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Critical Properties of the Potts Glass with many states

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[. . .] When I was a child
I caught a fleeting glimpse
Out of the corner of my eye [. . .]
D. Gilmour, R. Waters

To Chiara and Emma

Contents

Chapter 1

Overview

The main goal of this thesis is to investigate the critical properties of glassy systems and in particular of the Potts Glass.
It is in general very hard to study this model for a finite size systems, as it usually is for spin glass models, since we have just a few methods to move the exact results we can obtain from Mean Field Theory to finite dimensionality systems (and test their validity): the primary tool available in this case is the simulation, using Monte Carlo techniques, and its corresponding analysis, which is largely based on the Finite Size Scaling ansazt. In Mean Field Theory the Potts Glass exhibits a transition from a paramagnetic to a spin glass phase: the nature and the temperature of this transition depends on the number of states available for spin degree of freedom, p. For $p > 4$ this transition is expected to be discontinuous but without latent heat. There are basically no results known, except for a few ones which are not analytical, for finite dimensional systems, on whether this change in the nature in the transition holds or not, and if the transition happens at all, for different values of p. The aim of this thesis is to fill, at least in part, this gap, by studying the Potts Glass in three dimensions with $p = 4, 5, 6$.
As may appear evident in reading the thesis results are not incredibly precise and are not many: the simulation of these kind of systems is exceptionally hard not only from the physics' point of view, but also computationally. We were extremely lucky to be able to use the Janus computer to support us in the computation, otherwise we would not have been able to complete it. Nonetheless, the total timespan of the simulation campaign was a little more a year and a half. What we were able to obtain is a clear indication of the nature of the phase transitions under study and the critical temperatures at which they happen, together with the confirmation of an empirical equation on the temperature at which expect the spin glass transition given the number of available states, p. Moreover we were able to exclude the existence of a ferromagnetic phase, at least for the range of temperatures (which are L and p specific) we probed in our simulations: this confirms that we are looking at spin glass transition and that there are not "interferences" effects between ferromagnetic and spin glass ordering in the phase

and at the transition we are characterizing.
The results we obtain by all means are to be intended more like a roadmap for successive works on the Potts Glass: they seem to suggest that there could be a change in the nature of the transition for some value of p higher than the ones taken in consideration in this thesis. From the behaviour of Parallel Tempering, and considering also the evolution of the critical exponents as a function of p, there is also the possibility that the change in the nature of the transition happens for the values we are considering: it may be that the small sizes of the system we are able to simulate are rounding the first order transition and make it look like a continuous one. However, this is just a hint: the simulation of systems with larger sizes could resolve doubts on the matter. In this sense this work is more a start of future research than its end.
This is a theoretical thesis, based on theoretical models which describe complex systems. The model is parametric in p, which is more or less like having more models in one: for instance the $p = 4$ pure Potts Model has been used in the modeling of, in two dimensions, adsorption of N_2 on Kr in graphite layers. In three dimensions it describes the behaviour of FCC antiferromagnetic materials, such as NdSb, NdAs and CeAs, in a magnetic field oriented toward the $(1, 1, 1)$ direction. Its disordered counterpart, the Potts Glass, is used in the study of orientational glasses (examples are fullurene, $N_2 - Ar$ and CuCN). The Potts Glass shares many connections with other spin glass models, also due to the richness of behaviours given by p, such as the REM model and the p-spin model.
Our preliminary finding that the critical exponents of the phase transition change as p grows, even if the transition still is continuous, can be seen as an enrichment of the phenomenology associated with the model. From this point of view understanding the behaviour and critical properties for a large interval of p values is both important from the theoretical side and for the possible future applications of the model. This thesis works in this direction: producing results associated to the range of p form 4 to 6. Plans to go to even larger values of p have been stopped by unmanageable complexity of the simulation associated to an ever increasing thermalization time. We see this work as an important step into extracting the complete wealth of information available from Potts models.

The thesis is organized as follows: in the first chapter we will quickly review many concept related to spin glasses, starting from the Ising model and ending with Parisi theory and the Mean Field description of the Potts Glass. The purpose of this chapter is familiarize the reader with the main concepts of Spin Glass theory, in particular (non-trivial) broken ergodicity, frustration, the Parisi order parameter and, in general, the Mean Field Theory of spin glasses. We start from the Ising Model so that even the reader not familiar with the subject can get his bearings.
Chapter two is a (very) quick review of Monte Carlo methods: it cointains the main concepts of Monte Carlo methods, such as importance sampling and the Metropolis and Heat Bath algorithms. It presents also Parallel Tempering, that

we have been using extensively in simulations.
Chapter three describes the simulations that we ran on the Potts Glass: all the parameters are described in detail and all the methods, such as the Quotient Method, are explained.
Chapter four contains a description the analysis and of the results we obtained in regard to the critical temperatures and the critical exponents. It also contains a section in which we put together all the information we have been gaining from the simulations to form a coherent picture.
A conclusion, that wraps up the preceding chapters, ends the thesis.

Chapter 2

Introduction

Ferromagnetism is an interesting and fascinating subject in Condensed Matter Physics: a finite fraction of the magnetic moments of materials such as Fe or Ni spontaneously acquire a polarization (at a low enough temperature) and give rise to a macroscopic magnetization.
A simple model to describe the behaviour of this magnetic moments is the Ising model. In this chapter we will start from the Ising model to understand spin glasses.

2.1 A few initial pointers

Before analyzing some of the models that describe ferromagnetism, we shall devote a few moments to introduce a few of the most important tools to be used in the description of these models. While this is not by any means a complete approach to the subject, it's probably best to point them out here. A more complete discussion about models and observables can be found in [1] and [2].

2.1.1 The order parameter

When dealing with phase transitions, as we will, it is of paramount importance to understand and use currently a quantity called *order parameter*. This is a quantity which is defined to be 0 in one of the phases and to have some other value (non zero) in the other phase. There is no clear indication on which order parameter is better for a certain system, even thought quite often there is a close connection between the chosen order parameter and the symmetries of the Hamiltonian. For example: if we deal with magnetic dipoles, as in the case of the models discussed in this chapter, a clear example of a quantity that goes from zero to some value while the phase changes is the magnetization, which we will define formally in a moment. This quantity is linked to the symmetry of the Hamiltonian: if for example we describe the magnetic moment as a vector (of a dipole moment), the Hamiltonian has spherical symmetry and so is invariant

under a global rotation. In the non-magnetized phase each dipole is free to point anywhere, and so there is no preferred direction, the average of the spins is null. Once we reach the low temperature magnetized phase, then this is suddenly not true, and the spins prefer to point to one of the directions available: suddenly the magnetization reaches a non null value. In this case we have lost some of the initial "symmetry", this is often called a *natural symmetry breaking*. While continuing the example it is worth noting that initially, in the high temperature phase, the Hamiltonian had a $O(3)$ symmetry, while in the low temperature phase the symmetry is restricted to an $O(2)$ symmetry (rotations around the vector which is the one "preferred").
The notion that a system can find itself in states which break the symmetry of the Hamiltonian is very profound: it means that the ergodic hypothesis (that once it has reached equilibrium the system should be found in some configuration proportionally to the Gibbs probability $\propto e^{-\beta E}$) is violated. If, for example, we think of a ferromagnet with all its spins aligned in the "up" direction, it will *never* be found in the configuration in which all the spins point "down", in the limit $N \to \infty$ of course, and its motion is restricted to the part of the phase space in which the magnetization is positive. This situation we call *broken ergodicity*. It is important to stress that, strictly speaking, broken ergodicity and broken symmetry can only occur in infinite systems. In a finite system the entire configurations space is accessible: a finite ferromagnet in a configuration with "up" spins will eventually fluctuate over to a configuration with "down" spins (and then back again, many times) for any non zero temperature.

2.1.2 The correlations

A lot of information about phase transitions comes from diffusion experiments in which one send particles (photons, electrons or neutrons, for example) and then studies the diffusion to which they are subject. For the theory, and the simulation too, the correlation length and the correlation function play a pivotal role. In the phase transition of liquid mixtures one observes an opalescence, Einstein and Smoluchowski explained that are linked to the fluctuations of density and hence of the refraction index, due to an anomalous diffusion of light: we are basically probing the system with photons. In magnetic system one prefers to use neutrons since they tend to be more penetrating and to be able to avoid, at least on first approximation, multiple scatterings.
This scattering involves in this case the *two-point* correlation function of spins, which is defined as:

$$G^{(2)}(\vec{i},\vec{j}) = \langle \vec{\sigma}_i \cdot \vec{\sigma}_j \rangle, \tag{2.1}$$

where $\langle\,\rangle$ is a thermal average.
Since in most of the cases our systems are invariant for translation, this quantity really depends only on the difference $\vec{i}-\vec{j}$, and, if we can also assume isotropy, only on the distance $r = |\vec{i}-\vec{j}|$, which is like saying that $G^{(2)}(\vec{i},\vec{j}) = G^{(2)}(r)$. Obviously no real lattice is completely isotropic and invariant for translations,

but one can assume it is on scales which are big enough compared to the reticular distance, a.
From the definition of $G^{(2)}(r)$ we can see that it measures the relative alignment between two spins at a distance r: since in the ordered phase spins point for the biggest part in the same direction, if we want to study it fluctuations it's better to subtract, from $G^{(2)}$, its average, defining in this way the *connected* correlation function

$$G_c^{(2)}(r) = \langle(\vec{\sigma_i} - \vec{\sigma_0}) \cdot (\vec{\sigma_j} - \vec{\sigma_0})\rangle = \langle\vec{\sigma_i} \cdot \vec{\sigma_j}\rangle - |\vec{\sigma_0}|^2 \tag{2.2}$$

where $\vec{\sigma_0}$ is defined as $\vec{\sigma_0} = \langle\vec{\sigma_i}\rangle$. For $T > T_c$ the average value $\vec{\sigma_0}$ is null, so that from $G_c^{(2)}$ we recover the original $G^{(2)}$.
Nearby spins tend to be correlated: this correlation is, far from the critical point, extended only for some distance ξ, which is called *correlation length*, this is basically the extension of "blob" of spins who retain the same state. More formally we can define the correlation length as:

$$G_c^{(2)}(r) \approx e^{-r/\xi}, \;\; r \gg, a \;\; T \neq T_c. \tag{2.3}$$

Around T_c there's a change of dynamics and the correlation assumes another behaviour, the one of a power law:

$$G_c^{(2)}(r) \approx \frac{1}{r^{2-d+\eta}}, \;\; r \gg a, \;\; T = T_c, \tag{2.4}$$

where we have introduced our first critical exponent, η, also called the *anomalous dimension*. This power law behaviour indicates that at criticality fluctuations of the order parameter are correlated on all length, and that the correlation length around criticality becomes infinite (at least in second order phase transitions, while in first order ones it remains finite). If we indicate $t = (T - T_c)/T_c$, around the transition we can say that

$$\xi(T) = \begin{cases} \xi_+ t^{-\nu}, & T > T_c, \\ \xi_-(-t^{-\nu}), & T < T_c, \end{cases} \tag{2.5}$$

where ν is the critical exponent of the correlation length. We shall see some more critical exponents later in this chapter.
This two different behaviours can be actually merged in to one by writing

$$G_c^{(2)}(r) = \frac{1}{r^{d-2+\eta}} f\left(\frac{r}{\xi}\right) \tag{2.6}$$

where f is a *scale function* which depends only on the adimensional ratio r/ξ which behaves as $f(x) \sim e^{-x}$ when x if big, while $f(0)$ can be chosen to be 1, to fix the normalization. The dependency of this function from temperature is mediated only by $\xi(T)$.

2.1.3 Critical dimensions

Even if the real world is three dimensional it is sometimes useful to forget about it, and just consider the dimensions d of the model as one of the many variables of the system. In fact, there are some cases in which the systems which we try to model present, even in the three dimensional world, a two or even one dimensional behaviour: for example graphite's layers just barely interact, so to render the system, effectively, bidimensional. In another way, there could be a variation of the nature of the dimensional behaviour of the system depending on some parameter: an example of this could be a three dimensional system of magnetic dipoles in which different planes interact with couplings $J_z \ll J$, where J are the couplings between spins on the same plane. At high temperature, where the correlation length $\xi(T)$ is small, interaction between different planes is small, due to the definition of the coupling. But when the temperature is lowered ξ increases, with the effect that big areas of the plane is constituted of spins in the same state, which behave as a unique big magnetic dipole: in this case, even if J_z is small, the interaction between planes becomes relevant, changing the behaviour of the system from two to three dimensional.
Albeit these examples, there is at least another reason to consider the dimensionality of the system, d, as a parameter. The existence of a phase transition for a given Hamiltonian depends on the dimensionality of the system: in fact if we lower the number of dimensions in which the system lives, fluctuations become increasingly pronounced, destroying order and thus lowering the critical temperature, until eventually there is no longer a transition. Any given model, then, selects a *lower critical dimension*, d_l, such that for $d < d_l$ there is no phase transition for any T. In general one finds that for discrete symmetry models $d_l = 1$, while for models with continuous symmetry one has $d_l = 2$. Together with the lower an *higher critical dimension* d_s exists: critical exponents depend on the dimensionality of the system, too. When $d > d_s$, then the critical exponents are the same as the ones one can extract from the mean field theory treatment, which we will discuss briefly, of the system itself. The interval of values $d_l < d < d_s$ is the most interesting, and also the one where statistical fluctuations play a fundamental role.

2.2 The Ising and Potts models

2.2.1 The Ising model

The Ising model describes variables (which are the modelization of the magnetic dipoles we are dealing with in a ferromagnet), called *spins*, which sit on a regular d-dimensional lattice. Spins interact only with nearest neighbours, via coupling constants J, which can be positive (for a ferromagnet) or negative (antiferromagnet). Spins can have one of the two values ± 1, describing the magnetic moment pointing up or down respect to some axis, on which we take the projection. We

can then write the Hamiltonian as:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \quad + \quad h \sum_i .\sigma_i \tag{2.7}$$

The system can interact also with a constant external magnetic field, h. The notation $\langle i, j \rangle$ express the sum only over nearest neighbour: in another way we could have written the sum over $i < j$ and used the couplings as J_{ij} in which J_{ij} was non null only if the spins were nearest neighbours and null otherwise.
The magnetization of the system is calculated as:

$$m = \frac{1}{N} \left\langle \sum_i \sigma_i \right\rangle . \tag{2.8}$$

If we consider the model in $d \geq 2$ and null field, while the temperature is high enough, spins are randomly oriented either up or down, and the net magnetization of the system, in the thermodynamic limit, is null. Lowering the temperature, all of the spins tend to orient themselves in one of the two available directions, thus creating a spontaneous net magnetization for the whole system.

$$|m_s(T < T_c, h = 0)| > 0. \tag{2.9}$$

We are then in the presence of a phase transition (which is absent if $d = 1$) from a paramagnetic to a ferromagnetic phase. This transition happens at a temperature T_c.
For $h = 0$ we are in the presence of a twofold degeneracy, since both states in which all the spins are aligned in one of the two available directions are possible. To remove this degeneracy we can apply a small field to the system and then let the field go to zero, finding, for $T < T_c$:

$$m_s = \lim_{h \to 0} m(T, h), \tag{2.10}$$

which will be positive if we used a field pointing in the "up" direction, or negative otherwise. This comes from the fact that the Hamiltonian is invariant for global inversion of the sign: $\sigma_i \to -\sigma_i$.
The Ising model can be exactly solved for $d = 1$ and $d = 2$. In the latter the solution is quite lengthy and can be found on textbooks of Statistical Mechanics such as the already cited [1] and [2], so we won't cover it here. For $d = 3$ there is no known exact solution.

2.2.2 Mean Field Theory for the Ising model

Each spin in the Ising model interacts with both the external field and the field generated by neighbouring spins. The latter is obviously a dynamical variable of the system, which cannot be controlled externally, which fluctuates depending on

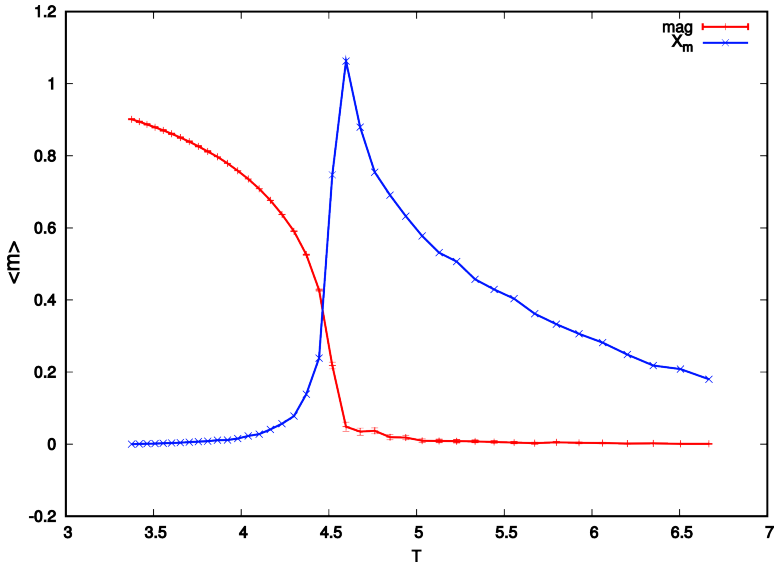


Figure 2.1: Magnetization (in red) for the three dimensional Ising model, from a Monte Carlo simulation of $L = 64$, using Parallel Tempering for 40 temperatures around the critical value, $T_c \approx 4.51$. In green a sketch of the magnetic susceptibility, rescaled to fit the graph, and hence completely out of scale.

the configurations that the system takes. The idea of the *mean field approximation* is to replace this interaction between neighbouring spins with the average of the field of all the spins of the system, except the one we are "looking at". In doing so we will let the spin interact, in some sense, with all the spins of the system, or, if we want to look at the thermodynamical limit, we are dealing with a $d = \infty$ system.
Even if this limit may appear very distant from the reality of the system we are trying to write a model for, we will see that some of the most essential features of magnets will be described in a quite accurate manner. This approximation was first tried by Braggs and Williams, so it's known by their names.
Let's now consider an Ising model defined on a d-dimensional lattice, with the same Hamiltonian as before:

$$\mathcal{H} = -\frac{J}{2}\sum_{\langle i,j\rangle}\sigma_i\sigma_j - h\sum_i \sigma_i, \tag{2.11}$$

where we consider each distinct pair i, j once. We define, again, the magnetization as:

$$m = \frac{1}{N}\left\langle \sum_i^N \sigma_i \right\rangle, \tag{2.12}$$

where by $\langle\rangle$ we express the thermal average. We can write the product $\sigma_i\sigma_j$ as:

$$\begin{aligned}\sigma_i\sigma_j &= (\sigma_i - m + m)(\sigma_j - m + m) \\ &= m^2 + m(\sigma_i - m) + m(\sigma_j - m) + (\sigma_i - m)(\sigma_j - m), \end{aligned} \tag{2.13}$$

where taking the thermal average of the last term basically measures the fluctuations of the spins. The mean field approximation basically consists in the "forgetting" of this last term, writing the Hamiltonian as:

$$\mathcal{H} = -\frac{J}{2}\sum_{\langle i,j\rangle}\sigma_i\sigma_j - h\sum_i \sigma_i \approx -\frac{J}{2}\sum_{\langle i,j\rangle}\left[-m^2 + m(\sigma_i + \sigma_j)\right] - h\sum_i \sigma_i. \tag{2.14}$$

If now we call z the *coordination number* of the lattice (the number of the nearest neighbour spins, $z = 2d$) we can now rewrite the first term in the sum over $\langle i, j\rangle$ as:

$$-\frac{J}{2}\sum_{\langle i,j\rangle} -m^2 = \frac{1}{2}\sum_i Jzm^2 = \frac{1}{2}JzNm^2, \tag{2.15}$$

while the second term in the same sum can be rewritten as:

$$-\frac{J}{2} = \sum_{\langle i,j\rangle}(\sigma_i + \sigma_j) = -Jzm\sum_i \sigma_i. \tag{2.16}$$

So now we can rewrite the whole Hamiltonian as:

$$\mathcal{H}_{MF} = \frac{1}{2}NJzm^2 - (Jzm + h)\sum_i \sigma_i. \tag{2.17}$$

In this view all spins are decoupled, and hence we can calculate the partition function as:

$$\begin{aligned} Z_N^{MF} = \sum_{\{\sigma\}} e^{-\beta\mathcal{H}_{MF}} &= e^{-\frac{1}{2}\beta Jzm^2}\left(\textstyle\sum_{\sigma=\pm1} e^{(\beta Jzm+\beta h)\sigma}\right)^N \\ &= e^{-\frac{1}{2}\beta Jzm^2}\left[2\cosh\left(2\,\beta Jm + \beta h\right)\right]^N. \end{aligned} \tag{2.18}$$

The free energy per spin will be then:

$$f^{MF}(T,h) = -\frac{1}{\beta N}\ln Z_N^{MF} = \frac{1}{2}Jzm^2 - \frac{1}{\beta}\ln\left[2\cosh\left(\beta Jm + \beta h\right)\right]. \tag{2.19}$$

Now, given that the magnetization is the derivative of f in respect to the field h, this satisfies the self-consistent relation:

$$m = -\frac{\partial f}{\partial h} = \tanh\left(\beta Jzm + \beta h\right) \tag{2.20}$$

If now we want to study the appearance of magnetized phases, we have to study the transcendent equation:

$$m = \tanh\left(\beta Jm\right) \tag{2.21}$$

which can be easily done in a graphic way: in fact we can plot the hyperbolic tangent and the line $y = m$ and look for intersection points. The point $m = 0$ is always a solution. If the derivative of tanh $(\beta J m)$ in the origin is bigger than 1 (or, equivalently, if $\beta J > 1$), then there are two more solutions, of opposite signs but with the same modulus, $\pm m_0$. So for $\beta J z = 1$, and hence the temperature is $T_c = Jz/k$, we have a phase transition from a disordered to an ordered phase. Spins are aligned to the field, if we had a field which we will let it go to 0: if we have $h \to 0^+$, then the magnetization will be $m = m_0$, otherwise if $h \to 0^-$, $m = -m_0$.
In the case of a non null expected value of the magnetization the symmetry Z_2 is spontaneously broken. In the ordered phase, the remnant of this symmetry is that we can change one solution in the other, $m_0 \to -m_0$ and viceversa.

2.2.3 The critical exponents of the Ising model

Using Mean Field Theory we can calculate the critical exponents for the Ising model. Let's write

$$t = \frac{T - T_c}{T_c} \tag{2.22}$$

and rewrite the autoconsistent relation as:

$$m = -\frac{h}{kT_c} + (1 + t) \operatorname{arctanh} m. \tag{2.23}$$

Let's start with the case of $h = 0$: in this case, for $T \approx T_c$, $t \approx 0$, the value of the magnetization is small, so that we can expand in series the right hand side of the last equation, obtaining:

$$m_0 = (1 + t) \operatorname{arctanh} m = (1 + t) \left[m_0 + \frac{1}{3} m_0^3 + \frac{1}{5} m_0^5 + \dots \right]. \tag{2.24}$$

If we now invert this to obtain m_0, we get:

$$m_0 = (-3t)^{\frac{1}{2}} \left[1 + O(t) \right]. \tag{2.25}$$

So, the critical exponent β has a value of $\frac{1}{2}$, since this critical exponent is the one that "regulates" the behaviour of m near the critical temperature in absence of an external field:

$$m = m_0 (-t)^{\beta}, \tag{2.26}$$

while in presence of an external field the system behaves as:

$$\mathcal{M}(h, T_c) = M_0 h^{\frac{1}{\delta}}. \tag{2.27}$$

The critical exponent γ is related to the magnetic susceptibility χ as:

$$\chi(h = 0, T) = \begin{cases} \chi_+ t^{-\gamma}, & T > T_c, \\ \chi_- (-t)^{-\gamma}, & T < T_c. \end{cases} \tag{2.28}$$

Since $\chi = \partial m_0/\partial h$, we differentiate the equation 2.24 to obtain:

$$\chi = -\frac{1}{kT_c} + (1+t)\left(\frac{1}{1+m^2}\right)\chi. \tag{2.29}$$

Now, for $h = 0$ and $T > T_c$ we have $m_0 = 0$, so that χ satisfies se equation

$$\chi = -\frac{1}{kT_c} + (1+t)\,\chi, \tag{2.30}$$

which results in

$$\chi = \frac{1}{kT_c} t^{-1}. \tag{2.31}$$

On the other hand, if we have $h = 0$ and $T < T_c$, we have:

$$\chi = \frac{1}{2kT_c}(-t)^{-1}, \tag{2.32}$$

so that we can conclude that the critical exponent $\gamma = 1$.
To calculate the critical exponent δ, we consider equation 2.24 again, expanding the hyperbolic function and simplifying we obtain:

$$\frac{h}{kT_c} \approx \frac{1}{3}m^3 + O(m^5) \tag{2.33}$$

or

$$m \approx h^{\frac{1}{3}} \tag{2.34}$$

yielding $\delta = 3$.
Mean field treatment of the Ising model in d-dimensions has let us understand the behaviour of the model around the phase transition, and have a rough value of the critical exponents, which we resume in the table 2.1: the values are approximate, and will not yield true for systems at a specific dimensionality.

	Exponent	Value in MFT
Specific Heat, C	α	0
Order parameter, $m(T)$	β	1/2
Susceptibility, χ	γ	1
$m(h)$	δ	3
Correlation Length, ξ	ν	1/2
Anomalous Dimension	η	0

Table 2.1: Critical exponents of the Ising model in the mean field approximation

2.2.4 The Potts model

The Potts model is a generalization of the Ising model: aside its theoretical importance, it is very useful when describing spins which cannot be assimilated to a 2-states system and more freedom is needed.
To do this, the Potts model prescribes, for each spin, p available states, instead of just the two of the Ising model. Also, as we can see in the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \delta(\sigma_i, \sigma_j) \tag{2.35}$$

the interaction is different: it takes place only when the spins σ_i and σ_j are in the same state, in which case the contribution to the energy of the system is $-J$. Whereas the Ising model was invariant under global spin inversion $\sigma_i \to -\sigma_i$, the Potts model is invariant under the group $\mathcal{S}_p$ of permutations of p variables, which is a non abelian group if $p \geq 3$. In the Potts model we regard the "states" of the spins as label, which are in this sense inessential, and could be anything: any set of numbers or colors or whatever else.
In the case $p = 2$, if we take ± 1 as the values of the spins, using the identity $\delta(\sigma_i, \sigma_j) = 1/2(1 + \sigma_i \sigma_j)$, we can see that, excluding a multiplicative constant, the Potts model is equivalent to the Ising model we just discussed.
The partition function of the Potts model for a lattice of N spins is :

$$Z_N = \sum_{\{\sigma\}} \left[\mathcal{K} \sum_{\langle i,j \rangle} \delta(\sigma_i, \sigma_j) \right], \tag{2.36}$$

where we have written $\mathcal{K} = \beta J = J/kT$.

