field systems. Strictly speaking, yes. However, in real system, like supercooled liquids at low temperatures, many of the following observations apply as well, provided that we pay great attention to the "states vs energy minima" issue. More precisely, in the temperature regime where T is low enough so that the dynamics is activated, but high enough so that the system is still ergodic and at equilibrium, the dynamics consists in vibrations inside a potential energy minimum, with some rare jumps among minima. In this regime, which is the one close to the Mode Coupling temperature, a phase space decomposition as the one we are going to explain below is applicable [58].

Let us compute the equilibrium partition function Z of the system,

$$Z = \int D\sigma \exp[-\beta H(\sigma)] = \sum_\alpha \int_{\sigma \in \alpha} D\sigma \exp[-\beta H(\sigma)] = \sum_\alpha Z_\alpha \qquad (195)$$

where Z_α is the partition function restricted to state α (stable or metastable it may be). We have,

$$Z_\alpha = e^{-\beta N f_\alpha} \qquad (196)$$

and thus,

$$Z = \sum_a e^{-\beta N f_\alpha} \qquad (197)$$

In these formulas the free energy density of state α is $f_\alpha = f(E_\alpha, T)$, where E_α is the bare energy of state α. We want to pass from a sum over all states to an integral over

all bare energies,

$$Z = \sum_\alpha \int dE \; \delta(E - E_\alpha) \; \exp[-\beta N f(E,T)] =$$

$$= \int dE \; \mathcal{N}(E) \exp[-\beta N f(E,T)] =$$

$$= \int dE \; \exp\{-\beta N[f(E,T) - T\Sigma(E)]\} \equiv$$

$$\equiv \int dE \; \exp[-\beta N \Phi(E,T)] \tag{198}$$

where we have defined,

$$\Phi(E,T) \equiv f(E,T) - T\Sigma(E) \tag{199}$$

and where we have used the very definition of the number of states at energy E,

$$\mathcal{N}(E) = \sum_\alpha \delta(E - E_\alpha) \tag{200}$$

In the equation above we can use the saddle-point method in the limit $N \to \infty$: the integral is concentrated on the value $E_{eq}(T)$ which minimize the exponent. The *total equilibrium free energy density* $F_{eq}(T)$ is therefore given by,

$$F_{eq}(T) = -\frac{1}{\beta N} \log Z = \min_E[f(E,T) - T\Sigma(E)] = \Phi(E_{eq}(T), T) \tag{201}$$

with

$$\frac{\partial \Phi}{\partial E}(E_{eq}(T)) = 0 \tag{202}$$

From its definition we see that Φ is clearly a sort of *generalized free energy*, with f playing the role of the energy, and the complexity playing the role of the entropy,

$$\begin{aligned} f &= \mathcal{E} - TS \quad \text{with} \quad S \quad \text{entropy} \\ \Phi &= f - T\Sigma \quad \text{with} \quad \Sigma \quad \text{complexity} \end{aligned} \tag{203}$$

and putting together these formulas we have,

$$\Phi = \mathcal{E} - T(S + \Sigma) \tag{204}$$

so the complexity is the extra contribution to the total entropy due to the presence of an exponentially large number of metastable states. We recall that $\mathcal{E}$ is the *finite temperature* energy density of the states, which is different from the bare (zero-temperature) energy E. In fact, $\mathcal{E} = \mathcal{E}(E,T)$ and $\mathcal{E}(E,0) = E$.

From what said above we see that the total equilibrium free energy density is found by minimization with respect to E of the potential $\Phi(E,T)$, in which the complexity plays a major role. The bare energy density $E_{eq}(T)$ obtained minimizing Φ, fixes the equilibrium states of the system. The free energy density of these equilibrium states will then be $f_{eq} = f(E_{eq}(T), T)$. What is a bit surprising is that,

$$F_{eq} = f(E_{eq}, T) - T\Sigma(E_{eq}) < f(E_{eq}, T) \tag{205}$$

since the complexity is positive. In other words, *the free energy density of equilibrium states is larger than the global equilibrium free energy density.* This funny thing is due to the presence of an exponentially large number of metastable states: equilibrium is given by an ensemble of states, each one with rather large free energy density f_{eq}, but whose *collective* contribution to equilibrium is enhanced by their complexity, which lowers the global free energy F_{eq}.

