ENERGY LANDSCAPE IN 3-DIMENSIONAL HEISENBERG SPIN GLASSES

SCENARIO ENERGETICO NEI VETRI DI SPIN DI HEISENBERG 3-DIMENSIONALI

TESI DI LAUREA SPECIALISTICA

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A mi mamá,
que me educó como mejor no era posible.
Abstract

**Italian Version**  Recenti lavori suggeriscono che i vetri di spin di Heisenberg possano appartenere alla stessa classe di universalità di vetri strutturali. Trovare un equivalente su reticolo per questo tipo di modelli consentirebbe probabilmente di semplificare lo studio sia dal punto di vista numerico che analitico, consentendo eventualmente di rispondere alle molte domande riguardanti la transizione vetrosa che sono irrisolte da decenni.

I liquidi sottoraffreddati hanno comportamenti peculiari che, nel caso in cui l’analogia tra i due tipi di sistema reggesse, dovremmo riscontrare nella fase paramagnetica dei vetri di spin di Heisenberg.

E’ con questo obiettivo che nel presente lavoro si affronta in maniera sistematica la caratterizzazione della fase paramagnetica. Si cerca di comprendere il ruolo del panorama energetico, con uno studio approfondito delle strutture inerenti (in analogia con i liquidi sottoraffreddati definiamo struttura inerente di una configurazione il minimo locale dell’energia più prossimo ad essa), che richiede lo sviluppo di un nuovo algoritmo di ricerca. Indaghiamo anche se si trovano tracce di una transizione dinamica nella fase paramagnetica. Di fatto sia l’esistenza di uno scenario energetico complesso, sia quella di una transizione dinamica, sono tratti caratteristici della fisica dei liquidi sottoraffreddati.
Abstract

**English Version**  Recent work suggests that Heisenberg spin glasses may belong to the same universality class than structural glasses. Indeed, finding a lattice equivalent for supercooled liquids would probably allow easier numerical and analytical studies, that may help to answer long standing questions on the glass transition. Supercooled liquids have many peculiar behaviors that should be found in the paramagnetic phase of Heisenberg spin glasses if the analogy between the two systems holds.

It is with this motivation that we undertake a study of the paramagnetic phase of Heisenberg spin glasses. We shall emphasize the role of the energy landscape, with a detailed study of the properties of the inherent structures (by analogy with supercooled liquids, we name inherent structure the local minimum of the energy function which is closest to the current spin configuration). Finding inherent structures will require the development of a new search algorithm. We shall investigate as well the existence of a dynamic ”phase transition” in the paramagnetic phase. As a matter of fact, both the existence of a complex energy landscape, as well as the existence of a dynamic transition, are distinguished features of the Physics of supercooled liquids.
## Contents

Abstract iv

Introduction 1

1 A brief summary on spin glasses 9
   1.1 Defining a spin glass model 10
   1.2 Order Parameters 12
       1.2.1 Ising Spins 13
       1.2.2 Heisenberg Spins 16

2 Update on developments in spin glasses 21
   2.1 Ising vs Heisenberg 22
       2.1.1 Ising ordering in zero field 22
       2.1.2 Heisenberg ordering in zero field and chirality sce-
           nario 23
   2.2 Dynamics 26
       2.2.1 Energy Landscape Scenario 26

3 Numerical Techniques 29
   3.1 Thermalization Dynamics 30
       3.1.1 Metropolis 30
       3.1.2 Heat Bath 31
3.1.3 Over Relaxation .......................... 32
3.2 Minimizing the Energy ....................... 32
  3.2.1 Gauss-Seidel ............................ 33
  3.2.2 Genetic Algorithms ....................... 35
  3.2.3 Successive Over Relaxation ............... 36
3.3 Computing Observables ...................... 38
  3.3.1 Energy .................................. 39
  3.3.2 Overlaps ................................ 39
  3.3.3 Correlation Lengths and Functions ....... 41
  3.3.4 Magnetic Susceptibility ................... 44
  3.3.5 Binder’s Cumulants ....................... 45
  3.3.6 Self-correlation Times and Functions ..... 46

4 Results ....................................... 49
  4.1 Using Gauss-Seidel ......................... 50
  4.2 Using Successive Over Relaxation .......... 51
    4.2.1 Parameter choice ....................... 51
  4.3 A comparison with genetic algorithms ...... 56
    4.3.1 Inherent structures at infinite temperature .... 58
  4.4 Inherent structures at finite temperature .... 62
  4.5 Dynamics ................................ 71
  4.6 Extrapolations ............................. 72
    4.6.1 An Estimate of $T_{SG}$ .................... 73
    4.6.2 An Estimate of the Exponent $\nu$ ....... 74
    4.6.3 Self-correlation times .................... 75
    4.6.4 A Lower Bound for the Dynamic Exponent $z$ .... 77
  4.7 Minima or Saddles? ......................... 78

Conclusions ................................... 81
Introduction

Spin and structural glasses are two completely different types of systems. Nevertheless, deep analogies can be found if one considers some dynamic properties, metastability, and the role of competing interactions in both types of systems. The main aim of this thesis is to try to give a good starting point for a solid correspondence between those two types of models. A similar job has been done with non-disordered systems, by making a one-to-one mapping between the Ising model and lattice gases. Although they represent systems that apparently have nothing in common, those two models have the exact same behavior if we recognize the correct relation between the quantities that appear in each model.