2.2.5 Mean Field Theory for the Potts model

We analyze the mean field theory for the Potts model, as we did for the Ising model. We shall see that the behaviour of this model is richer, in a sense, than in the Ising case: the nature of the phase transition changes depending on p. As said before in mean field theory each spin in the lattice interacts will all the other $N - 1$ spins, so that we can write the Hamiltonian as

$$\mathcal{H}_{MF} = \frac{1}{N} Jz \sum_{i<j} \delta(\sigma_i, \sigma_j) \tag{2.37}$$

where we have introduced for convenience a factor $1/N$ and z, as before, is the coordination number of the lattice.
To solve the model we will proceed in calculating the free energy, $F[\{\sigma\}] = U[\{\sigma\}] - TS[\{\sigma\}]$ as a function of configuration $\{\sigma\}$ and the look for its minimum. This approach is simplified by the fact that, even if to specify a configuration we have to indicate the state of each of the N spins, this function is degenerate,

since it can assume the same value for different configurations of the system: it is then useful to introduce variables which will make this propriety obvious. To do this we introduce, given a configuration $\{\sigma\}$ of the spins, $x_i = N_i/N$ the number of spins which are, for that configuration, in the state i, with $i = 1, 2, \ldots, p$. Obviously we need to impose

$$\sum_{i=1}^{p} x_i = 1. \tag{2.38}$$

Since there are $\frac{1}{2\,N_1\,(N_i-1)}$ coupling of type i in the Hamiltonian, the energy $U[\{\sigma\}]$ of this configuration is given by:

$$U[\{\sigma\}] = -\frac{1}{2N} Jz \sum_{i=1}^{p} N_i\,(N_i - 1). \tag{2.39}$$

Dividing now by the number of spins and considering the thermodynamic limit, $N \to \infty$, we obtain:

$$\frac{U[\{\sigma\}]}{N} \approx -\frac{1}{2} Jz \sum_{i=1}^{p} x_i^2. \tag{2.40}$$

Since there are

$$\frac{N!}{N_1!\,N_2!\,N_3!\ldots N_p!} \tag{2.41}$$

way of dividing the spins without an energy change, we have an entropy

$$S[\{\sigma\}] = k \log\left(\frac{N!}{N_1!\,N_2!\,N_3!\ldots N_p!}\right). \tag{2.42}$$

Using the Stirling approximation ($\log z! \approx z \log z$, if $z \gg 1$) for each term, and using the definition of x_i we can write:

$$\frac{S[\{\sigma\}]}{N} \approx -k \sum_{i=1}^{p} x_i \log x_i. \tag{2.43}$$

So that we can finally write the expression for the free energy per spin:

$$\frac{F(x_i)}{N} = f(x_i) = -\sum_{i=1}^{p} \left[\frac{Jz}{2} x_i^2 - k x_i \log x_i\right], \tag{2.44}$$

which we will minimize. We have also to keep in mind the condition expressed in (2.38): it will be automatically satisfied if we parametrize the x_i as [3]

$$\begin{aligned} x_1 &= \tfrac{1}{p}\,[1 + (p-1)s] \\ x_i &= \tfrac{1}{p}\,(1 - s)\,, \quad i = 2, 3, \ldots, p \end{aligned} \tag{2.45}$$

with $0 \le s \le 1$. If we assume $J > 0$ (the ferromagnetic case), this parametrization is mindful of the possible breaking of the symmetry of the group of permutations

$\mathcal{S}_p$ when we are in the phase of low temperatures. Substituting this expression for the x_i in the energy and in the entropy leads us to

$$\begin{aligned} \tfrac{\beta}{N} \quad & [F(s) - F(0)] = \\ = \quad & \frac{p-1}{2p}\mathcal{K}zs^2 - \frac{1+(p-1)s}{p}\log[1+(p-1)s] - \frac{p-1}{p}(1-s)\log(1-s) \\ \approx \quad & -\frac{p-1}{2p}(p-\mathcal{K}z)s^2 + \frac{1}{6}(p-1)(p-2)s^3 + \dots \end{aligned} \tag{2.46}$$

From this we can see that the cubic term of the free energy changes sign when $p = 2$. Let's consider the two cases in separate ways.
For $\mathbf{p < 2}$, the minimum condition for the free energy is expressed by

$$\mathcal{K}zs = \log\left[\frac{1+(p-1)s}{1-s}\right]. \tag{2.47}$$

$s = 0$ is always a solution for this equation, but for $\mathcal{K}z > q$ where q is the derivative of the right hand side of 2.47, we have another solution for $s \neq 0$. The two solutions coincide for $J\beta = \mathcal{K} = \mathcal{K}_c = q/z$, which is the critical point related to the transition for $p \leq 2$. In this case we have a continuous (or second order) transition.
For $\mathbf{p > 2}$, the situation is different, since changing $\mathcal{K}$, there is a critical value for which the free energy exhibits a *discontinuous* jump from $s = 0$ to $s = s_c$. This discontinuity is a characteristic of *first order* phase transitions (or discontinuous).In this case the critical values for $\mathcal{K}_c$ and s_c are obtained by solving simultaneously $F'(s) = 0$ and $F(s) = F(0)$:

$$\begin{aligned} z\mathcal{K}_c \quad &= \quad \frac{2(p-1)}{p-2}\log(p-1), \\ s_c \quad &= \quad \frac{p-2}{p-1}. \end{aligned} \tag{2.48}$$

Calculating the internal energy of the system,

$$U = -Jz\frac{p-1}{2p}s^2_{\min} \tag{2.49}$$

we see that for $\mathcal{K} = \mathcal{K}_c$ there's a jump in the function, corresponding to a value of the latent heat L per spin

$$L = Jz\frac{(p-2)^2}{2p(p-1)}. \tag{2.50}$$

2.3 Spin Glasses

Spin glasses are magnetic systems in which the interactions between magnetic moments are "in conflict" due to some quenched, or frozen in, structural *disorder*. This mean, among other things, that no conventional long range order

(ferromagnetic or antiferromagnetic) can be established. Nevertheless, these systems exhibit a transition into a phase in which spins are aligned with this random order. On the other hand these "conflicts" result in the other characteristic of spin glasses: *frustration*. Namely, we say a spin is in a frustrated state when, whichever state it is in, it cannot reach the lowest energy state, and so "agree" (where the meaning of "agree" depends on the sign of the coupling between the spin and the neighbours) with all its neighbours.
These two key elements, disorder and frustration, seem to suggest that the spin glass phase is intrinsically different from the forms of order we have been dealing until now, such as ferro or antiferromagnetic, and so new tools and concepts are needed to describe it. Experimentally it is not hard to find systems which behave as spin glasses, quite the contrary.
As it was the case with ferromagnets, we will employ models which will, hopefully, be simple enough to be used both theoretically and in simulation and still incorporate the necessary disorder and competing interactions that lead to frustration.
While we will consider spin glasses only of magnetic nature, which is to say that the "spin" degree of freedom is magnetic, it has been a while since people started to find spin glasses phases in different fields: properties analogous properties have been seen in ferroelectric-antiferroelectric mixtures (in which case the electric dipole moment takes the place of the magnetic dipole moment), in amorphous alloys and magnetic insulators (where the distances between magnetic moments is entirely different from that of the crystalline magnetic systems) and in disordered molecular crystals (where the electric quadrupole moment plays the role of the spin) in which a kind of orientational freezing has been observed.
Moreover a behaviour similar to the one of spin glasses has been observed not only in Physics: developments resulting from the study of spin glasses have found application in Computer Science, Biology and Mathematics.

A possible example of spin glass, which is well known, are alloys in the form $Eu_xSr_{1-x}S$. In the Eu-rich limit, this is a ferromagnet with ferromagnetic nearest neighbours and antiferromagnetic next-nearest neighbours interactions. The Sr is magnetically dead, so a substitution of Sr for Eu just dilutes Eu. We can write the Hamiltonian as

$$\mathcal{H} = -\frac{1}{2}\sum_{i,j} J_{ij}\, c_i c_j\, \vec{\sigma}_i \cdot \vec{\sigma}_j, \tag{2.51}$$

where c_i is 1 or 0 with probabilities x and $1-x$. This model has competing interaction, which, hopefully, will lead to frustration.

2.3.1 The Edwards-Anderson (EA) model

Starting form the Hamiltonian 2.51 we can simplify, if it turns out to be theoretically more convenient. The following Hamiltonian has been written first by

Edwards and Anderson in 1975 [5], in the paper that marks the start of spin glass Theory as an active area of Theoretical Physics. The model is defined on a translationally invariant regular lattice:

$$\mathcal{H} = -\frac{1}{2}\sum_{ij} J_{ij}\vec{\sigma}_i \cdot \vec{\sigma}_j, \tag{2.52}$$

where the J_{ij} are taken to be identically distributed independent random variables with distribution that depends only on the lattice vector separation $\vec{r}_i - \vec{r}_j$. In particular it's convenient to consider

$$P(J_{ij}) = \frac{1}{\sqrt{2\pi\Delta_{ij}}} \exp\left[-\frac{J_{ij}^2}{2\Delta_{ij}}\right], \tag{2.53}$$

a symmetric Gaussian distribution, or

$$P(J_{ij}) = \frac{1}{2}\delta(J_{ij} - \sqrt{\Delta_{ij}}) + \frac{1}{2}\delta(J_{ij} + \sqrt{\Delta_{ij}}), \tag{2.54}$$

a double delta function. In either case, the model is specified by

$$[J_{ij}^2]_{\text{av}} \equiv \Delta_{ij} \equiv \Delta(\vec{r}_i - \vec{r}_j), \tag{2.55}$$

where we have introduced the average $[\ ]_{\text{av}}$ as the average of the distribution of the random variables.
This model, in both the double delta and the Gaussian version, clearly has both the randomness and competing interactions we were looking for, but it turns out we can proceed to some further simplifications:

- instead of Heisenberg-like spins, $\vec{\sigma}_i$ we may consider Ising-like spins with a single component, $\sigma_{iz} \equiv \sigma_i$
- we can consider the interactions between spins to fall off very quickly, resulting in only nearest neighbours or next-nearest neighbours interactions
- we can "forget" to deal with a lattice, and just have spins interacting with a finite number of spins, which can be anywhere in the system

and still be able to obtain the spin glass phase. It's desirable that, even with any simplification, there should not be significant differences in the behaviour between models, given that all their forces fall off in the distance in the same way (eg. they are all nearest neighbours) and that the nature of the spins is the same (eg. we are dealing with Ising spins or Heisenberg spins).

2.4 How do we deal with disorder?

In the definition of the Hamiltonian of the EA model, we have introduced randomness, which in turn introduces special features in Statistical Mechanics. Basically we don't know all the parameters of the Hamiltonian we are trying to study, but only their distribution, for example of the J_{ij} or random fields h_i, so that we don't have a particular realization. We can, for example in simulation, simulate different distribution realizations, and then average over them, which corresponds to the $[\,]_{\rm av}$ average, but this is closer to experiments than to theory.
Also, we could calculate the quantities of interest for a given realization of the J_{ij}, but this is not what interests us: we want to calculate these quantities for the given distribution of these parameters.
Fortunately Statistical Mechanics comes in our help with the averaging in the limit of large systems. Just as it was the case with the ferromagnetic models, and in general, we know that the fluctuations of the energy of the system around the thermal average are of order $N^{-1/2}$, so we expect that the sample-to-sample fluctuations will go to zero in the limit of a large system. A quantity which exhibits this property is said the be *self-averaging*. If we know that the quantity that is of interest to us has this property, then we can expect different experiments to yield the same result, and even more interestingly, that the theoretical calculation in which we average over disorder agrees with the experiments. But there are some quantities which are not self averaging, for example the local internal field of a spin i which depends sensitively from the local environment. Most of the quantities which we want to measure are sums or integrals over the entire volume of the sample (so that we call them "extensive" quantities) and statistical fluctuations *will* become small for large systems.
We have thus two different kind of average to calculate: the first is the usual thermal average, which in principle is carried out in each sample, and the average over the disordered random parameters. As is often the case, the average that we want to calculate can be expressed as, or in terms of derivatives of, the free energy with respect to auxiliary fields. We then start with the partition function, which is the trace over the thermodynamic variables and function of the fixed interaction strengths for that sample:

$$F[J] = -T \ln Z[J]. \tag{2.56}$$

Now, $F[J]$ is an extensive variable, so we can think of it as self-averaging, and so the experimentally relevant quantity is

$$F \equiv [F[J]]_{\rm av} \equiv \int {\rm d}P[J]\, F[J] \;=\; -T \int {\rm d}P[J]\, \ln Z[J]. \tag{2.57}$$

It's important to note that it's $\ln Z$ which should be averaged, and not Z itself: the reason is that Z is *not* an extensive quantity, and so self-averaging cannot be expected to apply to it, and so $[Z]_{\rm av}$ is not a physically relevant quantity.

As an obvious extension of this argument one can calculate the magnetization in a macroscopic sample as

$$[M]_{\text{av}} = T\frac{\partial[\ln Z[J,h]]_{\text{av}}}{\partial h} \tag{2.58}$$

and in a similar fashion for other extensive quantities. For correlation functions we need to extend this definition (albeit just formally) to site-dependency:

$$[\langle\sigma_i\sigma_i\rangle - \langle\sigma_i\rangle\langle\sigma_j\rangle]_{\text{av}} = T^2\frac{\ln Z[J,h]]_{\text{av}}}{\partial h_i \partial h_j}. \tag{2.59}$$

How do we evaluate these averages? One way is to write down the formal expression for $F[J]$ or its derivative (for example obtained with perturbation theory) and average them, term by term, over the distribution of the J_{ij}. This procedure works, and it's practical. But it is also often very useful to be able to carry out the averaging formally from the beginning: this will leave us with a problem in which the disorder no longer appears explicitly. If the system is translationally invariant, we would end up with a nonrandom, translationally invariant Statistical Mechanics problem, which we would then be able to solve.
Since we want to average $\ln Z$ we cannot just write the integral in 2.57 as if we were dealing with Z: we basically want to "fix" the J_{ij} as *quenched* variables, and then let the spins σ_i just adapt to the couplings. If we were to write something like

$$[Z[J]]_{\text{av}} = \text{Tr}_{\ \sigma}\int\prod_{\langle i,j\rangle}\frac{\mathrm{d}J_{ij}}{\sqrt{2\pi\Delta_{ij}}}\exp\left(-\frac{J_{ij}^2}{2\Delta_{ij}} + \beta J_{ij}\sigma_i\sigma_j\right), \tag{2.60}$$

which can be solved by completing the square, we would be dealing, then, with the wrong Physics: we are in fact writing a nonrandom system in which both the spins and the coupling J_{ij} are thermodynamical variables, which are traced on the same footing. In the systems we will be dealing with, if we look at it from an experimental point of view, the J_{ij} are frozen in to their configuration when we prepare the sample to analyze by rapid cooling or, as we just mentioned, quenching. In this sense we may call the kind of average we want to do "quenched average".

2.4.1 The Replica Trick

We cannot write the integral as in 2.60, because we want to average over $\ln Z$ and not Z, since the free energy $F = -kT\ln Z$: we have a "trick", quite common in Statistical Mechanics of random systems, to deal with the complexity from that arising. It is called the replica method and it's based on the identity

$$\ln Z = \lim_{n\to 0}\frac{Z^n - 1}{n} \tag{2.61}$$

and the fact that the average of $[Z^n]_{\rm av}$ can be carried out almost as simply as $[Z]_{\rm av}$ if n is an integer. We write Z^n as

$$Z^n[J] = \mathrm{Tr}\ _{\{\sigma_1\},\{\sigma_2\},\ldots,\{\sigma_N\}} \exp\left(-\beta \sum_{\alpha=1}^{n} \mathcal{H}[\sigma^\alpha, J]\right). \tag{2.62}$$

We say then that we have replicated the system n times, and hence the terminology "replica method". The index α which appear in 2.62 identifies the replica and is called replica index. For the EA model, with Ising spins, the average of 2.62 over the Gaussian couplings is then

$$\begin{aligned} [Z^n]_{\rm av} &= \mathrm{Tr}\ _{\{\sigma_1\},\{\sigma_2\},\ldots,\{\sigma_n\}} \exp\left(\frac{1}{4}\beta^2 \sum_{ij} \Delta_{ij} \sum_{\alpha\beta} \sigma_i^\alpha \sigma_i^\beta \sigma_j^\alpha \sigma_j^\beta\right) \\ &\equiv \mathrm{Tr}\ _{\{\sigma\}} \exp\left(-\beta \mathcal{H}_{\rm eff}\right) \end{aligned} \tag{2.63}$$

which is basically like converting the disordered problem into a non-random one, involving four-spins interactions. For a general distribution of the J_{ij} we can write:

$$\beta\, \mathcal{H}_{\rm eff} = -\frac{1}{2} \sum_{ij} \sum_{p=1}^{\infty} \frac{1}{p!} [J^p]_c (\beta \sum_{\alpha=1}^{n} \sigma_i^\alpha \sigma_j^\alpha)^p, \tag{2.64}$$

where $[J^p]_c$ is the p-th cumulant of the distribution of the J_{ij}. After solving these effective problems in any way we can, we have to take the limit $n \to 0$ of the result.
The cumulants (here we report just the first two):

$$\begin{aligned} [J]_c &= [J_{ij}]_{\rm av} = \overline{J}, \\ [J]_c &= [J_{ij}^2]_{\rm av} - [J_{ij}]_{\rm av}^2 \equiv (\Delta J_{ij})^2 \end{aligned} \tag{2.65}$$

in terms with $p > 1$ introduce interactions, as to say: couplings, between different replicas of the disordered system.

2.5 Broken Ergodicity, the Spin Glass phase and order parameters

Since we don't know qualitatively how the spin glass phase is, we can't be sure that the order parameter we have defined for the ferromagnetic phase is still a good choice. In this section we will try to understand better what changes in the new phase, and it will turn out that we need a new order parameter.
In an Ising ferromagnet we do have broken ergodicity when we are dealing with an infinite system and a temperature that is below the transition temperature: as we said already, in this case the configuration space is basically divided in two (for two are the directions possible for the magnetization) and there is no way for

a system magnetized in one direction to go spontaneously into the region of the configuration space where the magnetization is in other direction. This has another very important consequence: when we write some quantity that is defined by a thermal average we have to be careful about what we mean. If we were to mean it as a conventional Gibbs average over all the spins configurations with the symmetric weight $\exp(-\beta\mathcal{H}[\{\sigma\}])$ then it would vanish by symmetry. Instead we restrict our averages over part of the configuration space: for example if in the ferromagnetic phase we restrict ourselves to one of the two halves just mentioned then the magnetizations would differ by sign, resulting in the two well known values of it. In this sense the broken ergodicity has to be put in "by hand" by restricting the trace we use to define the thermal averages to configurations near the chosen phase. In a ferromagnet we could restrict ourselves simply by applying a small field to the system (in the Hamiltonian) and then letting it go to zero once we have taken the thermodynamic limit. In this case it is crucial the order in which we take the limits: were we to take them in the opposite order (first $h \to 0$ and then $N \to \infty$) this would not, obviously, work. In another way, we could introduce the restriction over the trace by means of boundary conditions: if we want to end in the "up-spin" phase, we can set the spins on the boundary of the system to be fixed "up".
Another useful way to describe broken ergodicity is to interpret expectation values for quantities like $\langle\sigma_i\rangle$ as averages over time intervals $[0, t]$ taking the limit $t \to \infty$, noting that if there's broken ergodicity these long-time averages will not vanish.
In a spin glass we could suppose, as we did for the ferromagnet, to find two stable states related by an overall spin flip symmetry, but it turns out not to be the case: we have to take in account the possibility, given randomness and competing interactions, to find a *non trivial* broken ergodicity: in another way, we have to take into account the possibility to find many stable states. We could visualize the situation as a landscape where for each configuration we calculate the free energy F: in a ferromagnet there are just two states minimizing F below the transition. Under a temperature T_f, there will be many states that do the same for the spin glass: these minima will be the bottom of valleys of the energy separated by barriers which, in the limit $N \to \infty$ will become infinitely high, rendering impossible to move from valley to valley, thus breaking ergodicity. If we increase the temperature above T_f the valleys will become less deep and then just disappear, and there will be just one valley with the minimum at $m = 0$. The configurations $\{\sigma\}$ which contribute to the partition function inside a single valley (or phase, let's call a) all lie in the region of spin configurations space near the minimum (possibly comprising many sub-valleys).
When a system finds itself in one of these valleys it will exhibit the behaviour and the properties which is typical of that valley. In general, they will differ from true equilibrium properties, since these would include averaging over all valleys with appropriate relative thermal weights. If we wish to calculate the properties of the system inside a single valley (which as we said might differ, for example,

in the magnetization) we have to restrict our trace of the partition function only to the appropriate valley.
Since there many possible stable states, the trick to impose an external field, as we did in the ferromagnetic case, uncorrelated to the single spins magnetizations will not help in tentatively select out only a single phase: in this sense broken ergodicity makes the definition of "thermal averaging", and the notion of an order parameter for spin glasses, a non trivial task. In fact, different ways to project onto particular phases would lead to different values of the observables: this is also one of the main reasons why it is so difficult to write down a mean field treatment for Spin Glasses.
So far we have been dealing with what happens to a sample, but of course we want our results to be averaged over many samples, or, in another way, to be averaged over the disorder probability. The order parameter of a ferromagnet, the magnetization, even if averaged over the disorder will not do, for the reason outlined above, so we have to look for something else, even if it would clearly vanish in the limit of null external field: we have to look to some higher moments. If we were to consider the breaking of ergodicity as essentially a dynamical process, we could consider, as Edwards and Anderson did in their paper in 1975, [5], the order parameter as

$$q_{\mathrm{EA}} = \lim_{t\to\infty} \lim_{N\to\infty} [\langle \sigma_i(t_0)\, \sigma_i(t_0+t)\rangle]_{\mathrm{av}}\,, \tag{2.66}$$

where the average is over a long (infinitely long) set of reference times t_0. This would be null (in the limit of a vanishing external field) if the system is ergodic, and nonzero if the system is trapped inside a single phase. One must take the $N \to \infty$ limit before the $t \to \infty$ since the correlation will eventually die out, as a function of time, as true equilibrium is reached, for a finite system. Since, instead, an infinite system will never escape the valley it is in, the parameter q_{EA} measures the mean square single-valley local spontaneous magnetization, averaged over all possible valleys. In terms of thermal averages we would write it as

$$q_{\mathrm{EA}} = \left[\sum_a P_a (m_i^a)^2\right] \tag{2.67}$$

where

$$P_a = \frac{e^{-\beta F_a}}{\sum_a e^{-\beta F_a}}, \quad \text{and} \quad m_i^a = \langle \sigma_i^a \rangle \tag{2.68}$$

inside the valley (or phase) a. Assuming (it can be proved in mean field theory, and for single models) that this quantity is self-averaging we can write:

$$q_{\mathrm{EA}} = \frac{1}{N} \sum_a P_a \sum_i (m_i^a)^2. \tag{2.69}$$

This $q_{\rm EA}$ is not, of course, the mean square local *equilibrium* magnetization, for the reasons outlined above. If we consider

$$q = [\langle\sigma_i\rangle^2]_{\rm av} = [m_i^2]_{\rm av} = \left[\left(\sum_a P_a\, m_i^a\right)^2\right]_{\rm av} = \left[\sum_{ab} P_a P_b\, m_i^a m_i^b\right]_{\rm av} \tag{2.70}$$

this is the equilibrium (or Statistical Mechanics) order parameter, denoted simply by q. Equivalently we can write

$$q = \frac{1}{N}\sum_i \left[\sum_{ab} P_a P_b m_i^a m_i^b\right]_{\rm av}. \tag{2.71}$$

We can also define q for a single sample

$$q_J = \frac{1}{N}\sum_i m_i^2 = \frac{1}{N} P_a P_b\, m_i^a m_i^b. \tag{2.72}$$

We can see, from the definitions, that q differs from $q_{\rm EA}$ by having an inter-valley term. It is often useful to consider also

$$\Delta = q_{\rm EA} - q \tag{2.73}$$

(which is semidefinite positive, and zero only if there is just a single phase) which basically measures the degree of broken ergodicity. We can imagine the differences between $q_{\rm EA}$ and q by considering a non infinite system: on a long enough timescale (that could be *very* long) the system will, statistically, visit many valleys with their relative thermal weights, so that true equilibrium is reached and inter-valley terms in q contribute. On a shorter time scale there is no time for the system to change valley, so that only $q_{\rm EA}$ is the physically relevant quantity. Obviously we could imagine a somewhat intermediate picture, in which only a few valleys are "visitable" for the system (and so no true equilibrium is reached): in this case we should consider a quantity between these two limiting cases, q and $q_{\rm EA}$.
In ferromagnets the susceptibility can be written as

$$\chi_{\rm loc} = \frac{1}{N}\sum_i \chi_{ii} = \beta\left(1 - \frac{1}{N}\sum_i m_i^2\right) \tag{2.74}$$

where χ_{ii} is defined as $\chi_{ii} = \beta\,\langle(\sigma_i - \langle\sigma_i\rangle)^2\rangle$. We can then write, for a system in a single phase,

$$\chi_{\rm loc} = \beta(1 - q_{\rm EA}). \tag{2.75}$$

The average local equilibrium susceptibility, obtained with the equilibrium expression $m_i = \sum_a P_a m_i^a$, can be written as

$$\chi_{\rm loc} = [\chi_J]_{\rm av} = [\beta(1 - q_J)]_{\rm av} = \beta(1 - q), \tag{2.76}$$

where is worth noting that χ_J is not a self-averaging quantity if there is ergodicity breaking. While it's clear that in a macroscopic experiment χ, due to the fact that barriers are infinite, comes only from a single valley, since there is strict ergodicity breaking, if the barriers are not infinite one can hope to observe a crossover from single-valley to equilibrium in χ, from short to long observation times.
Another interesting quantity to look at, once we know we have many valleys, is the "overlap"

$$q_{ab} = \frac{1}{N}\sum_i m_i^a m_i^b, \quad \text{obviously for a single sample,} \tag{2.77}$$

when a and b run over the many different phases one can expect to observe values of q_{ab} in the range $[-1, 1]$. Following Parisi ([6], [7], [8] and [9]) is natural then to define the distribution

$$P_J(q) \equiv \langle \delta(q - q_{ab}) \rangle \equiv \sum_{ab} P_a P_b \delta(q - q_{ab}) \tag{2.78}$$

and its average over the couplings

$$P(q) \equiv [P_J(q)]_{\text{av}}\,. \tag{2.79}$$

For a system with just 2 phases, $P(q)$ is the sum of two deltas, and by introducing an external field, we can just simple it down to a single delta function. If there is strong ergodicity breaking $P(q)$ may have a continuous part, indicating there is, maybe, a continuum of possible overlaps between phases. Hence, by studying $P(q)$ we can tell systems in which we have a "conventional" broken symmetry from those where we have a non-trivial ergodicity breaking. Given the probability distribution we can then rewrite q and q_J as:

$$q = \int_{-1}^{1} P(q) q \,\mathrm{d}q, \quad \text{and} \quad q_J = \int_{-1}^{1} P_J(q) q \,\mathrm{d}q. \tag{2.80}$$

If we let the system be without an external field $P(q)$ is symmetric: it is in fact possible to find, for the overlap q_{ab}, the corresponding value $-q_{ab}$ by simply reversing all spins in a and b. If instead we apply a small field, then only the states with the magnetization aligned with the field will be selected, and therefore only positive overlaps will enter $P(q)$: the lower limit of the integral is then 0, and q is finite.
Until now we have devoted a lot of attention to different order parameters, even if we have not yet tried to represent them in the replica formalism we have introduced. We begin considering the ferromagnetic order parameter:

$$M = [m_i]_{\text{av}} \equiv [\langle \sigma_i \rangle]_{\text{av}} = \left[\frac{\text{Tr}_{\ \{\sigma\}} \sigma_i e^{-\beta \mathcal{H}[\{\sigma\}, J]}}{Z[J]} \right]_{\text{av}}, \tag{2.81}$$

and write $n-1$ factors of $Z[J]$ (applying the replica trick) on both numerator and denominator. In the limit $n \to 0$ the denominator goes to 1 so that we need to take the average over disorder only over the numerator. Introducing the replica indexes we find, then

$$M = \left[\text{Tr}_{\{\sigma_1\},\{\sigma_2\},\ldots,\{\sigma_n\}} \ \sigma_i^\alpha \exp\left(-\beta \sum_{\beta=1}^{n} \mathcal{H}[\{\sigma^\beta\}, J] \right) \right]_{\text{av}}, \tag{2.82}$$

where we can carry out the averaging over the disorder as we did for the calculation on $[Z^n]_{\text{av}}$, obtaining

$$M = \text{Tr}_{\{\sigma\}} \sigma_i^\alpha \exp(-\beta \mathcal{H}_{\text{eff}}), \tag{2.83}$$

which, taking the limit $n \to 0$, can be written as

$$M = \langle \sigma_i^\alpha \rangle, \tag{2.84}$$

where the "thermal" average is taken with the effective Hamiltonian $\mathcal{H}_{\text{eff}}$, since we can use the fact that

$$\text{Tr}_{\{\sigma\}} \exp(-\beta \mathcal{H}_{\text{eff}}) \equiv [Z^n]_{\text{av}} \to 1. \tag{2.85}$$

There is one big point that needs to be addressed here: our result should be independent from which replica α is the one chosen for σ_i^α, since all replicas are (supposedly) "created equal". What if they are not? What if some replicas are "more equal" than the others? If in the solution of our Hamiltonian all the $\langle \sigma_i^\alpha \rangle$ turn out to be equal then we have no problems, but what happens if it turns out they are not?
We turn our attention back to the equilibrium spin glass order parameter, finding

$$q = q^{\alpha\beta} \equiv \langle \sigma_i^\alpha \sigma_i^\beta \rangle \tag{2.86}$$

for any replicas $\alpha \neq \beta$, since otherwise we would obtain, for Ising spins, $(\sigma_i^\alpha)^2 \equiv 1$. Considering the possibility to have a broken replica symmetry, we have to average over all the possible ways to break it

$$q = \lim_{n \to 0} \frac{1}{n(n-1)} \sum_{\alpha \neq \beta} q^{\alpha\beta}. \tag{2.87}$$

In the same way we can express $P(q)$ as

$$P(q) = \lim_{n \to 0} \frac{1}{n-1} \sum_{\alpha \neq \beta} \delta(q - q^{\alpha\beta}). \tag{2.88}$$

If $P(q)$ is not a delta function but has a more complex structure, the matrix $q^{\alpha\beta}$ must depend on α and β in a non trivial way and the replica symmetry is

broken [18], which in turn signals the existence of many equilibrium states [11]. In another way, we can say that whenever averages depend on the indexes of the replicas they are calculated with, we have *broken replica symmetry.*

Comparing this to the expression of $P_J(q)$ in equation 2.78 we see that the distribution of values of the matrix elements $q^{\alpha\beta}$ in the replica symmetry breaking case and the distribution of the overlap between different states when there are many states must be the same.
Finally we can identify with q_{EA} the largest value of $q^{\alpha\beta}$ in a broken replica symmetry solution

$$q_{\mathrm{EA}} = \max_{\alpha\beta} q^{\alpha\beta}. \tag{2.89}$$

2.5.1 Susceptibilities

A quite important quantity in the study of spin glasses is the Spin Glass Susceptibility, which has the role corresponding to the one of the susceptibility for ferromagnets. This quantity is defined as

$$\chi_{\mathrm{SG}}(\vec{R}_{ij}) = [\chi_{ij}^2]_{\mathrm{av}} = \beta^2[(\langle\sigma_i\sigma_j\rangle - \langle\sigma_i\rangle\langle\sigma_j\rangle)^2]_{\mathrm{av}} \tag{2.90}$$

and its Fourier transform $\chi_{\mathrm{SG}}(\vec{k})$, evaluated for $\vec{k} = 0$.
Above the freezing temperature T_f this reduces to $\chi_{\mathrm{SG}} = \frac{\beta^2}{N}\sum_{ij}\langle\sigma_i\sigma_j\rangle^2$.
In a ferromagnet the susceptibility is the magnetization induced by an external field on the system per unit of external field, h. In a spin glass we can induce a non-zero q, even above T_f, by introducing random external fields h_i. We can then write

$$\langle\sigma_i\rangle = \sum_j \chi_{ij} h_j \tag{2.91}$$

and we can, by squaring and averaging over the disorder obtain

$$q = \sum_{ij}[\chi_{ij}^2]_{\mathrm{av}}\sigma^2 = \chi_{\mathrm{SG}}\sigma^2 \tag{2.92}$$

where σ^2 is the variance if the random field and where we have assumed that the random fields h_i are uncorrelated. We can see that σ^2 acts as a conjugate field for the order parameter q pretty much as the external constant field h did for the magnetization m in the ferromagnet. While above T_f we need h_i if we want have a non zero q, below T_f q is finite even if $\sigma^2 \to 0$, thus, by analogy with the ferromagnetic case, we expect the susceptibility, χ_{SG} to diverge when one approaches T_f from above: the correlation length of $\chi_{\mathrm{SG}}(\vec{r})$ diverges in the same way as the same quantity of the spin correlation function did in the ferromagnetic case.
One last important point: susceptibility is measurable, through what is called the non-linear susceptibility, which is defined as the coefficient of $-h^3$ in the expansion of the magnetization in powers of the external field:

$$m = \chi h - \chi_{\mathrm{nl}} h^3 + \cdots . \tag{2.93}$$

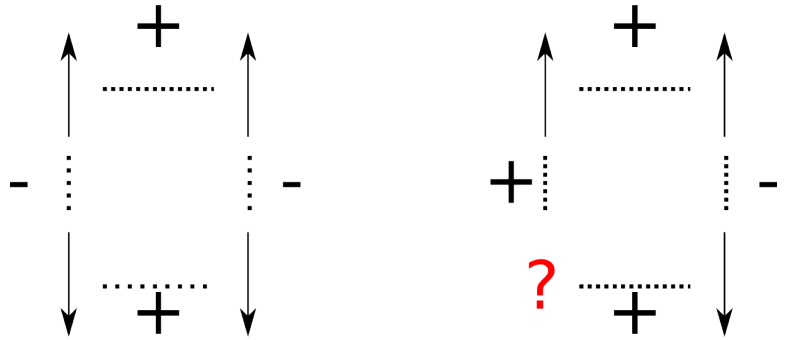


Figure 2.2: Plaquettes without and with frustrated spins: the spin at the site with the question mark cannot satisfy both its couplings at the same time.