This situation may seem paradoxical: equilibrium is given by a mixture of metastable states, but each of them is surrounded by infinite free energy barriers, so dynamically the system would not be able to exit from anyone of these states ! On the one hand, this is just a particular way of breaking the ergodicity, which is of course strictly valid only in mean-field. On the other hand, this situation makes much more sense in finite dimensions, where these metastable states may trap the dynamics for a time sufficiently long to allow us to define a complexity, but sufficiently short to make the system ergodic. This may indeed be the situation in structural glasses close to the glass transition [58, 59, 60].

5.7. Low temperatures, entropy crisis

The interval of definition of $\Phi(E, T)$ is the same as $\Sigma(E)$, that is $E \in [E_0 : E_{th}]$. Assuming that at a given temperature T the energy $E_{eq}(T)$ minimizing Φ lies in this interval, what happens if we lower the temperature ? Remember that the complexity is an increasing function of E, as of course is $f(E, T)$. When T decreases we favor states with lower free energy and lower complexity, and therefore E_{eq} decreases. As a result, it must exist a temperature T_0, such that,

$$E_{eq}(T_0) = E_0 \tag{206}$$

and thus,

$$\Sigma(E_{eq}(T)) = \Sigma(E_0) = 0 \tag{207}$$

Below T_0 the bare energy E_{eq} cannot decrease any further: there are no other states below the ground states E_0. Thus, $E_{eq}(T) = E_0$ *for each temperature* $T \le T_0$. As a result, if we plot the complexity of equilibrium states $\Sigma(E_{eq}(T))$ as a function of the temperature, we find a discontinuity of the first derivative at T_0, where the complexity vanishes.

A thermodynamic transition takes place at T_0: below this temperature equilibrium is no longer dominated by metastable states, but by the lowest lying states, which have zero complexity and lowest free energy density. The temperature T_0 can be computed by studying numerically equation (202). The following result should not be surprising at this point,

$$T_0 = T_s \tag{208}$$

The temperature where equilibrium is given for the first time by the lowest energy states, is equal to the static transition temperature. Above T_0 the partition function is

dominated by an exponentially large number of states, each with high free energy and thus low statistical weight, such that they are not captured by the overlap distribution $P(q)$. At T_0 the number of these states becomes sub-exponential and their weight nonzero, such that the $P(q)$ develops a secondary peak at $q_s \neq 0$.

In supercooled liquids, we can give an interesting interpretation of what is going on. As we have seen the total entropy is the sum of the entropy S inside each state and the complexity Σ. But in liquids the entropy of each energy minimum is (at low enough temperatures) very similar to the entropy of the crystal S_{CR}, while the total entropy is just the entropy S_{LQ} observed in the supercooled liquid phase. Thus we can write,

$$\Sigma(T) = S_{LQ}(T) - S_{CR}(T) \tag{209}$$

i.e. the complexity is the excess entropy of the liquid compared to the crystal. Therefore, the temperature T_0 is the temperature where the entropy of the liquid seems to become equal to the temperature of the crystal, as first observed by Kauzmann in 1948 [61]. This scenario (vanishing complexity at T_0) is normally known as *entropy crisis*.

Of course in real systems we cannot observe T_0, since it is far below the dynamical glass transition, where the system falls out of equilibrium. The possible existence of T_0 in real liquids relies on low temperature extrapolations of high temperature equilibrium data.

5.8. High temperatures, the threshold

When we raise the temperature we privilege states with higher free energy and complexity. Also in this case, thus, we must have a temperature beyond which we exit from our range of definition of the complexity. Indeed, there is a temperature T_{th}, such that,

$$E_{eq}(T_{th}) = E_{th} \tag{210}$$

i.e. the bare energy density of equilibrium states becomes equal to the threshold energy at T_{th}. What happens above T_{th}? If we close our eyes and insist minimizing the potential Φ, we see that the system would try to thermalize in an energy regime dominated by unstable saddles, and not by minima. This fact suggests that the dynamics above T_{th} is no longer trapped by minima, and that therefore it is ergodic. More precisely, we can argue that while below T_{th} equilibrium is in fact given by a superposition of metastable states with infinite barriers surrounding them, *above* T_{th} the system enters a phase dominated no longer by minima, but by saddles [62, 63, 56]. A crucial result, which can easily be proved, and which confirms this scenario, is the following,

$$T_{th} = T_d \tag{211}$$

The temperature T_{th} associated to the transition from minima to saddle (going up in temperature) is thus the same as the temperature T_d marking the passage from an ergodic to nonergodic dynamics (going down in temperature). In the light of this, it

becomes clearer the interpretation of the dynamics for $T > T_d$, but close to T_d: the landscape visited by the system in this phase is dominated by unstable saddle points, which have however a very small number of negative modes, since $T \sim T_d = T_{th}$ implies $E \sim E_{th}$. These objects cannot trap the dynamics for infinite times, but they can slow it down. In particular, the finite, but very long plateau of the dynamic correlation function $C(\tau)$, can be interpreted as a pseudo-relaxation of the system into a saddle with very few (order one) unstable modes [57]. At T_d the bare energy is E_{th} and unstable saddles turn into stable trapping minima. The plateau becomes infinite and ergodicity is broken.