Establishing a similar analogy between spin and structural glasses would probably be mutually beneficial for their study. In particular for spin models it is easier to demonstrate theorems, that could extend also to structural glasses and supercooled liquids. Besides, numerous approximation methods have been developed for spin glasses, and the numerical study of spin glasses is far more manageable than the one of structural glasses, since it is possible to apply very performing Monte Carlo algorithms on lattices, so that finding an eventual symmetry relating the former with the latter could make us extend the results of one model to the other, and vice versa.

Although it is several decades that supercooled liquids and structural
glasses are studied [1], their comprehension is far from being complete. In particular it is still not known if there exists a real thermodynamic glassy phase at low temperature. A salient feature is that lowering the temperature there is a very steep growth of the characteristic time scales $\tau$ of the system. The experimental approach is to define $T_g$ as the temperature at which $\tau \sim 10^2 - 10^3 s$, but this temperature has only a practical meaning. From the theoretical side, the Mode Coupling Theory (MCT) [2] offers a framework to describe quantitatively this dynamic slowdown. In fact, Mode Coupling Theory predicts a dynamic transition where the self-correlation times diverge with power law. Nowadays, the Mode Coupling Transition is known to be a crossover rather than a real transition. Nevertheless, the functional forms predicted by MCT are routinely used to fit experimental results when the autocorrelation times are in the range $10^{-13} s < \tau < 10^{-3} s$.

Recently, a topological interpretation has been given for the dynamic transition predicted by the MCT in which the role of the energy landscape, i.e. the topological aspect of the potential energy, assumes a determinant role in the dynamics of these systems. At high temperatures the typical configurations in which the system finds itself are closer to saddle points of the potential energy than minima, so there is always a negative direction in its hessian that permits to the system a fast movement in the configuration space. Decreasing the temperature the typical number of negative directions of these saddles starts falling too, so that the relaxation times increases as the system has always more difficulties in finding these more convenient directions. There is a temperature in which the density of negative directions of the hessian goes to zero. This change in the topology of the energy landscape is called topological transition, and it causes the dynamic transition, i.e. a high slowing down of the dynamics (but with no divergence and no real phase transition). Mode Coupling Theory predicts that the relaxation times diverge with
power law at this temperature. This is not what happens because when the saddles disappear we enter another regime of dynamics in which the system has to ‘jump’ from one minimum to the other, in which the typical times are much longer since they scale with the exponential of the energy barrier. We can so appreciate the divergence predicted by Mode Coupling Theory only until its characteristic time scales become comparable with those of activated dynamics. Another interesting feature that follows from the energy landscape scenario is the concept of inherent structure. It is possible to associate, to any state, the configuration corresponding to the local minimum where the system would find itself if the energy were to be lowered abruptly in some way. We call that configuration inherent structure. What is seen is that at high temperatures the energies of the inherent structures almost does not depend on $T$. On the contrary, at lower temperatures these energy suddenly start to decrease fairly quickly. The interpretation of this phenomenon is that there is an exponentially high number of minima at a certain level, and few with lower energy, so as long as we are at high temperature the probability of finding an exponentially numerous minimum is almost one, and to feel the presence of the lower energy inherent structures we need to be at lower temperatures.

On the other hand, we have a stronger hold on the physics of spin-glasses (the second partner in our intended analogy), specially for Ising spin glasses. Spin glasses [3, 4] are disordered magnetic alloys, such as $\text{Mn}_x\text{Cu}_{1-x}$, where magnetic moments (localized on the Mn atoms, typically) interact. If these magnetic moments may point basically anywhere, their interaction depending only on their relative orientation, one speaks of Heisenberg spin glasses. Yet, if the lattice anisotropies enforce the magnetic moments to point mostly to the North or South poles, we have Ising spin glasses.

It is since the beginning of the 90’s that there is clear evidence of a
thermodynamic spin glass phase at low temperatures for systems with Ising spins and finite-range interactions. Also, there is no dynamic transition, in the sense that there isn’t any temperature in the paramagnetic phase in which the relaxation times grow considerably. Moreover, Parisi’s solution of the mean field model yields an infinite-step replica symmetry breaking, that implies a continuous sequence of phase transitions once the threshold of $T_{SG}$ is passed, with a continuous fragmentation of the valleys of the free energy, and a macroscopically large number of different configurations that characterize the glassy phase. The slow down of the dynamics in the glassy phase would be due to this complexity of the phase space. It appears clear that Ising spins don’t offer the possibility of a correspondence with structural glasses.