As χ is proportional to the thermal variance $\langle(\sigma - \langle\sigma\rangle)^2\rangle$, one finds

$$\chi_{\rm nl} = -\frac{\beta^3}{3} N \left\langle \left(\sum_i \sigma_i \right)^4 \right\rangle_c \tag{2.94}$$

where we indicate with the subscript c a cumulant average. Above T_f the cumulant is expressed as

$$\begin{aligned} \left\langle \left(\sum_i \sigma_i \right)^4 \right\rangle_c &= \sum_{ijkl} \left(\langle \sigma_i\sigma_j\sigma_k\sigma_l \rangle - 3 \langle \sigma_i\sigma_j \rangle \langle \sigma_k\sigma_l \rangle \right) \\ &= 4N - 6 \sum_{ij} \langle \sigma_i\sigma_j \rangle^2 \end{aligned} \tag{2.95}$$

which leads to

$$\chi_{\rm nl} = \beta(\chi_{\rm SG} - \frac{2}{3}\beta^2) \tag{2.96}$$

and thus measurements of $\chi_{\rm nl}$ give us important information about the spin glass transition.

2.6 Frustration

It is safe to indulge in the thought that broken ergodicity is caused by the randomness and the frustration, at least the non trivial one, so it's a good idea to spend some time describing kinds of frustration, and it effects, since we already journeyed, even if only briefly, in the realms of randomness.
To clarify what we mean by frustration we turn our attention to an Edwards-Anderson model with Ising spins, $\sigma \in \{\pm 1\}$, on a square lattice, with couplings coming from a double delta function, so that, fixed J they can only take values from the set $\{\pm J\}$, and with only nearest-neighbours interactions. Instead of considering the whole lattice we focus for a moment only on four spins and their

four couplings: this elementary portion of lattice is commonly called a "plaquette". Since the couplings are taken randomly from the distribution there is an equal probability to end up with an odd or an even number of negative bonds. Now, if the number of negative bonds is even, then it is always possible to find an arrangement of the spins (and it's spin-flipped counterpart) which satisfy all the bonds. All one needs to do is to start at some point fixing a spin and then follow the couplings setting the spins so that the latter are satisfied, which basically means multiplying the spin by the value of the coupling and setting the result as the next spin. If, otherwise, the number of negative couplings is odd, then applying the same simple algorithm for setting the spins (or any other algorithm, for all that matters) will result in a conflict between the value of the spins, at some point. Trying to proceed by going back and flipping a spin previously set so to avoid this conflict will result in the spins at the ends of the other coupling in creating a new conflict. The term "frustration" refers to the inability to satisfy all the bonds simultaneously. The second plaquette in figure 2.2 exhibits frustration, and has an extra ground state degeneracy beyond the one that follows from global spin inversion. It is sometimes useful to think about it in terms of bonds variables instead of spins: we can define it as $A_{ij} = (\sigma_i \sigma_j \text{ sgn } J_{ij})$ and, if a bond is not satisfied, we see that $A_{ij} = -1$. Changing a spins, in a frustrated plaquette, moves the unsatisfied bond to the neighbouring bond.

2.6.1 Trivial and nontrivial disorder

A simple example, following Mattis [13], is helpful in describing what is meant by trivial and nontrivial disorder: not all kinds of disorder gives rise to frustration, and hence to spin glass behaviour. Let the bonds be

$$J_{ij} = H \xi_i \xi_j, \tag{2.97}$$

where the ξ_i are independent and take on the values ± 1 with equal probabilities. Half of the bond are indeed positive and half negative: this is what happens in competing ferromagnetic and antiferromagnetic interactions. But the J_{ij} are not independent: in fact, if we take the product of the J_{ij} around a plaquette (ie. $1 \to 2 \to 3 \to 4$):

$$J_{12}\, J_{23}\, J_{34}\, J_{41} = J^4 \xi_1 \xi_2 \xi_2 \xi_3 \xi_3 \xi_4 \xi_4 \xi_1 = J^4 \tag{2.98}$$

the result is always positive: plaquettes in the Mattis model are unfrustrated, even if we expected the contrary, since we had competing interactions. If we think that the spin glass behaviour has something to do with frustration then, by all means, the Mattis model is not a spin glass. If we make a change in how we define the "up" and "down" locally, for example by defining the new spins

$$\sigma_i' = \xi_i \sigma_i \tag{2.99}$$

the Hamiltonian of the Mattis model reduces to that of a ferromagnet.
From this example we can divide disorder in two kinds: the one that gives rise

to frustration and the one that does not, the latter being irrelevant to spin glass behaviour. It is possible to describe this separation mathematically by going over the bond variables in the partition function: for the $\pm J$ model the energy is a sum over bonds of $-|J|$ times the A_{ij} for that bond. What makes the problem nontrivial (and interesting) is that one must have a odd number of broken bonds around each frustrated plaquette (or an even number of broken bonds around an unfrustrated plaquette). We can then write:

$$Z[\Phi] = \mathrm{Tr}_A \ \exp\left(\beta \sum_{\langle i,j\rangle}\right) \prod_{\langle ijkl\rangle} \delta(A_{ij}A_{jk}A_{kl}A_{li}, \Phi_{ijkl}) \tag{2.100}$$

where we have set $|J| = 1$, $\langle ijkl\rangle$ labels the plaquette and Φ_{ijkl} is $+1$ or -1 depending if the plaquette is unfrustrated or frustrated, respectively. We can write the partition function as (see [14])

$$Z[\Phi] = \lim_{\beta'\to\infty} \mathrm{Tr}_A \ \exp\left(-\beta \mathcal{H}_{\mathrm{eff}}[A;\beta,\beta']\right) \tag{2.101}$$

where

$$\mathcal{H}_{\mathrm{eff}} = \beta \sum_{\langle i,j\rangle} A_{ij} - \beta' \sum_{\langle ijkl\rangle} (\Phi_{ijkl}A_{ij}A_{jk}A_{kl}A_{li} - 1). \tag{2.102}$$

We are writing $Z[\Phi]$ to emphasize that the partition function depends only on the frustration variables Φ_{ijkl}: in this formulation the J only determine the Φ's, and hence different sets of bonds which have the same Φ's have the same partition function. Hamiltonians similar to 2.102 appear in lattice formulation of gauge theories: there one has both an overall global symmetry and a local symmetry. In this way one can make different symmetry transformation in different points, and the Hamiltonian is still invariant. The simplest way to build such a theory is to define variables V_{ij} (in a particular group, in our case $\mathbb{Z}_2$) on the links of a lattice (just like the A_{ij}) and define them to transform as

$$V_{ij} = U_i^{-1} V_{ij} U_j \tag{2.103}$$

under an arbitrary, in general position dependent, operation U_i in the group. In our case U_i, as well as V_{ij}, can simply be $+1$ or -1. A gauge-invariant Hamiltonian must therefore be made up of a combination of the V's which are invariant under this transformation. The simplest such combination is a product of 4 elements around an elementary plaquette of the lattice, such as the one that appears in equation 2.102 in the β' term. The gauge transformation in 2.103 on the A_{ij} corresponds to the transformation $\sigma_i' = \xi_i \sigma_i$ of the spins in the original formulation of the problem, replacing ξ_i with U_i. It is worth noting that the first term in the Hamiltonian 2.102 is *not* gauge invariant. In this formulation we were able to achieve an interesting point: we were able to tell frustrating disorder, which *is* gauge invariant, from other disorder which we can consider less important and which is not gauge invariant. For example, if we were to change the magnitude

of the couplings, that would appear is the first term of the Hamiltonian, the one which is not gauge invariant.

We have argued that frustration is necessary to obtain spin glass behaviour. Now we could ask ourselves: is it also sufficient? Apparently, the answer is *no*: there has been a lot of work in this sense, on fully frustrated systems, for example, there is no result on a phase transition for any temperature different from zero. Some results point out that the energy landscape is too smooth to give rise to broken ergodicity. In other cases models exhibits periodic order below a non-zero temperature, but so far no one has found such a model with a phase resembling a spin glass state.

2.7 A replica-symmetric approach

In this section we will try to apply the replica method (based on the Replica Trick) to the SK model: the result we will obtain will be wrong, since we won't include in this treatment the replica symmetry breaking which we identified as an important ingredient of our treatment. We will, anyway, proceed to investigate the application of the replica method, ready to extend it to replica symmetry breaking problems. Also, we will find that often happens that the systems under study undergo a transition from a replica symmetric to a replica symmetry broken phase, so it's interesting to be able to describe both.
We basically want to calculate the free energy, as in 2.57, by means of the Replica Trick, as in 2.61 and 2.62. We will now generalize the treatment to the case where the couplings have nonzero mean, J_0:

$$P(J_{ij}) = \left[\frac{N}{2\pi J^2}\right]^{\frac{1}{2}} \exp\left[-\frac{N(J_{ij} - J_0/N)^2}{2J^2}\right]. \tag{2.104}$$

This distribution is assumed to be same for all pairs of spins, with $[J_{ij}]_{\text{av}} = J_0/N$ and $[J_{ij}^2]_{\text{av}} - [J_{ij}]_{\text{av}}^2 = J^2/N$. The parameter J_0 basically describes the tendency to find in the system ferromagnetic bonds: for $J_0 \gg J$ the model describes a ferromagnet. Starting from the SK model one can write, by means of the Replica Trick

$$[Z^n]_{\text{av}} = \text{Tr}_{\{\sigma\}} \exp\left[\frac{1}{N}\sum_{ij}\left(\frac{\beta J^2}{4}\sum_{\alpha\beta}\sigma_i^\alpha\sigma_i^\beta\sigma_j^\alpha\sigma_j^\beta + \beta J_0\sum_\alpha \sigma_i^\alpha\sigma_j^\alpha\right) + \beta\, h\sum_{i\alpha}\sigma_i^\alpha\right] \tag{2.105}$$

which, by successive manipulation, can be written as

$$\begin{aligned}[Z^n]_{\rm av} &= \exp\left[nN(\frac{1}{2}\beta J)^2\right]\int_{-\infty}^{\infty}\prod_{(\alpha\beta)}\frac{\beta J\sqrt{N}}{\sqrt{2\pi}}\,{\rm d}y^{\alpha\beta}\prod_{\alpha}\left(\frac{\beta J_0 N}{2\pi}\right)^{\frac{1}{2}}\,{\rm d}x^{\alpha}\cdot \\ &\cdot\ \exp\left[-\frac{1}{2}N(\beta J)^2\sum_{(\alpha\beta)}(y^{\alpha\beta})^2-\frac{1}{2}N\beta J_0\sum_{\alpha}(x^{\alpha})^2\right]\cdot \\ &\cdot\ {\rm Tr}_{\{\sigma\}}\exp\left[(\beta J)^2\sum_{i\alpha\beta}y^{\alpha\beta}\sigma_i^{\alpha}\sigma_i^{\beta}+\beta\sum_{i\alpha}(J_0x^{\alpha}+h)\sigma_i^{\alpha}\right]. \qquad (2.106)\end{aligned}$$

As we have seen earlier we can decouple spins interactions, paying the price of the inter-replica couplings in the single-spins problems. Now by means of

$${\rm Tr}_{\{\sigma\}}e^{\left[\sum_i g(\sigma_i^{\alpha})\right]}=e^{\left[N\ln{\rm Tr}_{\{\sigma\}}e^{g(\sigma^{\alpha})}\right]}, \qquad (2.107)$$

where g is an arbitrary function, we can write

$$[Z^n]_{\rm av}=\exp\left[nN(\frac{1}{2}\beta J)^2\right]\int_{-\infty}^{\infty}\prod_{(\alpha\beta)}\frac{\beta J\sqrt{N}}{\sqrt{2\pi}}{\rm d}y^{\alpha\beta}\prod_{\alpha}\left(\frac{\beta J_0 N}{2\pi}\right)^{2}{\rm d}x^{\alpha}\exp(-NG) \qquad (2.108)$$

where G contains the inter replica terms, being

$$\begin{aligned}G &= \frac{1}{2}(\beta J)^2\sum_{(\alpha\beta)}(y^{\alpha\beta})^2+\frac{1}{2}\beta J_0\sum_{\alpha}(x^{\alpha})^2 \\ &- \ln{\rm Tr}_{\{\sigma\}}\exp\left[\frac{1}{2}(\beta J)^2\sum_{(\alpha\beta)}y^{\alpha\beta}\sigma^{\alpha}\sigma^{\beta}+\beta\sum_{\alpha}(J_0x^{\alpha}+h)\sigma^{\alpha}\right], \qquad (2.109)\end{aligned}$$

where the trace ${\rm Tr}_{\{\sigma\}}$ extends over all states of a single replicated spin σ^{α}. The integral in 2.108 can be calculated, in the limit $N\to\infty$ using the steepest descents:

$$\int{\rm d}y\exp\left[-NG(y)\right]=\int{\rm d}y\exp\left[-NG(y_0)-\frac{1}{2}NG''(y_0)(y-y_0)^2+\ldots\right] \qquad (2.110)$$

where we can ignore the second term, provided that $G''(y_0)>0$, otherwise the resulting Gaussian integral diverges in the saddle point y_0, where $G'(y_0)=0$. The conditions

$$\begin{aligned}\frac{\partial G}{\partial\, y^{\alpha\beta}} &= 0 \\ \frac{\partial G}{\partial x^{\alpha}} &= 0 \qquad (2.111)\end{aligned}$$

lead to

$$\begin{aligned} y_0^{\alpha\beta} &= \langle \sigma^\alpha \sigma^\beta \rangle \equiv \tilde{Z}^{-1} \operatorname{Tr}_{\{\sigma\}} \left[\sigma^\alpha \sigma^\beta \exp \mathcal{H}_{\text{eff}} \right] \\ x_0^\alpha &= \langle \sigma^\alpha \rangle \equiv \tilde{Z}^{-1} \operatorname{Tr}_{\{\sigma\}} \left[\sigma^\alpha \exp \mathcal{H}_{\text{eff}} \right] \\ \tilde{Z} &\equiv \operatorname{Tr}_{\{\sigma\}} \exp \mathcal{H}_{\text{eff}} \end{aligned} \tag{2.112}$$

with the effective, single spin Hamiltonian

$$\mathcal{H}_{\text{eff}} = \frac{1}{2}(\beta J)^2 \sum_{(\alpha\beta)} y_0^{\alpha\beta} \sigma^\alpha \sigma^\beta + \beta \sum_\alpha (J_0 x_0^\alpha + h) \sigma^\alpha \tag{2.113}$$

where, in deriving the latest two results, we have basically interchanged the limits $n \to 0$ and $N \to \infty$: this could be very wrong, but we will see *a posteriori* that is the right thing to do. Now we can express the free energy (where we write $f = F/N$, and is hence a density) as

$$\beta f = \lim_{n \to 0} \left[(\frac{1}{2}\beta J)^2 \left(1 - \frac{1}{n} \sum_{\alpha\beta} (y_0^{\alpha\beta})^2 \right) - \frac{\beta J_0}{2n} \sum_\alpha (x_0^\alpha)^2 + \frac{1}{n} \ln \operatorname{Tr}_{\{\sigma\}} \exp \mathcal{H}_{\text{eff}} \right] \tag{2.114}$$

with

$$\frac{\partial f}{\partial\, y_0^{\alpha\beta}} = \frac{\partial f}{\partial x_0^\alpha} = 0 \quad (\text{all } \alpha \neq \beta). \tag{2.115}$$

Now, we can take the second derivative of the free energy with respect to h for $J_0 = 0$ and in the limit $h \to 0$, which is the local susceptibility

$$\chi_{\text{loc}} = \beta \lim_{n \to 0} \left(1 - \frac{1}{n} \sum_{(\alpha\beta)} y_0^{\alpha\beta} \right) \tag{2.116}$$

which agrees with the previous definition of the χ_{loc} given in 2.75 for $n \to 0$ if we identify $y_0^{\alpha\beta}$ with $q^{\alpha\beta}$, which we previously defined and

$$q = - \lim_{n \to 0} \frac{1}{n} \sum_{(\alpha\beta)} y_0^{\alpha\beta} \tag{2.117}$$

with the spin glass order parameter of 2.70. In the same fashion the quantity

$$M = \lim_{n \to 0} \frac{1}{n} \sum_\alpha x_0^\alpha \tag{2.118}$$

can be identified with the local magnetization.
Now, to solve the equations in the newly defined parameters, we use the so called "replica symmetric ansatz", which basically consists in considering the parameters $y_0^{\alpha\beta}$ and x_0^α as independent of the replica indices. So we write:

$$y_0^{\alpha\beta} = q^{\alpha\beta} = q \;\; (\alpha \neq \beta); \quad x_0^\alpha = M. \tag{2.119}$$

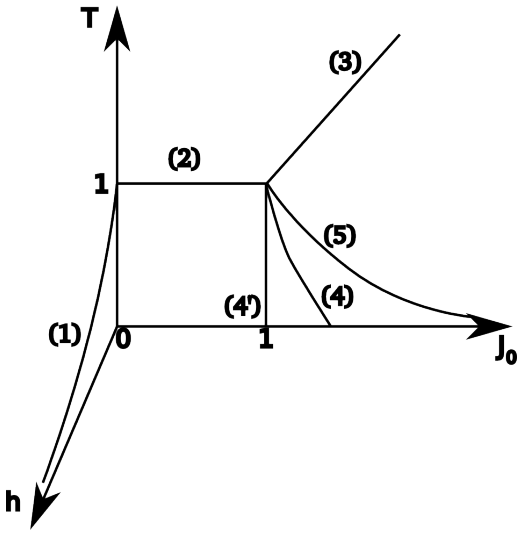


Figure 2.3: Phase diagram of the Ising SK model with infinite range interactions, as a function of T,h and J_0/J in units of $J = T_f$. Lines 1 and 5 are determined by the AT instability, 2 by $q \to 0$ and 3 by $M_s \to 0$, $q = 0$ and 4 by $q \neq 0$, $M_s \to 0$. Line 4, is the incorrect SK solution, line 4' the correct one, given by Parisi theory.

We note that $\sum_{(\alpha\beta)} 1 = n(n-1)$ and that

$$\mathrm{Tr}_{\{\sigma\}} \exp\left(A \sum_{\alpha} \sigma^{\alpha}\right) \approx 1 + n \ln\left(2\cosh\, A\right) \quad (n \to 0) \tag{2.120}$$

and we can express the free energy density as

$$-\beta f = (\frac{1}{2}\beta J)^2(1-q)^2 - \frac{1}{2}\beta J_0 M^2 + \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}z e^{-\frac{1}{2}z^2} \ln\cosh\, \eta(z) \tag{2.121}$$

where

$$\eta(z) = \beta\left(J\sqrt{q}z + J_0 M + h\right) \tag{2.122}$$

which can be interpreted as a random local field with mean $J_0 + M$ and variance $J^2 q$. Variation of the free energy 2.121 with respect to q and M leads to the SK equation for the equilibrium values of these quantities:

$$\begin{aligned} M(T,h) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}z\, e^{-\frac{1}{2}z^2} \tanh\, \eta(z) \\ q(T,h) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}z\, e^{-\frac{1}{2}z^2} \tanh^2 \eta(z). \end{aligned} \tag{2.123}$$

For these solutions we can identify various critical lines, which we will describe in some detail, the more important one being the AT line (from [17]). Below the AT instability lines (1 and 5 in figure 2.3) we find that the susceptibility χ_{SG} is

negative: this is somewhat disturbing, being a quantity defined as the average of the sum of the squares of integers. We will try to think about it, and try to cure this obviously wrong result, in a moment. Below line 2 we have a Spin Glass Phase, with the spontaneous magnetization, $M \neq 0$, and the enhanced susceptibility (see [15])

$$\chi(T) = \frac{1-q}{T - J_0(1-q)} \tag{2.124}$$

In the region above line 2, in zero external field, we have null q, so this susceptibility reduces to the ordinary Curie-Weiss law, which diverges as $T \to J_0 = T_c$, indicating the emergence of ferromagnetic behaviour. Thus one has, for $J > J_0$ below the Curie temperature T_c (line 3) a ferromagnetic state with a finite M as well as a finite q. The boundary between phases in which $M = 0$ and the one in which M has a finite value is given by the vanishing denominator in 2.124 in the Spin Glass Phase, using the SK equation above mentioned for q with $M = 0$. Anywhere below lines 1, 2 and 5, SK equations are not valid (because of the AT instability). An important point is the line 4: we follow in this Toulouse, [16]. In MFT the only change that happens in the thermodynamic potential in the presence of a non null J_0 is an addition to the ferromagnetic condensation energy:

$$A(T, M, J_0) = A(T, M) + \frac{1}{2} J_0 M^2, \tag{2.125}$$

where the first term in the sum refers to the case where $J_0 = 0$. Now, we assume that this is true below lines 2 and 5, for the whole $J - T$ plane. For small M the dependence of $A(T, M)$ is, generally

$$A(T, M) = A(T, M = 0) + \frac{1}{2} \chi^{-1} M^2 \tag{2.126}$$

where χ is the zero field susceptibility, with $J_0 = 0$. Combining the last two equations we see that the coefficient for M goes to zero when $J_0 = \chi^{-1}$, which indicates a ferromagnetic instability. Application of this criterion using the value of χ obtained from the SK equations gives line 4. We know that this is incorrect. Application of the Parisi theory, which we will tackle in the next section, gives instead the vertical continuous line indicated with number 4'.
In non zero field, lines 3 and 4 disappear. Apparently phases below lines 1 and 5 (respectively with $q \neq 0$, $M = 0$ and $q \neq 0$,$M \neq 0$) are different.
If from the free energy we calculate the specific heat we see that there is a a cusp at T_f and a behaviour proportional to T^{-2} above T_f: this is not observed. This discrepancy can be noted and resolved by noting that the MFT fails to take in account short range spin correlations, see [4] for more details on this.

All of the results we have obtained in this section (some wrong, as we noted) were obtained from the replica-symmetric SK saddle point in 2.119. But we are not sure of the validity of this treatment: this depends on whether the first corrections to the results in an expansion in $1/N$, which are obtained by expanding the exponent G in the integral for $[Z^n]_{\text{av}}$ to quadratic order in the deviations from the

saddle point value and then carrying out the remaining Gaussian integrals, can be ignored. Whether this theory based on the saddle point is sensible depends on whether the integral converges, and this will be true only if the eigenvalues of the Hessian matrix evaluated at the saddle point are all positive. The Hessian matrix is

$$\begin{aligned} A^{\alpha\beta\,,\,\gamma\delta} &\equiv \frac{\partial^2 G}{\partial\, y^{\alpha\beta}\, y^{\gamma\delta}} \\ &= \beta^2 J^2 \left[\delta_{\alpha\beta\,,\,\gamma\delta} - \beta^2 J^2 (\,\langle\sigma^\alpha\sigma^\beta\sigma^\gamma\sigma^\delta\rangle - \langle\sigma^\alpha\sigma^\beta\rangle\langle\sigma^\gamma\sigma^\beta\rangle\,)\right], \end{aligned} \tag{2.127}$$

we ignore here the case where $J_0 \neq 0$. In the more general case, we should consider also $\partial G/\partial x^\alpha \partial x^\beta$ and $\partial G/\partial x^\alpha \partial y^{\beta\gamma}$. Almeida and Thouless (in [17]) where able to calculate the eigenvalues of the matrix, which fall into three distinct classes: the first is related to the fully symmetric eigenvectors, which has value, in the limit $n \to 0$,

$$(\beta J)^{-2}\lambda_1 = 1 - (\beta J)^2(1 - 4q - 3r) \tag{2.128}$$

where

$$r = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}z\, e^{-\frac{1}{2}z^2} \tanh^4 \eta(z). \tag{2.129}$$

This mode consist in changes to the magnitude of the SK q without changing the structure of the matrix in replica space. This is called the "longitudinal" mode: eg. in an Heisenberg ferromagnet where the magnitude, but not the direction of the magnetization, is changed. The second class of eigenvectors corresponds to those which are symmetric under interchange of all but one index; these are called "anomalous" and in the limit $n \to 0$ the eigenvalue $\lambda_2 = \lambda_1$. The last eigenvector are called "replicons" which are symmetric under interchange of all but two indices, with eigenvalue

$$(\beta J)^{-2}\lambda_3 = 1-(\beta J)^2(1-2q-r) = 1-(\beta J)^2 \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}z\, e^{-\frac{1}{2}z^2} \mathrm{sech}^4 \eta(z) \tag{2.130}$$

which is equivalent the condition of χ_{SG} not be negative. So this is like saying that, while λ_1 and λ_2 are always positive, λ_3 is negative (as we said above) below the AT line: the SK saddle point is not a stable one in the $T-h$ plane below the AT instability.

Now we can imagine to have a stable solution ($\lambda_{1,2,3} > 0$, so we are in the case of the SK solution above the AT line). This means that if we move a little in the space of the $q^{\alpha\beta}$, the functional G increases a little, as we expected, since we are in the minimum of the free energy functional. The dimensionality of $\frac{1}{2}n(n-1)$ is negative in the limit $n \to 0$: due to this, if we calculate the correction to the free energy obtained by summing the fluctuations contributions from the Gaussian integrals in all the principal directions in space is *negative*. In this sense, we are sitting on a stable saddle point solution which is a *maximum*, rather than a minimum. This makes easier to understand why the free energy obtained in the

SK solution is higher than the extrapolation of the free energy of the paramagnetic phase to $T < T_f$. It could be said that in replica formalism one wants to maximize the free energy instead of minimizing it, but the relevant point of view is that outlined above: we want all the eigenvalues of the free energy fluctuation matrix to be positive. Another serious objection to the SK solution comes from the low temperature properties: the free energy in 2.121 leads to an entropy which is negative for $T \to 0$, a result that is clearly unphysical. In detail it is found that the entropy (which in a discrete system is proportional to the logarithm of the number of configuration, hence non negative by definition) is at $T = 0$, $S(0) = -1/(2\pi) \approx -0.17$.

In the end, we have applied the replica formalism to the SK model under the assumption of replica symmetry, and we found the result to be not satisfying, since they are wrong or unphysical. To correct these problems, we will now turn our attention to the possibility of breaking the replica symmetry and ergodicity: in the next section we will meet the Parisi solution.