The identification of T_d with T_{th}, and its resulting interpretation, is a crucial point in the physics of the PSM. It connects the dynamical and topological properties of the system in a very general way and it suggests that even in different systems where a glassy transition occurs, the topological properties of the underlying energy landscape may be the responsible for the slowing down of the system [68]. We have seen in the previous chapter that the dynamical equations of the PSM are just the Mode Couping equations, strongly suggesting that systems well described by MCT close to the glass transition, as fragile glasses, may have a dynamical behaviour similar to the PSM. As a consequence, one can try to extend to fragile glasses the topological approach developed in this chapter, which, as we have seen, is so closely related to dynamics. The cage effect, which as we have seen cannot explain the plateau in a mean-field model, can thus be reinterpreted in general as the effect of quasi-stable saddles probed by the system close to the glass transition [57].

A final remark. Mode coupling theory predicts a sharp transition at T_d, but this cannot be strictly true out of mean-field, where barriers are finite. In fact, even in fragile glasses, at T_d one just observes a very steep crossover, but not a transition [40]. However, it may be that the underlying description of the landscape, in terms of minima-to-saddle transition, is still valid [62]. In this way, a unique topological phenomenon would be responsible for the dynamical transition in the mean-field PSM, and of the sharp crossover in finite-dimensional fragile glasses [64, 66, 65, 67].

The complexity has at last unified all our results. The two transition temperatures are nothing else than the manifestation, at the static and dynamical level, of the lower and upper edges of the band of metastable states.

6. Conclusions

It was long enough, so let us be brief in these conclusions. We have seen that the PSM has two transitions. There is a thermodynamic transition at a temperature T_s, where the free energy switches from a paramagnetic state, to many spin-glass states. Moreover, T_s is also the temperature where the complexity of equilibrium states vanishes. What happens at T_s is a perfect realization of the entropy crisis scenario described by Kauzmann for supercooled liquids. Below T_s equilibrium is given by a non-exponential number of lowest free energy states, which are detected and described by a standard thermodynamic approach. Above T_s an exponentially large number of metastable states

dominates the partition function, due to their nonzero complexity. In this phase, we have the funny result that the free energy density of equilibrium states is larger than the global equilibrium free energy density. Thermodynamics is totally unaware of these states, and predicts a trivial paramagnetic state, with $P(q) = \delta(q)$.

At higher temperatures we have a purely dynamic transition $T_d > T_s$. When we arrive at this temperature coming from above, the dynamics gets trapped by metastable states, and the correlation time diverges. The equations describing such dynamical behavior are the same as the MCT equations for supercooled liquids. This suggests that what happens in the PSM at T_d is similar to what happens in real glasses close to the MCT temperature. The crucial difference, of course, is that in the PSM there can be no barrier crossing, since barriers are infinite, while in real glasses activation is present. On the other hand, the fact that standard MCT predicts a sharp dynamical transition at T_d seems to suggest that this theory too, as the PSM, does not account for activated events.

We have finally seen that there is a close relationship between the topological properties of the model and its dynamical behavior. In particular, the slowing down of the dynamics above but close to T_d is connected to the presence of saddles, whose instability decreases with decreasing energy. In fact, we have seen that the threshold energy level E_{th} separating saddles from minima, can be associated to the temperature $T_{th} = T_d$, marking the passage from ergodicity to ergodicity breaking. In this context the dynamical transition can be seen as a topological transition. The plateau of the dynamical correlation function, which has an interpretation in terms of cage effect in liquids, may be reinterpreted as a pseudo-thermalization inside a saddle with a very small number of unstable modes.

A very final warning. We should never forget that the PSM is a mean-field model, with no spatial structure at all. As a consequence, all physical modelizations and interpretations coming from the PSM, inevitably have a mean-field flavor. In particular, this is true for the topological interpretation of the dynamical transition: no fluctuations are taken into account, not to mention spatial heterogeneities, which may play a very important role. However, the arguments we gave in terms of phase space and topological concepts have at least the virtue of being simple and effective. If not pushed too far, they provide a nice tool to understand in a unifying way the physics of glassy systems.

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