2.8 Replica symmetry breaking: the Parisi solution

Until now we have been dealing with theories that do not break Replica Symmetry: that is, all replicas are created (and treated) as equal. In doing so we have obtained results which are, on one side, unphysical like a negative zero temperature entropy, or wrong, as for the value of the free energy at the same temperature. Obviously we should ask ourselves if something is wrong in this "equality" assumption, that is, if we should (or should not) break the assumption of the replica symmetric ansatz.
What we will do now, is exactly that: we will forget about the assumption we made in 2.119, and not suppose that $q^{\alpha\beta} = q$ for all $\alpha \neq \beta$. To do this we will proceed in steps: first we will see what is called One Step Replica Symmetry Breaking and then the full theory. We will follow, in this, Parisi. Also, we have already noted that there is a possible connection between ergodicity breaking and replica symmetry breaking, so the "non working" of the replica symmetric theory points us, again, in this direction. Last but not least, now we have enough tool to describe, in a formal way, by using the replica approach, broken ergodicity. Contrary to what we did in the preceding section, we will now restrict ourselves to the case where $J_0 = 0$ and in the proximity of T_f.
We try now to write a formulation of $\mathfrak{q} \equiv q^{\alpha\beta}$ which breaks replica symmetry: the first "natural" way to do it is to divide n replicas into n/m groups of m replicas each. As a first step, we will set $q^{\alpha\beta}$ equal q_1 if replicas α and β belong to the same group and equal to q_0 if they do not. On the diagonal, $q^{\alpha\alpha}$ is taken to be

identically zero. Hence we can write

$$\begin{aligned} q^{\alpha\beta} &= q_1 \text{ if } I(\alpha/m) = I(\beta/m) \\ q^{\alpha\beta} &= q_0 \text{ if } I(\alpha/m) \neq I(\beta/m) \end{aligned} \tag{2.131}$$

where $I(x)$ is an integer valued function: its value is the smallest integer which is greater or equal to x. We could stop here, and obtain what is called *One Step* replica symmetry breaking. But, if we keep going and repeat the same trick again and again, the final form of the matrix $\mathfrak{q}$ will be like this: introducing a set of integers m_i with $i = 0, \ldots, k+1$, such that $m_0 = 1$ and $m_{k+1} = 1$ and m_i/m_{i+1} is an integer (for $i = 1, \ldots, k+1$). Basically in this way we can divide the n replicas into n/m_1 groups of m_1 replicas each, then each group of m_1 replicas is divided into m_1/m_2 groups of m_2 replicas each and so on. Each off diagonal element of the $\mathfrak{q}$ matrix is then given by

$$\begin{aligned} \mathfrak{q} \equiv q^{\alpha\beta} = q_i \;\; \text{if } I(a/m_i) \neq I(b/m_i) \\ \text{and} \quad I(a/m_{i+1}) = I(b/m_{i+1}), \quad i = 0, \ldots, k \end{aligned} \tag{2.132}$$

the q_i are a set of $k+1$ real parameters. For $k = 0$ all replicas are equal: we recover the replica symmetric theory. For $k = 1$ we have the "One Step" replica symmetry breaking we were just discussing above. The matrix $\mathfrak{q}$ for $k = 2$ is sketched as

$$\begin{pmatrix} 0 & q_2 & q_1 & q_1 & q_0 & q_0 & q_0 & q_0 \\ q_2 & 0 & q_1 & q_1 & q_0 & q_0 & q_0 & q_0 \\ q_1 & q_1 & 0 & q_2 & q_0 & q_0 & q_0 & q_0 \\ q_1 & q_1 & q_2 & 0 & q_0 & q_0 & q_0 & q_0 \\ q_0 & q_0 & q_0 & q_0 & 0 & q_2 & q_1 & q_1 \\ q_0 & q_0 & q_0 & q_0 & q_2 & 0 & q_1 & q_1 \\ q_0 & q_0 & q_0 & q_0 & q_1 & q_1 & 0 & q_2 \\ q_0 & q_0 & q_0 & q_0 & q_1 & q_1 & q_2 & 0 \end{pmatrix} \tag{2.133}$$

with $n = 8$, $m_1 = 4$, $m_2 = 2$. Eventually we shall consider the limit for $k \to \infty$, which will lead to interesting results. If we now examine $P(q)$ in the case of $k = 2$ we have that, in the limit $n \to 0$ is

$$P(q) = m\,\delta(q - q_0) + (1 - m)\,\delta(q - q_1), \tag{2.134}$$

from which we see immediately that is non negative (being a probability) if

$$0 \leq m \leq 1. \tag{2.135}$$

It is obvious from this that, if we exclude the cases $m = 0$ and $m = 1$ which correspond to the replica-symmetric solution, m cannot be an integer and satisfy 2.135, but since we are taking the limit $n \to 0$, and this is obtained by an analytic continuation, nothing seems to forbid, in such a process, for m be non integer. Now, increasing k we can write

$$P(q) = \sum_{i=0}^{k} (m_i - m_{i+1})\,\delta(q - q_i) \tag{2.136}$$

and

$$\lim_{n\to 0}\left\{\frac{1}{n}\sum_{a,b=1}^{n}\mathfrak{q}^2\right\} = -\sum_{i=0}^{k}(m_{i+1}-m_i)q_i^2. \tag{2.137}$$

This second $P(q)$ is positive definite only if

$$0 \le m_i \le m_{i+1} \le 1 \tag{2.138}$$

is satisfied. In the limit of $k \to \infty$, we are basically repeating the procedure of breaking the replicas in infinitely many blocks, the m_i become continuous, $m_i \to x$, $0 < x < 1$: we are encoding the information contained originally in m_i and q_i in a function $q(x)$ in the unit interval.
It is now time to try to write the energy functional, as we did in the Replica Symmetric case, and then try to minimize it (if $n > 1$) or maximize it (in the case where $0 < n < 1$, while $n \to 0$). Following [9], [18], [19] and [20] we write (in the vicinity of T_f)

$$F[\mathfrak{q}] = \lim_{n\to 0}\frac{1}{n}\left[\tau\ \mathrm{Tr}\ \mathfrak{q}^2 + \frac{1}{3}\mathrm{Tr}\ \mathfrak{q}^3 + \mathsf{y}\sum_{\alpha,\beta}\mathfrak{q}^4 + O(\mathfrak{q}^4)\right] \tag{2.139}$$

where, out of the various possibile terms of fourth order, we have kept, according to [7], the one responsible of breaking replica symmetry. By τ we have indicated $(T - T_c)/T_c$. In the SK model y is negative, and replica symmetry is broken: we will set $\mathsf{y} = -1/6$. This can be written also as, keeping in mind that [21]

$$\begin{aligned}
\mathrm{Tr}\ \mathfrak{q}^2 &= \sum_{\alpha\beta}(q^{\alpha\beta})^2 = n\sum_{i=0}^{k}(m_i - m_{i+1})q_i^2 = -n\int_0^1 q^2(x)\mathrm{d}x \\
\mathrm{Tr}\ \mathfrak{q}^4 &= \sum_{\alpha\beta}(q^{\alpha\beta})^4 = n\sum_{i=0}^{k}(m_i - m_{i+1})q_i^4 = -n\int_0^1 q^4(x)\mathrm{d}x \\
\mathrm{Tr}\ \mathfrak{q}^3 &= \sum_{\alpha\beta\gamma}q^{\alpha\beta}q^{\beta\gamma}q^{\gamma\alpha} = n\int_0^1 \mathrm{d}x\left[xq^3(x) + 3q(x)\int_0^x q^2(x')\mathrm{d}x'\right]
\end{aligned} \tag{2.140}$$

as

$$F(\mathfrak{q}) = \frac{1}{2}\int_0^1 \mathrm{d}x\left[\tau q^2(x) + \frac{1}{6}q^4(x) - \frac{1}{3}xq^3(x) - q(x)\int_0^x q^2(x')\mathrm{d}x'\right]. \tag{2.141}$$

In all this we have considered the function $q^{(k)}(x)$ as

$$q^{(k)}(x) = q_i \quad \text{if } m_i < x < m_{i+1}. \tag{2.142}$$

We can write the free energy also as

$$F(q_i, m_i) = \sum_{i=0}^{N}(m_i - m_{i+1})\left[\tau q_i^2 + \frac{1}{6}q_i^4 - \frac{1}{3}(2m_i - mi + 1)q_i^3 + q_i\sum_{j=i+1}^{N}(m_j - m_{j+1})q_j^2\right] \tag{2.143}$$

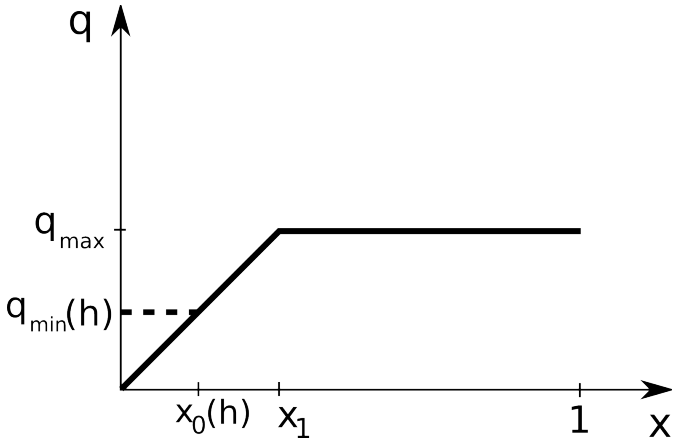


Figure 2.4: Parisi solution for $q(x)$ close to T_f. Dashed line is for small $h \neq 0$, solid lines for $h = 0$.

as a function of the parameters q_i,m_i.

If we now vary 2.141 with respect to $q(x)$ we obtain

$$2|\tau|q(x) - xq^2(x) - \int_0^x q^2(x')\mathrm{d}x' - 2q(x)\int_x^1 + \frac{2}{3}q^3(x) = 0. \tag{2.144}$$

Differentiating this equation gives:

$$|\tau| - xq(x) - \int_x^1 q(x')\mathrm{d}x' + q^2(x) = 0 \quad \text{or} \quad \frac{\mathrm{d}q}{\mathrm{d}x} = 0 \tag{2.145}$$

and again:

$$q(x) = \frac{1}{2}x \quad \text{or} \quad \frac{\mathrm{d}q}{\mathrm{d}x} = 0. \tag{2.146}$$

Assuming now that $q(x)$ is a continuous function we find a solution by taking the first solution for small x and a constant for $x > 2q(1)$. This, with 2.145, lets us solve for the plateau value $q(1) = |\tau| + O(|\tau|^2)$. From the point of view of physics, $q(1)$ being the largest overlap must be the single phase order parameter, q_{EA}.

It is interesting to consider this result, following [21], for a non zero external field, h: one has

$$q(0) = \frac{3}{4}\left[\frac{h^2}{J^2}\right]^{\frac{2}{3}}. \tag{2.147}$$

As the field increases the value of $q(0)$ increases, until in reaches the second plateau for $q(1)$, and hence the replica symmetry breaking is removed, and one obtains, again, the SK replica symmetric solution. This effect is recognizable with the passage over the AT instability line that we mentioned earlier.

We were firstly moved to formulate a replica symmetry breaking theory from the fact that our replica symmetric theory did not work: the eigenvalues of the Hessian matrix were not all positive (one of them, the one related to χ_{SG}, would turn negative below the AT line) and from the fact that the entropy was negative at $T = 0$, we will now check if these maladies have been cured by this new theory. The diagonalization of the Hessian matrix at the Parisi saddle point has been carried out by De Dominicis and Kondor: they found two families of eigenvectors (which in some sense resemble the ones we have already met before) each with now a spectra of eigenvalues. Some of these spectra have support only in the positive real axis (which can be, even if roughly, associated with he λ_1 we met before) while other spectra extend to zero. There are, also, some isolated zero eigenvalues. The important thing is: we have now *no negative* eigenvalues: the instability below the AT line has been cured. Having some zero eigenvalues tells us that the system is marginally stable, like a system at a critical point: both intervalley contributions and locally stable phases contribute to this result. The problem of negative entropy is also cured by this solution: for $T < 1$, from [9] we find that the entropy is -0.01 for $k = 1$, a significant improvement over $k = 0$. It is expected to find $S(0) = 0$ only for $k = \infty$.
We now turn our attention to $P(q)$, hoping to gain some insight also about broken ergodicity. With the Parisi parametrization of $q^{\alpha\beta}$ we have

$$P(q) = \lim_{n\to 0} \frac{1}{n(n-1)} \sum_{\alpha\neq\beta} \delta(q - q^{\alpha\beta}) = \int_0^1 \delta(q - q(x))\mathrm{d}x = \frac{\mathrm{d}x(q)}{\mathrm{d}q} \qquad (2.148)$$

where $x(q)$ is the inverse function of $q(x)$. To be able to perform the inversion, $q(x)$ must be a non decreasing function. Moreover, we can write as the sum of two deltas, one for $q(1) \equiv q_M$ (which is the "second" plateau) and for $q(0) \equiv q_m$ (whose value depends on the external field)

$$P(q) = x_m\delta(q - q_m) + x_M\delta(q - q_M) + \tilde{P}(q) \qquad (2.149)$$

where $\tilde{P}(q)$ is a smooth function with support in the interval

$$q(0) \equiv q_m \leq q \leq q(1) \equiv q(1). \qquad (2.150)$$

In other words, if we choose two states, α and β at random, there is a probability $x_M = x(q_M)$ that these two states are the same one, in which case $q_{\alpha\beta} = q_M$, a probability x_m that they have the minimum allowed overlap q_m and a probability, finally, $1 - x_m - x_M$ to be in an intermediate situation. In [12] is shown a direct measure of $P(q)$: what is interesting is to note, together with the presence of a continuous part is the presence of the spike (the delta function), which tells us that only an handful of the states dominate the thermodynamic sum. From [22] and [23] we gain insight on how the barriers between the different phases scale with the size of the system, N: they find that the logarithm of the longest relaxation time τ (which is proportional to the largest energy barrier) in the

system is proportional to $N^{\frac{1}{4}}$: there is also a so called ergodic time, which is the time in which the magnetization typically changes in sign, which diverges also for ferromagnets, usually like N, and in SK is found to be diverging like $N^{\frac{1}{2}}$. Hence we can conclude that barriers between phases are, in the thermodynamic limit, infinite.

2.9 The Potts Glass

Until now we have been focusing only on spins glasses that possess total inversion symmetry. It is interesting, not only for the aim of this thesis, to investigate whether the proprieties we have seen until now are a special feature of this kind of models or is something that is shared between different models with different symmetries (or lack of thereof). Also, there are glasses, like Quadrupolar Glasses, which cannot be described by models such as EA or SK, exactly because they do not possess the kind of symmetry these models have: in some sense they are more general. One class of such models is the Potts Glass, which is basically the disordered version of the Potts model we already met. We will now see that, as was the case between Ising and Potts models, we find a richer behaviour in the Potts Glass than in EA or SK models.
Being J_{ij} random variables as in the EA or SK models, we write, with slight differences from the Potts model, the Hamiltonian as

$$\mathcal{H} = -\frac{1}{2}\sum_{ij} J_{ij}(p\,\delta(\sigma_i,\sigma_j) - 1). \tag{2.151}$$

As before, $p = 2$ is related the Ising case. We can measure the ferromagnetic order by defining a magnetization, for a particular state r,

$$m_r = \langle \delta(\sigma_i, r)\rangle \; - \; \frac{1}{p} \tag{2.152}$$

where $1/p$ is basically the correlation we would have if the configurations were completely random. In a Potts Glass we have randomly frozen m_r characterized by a spin glass order parameter

$$q_{r,r'} = \left[(\langle \delta(\sigma_i, r) - \frac{1}{p})(\delta(\sigma_i, r') - \frac{1}{p})\right]_{\text{av}}. \tag{2.153}$$

This quantity has the symmetry $q_{r,r'} = q(\delta(r, r') - 1)$ and it can be completely characterized by a single number, q. If we move now to Replica Theory this number becomes a matrix

$$q^{\alpha\beta} = \langle \delta(\sigma^\alpha, \sigma^\beta)\rangle - \frac{1}{p} \tag{2.154}$$

where, just to be precise, we need as before to take the thermal average over an effective Hamiltonian.

We can now proceed and write the expansion as we did for the SK model: it's worth noting that now we will need to write a term for $\sum_{\alpha\beta}(q^{\alpha\beta})^3$ that was missing before, since we do not have anymore the inversion symmetry:

$$F[\mathfrak{q}] = \lim_{n\to 0} \frac{p-1}{2n} \left[\tau \mathrm{Tr}\ \mathfrak{q}^2 - \frac{1}{3}\mathrm{Tr}\ \mathfrak{q}^3 - \frac{p-2}{6}\sum_{\alpha\beta}(q^{\alpha\beta})^3 + \frac{\mathsf{y}(p)}{6}\sum_{\alpha\beta}(q^{\alpha\beta})^4 \right]. \tag{2.155}$$

We know from the SK model that $\mathsf{y} = -1$ for $p = 2$, in the same case the term $\sum_{\alpha\beta}(q^{\alpha\beta})^3$ disappears, due to symmetry considerations. Gross, Kanter and Sompolinski, in [24], found two different regimes, depending on the value of p, since $\mathsf{y}(p)$ changes sign, from negative to positive. This change of sign is responsible for the lack of a solution which has the Parisi function $q(x)$ continuous. In SK, the y-term was responsible for replica symmetry breaking, so its presence here makes us think that we will have replica symmetry breaking too. In fact, if one looks at the replica symmetric solution for the Potts Glass finds it more unstable than it was in SK.

In [24] the change of sign of $\mathsf{y}(p)$ is found to happen for $p^* \simeq 2.8$.

For $p < p^*$ one finds a solution with features similar to those of the SK solution: figure 2.5 in the first panel on the left, *(a)*, shows q and $P(q)$ in this case. It resembles the one of the SK solution in a field, only that the first part is at $q = 0$, instead of a minimum $q_{\min}$. The corresponding $P(q)$ shows two deltas, one at zero that signal the existence of many uncorrelated replicas. As in the SK solution we have a continuous part, between zero and the plateau. One step replica symmetry breaking is sufficient to recover a correct mean field solution.

As y changes sign (for $p > p^*$) the situation changes: no Parisi-like solution with a continuous $q(x)$ is possible anymore. What works here is a solution similar to the one found in the Random Energy Model (REM) [25] [26], also with one step replica symmetry breaking: $q(x)$ has a discontinuous jump at $\tilde{x} \simeq (p-2)/2$ and a plateau value proportional to $(T - T_f)/(4 - p)$ for T near T_f, also sketched in figure 2.5 *(b)*. All eigenvalues are positive about the saddle point [27] [28].

As $p > 4$ the jump point $\tilde{x}(T \to T_f^-) \to 1$. The solution outlined above ceases to exists (this happens also whenever the second cubic term is larger than the first). In this case one must consider a discontinuous jump of q as a function of temperature. Since q is no longer a small parameter, equation 2.155 is no longer valid, but we still can consider the limit $p = 4 + \epsilon$, $\epsilon \to 0$: a stable glass phase is found [24] [27] with broken replica symmetry, similar to the one found for $p < 4$ (eg. one step replica symmetry breaking). This glass phase appears below $T_f - 1 \propto \epsilon$, with $q(T_f) \propto \epsilon$ and $\tilde{x}(T \to T_f) \to 1$. Fluctuations around both this saddle point and the paramagnetic phase are all finite near T_f. The crucial point of this transition is that $\tilde{x}(T \to T_f) \to 1$ and it holds order by order in expansion of powers of ϵ and in the limit of large p.

Solving for $p \to \infty$ the full mean-field theory of the glass phase we find a discontinuous transition from the paramagnetic phase at the temperature at which its

entropy vanishes: $T_f = 1/2J(p/\ln p)^{1/2}$. Below T_c a Potts Glass phase appears with order parameter $q(T) = 1$, $\tilde{x}(T) = T/T_f$. The free energy is constant and equal to the ground state energy. This phase transition is identical to the one found in the already cited Random Energy Model.
In the large-p limit the Potts Glass phase exists down to $T = 0$, however, as soon as $p > 2$, this phase has a negative entropy at $T = 0$. There is, in fact, a second phase transition at a temperature $T_2 < T_f$ to inducing replica symmetry breaking in the region $\tilde{x} < x < 1$. This gives rise to a second glass phase, commonly called *PG2*, in which $q(x)$ is continuous for some range of x. This phase is marginal and has entropy zero at $T = 0$. This phase transition can be studied with the expansion at the fifth order [24] in $p - p^* \to 0$: one sees the instability explicitly at T_2 and the rise of the new phase. This second transition is always continuous, as a function of T, even for $p > 4$. According to [31], the fact that the entropy becomes negative is related to the fact that the one step replica symmetry breaking scheme does not suffices anymore and it is necessary to move to continuous breaking. This situation is sketched in figure 2.5, *(c)*.
To resume, in the Potts Glass (in mean field theory):

- we have a stable glass phase (PG) for all values of p
- for $p \geq 3$ the order function $q(x)$ is discontinuous
- for $p > 2$ the glass phase PG becomes unstable below $T_2 < T_f$ and a new phase is formed, *PG2*. Here each of the pure states in the aforementioned phase splits in a hierarchical manifold of infinite partially correlated states. The order function is then a step plus a continuous part (see figure
- in $p = 3$ and $p = 4$ *both* phase transitions (PM $\to$ PG and PG $\to$ PG2) are continuous
- for $p > 4$ the transition PM $\to$ PG is discontinuous
- the discontinuous transition for $p > 4$ has unusual properties: in particular there is no latent heat at the transition.

A similar situation is also reported by Gardner in [30] in the case of the p-spin spin glass that is basically a generalization of the SK spin glass to include interactions between every set of p spins: there is then a transition with a jump of the order parameter (but without latent heat), and, at a lower temperature there is another transition (the PG phase becomes unstable) where the order parameter changes smoothly.

In the Potts Glass, below T_f the dependence of the singular part of the free energy on T and external *static* sources obeys ordinary scaling laws with the critical exponents [24]

$$\beta = 1, \;\; \gamma = 0, \;\; \alpha = 0, \;\; \delta = 1. \tag{2.156}$$

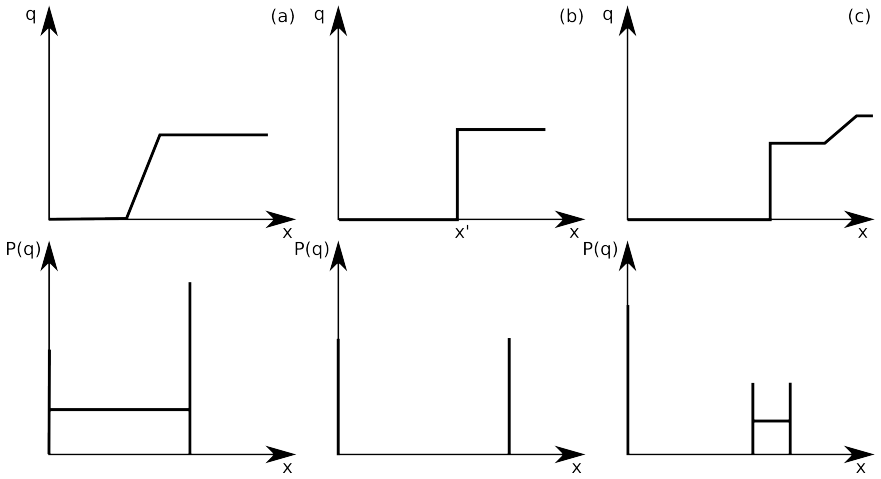


Figure 2.5: Schematic plot of $q(x)$ and $P(q)$: a. $p < p^*$, q roughly looks like in the SK model in a field, but with $q_0 = 0$ instead of $q_0 = q_{\min}$; b. $p > p^*$, $T_2 < T < T_f$: q is discontinuous, $x' \equiv \tilde{x} = (p-2)/2$, the plateau's height is proportional to $(T-T_f)/(4-p)$; c. $p > p^*$, $T < T_2$. Lower is $P(q)$: a. $p < p^*$, the spike at $q = 0$ signals the presence of many uncorrelated replicas; b. $p > p^*$,$T_2 < T < T_f$; c. $p > p^*$, $T < T_2$.

If this holds also for short-range systems in some range of dimensionality d, then the hyperscaling law $\nu d = 2 - \alpha$ suggests that the thermal exponent that determines the rounding at the transition due to the finiteness of the system size obeys $1/\nu = d/2$, which should be compared with $1/\nu = d$ that holds for ordinary first-order transitions.
It is worth noting, also, that in [24], [29] and [31] is reported that in the Potts Glass, for sufficiently low temperatures, ferromagnetic order is preferred to the spin glass phase. The temperature below which ferromagnetic order appears, from [31] is

$$\frac{1}{T_{\rm FM}}\left(J_0 + \frac{p-2}{2\,T_{\rm FM}}\right) = 1. \tag{2.157}$$

In the case $J_0 = 0$, the ferromagnetic transition appears below $T_{\rm FM} = 1$ for $p < 4$ and above that temperature for $p > 4$.
In [29], the order parameter q is written as

$$q_{\rm r\,s}^{\alpha\beta} = q_{\rm L}^{\alpha\beta} I_{\rm r\,\lambda} I_{\rm s\,\lambda}/(p-1) + q_{\rm T}^{\alpha\beta}\left[I_{\rm r\,\lambda} I_{\rm s\,\lambda}/(p-1)\right] \tag{2.158}$$

and the magnetization

$$m_{\rm r}^{\alpha} = m^{\alpha} I_{\rm r\,\lambda}, \tag{2.159}$$

where it has been used the invariant tensor

$$I_{\rm r\,s} = p\delta({\rm r,s}) - 1. \tag{2.160}$$

The order parameters $q_{\rm L}^{\alpha\beta}$ and $q_{\rm T}^{\alpha\beta}$, which represent respectively longitudinal and transverse spin glass ordering, are related directly to the structure of the local

susceptibility

$$\chi^l_{\mathrm{r\,s}} = \chi^l_{\mathrm{L}} I_{\mathrm{r}\,\lambda} I_{\mathrm{s}\,\lambda}/(p-1) + \chi^l_{\mathrm{T}} \left(I_{\mathrm{r\,s}} - I_{\mathrm{r}\,\lambda} I_{\mathrm{s}\,\lambda}/(p-1)\right). \tag{2.161}$$

In this reference different phases are identified: paramagnetic ($q_L, q_T, m = 0$), isotropic spin glass ($q_L = q_T = q \neq 0, m = 0$), collinear ferromagnetic ($m, q_L \neq 0, q_T = 0$) and mixed ($m, q_L, q_T \neq 0, q_L \neq q_T$), this last phase being a combination of a collinear ferromagnet and a transverse spin glass corresponding to a canted ferromagnet in simplex space. In the same reference, phase transitions between the phases just described are analyzed.
See [24], [29], [31] and [32] for a broader discussion on the topic.
Another interesting feature pointed out in [28] is the presence, for $p > 4$, of the another transition for a temperature $T_A > T_F$ signaled by the slowing down of the dynamical correlations as $T \to T_A^+$. Below T_A the system gets stuck in a metastable state. In the mean field theory barriers separating different phases become infinite and a transition from ergodic to non-ergodic behaviour takes place.

Chapter 3

Monte Carlo Methods

Once we move our quest for answers from infinite systems to finite sizes and from mean field to short range interactions, our "toolbox" becomes less furnished, and we have to accept that we cannot succeed with theory only anymore. For a very simple Ising ferromagnet, for example, we have results for a two dimensional short range system, but as we begin investigating the three dimensional one, we are left without a solution. We have to use a different set of tools, the most prominent of which is the Monte Carlo Method.
While the purpose of this chapter is just to introduce a few elements which will be used in the subsequent discussion, it necessarily just skims the surface: for a thorough discussion of Monte Carlo methods, see [33] or [34].

3.1 A first glance

If we want to simulate a system, as the Ising or the Potts model we can sum up the situation like this: we have a function, the Hamiltonian, which, given a configuration of the spins, gives us the energy of the system (in some appropriate units). We also know, from Statistical Physics, that a given configuration $\{\sigma\}$ will be realized, at a given temperature, with a probability that is proportional to $\exp[-\beta E(\{\sigma\})]$. This is *all* we basically need to do Monte Carlo, although the picture, as often happens in Physics, can be complicated some more, as we shall see. Now, let's suppose that, at a given time t_0, our system is in a configuration μ. If we define $R(\mu \to \nu)$ the transition rate from state μ to state ν there is a probability $R(\mu \to \nu)\,\mathrm{d}t$ to find the system in the configuration ν after a time $\mathrm{d}t$. Now, our system will have many possible configurations, and we can define a rate of change to any of these configuration: to continue the example, if we start from μ and wait for a sufficiently long time, the system could be in one of the (possibly many) configurations available. If we define a weight, w_μ, for the probability of the system to be in configuration μ at a time t, we can write a master equation

of sorts for the evolution of $w_\mu(t)$:

$$\frac{\mathrm{d}w_\mu(t)}{\mathrm{d}t} = \sum_\nu \left[w_\nu(t) R(\nu \to \mu) - w_\mu(t) R(\mu \to \nu) \right], \tag{3.1}$$

with the constraint

$$\sum_\mu w_\mu(t) = 1, \quad \text{for all } t \tag{3.2}$$

since the system is always in some configuration. In 3.1 the first term on the right hand side is the probability of the system to end up in configuration μ while being in a state ν and the second term is the probability to move away to any state ν from μ. The solution of 3.1 shines light on how the weights w_μ change over time. Now, let's say that we want to calculate some quantity A which depends on the configuration we are in, for example μ, so that we can write A_μ. How to we calculate the expectation of A at a time t for the system? We can write it down as:

$$\langle A \rangle = \sum_\mu A_\mu \, w_\mu(t). \tag{3.3}$$

We can look at this equation in different way: one way would be to imagine, having many realization of the system under study, each not interacting with the other and with its own reservoir that keeps the temperature constant: the average then would be done "reading" the value of A for each copy. Since each value A_μ will be presented with a probability w_μ, then we are executing a "correct" average. Another way, which is undoubtedly more convenient in terms of realization, is to read the value of A in a sufficiently long interval of time and then averaging: again, we would have the correct weights. In this second case we are integrating over time the measure. This would work as long as the system visits each state μ with the correct weight in the given time: one easy way out would be to increase the observation time. Of course, something could go wrong: for example, the rate of change of state could be very slow (and this could be cured by simply prolonging the time in which we do the measures), or it could be that the system changes a few configurations very slowly and passes through the other very quickly, so that we have more probability of our measures be taken in the "slow part". Last but not least, they weights could change in the time scale of our measures, and we would be measuring something that is itself changing over time. We will see that for equilibrium system this is not the case: in fact once we reach equilibrium the two term in the right hand side of 3.1 cancel out, and weights become constant over time. The do not take just any value: they take the value of the Boltzmann probability for a given configuration

$$p_\mu = \frac{1}{Z} e^{-\beta E_\mu} \tag{3.4}$$

in the limit in which the weights, if we wait for a sufficient long time, become constant. We can then rewrite the measure of a quantity A as

$$\langle A\rangle = \sum_\mu A_\mu w_\mu = \frac{1}{Z}\sum_\mu A_\mu e^{-\beta E_\mu}. \tag{3.5}$$

The important point here to note is that we know the probabilities for each configuration, now, *a priori*, once we know how to calculate the energy for a given configuration, which we know how to do if we have the Hamiltonian of the system.

3.2 Measures and Fluctuations

Armed with what we just saw we can now write, for example for the internal energy:

$$U = \frac{1}{Z}\sum_\mu E_\mu e^{-\beta E_\mu} \tag{3.6}$$

which of course is also

$$U = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = -\frac{\partial \log Z}{\partial \beta}. \tag{3.7}$$

Albeit quantities like U are definitely very interesting, we are deeply curious also about fluctuations such as (we write $U = \langle E\rangle$)

$$\left\langle (E - \langle E\rangle)^2\right\rangle = \langle E^2\rangle - \langle E\rangle^2. \tag{3.8}$$

We can calculate $\langle E^2\rangle$ as

$$\langle E^2\rangle = \frac{1}{Z}\sum_\mu E_\mu^2 e^{-\beta E_\mu} = \frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2} \tag{3.9}$$

and hence we find

$$\langle E^2\rangle - \langle E\rangle^2 = \frac{1}{Z}\frac{\partial^2 Z}{\partial \beta^2} - \left[\frac{1}{Z}\frac{\partial Z}{\partial \beta}\right] = \frac{\partial^2 \log Z}{\partial \beta^2}, \tag{3.10}$$

and since we know that

$$C = -k\beta^2\frac{\partial^2 \log Z}{\partial \beta^2} \tag{3.11}$$

we can finally write

$$\langle E^2\rangle - \langle E\rangle^2 = \frac{C}{k\beta^2} \tag{3.12}$$

which is like saying that the variance of the energy that we measure using Monte Carlo techniques is proportional to the specific heat of the system. Now, this has an obvious practical application, since C is a very interesting quantity, but also

tells us a few things about what to expect. Since C is an extensive quantity, the RMS energy fluctuations scale as $\sqrt{V}$ where V is the size of the system. Now, the internal energy scales like V, so that the relative size of the fluctuations compared to the internal energy decreases as $1/\sqrt{V}$: if $V \to \infty$, in the thermodynamic limit, relative fluctuations go to zero. With Monte Carlo simulations we cannot, however, simulate infinite systems, but we will see how to learn something from this behaviour. To generalize a little this discussion we will say that every parameter of the system, X, we can consider a conjugate variable, Y. For example we could consider the magnetization, m and the external field, h. Now:

$$\langle X \rangle = \frac{1}{\beta} \frac{\partial \log Z}{\partial Y} \tag{3.13}$$

and so we can write

$$\frac{1}{\beta} \frac{\partial \langle X \rangle}{\partial Y} = \langle X^2 \rangle - \langle X \rangle^2 \tag{3.14}$$

which is the mean square fluctuation in the variable X. Now we can call

$$\chi = \frac{\partial \langle X \rangle}{\partial Y} \tag{3.15}$$

the *susceptibility* of X to Y, which is the response of X to a change in Y. Hence we can write:

$$\langle X^2 \rangle - \langle X \rangle^2 = \frac{1}{\beta} \chi, \tag{3.16}$$

the fluctuations in a variable are proportional to the susceptibility of that variable to its conjugate field, which is a fact know as linear response theorem. We can extend this reasoning to a parameter that is defined on a particular site of the lattice we are studying and ask ourselves what kind of effect a change for it has in the conjugate variable at other positions.
In the first chapter we already mentioned susceptibilities: now we also know, in a simulation, how to calculate them.

3.3 Importance Sampling

We have found a way in which we can calculate the value of an observable A in Monte Carlo simulation. Obviously, we are not going to go through all the possible configurations, or states, and the just calculate the correct average with correct weights. There is a simple reason for that: for a very simple Ising ferromagnet defined on a cubic lattice of linear size L, there are 2^{L^3} possible configurations. If L is big enough to do something useful with it (in terms of Physics) that number is definitely too large to be handled. So a smart idea would be to take only configurations which have an higher weight: in some sense the real system will do the same, since in equilibrium it will present itself in a configuration

accordingly with its Boltzmann probability. So our strategy will be to measure A with probability $p_\mu = \frac{1}{Z} e^{-\beta E_\mu}$, and hence our estimator for $\langle A \rangle$ will be:

$$A_M = \frac{1}{M} \sum_{i=0}^{M} Q_{\mu_i} \tag{3.17}$$

3.4 Markov processes

It's clear from previous section that the trickiest part of our Monte Carlo simulation will be to generate configurations which agree with the correct probability. To do this most Monte Carlo schemes use a Markov process: for our purposes this is nothing more than a way, starting from a configuration μ to obtain a new configuration ν, in some random fashion. Which is like saying that, if we are in a state μ this gives us the probability to move to a state ν, $P(\mu \to \nu)$. In a true Markov process $P(\mu \to \nu)$ has to satisfy two requirements: the probabilities should not change in time and they should depend only on the two states μ and ν, not on other states the system has passed through. This means that given a state the probability to end in any other state is the same all the time we repeat this change. Also, probabilities should satisfy

$$\sum_{\mu} P(\mu \to \nu) = 1 \tag{3.18}$$

which says that the Markov process generates always *some* state when fed with another one, and also that the probability to stay in the same state, $P(\mu \to \mu)$ need not to be zero. In our Monte Carlo we will use the Markov process to generate a Markov chain of states. Our Markov Chain, starting from some arbitrary state, will lead us to a succession of states which appear with probability given by the Boltzmann distribution.
But aside from these requirements we have asked for on the Markov process, we need to impose a few more to achieve this.

3.4.1 Ergodicity

In the last chapter we have been spending a lot of time on the concept of ergodicity. We see now that also our Monte Carlo simulation must agree with this: since every state in which our system can be found has some non-zero probability attached then we must be able in our simulation, to move from any given state to any other given state, no matter how long this could require. If some configuration in the Markov chain has a null probability then, no matter how hard we try, we will not be able to reach it, and so our simulation will not be ergodic.

3.4.2 Detailed Balance

Another condition we wish to impose to our Monte Carlo simulation is that it satisfies the Balance equation:

$$\sum_{\nu} p_\mu P(\mu \to \nu) = \sum_{\nu} p_\nu P(\nu \to \mu) \tag{3.19}$$

which is like saying that the rate at which we enter state μ is equal to the rate at which we leave it: the system is in equilibrium. By using 3.18 we can write this as

$$p_\mu = \sum_{\nu} p_\nu P(\nu \to \mu). \tag{3.20}$$

For any set of transition probabilities satisfying this equation the probability distribution p_μ will be an equilibrium of the dynamics of the Markov process. However, simply satisfying this equation will not guarantee that the probability distribution will tend to p_μ from any state of the system if we run the process long enough. To avoid, for example, that the system gets trapped in a closed loop of configurations, which would violate ergodicity, we have to ask for

$$p_\mu P(\mu \to \nu) = p_\nu P(\nu \to \mu), \tag{3.21}$$

known as Detailed Balance, to be satisfied. This last equation basically tells us that the probability to be in state μ and then be moved to state ν equals the reverse probability to be in state ν and be moved to state μ. This avoids limit cycles.
Now, given we are respecting 3.21, we are free to choose the transition probabilities as we please, but given that we want the p_μ to tend to the Boltzmann distribution, we can take

$$\frac{P(\mu \to \nu)}{P(\nu \to \mu)} = \frac{p_\nu}{p_\mu} = e^{-\beta(E_\nu - E_\mu)}. \tag{3.22}$$

This equation together with 3.18 are the constraints we impose to our transition probabilities: if we respect these, and ergodicity, then the equilibrium distribution of states in the Markov chain will be the Boltzmann distribution[1].

3.5 Acceptance Ratios

The Markov chain let us free to choose the transition probabilities as we want. A step further to actually define the probabilities, as we will see in the Metropolis algorithm, is to break them in two parts as:

$$P(\mu \to \nu) = g(\mu \to \nu) A(\mu \to \nu) \tag{3.23}$$

[1] For a demonstration see the note by prof. A.P. Young, and references therein, on "Monte Carlo Simulations in Statistical Physics" available on his homepage.

in which the transition probability is divided in two step: first we propose, starting from configuration μ, an arrival configuration, ν with probability $g(\mu \to \nu)$ and then we accept the change with probability $A(\mu \to \nu)$, which we call the *acceptance ratio*, while $g(\mu \to \nu)$ is usually called *selection probability*. The acceptance ratios says that if we start in a state μ and our algorithm generates a new state ν from it, we should accept the state and change our system to the new state with probability $A(\mu \to \nu)$. The rest of the time we will stay in state μ. We are free to choose acceptance ratios to be in the interval between zero and one: obviously if we set it to zero, then our system will stay forever in the original state μ. This gives use absolute freedom on how to choose the selection probability, since the constraint 3.22 only fixes the ratio

$$\frac{P(\mu \to \nu)}{P(\nu \to \mu)} = \frac{g(\mu \to \nu)}{g(\nu \to \mu)} \frac{A(\mu \to \nu)}{A(\nu \to \mu)}. \tag{3.24}$$

The ratio of the acceptance probabilities, hence, can take any value between zero and infinity, which means that both $g(\mu \to \nu)$ and $g(\nu \to \mu)$ can take any values we like.
While this could sound "easily" done, there is a catch: we have design out Monte Carlo simulation algorithm in such a way that it doesn't get stuck. If the acceptance ratios are too low, then the algorithm will refuse to move in to the new state most of the time and will not go anywhere, wasting a lot (our) of time.

3.6 The Metropolis algorithm

Armed with all the tools we have seen until now we turn now our attention to the Metropolis algorithm, developed in 1953 by Metropolis and co-workers. This is not the only algorithm available (by far) but we will use it to clarify the concept, and refer to [33] and [34] for an extensive treatment. The idea is to propose a change in the configuration of the system by flipping a single spin (chosen at random), changing its state. In an Ising model that would mean invert its sign, in a Potts model, select a new state between the p available. This is the new configuration: having $N = L^d$ spins this means that we have N non zero selection probabilities and each takes the value

$$g(\mu \to \nu) = \frac{1}{N}. \tag{3.25}$$

With these selection probabilities 3.22 becomes

$$\frac{P(\mu \to \nu)}{P(\nu \to \mu)} = \frac{g(\mu \to \nu)}{g(\nu \to \mu)} \frac{A(\mu \to \nu)}{A(\nu \to \mu)} = \frac{A(\mu \to \nu)}{A(\nu \to \mu)} = e^{-\beta(E_\nu - E_\mu)}. \tag{3.26}$$

So we have now to choose the acceptance ratios: even if we still have some maneuver space, we must be careful, otherwise our algorithm will end up being highly inefficient. A clever trick is to set one of the two acceptance ratio in their

ratio to 1 (ideally the largest) and then adjust the other to satisfy the constraints. In our case the optimus would be

$$A(\mu \to \nu) = \begin{cases} e^{-\beta(E_\nu - E_\mu)}, & \text{if } E_\nu - E_\mu > 0 \\ 1, & \text{otherwise.} \end{cases} \tag{3.27}$$

We choose one "direction" (the one that makes the energy go downhill) and set its acceptance ratio to one and then fix the other. This tells us also that the Metropolis algorithm will accept increases in energy of the system with a probability proportional to the length of jump uphill (in energy): the longer the jump, the lower the probability.
It is worth mentioning that we can also choose not to select a spin at random, but instead update the spin in a sequential order, starting from one corner of the d-dimensional hypercube and ending at the opposite one. In this case, even if the single spin updates probability respect detailed balance, their product (the update probability of the whole lattice) does not, even if the probabilities are still stationary: this is because the probability of the reverse transition is related to the probability of the forward transition in the "correct way" only if the spins are updated in reverse order[2].

Another algorithm which is commonly used is Heat Bath. In this case we select the new value directly with a probability proportional the Boltzmann factor, regardless to the actual state of the spin we are updating. The probability to assign a given spin σ_i a value ± 1 (in a EA model) is:

$$\begin{aligned} p_{\mathrm{HB}}(\sigma_i = 1) &= \frac{e^{-\beta E_+}}{e^{-\beta E_+} e^{-\beta E_-}} \\ p_{\mathrm{HB}}(\sigma_i = -1) &= 1 - p_{\mathrm{HB}}(\sigma_i = 1). \end{aligned} \tag{3.28}$$

The quantities $E_\pm$ are the local energies in the case the spin σ_i is 1 or -1, respectively: this can be calculated as the sum of the products of the spins with the respective couplings. It is possible to generalize the HB algorithm for the Potts spins as:

$$p_n = \frac{e^{-\beta E_n}}{\sum_{l=1}^{p} e^{-\beta e_l}}. \tag{3.29}$$

Since the function returning the energy is simpler, in general the HB algorithm is preferred where there is need to keep the computational load low. Also, in the case of the Potts models the HB algorithm is sometime preferred, especially in the case of high p. We can see why considering a two dimensional Potts model (eg. ferromagnetic) in a case with p high. As long as we are in the high temperature phase the acceptance ratio is close to one, but as we go to lower temperatures it is not the case anymore. Consider a case in which all the four neighbours of a spin have different values. There are four cases in which the spin is aligned with

[2] See, again, prof. Young's note on this.

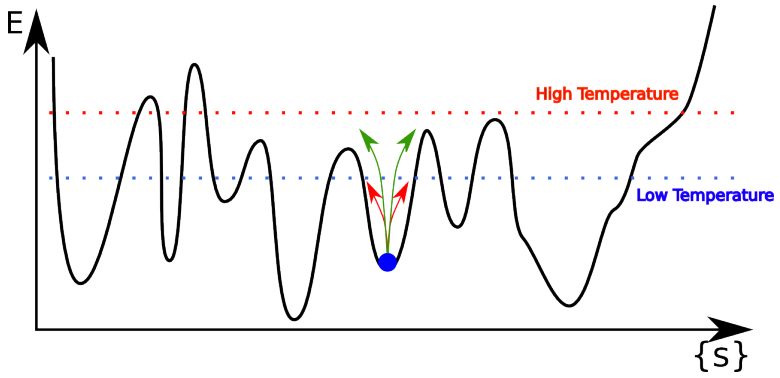


Figure 3.1: Energy as a function of the configuration space $\{s\} \equiv \{\sigma\}$, the energy landscape is rugged and complex. The configuration (blue point) is trapped in a local minimum: if the temperature is low, then it cannot exit the minimum (red arrows), while if temperature is higher (due to Parallel Tempering) it can exit the local minimum (green arrows) and continue the quest for the global minimum.

one of its neighbours which have a lower energy (and hence an higher Boltzmann weight) and $p-4$ equivalent cases in which the energy is higher: all these states in which the spin passes through in its MC evolution will have the same energy, hence the Metropolis acceptance ratio will be one. On average then, it will take $p/4$ steps to find one of the four desirable states. As p increases, this time will increase and it will take longer and longer for the to find the low-energy states, even if the acceptance ratios of the Metropolis algorithm is one, only because there are many states to go through. The HB algorithm may use less time in finding the appropriate state, by partitioning the interval $[0, 1]$ of the probability according to the Boltzmann weight: the more favorable state (or configuration) will be more probable.

3.7 Parallel Tempering

While the Metropolis algorithm is a very clever way to simulate spin systems (and not only these), we face a difficulty: once we start the simulation, if the energy landscape is rugged, the system could get trapped inside a local minimum of the energy quite easily. In fact, since the Metropolis algorithm favours the "downhill" direction of the energy, if the well in which the system has fell is deep enough, we will not be able, easily, to get it out. Parallel Tempering algorithm [37] tries to solve this problem by simulating, in parallel, N_β exact copies of the system at different temperatures usually on both sides of the transition. Once every M MC sweeps an exchange between two copies at different temperatures is proposed and accepted with probability

$$p \propto e^{\Delta E \Delta \beta}, \tag{3.30}$$

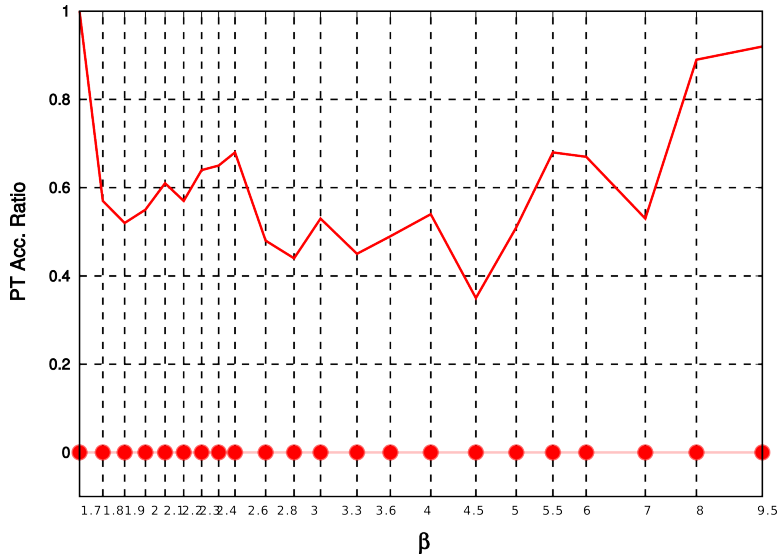
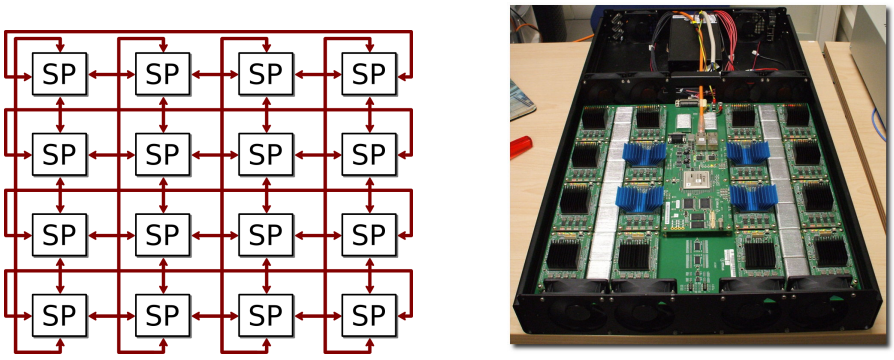


Figure 3.2: Acceptance ratio for a short simulation, performed only for illustrational purposes, of the Potts Glass $p = 5$, $L = 6$. The circles on the bottom show the temperature's positions. The β axis is logarithmic.

which has the same form (except for $\Delta\beta$) of the Metropolis acceptance probability, and respects the detailed balance condition. Choosing the temperatures in a skillful way allows copies at low temperatures, with a slow dynamic, to reach higher temperatures and decorrelate. Once brought back to low temperatures such copies will likely end in a different valley of the complex energy landscape, which was our original aim. As a bonus, simulating in parallel copies of the system lets us, in just one run, to have all the data points we need. If we try to swap temperatures which are far away we might end up proposing a lot of exchanges and accepting a very small part of them, so usually one proposes exchanges only between adjacent temperatures. The details, such as in which order we select temperatures to swap or in which direction we want to exchange copies, are not fixed, and one can experiment: questions like how often do we do a Parallel Tempering step or how we select temperatures require a trial-and-error approach for the system under study. There are, though, some results that we can use to understand better what is going on. Between these it is worth nothing the Incomplete Beta Law [38], which can help us understanding what to expect in terms of acceptance ratio of the swaps in some cases. There is an extensive literature which aim is to improve Parallel Tempering: increasing the acceptance ratio is not the whole point, we also want the copies to be able to move from one end to the other of the spectra of temperatures: various approaches are being tried, see for example [39], [40], [41], [42], [43], [44] and [45].



(a) (b)

Figure 3.3: (a) Topology of a Janus board: each SP communicates with its nearest neighbours in the plane of the board. (b) Janus board in a Janus box, commonly called "the coffin".

3.8 The Janus computer

Janus is a dedicated computer for the simulation of discrete spin systems such as Ising and Potts models. It makes possible, as we will see in the next chapters, to simulate these for an unprecedented Monte Carlo time. In the first run of the Janus computer we were able to simulate an EA model for a "real time" of a tenth of a second, several orders of magnitude more than any previous work [46]. It is the product of a collaboration between BiFi (Institute for Biocomputation and Physics of Complex Systems) of the University of Zaragoza, universities of Madrid, Badajoz, Rome and Ferrara together with an industrial partner, Eurotech.

Janus is designed as an heterogeneous system comprising conventional processor and FPGAs and to be modular: each board contains 17 FPGA-based miniboards called *nodes*, of which 16 are used for computation, called Scientific Processors (SPs), and one for input/output operations, called Input/Output Processor (IOP). Each board is driven by a conventional computer, called the Janus Host. The first system installed is composed of 16 boards and 8 Janus hosts, for a total of 256 SPs, 32 conventional computer's core, 32 GB of RAM and several TB of disk space.

In a single board each SP is linked to its nearest-neighbours SPs with periodic boundary condition, in such a way that the SPs form a 2-dimensional mesh toroidal network: this allows for communication between SPs, that in turn allows parallelization at the SPs level. Each SP is also connected with a point-to-point connection to the IOP for initialization purposes and for input/output operations, for example in communicating with the Janus host: the latter is connected to the boards via a Gigabit Ethernet connection, using a set of specifically crafted low-level C libraries accessing the raw Gigabit Ethernet level.

Programming the Janus machine can be accomplished by either an interactive Perl shell, mostly used for debugging and testing purposes, or physics-oriented C libraries, which make relatively easy to access hardware resources without the necessity of extensive hardware knowledge.
SPs are programmed using VHDL code which is in turn compiled to obtain a firmware to load onto the FPGAs, and as of writing there are several firmwares available: spin glasses mostly , such as EA and Potts, for different linear sizes and different p, as well as an implementation of the Graph Coloring problem using an antiferromagnetic Potts model and Simulated Annealing. For each of these models both Metropolis and Heat Bath update algorithms are available. In these firmwares all the available parallelisms are exploited: at the sample level, simulating different realizations of the disorder on different SPs and at replica and spin level, using an efficient checkerboard scheme which updates the whites of one replica at the same time of the black of the other replica. This allows for the update of as many as 1024 spin sites per clock cycle.
Parallel Tempering can be implemented in Janus in two ways: one can have all the N_β copies of the system in the same SP. This is feasible as long as the system is not too big: for a $L \leq 32$ and a reasonable number of temperatures, there are no problems of space: we can trade lattice size for number of copies, given that the space inside the FPGA is limited. Also, we need two replicas (in some cases four) of the same system at the same temperature, to calculate the overlap, so we need a total of $2N_\beta$ copies of the system in the same SP. In another way we could, for bigger systems, simulate more replicas of the same system on one SP and then implement Parallel Tempering between different SPs, using the IOP to decide about temperature swaps.
The Janus project was started in 2004, the first prototypes were available around the summer of 2007, and the first system built later the same year: in March 2008 the first run (a 25 days simulation with just one system crash due to severe weather condition that cause a power failure) with results submitted to the Gordon Bell Prize, and producing already relevant physics. In May 2008 the system was installed in Zaragoza and it has running several physics simulations codes ever since.

Chapter 4

Monte Carlo Simulations and Observables

In this chapter we will define and discuss the observables used in the Monte Carlo simulations. We will also detail the simulations themselves, and describe the methods used in the analysis.

4.1 A few initial words

The simulations that have been performed on the Potts Glass had the purpose of studying the paramagnet-glass phase transition. We know that in mean field theory there is a transition, and its character depends on p, and we want to investigate its existence and nature in finite size systems (in detail in $d = 3$). To do this we are run Monte Carlo simulations and analyze the results, since there is no way, in a three-dimensional system, to look for the transition temperature analytically. Simulations and analysis let us locate the transition and at the same time study the critical exponents of the system.
We were able to simulate lattices of linear dimension $L = 4, 6, 8, 12, 16$ (not all sizes for all p) and to thermalize most of them: we will see where thermalization failed, and we will try to understand why. The smaller lattices were simulated on a traditional computer cluster, while for linear size equal or above 8 we used the Janus dedicated machine (see previous chapter, but also [47], [48] and [49]): as a comparison the simulation of the Potts Glass for $L = 16, d = 3, p = 4$ on an Intel Core2Duo running at 2.4 GHz would have taken thousands of CPU-years, while it was manageable on the Janus system.
The model we simulated is described by the Hamiltonian

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{i,j}\delta(\sigma_i, \sigma_j) \tag{4.1}$$

with bimodal couplings $J_{ij} = \pm 1$ with equal probability, defined on a cubic lattice, with periodic boundary condition.

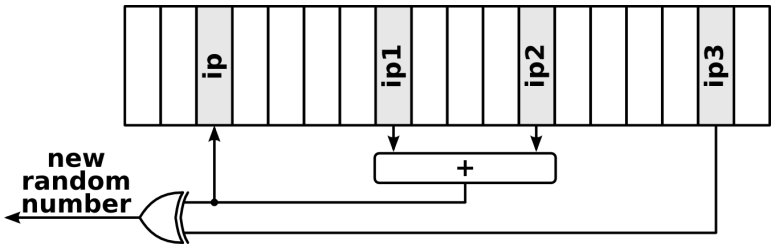


Figure 4.1: The Parisi-Rapuano shift register Random Number Generator (RNG): a set of 32-bits words (the *wheel*): $R(k)$ is the new random number, produced by $I(k) = I(k-24) + I(k-55), \quad R(k) = I(k)I(k-61)$. We initialize the wheel with externally generated random values. $I(k)$ is the new element of the updated wheel: $ip1 = 24$, $ip2 = 55$, $ip3 = 61$: hence $ip = ip1 + ip2$ and the new random is $ip \cdot ip3$. At each step the value of k is incremented by one, modulo the length of the wheel.

In all the simulations we have used the Heat Bath and the Parallel Tempering algorithms. We define a Monte Carlo Sweep (MCS) as the subsequent spin update of $N = L^3$ spins in sequential order. In Monte Carlo simulations we use, as it may appear evident from the discussion of the latest chapter, a very big number of random numbers: for each spin sweep update, we need, at most, N of them. It is of paramount importance that the pseudo random numbers are of really good quality: we used the Parisi-Rapuano [50] pseudo random number generator (see figure 4.1), which has, so far, been satisfying. The implementation on the Janus computer produces one random number per clock cycle: up to 10^{13} random numbers we were not able to appreciate any correlation in the random numbers produced. Even given this, to be sure to avoid dangerous correlations, we refresh every 10^6 MCS the random wheel.

4.2 Observables

The first observable that we will define for the Monte Carlo runs is the magnetization. As a first step we need to change the labeling of the spins to something more "handy" to use. We will use the *simplex* [51] representation, in which one associates to each state p a unit length vector pointing to the p vertices of the $(p-1)$-dimensional hypertetrahedron. A few examples are in figure 4.2, for $p \leq 4$. These vectors satisfy the relation:

$$\vec{S}_a \cdot \vec{S}_b = \frac{p}{p-1}(\delta(a,b) - 1). \tag{4.2}$$

For example, for $p = 3$, the simplex vectors lie on a two dimensional plane,

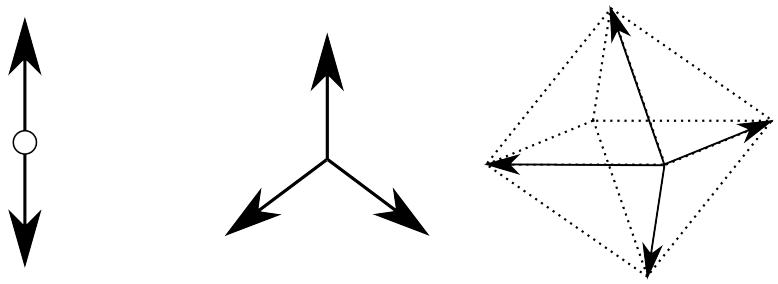


Figure 4.2: p unit vectors pointing in the p symmetric directions of the $p-1$-dimensional hypertetrahedron, used to represent Potts spins: from left to right $p = 2$, $p = 3$ and $p = 4$.

and they take to form:

$$\begin{aligned} \vec{S}_1 &= (0,1) \\ \vec{S}_2 &= \left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \\ \vec{S}_3 &= \left(-\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \end{aligned} \tag{4.3}$$

$$\tag{4.4}$$

The simplex representation lets us, as a first thing, rewrite the Hamiltonian in a more familiar way:

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J'_{ij}\ \vec{S}_i \cdot \vec{S}_j \tag{4.5}$$

where we have rescaled the couplings as

$$J'_{ij} = \frac{p-1}{p} J_{ij}. \tag{4.6}$$

In this way we can easily study the magnetization as:

$$\vec{m} = \frac{1}{N} \sum_{i=1}^{N} \vec{S}_i. \tag{4.7}$$

We also define the ferromagnetic susceptibility, which will signal to us the onset of ferromagnetic order and hence the possible presence of a para-ferromagnetic transition as

$$\chi_{\mathrm{M}} = N \left[\langle |\vec{m}|^2 \rangle \right]_{\mathrm{av}} \tag{4.8}$$

where we have averaged both in the thermal sense and on the disorder.
In a different way from what we did in the first chapter, we will use the Fourier transform of the spin glass order parameter:

$$q^{\mu\nu}(\vec{k}) = \frac{1}{N} \sum_{i=1}^{N} S_i^{\mu(1)} S_i^{\nu(2)} e^{i\vec{k}\cdot\vec{R}_i} \tag{4.9}$$

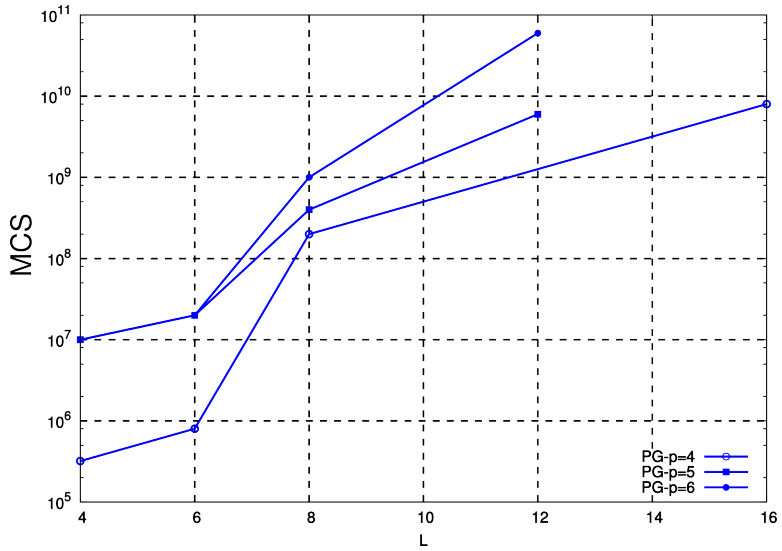


Figure 4.3: A schematic semilog plot of the number of MCS per L for different p.

where $S_i^{\mu(1)}$ is the μ^{th} component of the i^{th} spin in the first replica, and $S_i^{\nu(2)}$ is the ν^{th} component of the same spin in the second replica: as it may appear now obvious, and as we noted earlier, we are simulating two replicas of the same realization of the coupling with different random numbers (with different time evolutions). We also use the Fourier transform of the spin glass susceptibility as

$$\chi_{\text{q}}\left(\vec{k}\right) = N \sum_{\nu\mu} \left[\langle |q^{\mu\nu}(\vec{k})|^2 \rangle \right]_{\text{av}} . \tag{4.10}$$

Finally we define the correlation length, ξ, in terms of the ratio of Fourier transform of the spin glass susceptibility

$$\xi = \frac{1}{2\sin\left(\frac{\vec{k}_{\text{m}}}{2}\right)} \left(\frac{\chi_{\text{q}}(0)}{\chi_{\text{q}}(\vec{k}_{\text{m}})} - 1 \right)^{\frac{1}{2}} \tag{4.11}$$

where $\vec{k}_{\text{m}}$ is the minimum wave vector allowed in the lattice, which with periodic boundary condition is $\vec{k}_{\text{m}} = \left(\frac{2\pi}{L}, 0, 0\right)$ or any of the other two vectors obtained permuting the indexes [52]. We are very interested in ξ since it will give us a reliable method for estimating the transition point by simulating different sizes of the system and looking for the intersection point of ξ/L.

4.3 Details of the simulations

We ave used the Heat Bath algorithm and PT in our simulations. The first question which arises is: what is the best number of HB sweeps between PT

steps? A correct answers should be dependent on the details of the system we are simulating. We have performed testing to understand this dependence not only for Potts models but also for the EA spin glass. Starting from 1 HB/PT (each HB step perform a PT step), to 10 HB/PT and then to 100 HB/PT results do not really significantly. We decided for 5 HB/PT when simulating on the cluster and 10 HB/PT when simulating on Janus. The difference is driven by the fact that while a PT step on a conventional computer does not "cost" more than an HB step (in terms of time they are equal), on Janus a PT step is approximately 60% more expensive, in terms of time, than the HB step, due to the architecture used. Reducing the frequency of PT steps, having first checked that the Physics is all right with it, lets us decrease the total wall clock time of the simulation.
The second question regards the temperatures we simulate: how to select them? Of course this decision has two important sides we should consider. In the first place we have to ensure that Parallel Tempering is doing its job: the copies of the system must be able to move freely from one end to the other of the spectra of temperatures, otherwise we would be calculating averages in the wrong way. This is particularly hard when the system we are simulating exhibits a discontinuous phase transition, or a continuous phase transition with critical exponents very near to the discontinuous boundary (see [43] for an example). Secondly, we wish to simulate a range of temperatures which lets us gather information on both the sides of the transition. In doing this one has to be extremely careful since, we noticed, going too deep in the cold region, where the dynamic is slow, could mean trap copies there, making very hard for them to exit the region to decorrelate. In general we started using uniformly distributed inverse temperature, increasing the temperature's density near the transition. This is typically an iterative procedure, where one checks the behaviour of the copies of the system in Parallel Tempering, and looks for a temperatures' density which lets the copies freely move from one side to the other of the transition, keeping an eye on the acceptance ratios and on the average round trip time (or, in another way, to the number of round trips from low to high temperatures and back that a copy performs).
Details for the simulation of the Potts Glass $p = 4, 5, 6$ are summarized in table 4.1. While one could argue that for the different values of p the parameters are, more or less, the same there are a few important differences. What one notes first is that the thermalization of $L = 16$ was possible only for $p = 4$, while for $p = 5$ we were able to reach it just a few samples: enough to gain some insight on the behaviour of the system, but not enough to have good data. If we look at the $p = 4$ case we can note that the interval between temperatures for $L = 4$ is approximately 0.44, for $L = 6$ is 0.35, for $L = 8$ is 0.09375 and for $L = 16$ is 0.075: the temperature density increases with L, and the upper temperature lowers in agreement to what we just said. The temperature density, anyway, tells just half of the story: the other half is in the disposition around the critical point.
If we turn our attention to the total number of Monte Carlo Sweeps per sample, we note immediately that for increasing p the difficulty in reaching a thermalized phase increases: while for $p = 4$ thermalizing $L = 16$ required 8×10^9 mcs we

p	L	N_{samples}	MCS	$[\beta_{\min}, \beta_{\max}]$	N_β	N_{HB}	N_m
4	4	1000	3.2×10^5	[2.0,6.0]	9	5	10^3
	6	1000	8×10^5	[2.5.5.0]	7	5	10^3
	8	1000	2×10^8	[2.7,4.2]	16	10	2×10^5
	16	1000	8×10^9	[1.7,4.1]	32	10	2×10^5
5	4	2400	10^7	[1.6, 9.5]	18	5	10^3
	6	2400	2×10^7	[1.6, 9.5]	22	5	10^3
	8	2448	4×10^8	[1.7, 6.5]	24	10	2×10^5
	12	2451	6×10^9	[1.8, 5.5]	20	10	2×10^5
6	4	2400	10^7	[2.1, 9.8]	10	5	10^3
	6	2400	2×10^7	[2.0, 9.65]	16	5	10^3
	8	1280	10^9	[1.7, 7.5]	30	10	2×10^5
	12	1196	6×10^{10}	[1.6, 6.5]	22	10	2×10^5

Table 4.1: For $p = 4, 5, 6$ and for each lattice size, number of disorder samples analyzed, number of MCS per sample, range of simulated inverse temperatures, number of (uniformly distributed) β values used for PT, number of MCS performed between two PT steps (N_{HB}) and the number of MCS between measurements (N_m).

needed 6×10^{10} to thermalize $L = 12$ in $p = 6$. A schematic plot of the MCS as a function of L is in figure 4.3.
In the end we note that, for each temperature, we simulate two different replicas (identical realization of the disorder), to be able to calculate q.

4.4 Thermalization

Before proceeding with the analysis, we have to be sure that the data we are looking at comes from systems which are well thermalized. A common test is to consider a physical quantity and average (thermally first, then on disorder, in this order) over logarithmically increasing time windows. In this way the last point of our thermalization check, if we have a total N_{sweep} sweeps, will represent the time between $N_{\text{sweep}}/2$ and N_{sweep}, averaged, the previous point the average of the data from the time between $N_{\text{sweep}}/4$ and $N_{\text{sweep}}/2$ and so on. Ideally we can say the system has reached thermalization once the value of the quantity we are measuring doesn't change over the last few (3, in our case) points, corresponding to the three last time windows. There is no need to apply this kind of analysis to all the temperatures configuration: if we do this only for the coldest temperature we can be sure that all the others will be thermalized too, since the lowest temperature is the slowest to thermalize. This also gives us a pretty clear idea on how much we have discard of the first part of the simulation

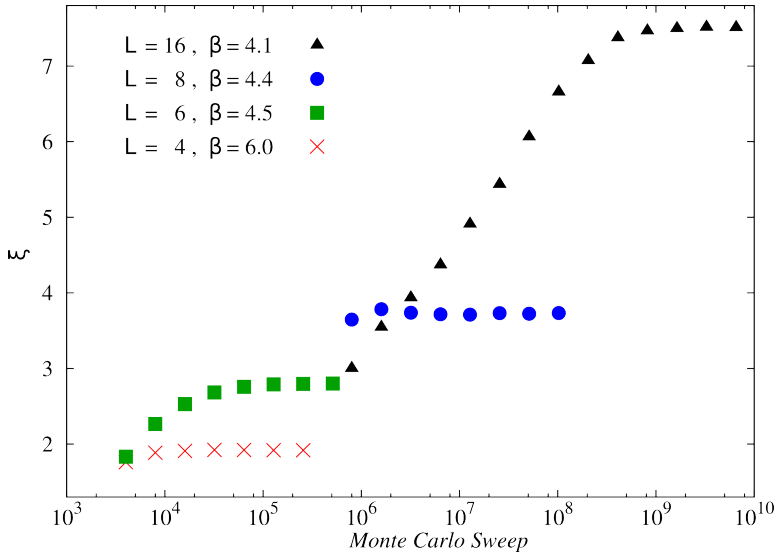


Figure 4.4: ξ as a function of the Monte Carlo sweeps for the Potts Glass $p = 4$. Data are log binned. All error bars are smaller than the point size. We can see the transient and the plateau.

to be sure to average only on well thermalized data, since we can tell the plateau, that we keep, from the transient, that we throw away. Thermalization tests for the Potts Glass, $p = 4, 5, 6$, are shown in figures 4.4, 4.5 and 4.6. In all of them, the last three points (or more) agree within error bars: we can be sure to be dealing with well thermalized data.

4.4.1 Temperature-temperature time correlation function

In order to check the time scales of the dynamical process and to asses the thermalization and the statistical significance of our statistical samples, we compute a few dynamical observables that characterize the Parallel Tempering dynamics. One of them is the temperature-temperature time correlation function as introduced in [53] (and in references therein): this will tell us if we have simulated each single sample for a MC time long enough for it to thermalize. Doing this we can investigate thermalization on a *sample per sample* basis, whereas in studying ξ's plateau we were looking at the problem using the whole sample group.
Let $\beta^{(i)}(t)$ be the inverse temperature of the system (i) at time t, where $i \in \{0, 1, \ldots, N_\beta - 1\}$ and with N_β equal to the number of systems (and hence temperatures) evolving with Parallel Tempering. Let $f(\beta)$ be an arbitrary function of the temperatures which changes sign at β_c, the temperature where the transition is. Let $f_t^{(i)}$ be

$$f_t^{(i)} = f(\beta^{(i)}(t)). \tag{4.12}$$

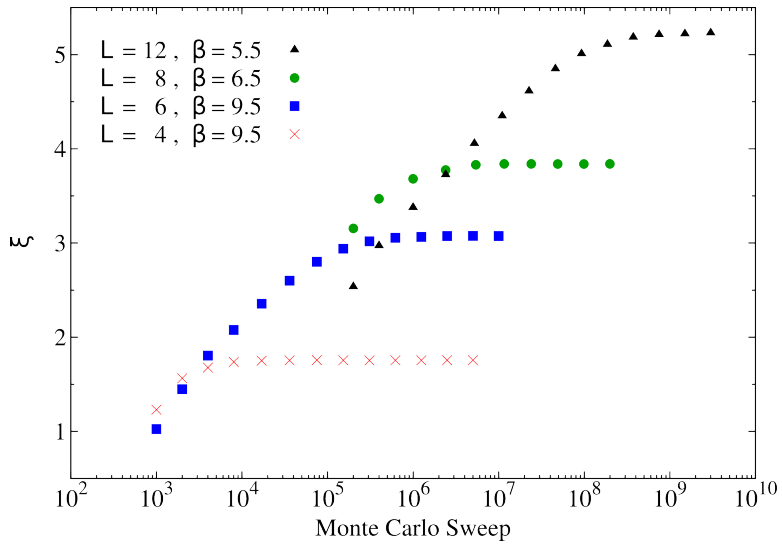


Figure 4.5: ξ as a function of the Monte Carlo sweeps for the Potts Glass $p = 5$. Data are log binned. All error bars are smaller than the point size.

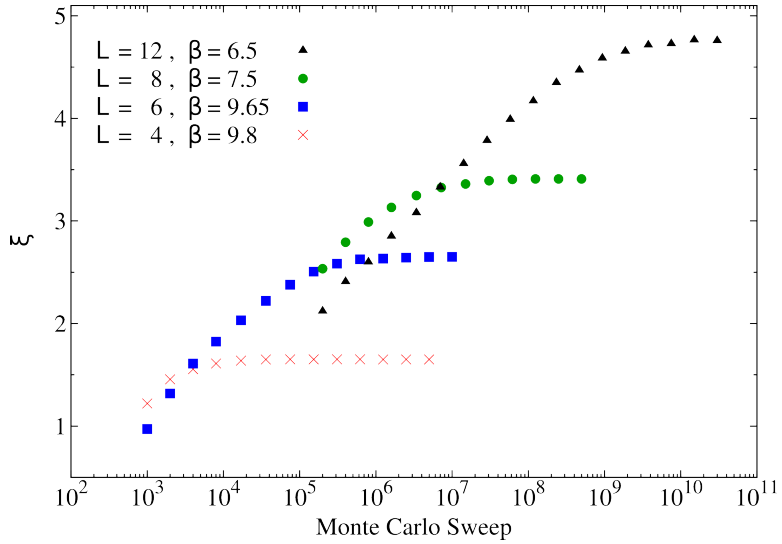


Figure 4.6: ξ as a function of the Monte Carlo sweeps for the Potts Glass $p = 6$. Data are log binned. All error bars are smaller than the point size.

In equilibrium, system i can be found at any of the N_T temperatures, for all i and all t, hence

$$\langle f_t^{(i)} \rangle = \sum_{k=0}^{N_T-1} \frac{f(\beta_k)}{N_T} \tag{4.13}$$

The function f must be as simple as possible ([53] chooses it to be a cubic polynomial) such that

$$\sum_{k=0}^{N_\beta-1} \frac{f(\beta_k)}{N_\beta} = 0. \tag{4.14}$$

In [55] we choose a slightly different function:

$$f(\beta) = \begin{cases} a(\beta - \beta_c), & \text{for } \beta < \beta_c \\ b(\beta - \beta_c), & \text{for } \beta > \beta_c. \end{cases} \tag{4.15}$$

where the ratio of the slopes, a/b is fixed by the condition 4.14. Since the overall normalization is irrelevant we choose $a = 1$.
Now we can define the correlation function

$$C_f^{(i)}(t) = \frac{1}{M - |t|} \sum_{s=1}^{M-|t|} f_s^{(i)} f_{s+|t|}^{(i)}, \tag{4.16}$$

where M is the total simulation time. $C_f^{(i)}(t)$ in 4.16 can be normalized as

$$\rho_f^{(i)}(t) = \frac{C_f^{(i)}(t)}{C_f^{(i)}(0)}. \tag{4.17}$$

To gain statistics we consider

$$\rho_f(t) = \frac{1}{N_\beta} \sum_{i=0}^{N_T-1} \rho_f^{(i)}(t). \tag{4.18}$$

We have characterized the correlation function through its integral autocorrelation time

$$\tau_{\text{int}} = \int_0^{\Lambda_{\text{int}}} \mathrm{d}t \rho_f(t) \tag{4.19}$$

where $\Lambda_{\text{int}} = \omega \tau_{\text{int}}$ and where it is convenient to set $\omega = 10$. In figure 4.7 is shown the typical behaviour of the correlation function: an initial fast (exponential) decay and, later in time, fluctuations around zero.

This is also important since sample fluctuations of τ_{int} are very large as we can see in figure 4.4.1. To be sure that we are dealing with thermalized data, we can increase the number of Monte Carlo sweeps (the Monte Carlo time)[55]: we increase the total number of MCS if the estimated τ_{int} is bigger than M/c (where M is the length of the simulation in MCS and c is a constant of order 20 for $L = 8$ and 15 for $L = 12$ in the $p = 5$ case).

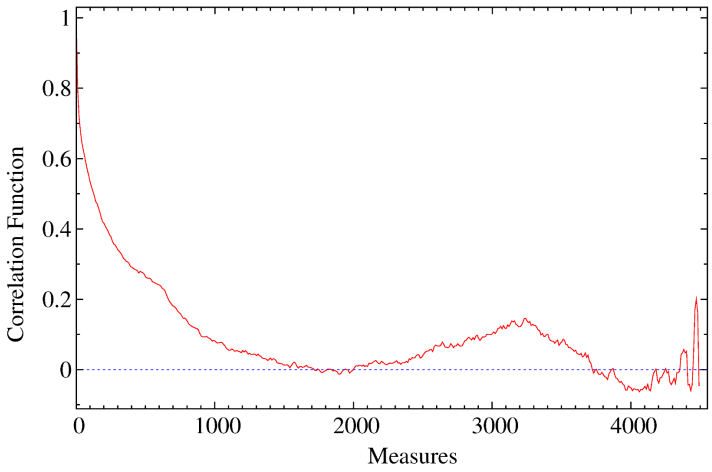


Figure 4.7: The Correlation function for a generic sample ($p = 6$, $L = 8$) as defined in 4.18.

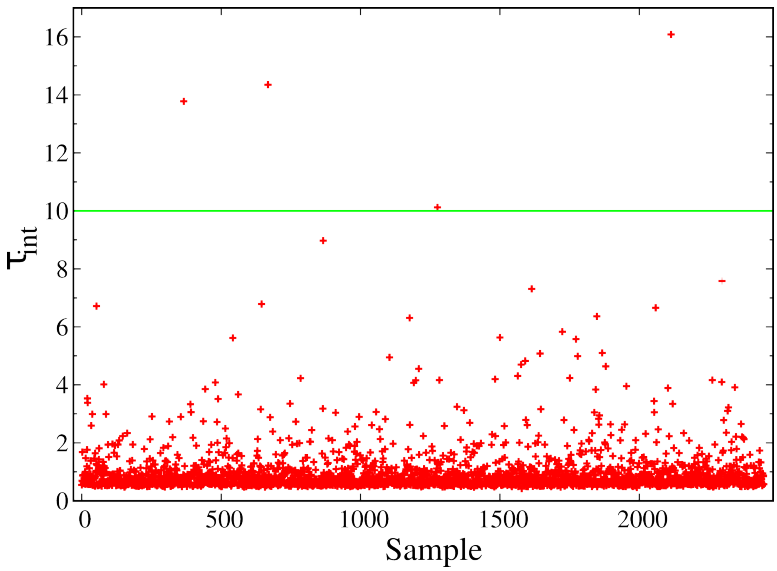


Figure 4.8: τ_{int} for all $p = 5$, $L = 8$ samples simulated, in units of blocks of ten measures (corresponding to $\approx 2000^3$ MCS). Those samples whose τ_{int} is above the green have been simulated for a longer Monte Carlo time

4.5 The critical temperature and the critical exponents

Consider an intensive quantity, O, for example the energy density or magnetization density or magnetization susceptibility, which behaves in the thermodynamic limit as

$$\langle O \rangle_{L\to\infty} \propto |t|^{-x_O} \tag{4.20}$$

when $|t| \equiv \frac{T-T_c}{T_c} \approx \frac{\beta-\beta_c}{\beta_c} \to 0$. The Finite Size Scaling ansazt (FSS) lets us write that the mean value for a lattice of size L behaves like

$$\langle O \rangle_L = L^{x_O/\nu} f_O(L/\xi_\infty). \tag{4.21}$$

This is based on the assumption that the finite size behaviour is governed by the ratio L/ξ_∞, where ξ_∞ is the correlation length of the infinite system. f_O is an analytic function of its argument, that depends on the particular quantity we consider. It is expected to be universal, even if dependent on the boundary conditions we impose on the system. We have also to consider corrections to scaling, writing

$$\langle O \rangle_L(\beta) = L^{x_O/\nu} \left[f_O(L^{1/\nu}t) + L^{-\omega} h_O(L^{1/\nu}t) + \ldots \right] \tag{4.22}$$

where ω is the corrections-to-scaling exponent. The derivation of this, quite lengthy, can be found in [52]: the basic idea is that one can write corrections to $\langle O \rangle_L$ in an asymptotic expansion. We can say that we are in the FSS regime if $L \leq \xi_\infty$, or, equivalently, if $|t|L^{1/\nu} \sim 1$. It is interesting to note the correspondence between $\xi_L(t)/L$ and $tL^{1/\nu}$. In the FSS regime

$$\xi_L = L f_\xi(L^{1/\nu}t) \left[1 + L^{-\omega} h_\xi(L^{1/\nu}t) + \ldots \right]. \tag{4.23}$$

We can equivalently write, for 4.22,

$$\langle O \rangle_L(\beta) = L^{x_o/\nu} \left[\tilde{f}_O(\xi_L/L) + L^{-\omega} \tilde{h}_O(\xi_L/L) + \ldots \right]. \tag{4.24}$$

We can use the FSS ansatz (with corrections) to extrapolate results from finite size simulations to infinite volume (which is absolutely necessary to compare results from simulations to experiments). There is a variety of ways to perform such extrapolations, we will consider here the method described in [35]. We fix s ($s > 1$) the scaling factor, and then form a ratio

$$R_O(\beta, L, s) = \frac{\langle O \rangle(\beta, sL)}{\langle O \rangle(\beta, L)} \tag{4.25}$$

Note that nothing forbids to use $O \equiv \xi$. From equation 4.24 we can obtain

$$R_O(\beta, L, s) = f_{s,O}(\xi_L/L) \left[1 + L^{-\omega} h_{s,O}(\xi_L/L) + \ldots \right], \tag{4.26}$$

with $f_{s,O}$ a universal function that tends to one in the thermodynamic limit, for periodic boundary condition:

$$f_{s,O}(x) \sim 1 + A_O e^{-1/x} + \dots \tag{4.27}$$

where A_O is a constant. The extrapolation to the thermodynamic limit can be done by first obtaining an estimate of the scaling functions $f_{s,O}$ and $f_{s,\xi}$, for example from Monte Carlo simulations: from data pairs $(\xi_L(\beta), R_O(\beta, L, s))$ we can obtain $f_{s,O}$ by plotting $R_O(\beta, L, s)$ as a function of $(\xi_L(\beta)/L)$ and by fitting $R_O(\beta, L, s)$ to a polynomial in e^{-L/ξ_L}. Once we have these estimates from data pairs $(\xi_L(\beta), \langle O\rangle_L(\beta))$ (obtained at size L) we can obtain the corresponding pair for lattices of size sL with

$$\begin{aligned} \langle O\rangle_{sL}(\beta) &= \langle O\rangle_L(\beta) f_{s,O}\left(\frac{\xi_L(\beta)}{L}\right), \\ \xi_{sL}(\beta) &= \xi_L(\beta) f_{s,\xi}\left(\frac{\xi_L(\beta)}{L}\right). \end{aligned} \tag{4.28}$$

From this, one can move to lattices of size s^2L in the same way, using the data of sL just obtained.

We do not know beforehand the value of the critical temperature and the idea is to employ a similar method to bypass the problem. We consider a pair of lattices of size L and sL, with $s > 1$ as before. A typical value of s is 2. As before we consider the ratios defined in equation 4.25. It is of particular interest the ratio R_ξ at the temperature $\beta_c^{L,s}$ at which

$$R_\xi(\beta_c^{L,s}, L, s) = s, \tag{4.29}$$

which can be rewritten as

$$\frac{\xi_L(\beta_c^{L,s})}{L} = \frac{\xi_{sL}(\beta_c^{L,sL})}{sL}. \tag{4.30}$$

At this temperature the correlation length in unit of lattice size is independent of the latter: it coincides for both systems. This is an expression of scale invariance which should be true only at the critical temperature. Nonetheless, due to scaling corrections, $\beta_c^{L,s}$ differs slightly from the true critical temperature by a quantity proportional to both $s^{-\omega}$ and $L^{-\omega-\frac{1}{\nu}}$. An interpretation of the coincidence of ξ_L/L and ξ_{sL}/sL can be given in terms of a kind of renormalization, due to Nightingale [36]: one considers a kind of real space renormalization group which maps a system of size sL into a system of size L which the same Hamiltonian. The temperature in the renormalized system is obtained from the temperature in the original system via:

$$\beta_{sL} \to \beta_L \quad : \quad \frac{\xi_L(\beta_L)}{L} = \frac{\xi_{sL}(\beta_{sL})}{sL}. \tag{4.31}$$

Hence, $\beta_c^{L,s}$ is the fixed point of this transformation. This enforces scale invariance, as expressed before.
Recalling 4.24 and considering the ratio for a generic observable at $\beta_c^{L,s}$ we can write:

$$\begin{aligned} R_O(\beta_c^{L,s}, L, s) &= s^{x_O/\nu} \frac{\tilde{f}_O(\xi_L/L)\left[1 + s^{-\omega}L^{-\omega}\tilde{h}_O(\xi_L/L) + \ldots\right]}{\tilde{f}_O(\xi_L/L)\left[1 + L^{-\omega}\tilde{h}_O(\xi_L/L) + \ldots\right]} \\ &= s^{x_O/\nu} + A_O L^{-\omega} + \ldots, \end{aligned} \tag{4.32}$$

where A_O is a constant and the dots stand for higher order corrections. Equation 4.32 lets us extract the exponent x_O/ν by means of an extrapolation in $L^{-\omega}$: by applying this to different observables we can obtain different the critical exponents. By using it with $O = \partial_\beta \xi$ we obtain $1 + \nu$, while applying it to χ_m we can obtain $2 - \eta_m$. The same holds for χ_q, resulting in η_q.
This work is well described in [56]: even if the model has no analytical solution, we can obtain the critical exponents by means of the FSS ansatz and this technique, which goes by the name of Quotient Method.

4.6 The ferromagnetic phase

As we noted in the first chapter, the Potts Glass can enter, for sufficiently low temperature, a ferromagnetically ordered phase. We need to check whether the system is in such a phase, since we want to be sure that we are characterizing a spin glass phase transition, and the corresponding phase, and not a para-ferro transition. Ferromagnetic ordering could influence the spin glass phase even close to the glass transition, hence biasing our analysis. The problem is very serious if the temperatures of the two transitions (para-ferro and para-glass) are expected to be very close. It is then very important to check whether there is a region with nonzero spontaneous magnetization close to the spin glass critical region. We have all the tools to study this: the critical exponent of the magnetic susceptibility, η_{m}, first. If this exponent has value close to 2 then we expect no divergence, hence no transition, since χ_{m} diverges as $2 - \eta_{\mathrm{m}}$. But we can also study the magnetization and magnetic susceptibility for the whole range of temperatures: in the paramagnetic region the m is random in sign and so it modulus $\overline{\langle|\vec{m}|\rangle}$ is proportional to $1/\sqrt{N}$, $N = L^d$ in our case $d = 3$, and the magnetic susceptibility is independent of size. By contrast in the ferromagnetic phase $\overline{\langle|\vec{m}|\rangle}$ tends to a positive value at large N so that χ_{m} diverges, proportionally to N.
Checking both of these two ways of controlling the ferromagnetic ordering will let us keep the situation under control: a value of η_{m} around 2 and the non-divergence of χ_{m} will make us sure that we are not dealing with a ferromagnetic phase, and hence we are characterizing a spin glass transition.

Chapter 5

Results

In this chapter results from the simulations will be presented: before that we will quickly review what to expect, by reviewing results from literature about Monte Carlo simulations, and in the end we will try to put together all the insights we obtained from the simulations.

5.1 Overview of known results

The complexity of the simulation of the Potts Glass, in some sense, kept the probing of the critical behaviour of the model at bay, even if there have been attempts to tackle it. Without any particular order we will try to review the results, mostly from Monte Carlo simulation, on the short-range three-dimensional Potts Glass with both Gaussian and Bimodal couplings. Some of these results will also be from Mean-Field Potts Glass, such as some papers from Brangian, Kob and Binder.
In 1988, [58], Carmesin and Binder simulated a three-dimensional, short-range, three-states Potts Glass with Gaussian couplings, without having the possibility to distinguish if there was a phase transition for $T_c > 0$, but stating, anyway, that a non zero transition temperature is doubtful. Scheucher, Reger, Binder and Young in 1990, [59], simulated the same model, applying a finite-size-scaling study. They, too, suggest a zero-temperature phase transition, with exponentially diverging correlation length, implying a lower critical dimension of 3. Scheucher and Reger, in 1992, simulates a three-state three-dimensional Potts Glass with Bimodal couplings, [60]: they find, too, no signs of transition for $T_c > 0$, and conclude that 3 is the critical lower dimension. They conclude, too, that the Bimodal three-state Potts Glass has not a different behaviour from the Gaussian three-state Potts Glass. In the meantime, in 1989, Cieplak and Banavar, see [61] and [62], studied the same model, the three-state, three-dimensional Potts Glass: they conclude, using domain-wall renormalization group calculation (at $T = 0$) and found that the lower critical dimension is $d_l < 3$ for Gaussian couplings and $d_l > 3$ for Bimodal couplings, with a transition temperature $T_c \simeq 0.27$ for the

Gaussian couplings. In 1998 Dillmann, Janke and Binder, see [63], studied the mean-field Potts glass with Bimodal couplings for $p = 3$ and $p = 6$. They state: "Another unsatisfactory feature of our results is that they cannot distinguish the difference in character of the transition for $p = 3$ and $p = 6$" [63]. They also study the self-averaging properties of the moments of the magnetization distribution and their conclusion is that it seems to imply weak self-averaging for $p = 3$ and strong self-averaging for $p = 6$. The same year Reuhl, Nielaba and Binder, [64], study the three-dimensional, three-state Bimodal coupling Potts Glass using Monte Carlo simulations finding results compatible with a zero-temperature phase transition, even if, in their own words, "they do not prove it" [64]. They also reconsider the simulations of [58] as suffering from possibly insufficient thermal equilibrium: in their work they have reached 4.6×10^6 MCS for $L = 16$ lattices. In a series of works, [65] [66] [67] [68] [69] [70], Brangian Kob and Binder study both the mean-field and the short-range ten-states Potts Glass with $J_0 < 0$ to suppress ferromagnetic ordering. They find no plateau for $C(t)$ at $T = T_D$ revealing that no dynamic transition is observed and no signs of the static transition. They use the Heat-Bath algorithm for up to 10^8 MCS for sizes up to $L = 16$. Basically, they state that in the $p = 10$ Potts Glass both transitions, dynamic and static, are wiped out. Lee, Katzgraber and Young, in 2006, see [71], studied the three-states and ten-states three-dimensional Potts Glass using Finite Size Scaling. Simulations were carried out using Parallel Tempering. Results indicate a phase transition for the Gaussian couplings around $T_c \simeq 0.273$ (which is curiously similar to the one of Banavar and Cieplak in [61] and [62]) and $T_c \simeq 0.377$ for Bimodal couplings, in the case $p = 3$. For the $p = 10$ case they find no phase transition for three-dimension and a transition temperature $T_c \simeq 0.536$ for the four-dimensional model. Hence, their results for the ten-states Potts Glass with nearest neighbours of this work agree with the ones of Brangian, Kob and Binder: there is no phase transition. Recently, Andrist, Larson and Katzgraber, using a slightly different model, simulated the ten-states non-mean-field Potts glass [72]. They used a one-dimensional model (with periodic boundary conditions, so that is basically a ring of circumference L), with interactions between spins that fall off as

$$J_{ij} = \frac{\varepsilon_{ij}}{r_{ij}^{\sigma}} \tag{5.1}$$

with ε Normal distributed random variables and

$$r_{ij}^{\sigma} = \left(\frac{L}{\pi}\right) \sin \frac{\pi |i - j|}{L} \tag{5.2}$$

which represents the distances of the spins i and j on the ring. By tuning the parameter σ they are hence able to change the behaviour of the model from mean-field to non-mean-field, from above the upper critical dimension ($d_s = 6$) to an effective short-range hypercubic model below 6 dimensions. In their work they set $J_0 = -1$, and reach up to $10^7(2^{26})$ MCS. They do see a phase transition, for values of σ compatible with the Potts Glass below d_s, at a very low temperature

($T_c \simeq 0.025$ for $\sigma = 0.85$). They do not see any hint of a discontinuous phase transition: by analyzing the distribution functions of the energy they do not find any sign of the double peak which is indicative of a first order phase transition and they also note that setting $J_0 = 0$ would have increased ferromagnetic ordering in respect to $J_0 = -1$. Also, they note, the critical temperature seems to be affected by this change: it seems to be reduced by a factor $2 - 3$ and the change of J_0 does not change the complexity of the simulation.
It is worth mentioning also the study of a different model, even if only briefly, which goes by the name of Commutative Random Permutation Glassy Potts. Introduced originally in [73] by Marinari, Mossa and Parisi, with the explicit purpose of avoiding ferromagnetism, it was studied extensively in [74] by Fernandez, Maiorano *et al.*. In the latter the model was studied in three and four dimensions (the four dimensions version was studied also in the original work, finding a critical temperature $T_c \simeq 1.5$). In [74] the authors were able to refine the estimate of the transition temperature, for $d = 4$, as $T_c \simeq 1.41$, while for $d = 3$ the transition was found to be compatible with a Kosterliz-Thouless behaviour, but, it was not clear to them if they were dealing with a transient effect due to the vicinity of the lower critical dimension.

5.2 A quick reminder

What to expect from our simulations? How to decide the range of the temperatures to study? Which scenario between those outlined in literature do we expect to deal with? These questions, innocent at first look, require attention. We know from chapter one that the Potts Glass in MFT undergoes a phase transition, in which replica symmetry is broken, at a temperature that depends on the number of available states, p. Empirically, we expect this transition to happen at an inverse temperature $\beta_c(p) \approx p$. This comes from [75]: in that work they use an expansion in $1/d$ for K_c (that is thereby defined as $K_c = J/k_B T_c$, and is thus equivalent to our β_c) as a consistency check for the series expansion of χ_q finding $\beta_c^2 = p^2/2d + \ldots$, where the dots represent other terms of the expansion, whose coefficient are reported in the paper cited. If we look at the model for $p = 2$ the transition temperature is $\beta_c(2) \approx 1.80$ and for $p = 3$, we know from literature, $\beta_c(3) \approx 2.65$, so, roughly, we wonder if the slope, which in [75] should be $1/6$ for $d = 3$, is correct. We will check in the last section of this chapter if this empirical law holds, and if the slope, which just by plotting these two critical inverse temperatures outlines looks suspicious, is correct (or not).
The selection of the temperatures to simulate has a fundamental role for two reasons: firstly we will take measures on these temperatures, so we need them to gives us enough details, but, secondly, we absolutely need Parallel Tempering to be able to move copies of the system up and down in the temperature range: in high temperatures the system will decorrelate, giving us the ability, as we already pointed out, to obtain averages from a system who has visited many valleys. The

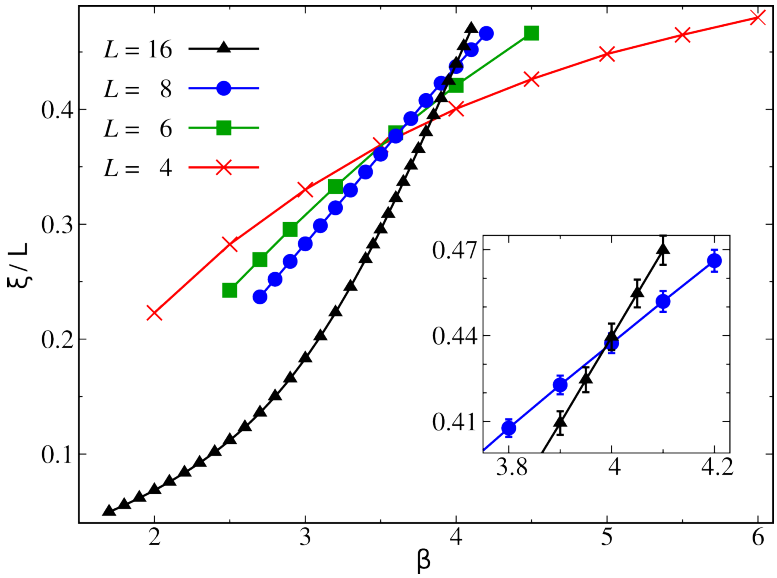


Figure 5.1: Plot of the spin glass correlation length over the system size as a function of β for all linear sizes of the Potts Glass $p = 4$. In the inset: magnification of the crossing between $L = 8$ and $L = 16$. Lines are just a guide for the eye.

choice, hence, is a bit of trial and error. Ideally we start with equally spaced temperatures in a range from very hot temperatures (low β) to temperatures which are not too advanced in the cold region: this "extension" in the cold region gets, in the simulations hereby described, smaller and smaller as the size of the system increases. Meanwhile, when the size of the system increases, we add temperatures near the temperature that we suspect, following the empirical rule pointed out above, to be critical. As said there is no clear rule for this: we basically try to obtain a sufficient acceptance ratio in Parallel Tempering to allow copies to perform the correct random walk in temperature space.
We expect the ferromagnetic transition temperature to follow

$$T_{\mathrm{FM}} = \left(\frac{p-2}{2}\right), \tag{5.3}$$

so that, since we want to investigate the para-spin-glass transition, we have to be sure that we have no ferromagnetic effects.

5.3 The $p = 4$ Potts Glass

The $p = 4$ case in of particular interest for various reasons: firstly for $p = 4$ we expect a continuous transition, while for $p \geq 4$ this should change. Secondly, the spin glass and ferromagnetic transition should be at same temperature, $T_{\mathrm{FM}} = T_{\mathrm{RSB}} = 1$, so in this sense the $p = 4$ case is marginal. Whether, or not, these prediction of Mean Field Theory apply to a three dimensional system it is

(L_1, L_2)	$\beta_{\rm cr}(L_1, L_2)$	$\nu(L_1, L_2)$	$\eta_q(L_1, L_2)$	$\eta_m(L_1, L_2)$
$(4, 8)$	3.59(4)	0.83(5)	0.15(4)	1.84(3)
$(8, 16)$	4.00(4)	0.96(8)	0.12(6)	2.06(3)

Table 5.1: Results for the critical exponents using the Quotient Method for the Potts Glass $p = 4$. (L_1, L_2) are the two lattice sizes used and $\beta_{\rm cross}$ is the inverse temperature where the two curves ξ/L cross. The values for ν and η_q are extracted from measurements involving q, whereas η_m has been computed from the magnetization.

the main point of interest.
After having checked for correct thermalization, as we did in the previous chapter, we proceed in looking for the spin glass transition temperatures, using ξ/L, where L is the linear size of the system. A complete plot of ξ/L as a function of β for all simulated system sizes is reported in figure 5.1. There is not an obvious crossing point common to all system sizes, due to correction to scaling: we see that, anyway, there are crossing points, so that we can quite sure in saying that we are looking at a phase transition. There is, of course, the possibility that for $L \to \infty$ the critical temperature goes to zero, and in that case there would be no transition. Looking at the critical exponents we think this is not the case.
We proceed, as we discussed, using the Quotient Method: we select two linear sizes whose ratio is $s = 2$, and we look for the crossing point. To do this we interpolate the curves using cubic splines. Since we cannot be sure that our results are independent of the interpolation, a linear interpolation around the crossing point has been implemented and the results checked with the cubic splines' one: they do agree within statistical precision. From the same Quotient Method we can also estimate the values of the critical exponents, computing the spin glass susceptibility and the derivative of ξ at the crossing points. Results are in table 5.1.
Even thought simulating the Potts Glass $p = 4$ for $L = 4, 6, 8, 16$ is a notable computing effort, we do not have, as of now, enough information to extrapolate the critical temperature in the thermodynamic limit. The two values of $\beta_{\rm cr}$ are quite different: this suggest a small value of ω (the leading correction to scaling exponent) in equation 4.32, which says we cannot reliably compute the asymptotic critical exponents. From table 5.1 we can infer that, given the behaviour of $\eta_{\rm q}$ as a function of the size of the systems involved in its computation, there is a transition: were $\eta_{\rm q}$ to tend to a value of 2 it would be the opposite. So far, data suggest the existence of a spin glass phase transition at finite temperature, but we also need to check for ferromagnetic effects around the transition which could bias our analysis.
Since the ferromagnetic and the spin glass transitions are expected, in MFT, to happen at the same temperature, in $p = 4$, these effects could be very strong. Magnetic susceptibility and $\overline{\langle |m| \rangle}$ are represented in figure 5.2: we see no divergence of $\chi_{\rm m}$ around the spin glass critical point, in agreement with the fact that

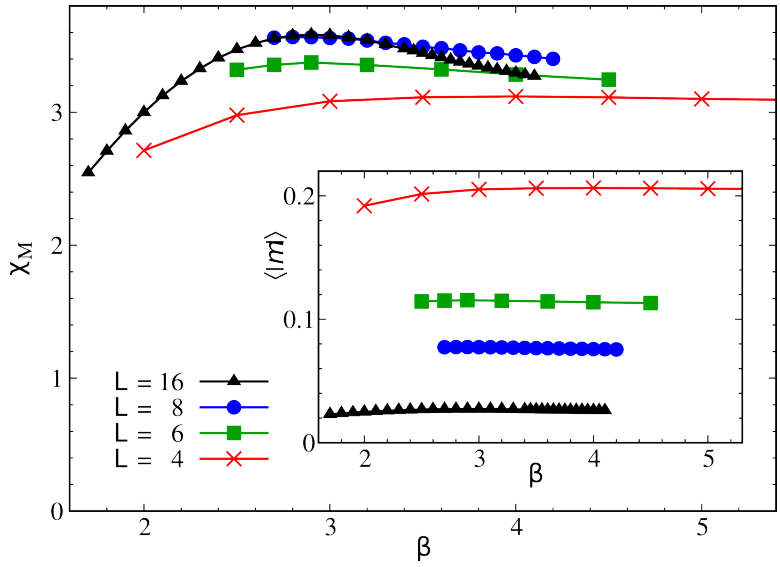


Figure 5.2: Plots of $\chi_{\rm m}$ and $\overline{\langle|m|\rangle}$ as a function of temperature, to check for ferromagnetic ordering in proximity of the spin glass transition, for the $p = 4$ Potts Glass.

(L_1, L_2)	$\beta_{\rm cr}(L_1, L_2)$	$\nu(L_1, L_2)$	$\eta_q(L_1, L_2)$	$\eta_m(L_1, L_2)$
$(4, 8)$	4.83(5)	0.82(3)	0.13(2)	1.72(2)
$(6, 12)$	5.01(4)	0.81(2)	0.16(2)	1.94(2)

Table 5.2: Numerical values of the estimates for the crossing point of the curves ξ/L, together with the critical exponents, as in 5.1, for the case $p = 5$.

$\eta_{\rm m}$ is around 2, and, in the inset of the same figure, we see that the behaviour of $\overline{\langle|m|\rangle}$ is proportional to $1/\sqrt{L^3}$, as it should be in the paramagnetic phase.

What is of most interest to us in the $p = 5$ and $p = 6$ cases is to study if, and when, the spin glass transition changes nature, in the three-dimensional short-ranged model, and how the critical exponents change as a function of p. We proceed, in the next two sections, in a fashion similar to the $p = 4$ case.

5.4 The $p = 5$ Potts Glass

We proceed in our analysis with the $p = 5$ case: as before, we look for crossings, calculate critical exponents, check for the absence of magnetization. Figure 5.3 is the equivalent of figure 5.1 in the $p = 5$ case: crossings for all lattice sizes are neatly in just one point in this case, and, since we already assessed thermalization and transient length, we can proceed in calculating the critical exponents, once we have looked for the crossing points. Scaling corrections are again visible, in

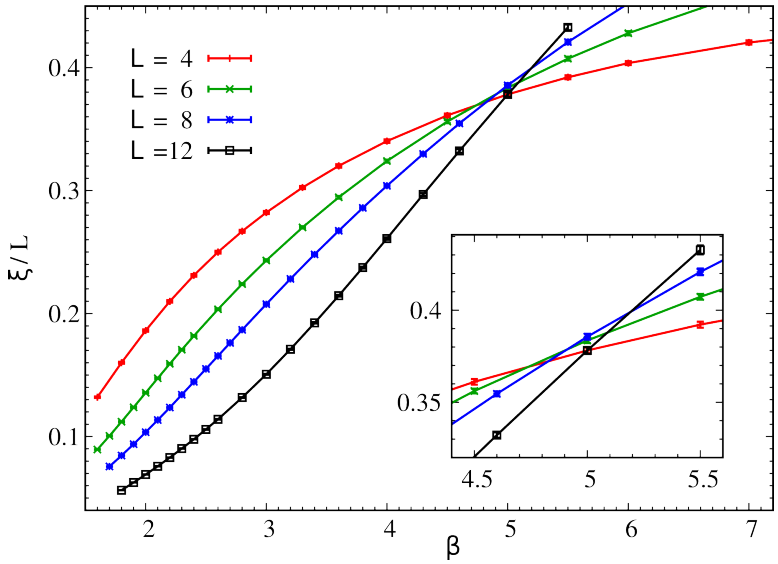


Figure 5.3: As in figure 5.1, plot of the spin glass correlation length over the system size as a function of β for all linear sizes of the Potts spin glass, $p = 5$. Lines are just a guide for the eye.

the small but steady drift of the crossing temperature to the lower side (increasing β), as the linear size of the lattices increases. The results for the crossing temperatures and critical exponents, as before using the Quotient Method (we set $s = 2$), are resumed in table 5.2. We do not have enough data to extrapolate to $L \to \infty$, or to evaluate ω, but there is strong evidence of a phase transition, and we are quite sure about the absence of ferromagnetic ordering, given that η_{m} is around 2. The values of η_{q} is compatibile with a spin glass phase transition. To be sure, we plot, in figure 5.4, χ_{m} and $\overline{\langle |m| \rangle}$ where it is clear that we do not have divergence around the critical point for the former and that the latter behaves like $1/\sqrt{L^3}$, imprint of a paramagnetic phase.
We can see that the behaviour of χ_{m} and $\overline{\langle |m| \rangle}$ are consistent with the absence of ferromagnetic ordering around the spin glass transition temperatures, signaling, again, that we are looking only at a spin glass transition.

5.5 The $p = 6$ Potts Glass

At last, we analyze the $p = 6$ Potts Glass. If we consider for a moment again table 4.1 we can see how hard it is to simulate $p = 6$ compared to $p = 5$ and $p = 4$. This may be a first hint in explaining why we were not able to simulate $L = 16$ in these cases, but we will see that there is more than this. As we did before, we proceed in looking for the crossing points for ξ/L as a function of temperature, looking thus for the spin glass transition temperatures. As we can see in figure 5.5 the curves meet in a unique point (with good approximation).

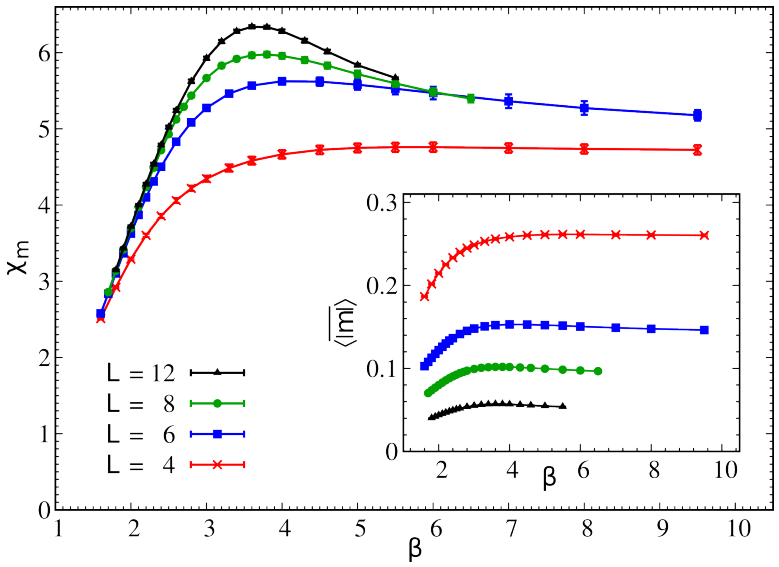


Figure 5.4: As in figure 5.2, χ_{m} and $\overline{\langle |m| \rangle}$ as a function of temperature for the $p = 5$ Potts Glass.

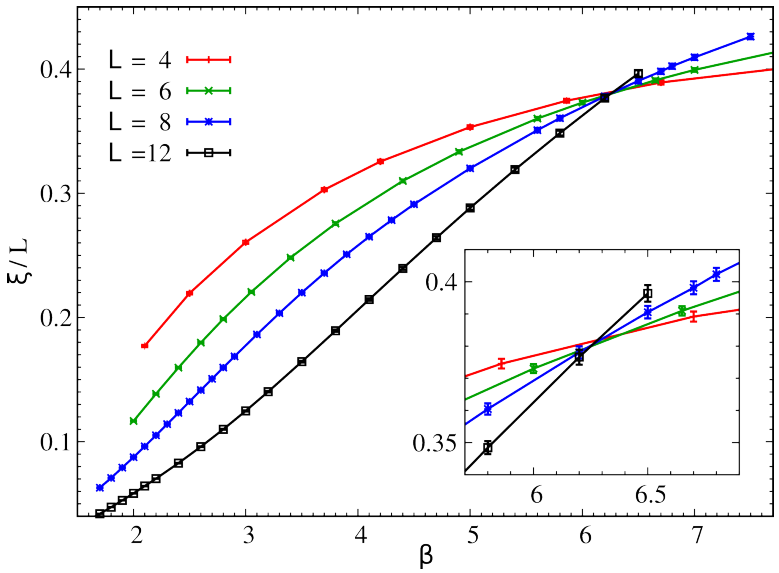


Figure 5.5: As in figure 5.1, plot of the spin glass correlation length over the system size as a function of β for all linear sizes of the Potts spin glass, $p = 6$. Lines are just a guide for the eye.

(L_1, L_2)	$\beta_{\text{cross}}(L_1, L_2)$	$\nu(L_1, L_2)$	$\eta_q(L_1, L_2)$	$\eta_m(L_1, L_2)$
$(4, 8)$	6.30(9)	0.80(2)	0.10(2)	1.453(19)
$(6, 12)$	6.26(7)	0.80(4)	0.16(2)	1.971(19)

Table 5.3: As in table 5.2, but $p = 6$.

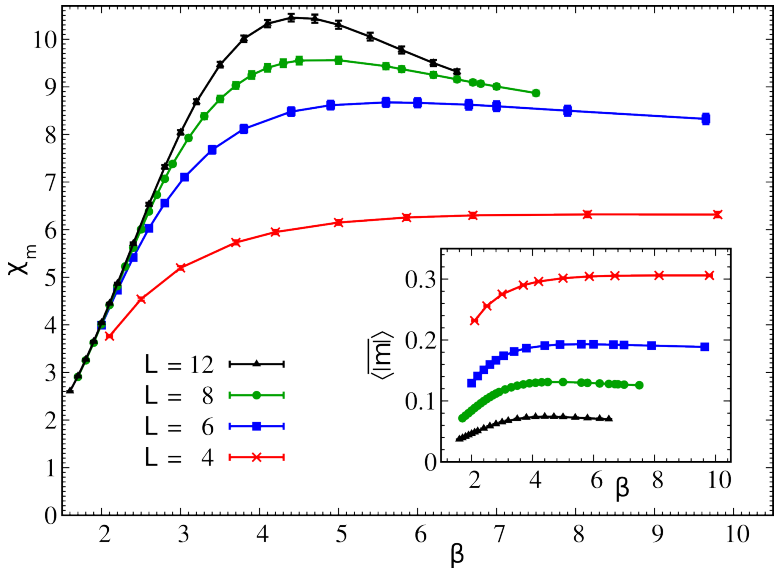
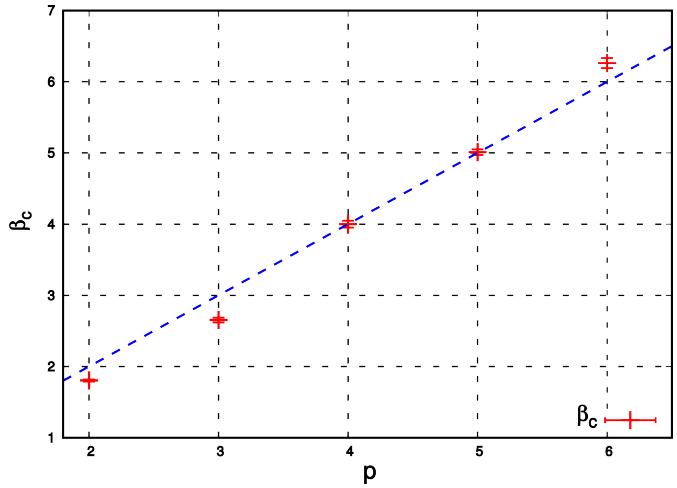


Figure 5.6: As in figure 5.2, χ_{m} and $\overline{\langle |m| \rangle}$ as a function of temperature for the $p = 6$ Potts Glass.

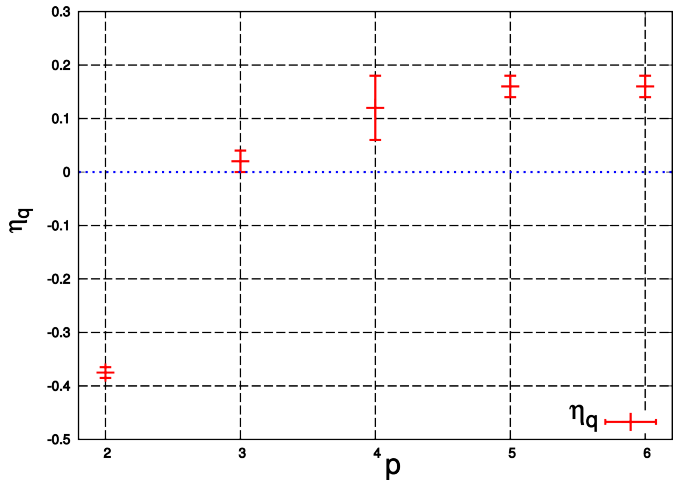
Since the curves meet in one point and then splay out, it is natural to think that we are looking at a continuous transition, eg. not a Kosterliz-Thouless transition. In table 5.3 results from the Quotient Method for the crossing temperatures and critical exponents ν, η_{q} and η_{m}. As before we have set $s = 2$. Correction to scaling is smaller in this case, even if it is present. We do not have, again, enough data to extrapolate critical temperatures and exponents to the thermodynamical limit, nor to calculate ω, nonetheless data strongly suggest a phase transition. Critical exponents are compatible with a continuous phase transition, and η_{m}, which seems to converge to 2 as lattices size increase, suggest that there is not ferromagnetic ordering. To check this last information, as before, we plot χ_{m} and $\overline{\langle |m| \rangle}$ as a function of β and check for divergence of the former and the asymptotic behaviour of the latter, in figure 5.6 we plot them: since the first shows no divergence and the second goes like $1/\sqrt{L^3}$ we conclude that there are ferromagnetic phase effects in the region of the critical spin glass temperature, and hence, as in the $p = 4, 5$ cases, that we are dealing with a spin glass transition.

5.6 Piercing it all together

It is interesting to put together all the information we have obtained about the transitions of the Potts Glass with different number of states, consider it as a function of p and compare it with know results in literature. In MFT we would expect the nature of the transition to change for $p > 4$. In the large p limit a discontinuous disordered phase transition should be observed. Does this change in lowering the number of dimensions of the system to three? Also, in other works, for example [71], [65], [66], [67], [68], [70] and [75] different behaviours for the Potts Glass, albeit with a few difference we will see in a moment, have been described. The main difference with some of the works just cited is that, in their case, J_0 is negative, to suppress ferromagnetic ordering, whereas in our simulations is zero. This might be a small difference or not so small: in their paper Lee, Katzgraber and Young do not observe a spin glass phase transition for a $p = 10$ Potts Glass with Gaussian couping with, as said, $J_0 = -1$, the correlation length remains well small for all temperatures.
In figure 5.7 the critical temperature β_c and the critical exponents ν and η_q are represented as a function of p. The dashed line in the plot of ν versus p is the value of 2/3: using finite size scaling to study a disordered first-order phase transition one expects to find [54], $\nu = 2/d$. In our $d = 3$ case this means $\nu_{\text{first}} = 2/3$ and $\eta_{\text{q, first}} = 1/2$, since the spin glass susceptibility grows like $L^{d/2}$. In the plot of β_c versus p the dashed line represents the function $\beta_c(p) = p$. We notice immediately that this fit holds very well.
We have used, in the plot, data from table 5.4: some are from literature, some from the best estimates of this analysis, to say: the ones with the biggest lattices sizes. The value of ν from [76] is from the analysis of ξ_L/L. It is different, and more reliable, than the one obtained from the spin glass susceptibility, that, because of large scaling corrections, would severely depend on the kind of analysis. In the table, from the same reference, the value of η_q is from the study of the spin glass susceptibility. From figure 5.7 we see that is confirmed our empirical relation about β_c: it increases linearly in p. η_q increases in value for increasing p reaching a plateau (which should go to 1/2, limit value for the first order phase transition), while ν lowers its value for increasing p leaning towards the value of 2/3, without reaching it. This signals to us that, while the boundary value of the spin glass susceptibility exponent is not reached, the nature of the continuous disordered phase transition changes, becoming increasingly stronger. The trend of η_q as a function of p is as well compatible with the tending, increasing p, to a change of the nature of the phase transition from continuous to discontinuous, for some value of $p > 6$. For $p < 6$ the transition is still continuous, but gets, as we said, stronger. There are two possible explanation for what happens to the system increasing p: the first is the one we just dealt with (the transition for some value of p changes from continuous to discontinuous, even if it is possible that there is a rounding due to finite size) and the second is that, for all values of p, the three dimensional Potts Glass has a continuous disordered phase transition,



(a)



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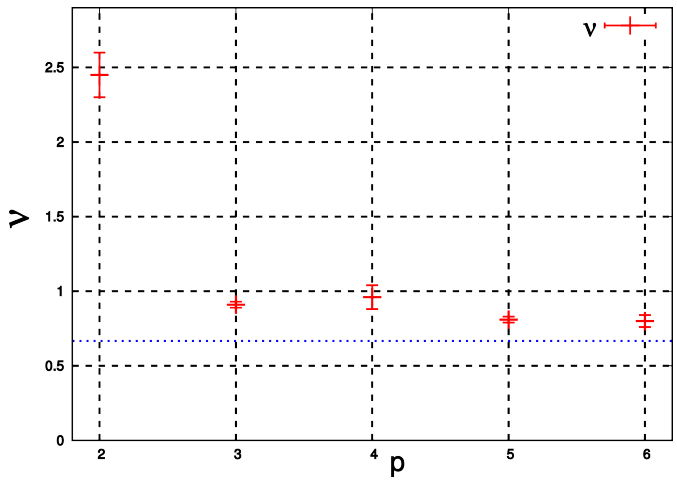

(c)

Figure 5.7: β_c, ν and η_q as a function of p, from the results we obtain in the simulations of the Potts Glass for $p = 4, 5, 6$ plus some results know from literature. The dashed horizontal line in ν vs. p is $\nu_{\text{first}} = 2/3$, while the dashed line in β_c vs. p is a fit with the function $\beta_c(p) = p$. Data for β_c for $p = 4, 5, 6$ are our best estimates: the ones for the biggest lattices sizes.

p	β_c	ν	η_q	R
2 (from [76])	1.786(6)	2.39(5)	−0.366(16)	2.187(8)
2 (from [77])	1.804(16)	2.45(15)	−0.375(10)	2.209(20)
3 (from [71])	2.653(35)	0.91(2)	0.02(2)	2.17(3)
4	4.000(48)	0.96(8)	0.12(6)	2.45(3)
5	5.010(40)	0.81(2)	0.16(2)	2.51(2)
6	6.262(71)	0.80(4)	0.16(2)	2.69(3)

Table 5.4: Critical parameters as a function of p. All data are for binary couplings, with $J_0 = 0$. R denotes the ratio between the critical β in three dimensions and the one computed in Mean Field Theory.

with exponents that show a strong transition (with the values of ν and η_q close to the ones of a discontinuous transition). The fact that in literature the Potts Glass with a big p has been found not to have a phase transition could depend on the fact that in those simulations, such as the ones in [71], the expectation value of the couplings was negative, while in our simulation was zero. On the other hand, if the empirical rule $\beta_c(p) \approx p$ holds it would be necessary, to see the transition, to reach an inverse temperature $\beta_c = 10$, which, in [71] was not reached.

5.7 The curious case of $p = 5$, $L = 16$

It is interesting for a moment to consider the $p = 5$, $L = 16$ case which was not included in the calculations above. The reason why is that we were not able to thermalize the system, even though we simulated it for $10^{12} - 10^{14}$ Monte Carlo Sweeps, $2 - 4$ orders of magnitude more than $L = 12$ with the same number of available states. It is possible to appreciate its non-thermalization in figure 5.10: the two curve come from two different trials. In the first curve, the one for $\beta = 5.2$ we employ PT with a set if 32 inverse temperatures, simulating 280 samples. The second one, for $\beta = 5.1$, is another test we did, using 46 inverse temperatures. The first one was simulated for a longer time than the second and with different frequency of HB steps between PT steps. Following the thermalization criteria we defined, a sample set is said thermalized if the last three measures in log binning of the data agree within errors, we say that these data come from systems which are not thermalized. What is interesting to investigate is the reason *why* this happens.
If we look at the evolution of configurations in temperature space in the Parallel Tempering evolution, what we see is a bottleneck around the critical temperature, even if we increase the number of temperatures around the critical one, systems are not able to perform a complete random walk from low to high, and back, temperatures, and they just stay in one phase, with high probability. Occasionally

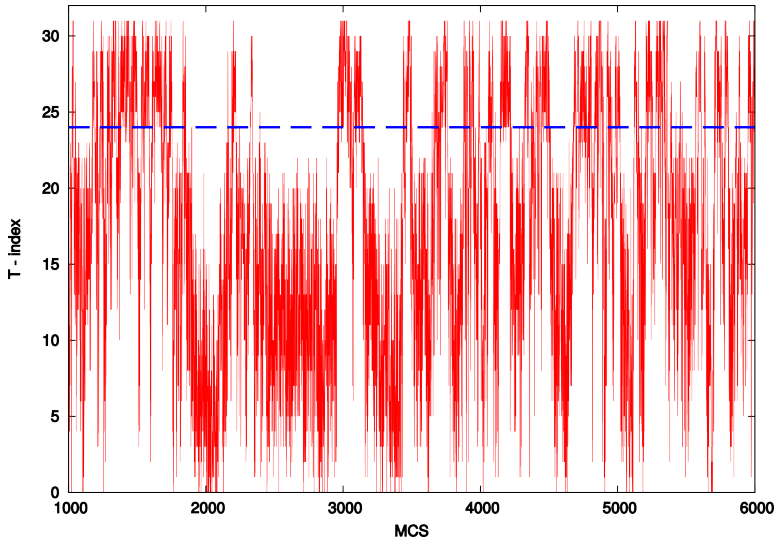

Figure 5.8: Example of an almost good looking random walk in temperature space, at least for the last part. In the first part even if the system moves, complete round trip from low to high β happen, the system is not completely stuck. In the second part the situation gets better, and round trips are more frequent. MCS on the x axis and Temperature Index in the y axis. The dashed line is, approximately, where the transition temperature should be.

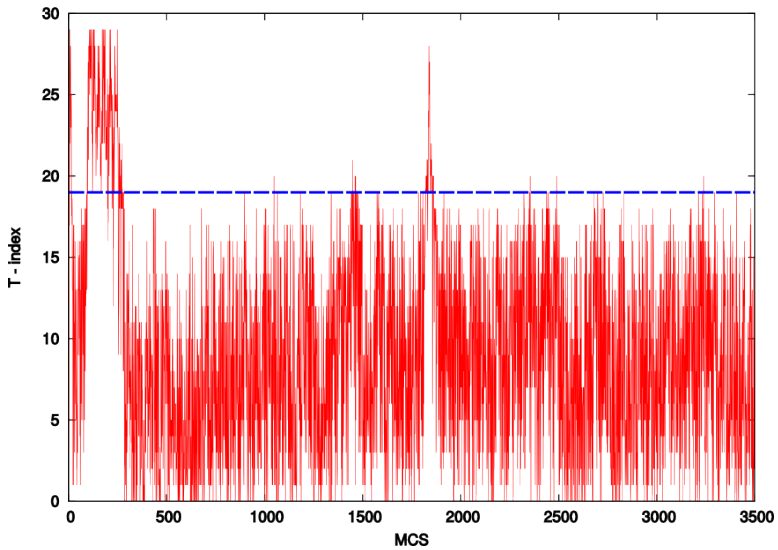

Figure 5.9: A bad random walk in temperature space. MCS on the x axis and Temperature Index in the y axis. The dashed line is, approximately, where the transition temperature should be. The configuration, after a very short transient where it moves up and down, gets trapped in a phase. The part of the "T-index" axis above the dashed line is the high β zone.

they do change phase, but in doing this a configuration gets trapped inside that phase, and with high probability they almost never go from end to end in their random walk. A situation somewhat intermediate between completely stuck in a phase and correctly mobile configurations, is quite frequent, too. Some examples of walks in temperature space, obtained for the $p = 5$, $L = 16$ Potts Glass, are shown in figure 5.8 and 5.9.
Why does this happen? We have tried many different configurations of Parallel Tempering: we changed the temperatures' distribution, the range, the frequency of PT updates, but somewhat it eludes us why we keep seeing the same behaviour. We know, from the first chapter, that the Potts Glass in MFT, in the case of a first-order phase transition, does not have a latent heat, but nonetheless suggestions like the ones found in literature (for example, [38]) come to mind. The basic idea in [38] is that acceptance ratio is proportional to the inverse of the latent heat: if we had latent head, we could explain the drop in acceptance ratio by this.
What we can hypothesise is that there might be a crossover between continuous and discontinuous transition behaviour: for smaller sizes the discontinuous transition is rounded to to finite size effects, while for larger sizes this rounding disappears, showing the true nature of the transition. As we said in the previous section, this must be added with the two possibilities of not having a change in the phase transition depending on p, or to have the nature change for some $p > 6$, which remain both available at this stage. The only way to probe what is happening is to perform simulations with larger systems.

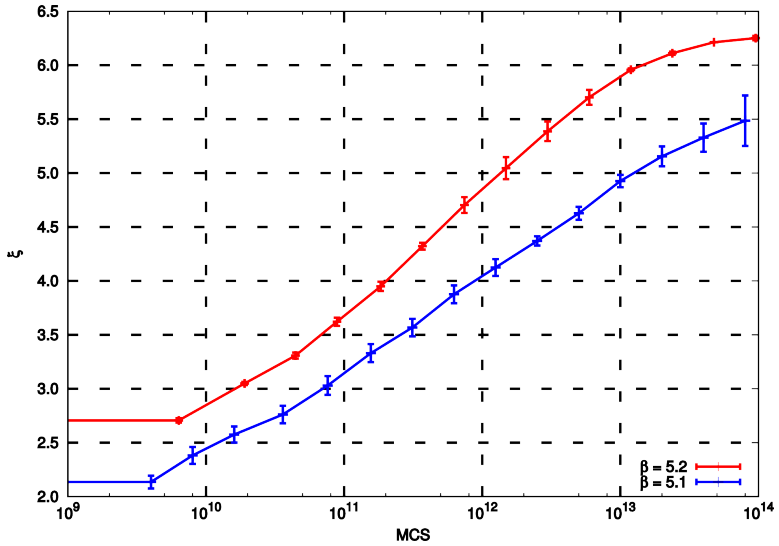

Figure 5.10: ξ vs. MCS for the $L = 16$, $p = 5$ Potts Glass. Represented are the curve for understanding thermalization of the system for two different temperature, from different simulations. The red curve ($\beta = 5.2$) is the result of a simulation of 280 samples, using 32 betas for PT. The blue one ($\beta = 5.1$) is from the simulation of 32 samples, using 46 betas.

Chapter 6

Conclusion

The main aim of this thesis was to fill the gap in the simulation of the Potts Glass, for $p = 4, 5, 6$ in three dimensions. In this range of p many things in the behaviour of the model changes: the most striking change being, for the ∞-dimensional case of Mean Field Theory, the different nature of the phase transition which is expected to be discontinuous for $p > 4$ and continuous in all other cases.

Our progress was tainted by the impressive computational requirements of the simulation of this model, requirements that kept growing as p increased, so much that – in spite of state-of-the-art computing facilities – we were not able to thermalize systems greater than $L = 12$ for $p \geq 5$. Nonetheless we have used all available information to understand the behaviour of the system and to formulate educated guesses of what might happen for $p > 6$ which is, also, the target of the next round of simulations, possibly using the next generation of dedicated computers.
We gained insight on the Potts Glass: the indications of the existence of the para-spin glass phase transition for all the p we studied, and the nature of the phase transition which, according to the critical exponents we have calculated, well rests in the range of a continuous transition, albeit drifting, as p increases, toward the lower bound values for the transition to stay continuous.
While these results need more simulations to be confirmed, we can look beyond the mere numbers and infer what to expect from future simulations: there are basically two different scenarios. In the first, the transition as p increases beyond 6 might continue to be continuous, or, as a second option, for some value of $p > 6$ it might change and become discontinuous.
In our simulations, up to $p = 6$, we have a strong hint that the transition stays continuous, but there is one point that might suggest that, as opposed to what we have identified as two different possibilities, the change in the nature of the transition might have happened in the range of p between 4 and 6 so that we are effectively looking at a discontinuous transition, rounded by the small sizes of the lattices.

Unfortunately there is no way, right now, to understand what is going on, but we can have some hints: it is of particular interest the behaviour of Parallel Tempering, as p increases. Despite our efforts in trying to make the Parallel Tempering well behave in letting configurations visit the whole range of temperatures, we were not able to reach an optimum: we tried to change in different ways the values (and intervals in between) inverse temperatures and increase (as much as acceptable) the total simulation time. In all our efforts, there is a bottleneck around the critical temperature, which is the mark of a discontinuous phase transition as seen from the Parallel Tempering perspective. In this sense, we may suppose that there is a rounding in the nature of the transition, and it may well already be discontinuous: only the ability to simulate bigger system sizes will shine light on this point.

In conclusion this work enriches the phenomenology of the Potts Glass, and this has been a "good excuse" to understand better the Parallel Tempering method and its applicability, too. While the results obtained are not conclusive on the matter, they are to be intended as a roadmap for further steps in the simulation of this model in order to deepen our knowledge and to understand if the Potts Glass can be a relevant candidate for the description of orientational glasses.

In the future we might be able to increase both the values of p we simulate and the size L of the systems: only then we will have definitive results. This thesis tries to set the right direction to follow.

References

[1] G. Mussardo, *Il modello di Ising: introduzione alla teoria dei campi e delle transizioni di fase*, Bollati Boringhieri, 2007

[2] K. Huang, *Statistical Mechanics*, Wiley, 1963 and 1988 (2nd ed.)

[3] T. Kihara, Y. Midzuno, T. Shizume, *Statistics of two-dimensional lattices with Many-Components*, J. Phys. Soc. Jpn., 9, 5, 1954

[4] K.H. Fischer, J.A. Hertz, *Spin Glasses*, Cambridge University Press, 1991

[5] S.F. Edwards, P.W. Anderson, *Theory of spin glasses*, Journal of Physics F, Met. Phys. 5 965, 1975

[6] M. Mezard, G. Parisi, M. Virasoro, *Spin Glass Theory and Beyond*, World Scientific Lecture Notes in Physics - Vol. 9, 1986

[7] G. Parisi, *The order parameter for spin glasses: A function on the interval 0-1*, J. Phys. A: Math. Gen. 13, 1101-1112, 1980

[8] G. Parisi, *Order parameter for spin glasses*, Phys. Rev. Lett., 50, 24, 1946, 1983

[9] G. Parisi, *A sequence of approximated solutions to the S-K model for spin glasses*, J. Phys. A: Math. Gen., 13, L115-L121, 1980

[10] G. Parisi, *Spin Glasses Theory*, Physica A, 140, 312-318, 1986

[11] G. Parisi, *Spin Glasses, Complexity and all that*, Physica A, 194, 28-40, 1993

[12] C. De Dominicis, A. P. Young, *Weighted averages and order parameters for the infinite range Ising spin glass*, J. Phys. A: Math. Gen. 16, 2063-2075, 1983

[13] D. C. Mattis, *Solvable spin systems with random interactions*, Physics Letters A, Volume 56, Issue 5, 421-422, 1976

[14] S. Kirkpatrick, *Frustration and ground-state degenerancy in spin glasses*, Phys. Rev. B., 16, 4630, 1977

[15] D. Sherrington, S. Kirkpatrick, *Solvable Model of a Spin-Glass*, Phys. Rev. Lett., 45, 1792-1796, 1975

[16] G. Toulouse, *On the mean field theory of mixed spin glass-ferromagnetic phases*, J. Physique Lett. 41, 447-449, 1980

[17] J.R. de Almeida, D.J. Thouless, *Stability of the Sherrington-Kirkpatrick solution of a spin glass model*, J. Phys. A: Math. Gen., 11, 983, 1978

[18] G. Parisi, *Infinite Number of Order Parameters for Spin-Glasses*, Phys. Rev. Lett., 43, 17541756, 1979

[19] A.J. Bray, M.A. Moore, *Replica-Symmetry Breaking in Spin-Glass Theories*, Phys. Rev. Lett., 41, 1068-1072, 1978

[20] E. Pytte, J. Rudnick, *Scaling, equation of state, and the instability of the spin-glass phase*, Phys. Rev. B, 19, 36033621, 1979

[21] D.J. Thouless, J.R.L. de Almeida, J.M. Kosterlitz, *Stability and susceptibility in Parisi's solution of a spin glass model*, J. Phys. C: Solid State Phys., 13, 3271, 1980

[22] N.D. Mackenzie, A.P. Young, *Lack of Ergodicity in the Infinite-Range Ising Spin-Glass*, Phys. Rev. Lett. 49, 301304, 1982

[23] N.D. Mackenzie, A.P. Young, *Statics and dynamics of the infinite-range Ising spin glass model*, J. Phys. C: Solid State Phys., 16, 5321, 1983

[24] D.J. Gross, I. Kanter, H. Sompolinski, *Mean-Field theory of the Potts Glass*, Phys. Rev. Lett., 55, 3, 304, 1985

[25] B. Derrida, *Random-energy model: An exactly solvable model of disordered systems*, Phys. Rev. B, 24, 26132626, 1981

[26] D.J. Gross, M. Mezard, *The simplest Spin Glass*, Nucl. Phys. B, 240, [FS12], 431-452, 1984

[27] G. Cwilich, T.R. Kirkpatrick, *Mean-Field theory and fluctuations in Potts spin glasses: I*, J. Phys. A: Math. Gen., 22, 4971, 1989

[28] G. Cwilich, *Mean-Field theory and fluctuations in Potts spin glasses: II*, J. Phys. A: Math. Gen., 23, 5029, 1990

[29] D. Elderfield, D. Sherrington, *Spin glass, ferromagnetic and mixed phases in the disordered Potts model*, J. Phys. C: Solid State Phys., 16, L971-977, 1983

[30] E. Gardner, *Spin Glasses with p-spin interactions*, Nucl. Phys. B, 257, [FS14], 747-765

[31] E. De Santis, G. Parisi, F. Ritort, *On the static and dynamical transition in the mean-field Potts glass*, J. Phys. A: Math. Gen., 28, 3025-3041, 1995

[32] D.M. Cragg, D. Sherrington, M. Gabay, *Instabilities of an m-vector Spin-Glass in a Field*, Phys. Rev. Lett, 49, 158161, 1982

[33] M.E.J. Newman, G.T. Barkema, *Monte Carlo Methods in Statistical Physics*, Oxford University Press, 2002

[34] D.P. Landau, K. Binder, *A guide to Monte Carlo simulations in statistical physics*, Cambridge University Press, 2005

[35] S. Caracciolo, R.G. Edwards, A. Pelissetto, A.D. Sokal, *Extrapolating Monte Carlo Simulations to Infinite Volume: Finite-Size Scaling at* $\xi/L \gg 1$, Phys. Rev. Lett., 74, 29692972, 1995

[36] P. Nightingale, *Scaling theory and finite systems*, Physica A: Statistical and Theoretical Physics, 83, 3, 561-572, 1975

[37] K. Hukushima, K. Nemoto, *Exchange Monte Carlo method and application to spin glass simulations*, J. Phys. Soc. Jpn., 65, 1604, 1996

[38] C. Predescu, M. Predescu, C.V. Ciobanu, *The incomplete beta function law for parallel tempering sampling of classical canonical systems*, J. Chem. Phys., 120, 4119, 2004

[39] H.G. Katzgraber, S. Trebst, D.A. Huse, M. Troyer, *Feedback-optimized parallel tempering Monte Carlo*, J. Stat. Mech., P03018, 2006

[40] W. Nadler, U.H.E. Hansmann, *On Dynamics and Optimal Number of Replicas in Parallel Tempering Simulations*, Phys. Rev. E, 76, 065701(R), 2007

[41] E. Bittner, A. Nussbaumer, W. Janke, *Make life simple: unleash the full power of the parallel tempering algorithm*, Phys. Rev. Lett., 101, 130603, 2008

[42] J. Machta, *Strengths and Weaknesses of Parallel Tempering*, Phys. Rev. E, 80, 056706, 2009

[43] B. Bauer, E. Gull, S. Trebst, M. Troyer, D.A. Huse, *Optimized broad-histogram simulations for strong first-order phase transitions: Droplet transitions in the large-Q Potts model*, J. Stat. Mech., P01020, 2010

[44] F. Hamze, N. Dickson, K. Karimi, *Robust Parameter Selection for Parallel Tempering*, accepted in International Journal of Modern Physics C, available as arXiv:1004.2840, 2010

[45] M. Hasenbusch, S. Schaefer, *Speeding up parallel tempering simulations*, Phys.Rev.E, 82, 046707, 2010

[46] F. Belletti, M. Cotallo, A. Cruz, L.A. Fernandez, A. Gordillo-Guerrero, M. Guidetti, A. Maiorano, F. Mantovani, E. Marinari, V. Martin-Mayor, A. Munoz Sudupe, D. Navarro, G. Parisi, S. Perez-Gaviro, J.J. Ruiz-Lorenzo, S.F. Schifano, D. Sciretti, A. Tarancon, R. Tripiccione, J.L. Velasco, D. Yllanes (the Janus collaboration), *Nonequilibrium spin glass dynamics from picoseconds to 0.1 seconds*, Phys. Rev. Lett., 101, 157201, 2008

[47] F. Belletti, I. Campos, A. Cruz, L. A. Fernandez, S. Jimenez, A. Maiorano, F. Mantovani, E. Marinari, V. Martin-Mayor, D. Navarro, A. Munoz-Sudupe, S. Perez Gaviro, G. Poli, J. J. Ruiz-Lorenzo, F. Schifano, D. Sciretti, A. Tarancon, P. Tellez, R. Tripiccione, J. L. Velasco, *Ianus: an Adpative FPGA Computer*, Computing in Science & Engineering, 8, 41-49, 2006

[48] F. Belletti, M. Cotallo, A. Cruz, L. A. Fernandez, A. Gordillo, M. Guidetti, A. Maiorano, F. Mantovani, E. Marinari, V. Martin-Mayor, A. Mu oz-n Sudupe, D. Navarro, G. Parisi, S. Perez-Gaviro, M. Rossi, J. J. Ruiz-Lorenzo, S. F. Schifano, D. Sciretti, A. Tarancon, R. Tripiccione, J. L. Velasco, *Janus: an FPGA-based System for High Performance Scientific Computing*, Computing In Science and Engineering, 11, 1, 48-58, 2009

[49] F. Belletti, M. Cotallo, A. Cruz, L. A. Fernandez, A. Gordillo-Guerrero, M. Guidetti, A. Maiorano, F. Mantovani, E. Marinari, V. Martin-Mayor, A. Mu oz Sudupe, D. Navarro, G. Parisi, S. Perez-Gaviro, M. Rossi, n J. J. Ruiz-Lorenzo, J. F. Saenz-Lorenzo, S. F. Schifano, D. Sciretti, A. Tarancon, R. Tripiccione, J. L. Velasco, D. Yllanes and G. Zanier, *Monte Carlo Simulations for Statistical Physics: Janus*, Il Nuovo Cimento B, 123, 6, 972-974, 2008

[50] G. Parisi and F. Rapuano, *Effects of the random number generator on computer simulations*, Phys. Lett. B, 157, 301, 1985

[51] Zia and Wallace, *Critical behaviour of the continuous n-component Potts model*, J. Phys. A: Math. Gen., 8 1495, 1975

[52] D. J. Amit and V. Martin-Mayor, *Field Theory, the Renormalization Group and Critical Phenomena*, World-Scientific Singapore, Third Edition, 2005

[53] L.A. Fernandez, V. Martin-Mayor, S. Perez-Gaviro, A. Tarancon, A. P. Young, *Phase transition in the three dimensional Heisenberg spin glass: Finite-size scaling analysis*, Phys. Rev. B, 80, 024422, 2009

[54] A. Cruz, L.A. Fernandez, A. Gordillo-Guerrero, M. Guidetti, A. Maiorano, F. Mantovani, E. Marinari, V. Martin-Mayor, A. Munoz Sudupe, D. Navarro, G. Parisi, S. Perez-Gaviro, J.J. Ruiz-Lorenzo, S.F. Schifano, D. Sciretti, A. Tarancon, R. Tripiccione, J.L. Velasco, D. Yllanes, and A.P. Young, *Spin glass phase in the four-state three-dimensional Potts model*, Phys. Rev. B, 79, 184408, 2009

[55] R. Alvarez Banos, A. Cruz, L. A. Fernandez, A. Gordillo-Guerrero, J.M. Gil-Narvion, M. Guidetti, A. Maiorano, F. Mantovani, E. Marinari, V. Martin-Mayor, J. Monforte-Garcia, A. Munoz Sudupe, D. Navarro, G. Parisi, S. Perez-Gaviro, J. J. Ruiz-Lorenzo, B. Seoane, S. F. Schifano, A. Tarancon, R. Tripiccione, D. Yllanes, *Critical Behavior of Three-Dimensional Disordered Potts Models with Many States*, J. Stat. Mech. P05002, 2010

[56] H.G. Ballesteros, L.A. Fernandez, V. Martin-Mayor, A. Munoz Sudupe, G. Parisi, J.J. Ruiz-Lorenzo, *Scaling corrections: site percolation and Ising model in three dimensions*, J. Phys. A: Math. and Gen., 32, 1, 1999

[57] D.J. Amit, V. Martin-Mayor, *Field theory, the renormalization group, and critical phenomena: graphs to computers*, World Scientific, 2005

[58] H-O Carmesin, K. Binder, *Monte Carlo study of the Potts glass with nearest-neighbout random Gaussian interaction*, J. Phys. A: Math. Gen., 21, 4053-4065, 1988

[59] M. Scheucher, J.D. Reger, K. Binder, A.P. Young, *Finite-size-scaling study of the simple cubic three-state Potts glass: Possible lower critical dimension* $d = 3$, Phys. Rev. B, 42, 10, 6881, 1990

[60] M. Scheucher, J.D. Reger, *Monte Carlo study of the bimodal three-state Potts glass*, Phys. Rev. B, 45, 5, 2499, 1992

[61] J.R. Banavar, M. Cieplak, *Zero-temperature scaling for Potts spin glasses*, Phys. Rev. B, 39, 13, 9633, 1989

[62] J.R. Banavar, M. Cieplak, *Nature of ordering in Potts spin glasses*, Phys. Rev. B, 40, 7, 4613, 1989

[63] O. Dillmann, W. Janke, K. Binder, *Finite-size Scaling in the p-State Mean-Field Potts Glass: A Monte Carlo Investigation*, J. Stat. Phys., 92,1/2, 57, 1998

[64] M. Reuhl, N. Nielaba, K. Binder, *Slowing down in the three-dimensional three-state Potts glass with nearest neigbor exchange* $\pm J$*: A Monte Carlo study*, Eur. Phys. J. B, 2, 225-232, 1998

[65] C. Brangian, W. Kob, K. Binder, *Finite-size scaling at the dynamical transition of the mean-field 10-state Potts glass*, Europhys. Lett., 53, 756-76, 2001

[66] C. Brangian, W. Kob, K. Binder, *The High Temperature Dynamics of a mean field Potts glass*, Phil. Mag. B, 82, 663, 2002

[67] C. Brangian, W. Kob, K. Binder, *Statics and Dynamics of the 10-state mean-field Potts glass model: A Monte Carlo study*, J. Phys. A : Math. Gen., 35, 191, 2002

[68] C. Brangian, W. Kob, K. Binder, *Evidence against a glass transition in the 10-state short range Potts glass*, Europhys. Lett., 59, 546, 2002

[69] C. Brangian, W. Kob, K. Binder, *Ergodicity breaking in a mean field Potts glass: A Monte Carlo investigation*, Comp. Phys. Comm. 147, 154, 2002

[70] C. Brangian, W. Kob, K. Binder, *Statics and dynamics of the ten-state nearest-neighbour Potts glass on the simple-cubic lattice*, J. Phys. A: Math. Gen., 36, 10847, 2003

[71] L.W. Lee, H.G. Katzgraber, A.P. Young, *Critical behavior of the three- and ten-state short-range Potts glass: A Monte Carlo study*, Phys. Rev. B, 74, 104416, 2006

[72] R.S. Andrist, D. Larson, H.G. Katzgraber, *Evidence of a glass transition in a 10-state nonmean-field Potts glass: A step towards an effective understanding of structural glasses using spin models*, available as arXiv:1009.1916v1 [cond-mat.dis-nn], 2010

[73] E. Marinari, S. Mossa, G. Parisi, *The Glassy Potts Model*, Phys. Rev. B, 59, 8401, 1999

[74] L.A. Fernandez, A. Maiorano, E. Marinari, V. Martin-Mayor, D. Navarro, D. Sciretti, A. Tarancon, J.L. Velasco, *Critical properties of the four-state Commutative Random Permutation Glassy Potts model in three and four dimensions*, Phys. Rev. B 77, 104432, 2008

[75] B. Lobe, W. Jankea, K. Binder, *High-temperature series analysis of the p-state Potts glass model on d-dimensional hypercubic lattices*, Eur. Phys. J. B, 7, 283291, 1999

[76] H.G. Katzgraber, M. Körner and A.P. Young, *Universality in three-dimensional Ising spin glasses: A Monte Carlo study*, Phys. Rev. B, 73, 224432, 2006

[77] M. Hasenbusch, A. Pelissetto and E. Vicari, *Critical behavior of three-dimensional Ising spin glass models*, Phys. Rev. B, 78, 214205, 2008

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