In spite of the fact that they are a much more reasonable representation of real spin glasses, extremely little is known about Heisenberg spins glasses. Although it is assumed that a phase transition takes place at finite temperature, its nature is not clear yet, since there is a degree of freedom that was absent in Ising spins, called chirality, that represents the handedness of the non-collinear orientation, and that could yield another phase transition. It is reason of intense debate whether spin and chirality transitions are two distinct phenomena, or if they take place at the same temperature. Not much more has been investigated, so it is worth to make an investigation to see if Heisenberg spin glasses have features in common with structural glasses.

There are some reasons to conceive an analogy between structural glasses and some types of spin-glasses. In 1987, Kirkpatrick and Thriumalai [5] pointed out the formal identity between the Mode Coupling equations and the exact equations for the dynamics of a particular type of spin-glasses, with p-body interactions (the so called p-spin models). Unfortunately, this analogy has been established so far only for models with long range interactions, where the mean field approximation is ac-
Section of the document

Introduction

In their intuition, in the year 2000 G. Parisi and M. Mézard [6] made a replica study of structural glasses for finite-size systems that suggested that the structural glass transition belongs to the same Universality Class of the systems with one step of replica symmetry breaking. That means that the order parameter’s distribution is not continuous as in the Ising spin glasses, but it is takes only two values, because there is only one step of fragmentation of the free energy landscape. Unfortunately, a simple model, with short range interactions, undergoing a 1-RSB glass transition, is yet to be found.

There are a couple of clues that make us think that finite-range interaction Heisenberg spin glasses are a good candidate for the correspondence with spin glasses that we have exposed. The first is that H. Kawamura in 2005 [7] found a double-peak distribution of the order parameter typical of the one-step replica symmetry breaking, so the universality class may be the same. The second is that up to our knowledge the only dynamic study of the paramagnetic phase done up to now [8] estimates the phase transition at a temperature 50% higher than its actual position, and in an optimistic scenario this overestimation could be explained if what they found was actually the dynamic transition predicted by Mode Coupling Theory.

The above mentioned clues clearly do not suffice to establish our sought analogy. Hence, if one wants to have stronger evidence of the similarities between the two models it is necessary to make a systematic research of the aspects under which we would like to remark the analogy. We conducted our research under two main aspects:

1. Since the Mode Coupling Transition is best understood through the topological properties of the energy landscape, it is absolutely natural to start our investigation concentrating ourselves on the energy landscape.

\footnote{In absence of spacial symmetries we have two peaks: one at zero, and one at a finite value \(q_{EA}\). If, the system is symmetric under reflection there are three peaks because we have the reflection of \(q_{EA}, -q_{EA}\).}
landscape of the Heisenberg spin glasses, so we disposed ourselves to a systematic research of inherent structures. This type of investigation has never been done, because Ising spins are discrete variables, and Heisenberg spin glasses are still a largely unexplored topic. The only energy-lowering routine used in bibliography is the quench, which is known to be very badly performing. Hence we had to find a better performing algorithm to find inherent structures, and we made a deep study of their spatial correlation functions. We succeeded in finding a fast algorithm that permitted us to make our research with very large samples, compatible with the thermodynamic limit, and we noticed that the inherent structures are indeed relevant for the physics. First, we found the anharmonic term was rather small, so we can explain the energy of a thermalized state as harmonic fluctuations around a minimum. Second, lowering the temperature the correlation lengths of thermal states and the relative inherent structures converge.

2. Mode Coupling Theory predicts a divergence of the relaxation times in the paramagnetic phase, so we investigated the equilibrium dynamics of the Heisenberg spin glass model to see if we would encounter the same behavior. In conformity with the former point, we wanted to be in the thermodynamic limit, so we had to use non-physical algorithms to obtain thermalized configurations, and then we switched to physical dynamics. We wanted to verify if the relaxation time admitted a power law scaling for 3-4 decades that predicts a transition significantly over the critical temperature, as it happens in structural glasses. Also this analysis was successful: we found a scaling with exponents of the same order, in the same range of times, and the estimate of the possible dynamic transition was consistently over the spin glass transition, and two standard deviations under the previous estimate given in [8].
After these results the analogy between the two systems looks definitely more solid. Stronger data for this hypothesis could be given by an analysis of the variation with temperature of the density of negative directions in the hessian, which is a work actually in progress, and of the configurational entropy.
# Chapter 1

A brief summary on spin glasses

## Contents

| Section | Title                             | Page |
|---------|-----------------------------------|------|
| 1.1     | Defining a spin glass model      | 10   |
| 1.2     | Order Parameters                  | 12   |
| 1.2.1   | Ising Spins                       | 13   |
| 1.2.2   | Heisenberg Spins                  | 16   |
1.1 Defining a spin glass model

In the last decades particular attention has been given to a set of models which were meant to describe random magnets with co-presence and competition of ferromagnetic and anti-ferromagnetic interactions.

From the pure modelisation point of view a spin glass has two key ingredients: disorder and frustration. A simple example is given in figure 1.1, where we have 4 Ising spins (they can point only up or down) interacting in a loop. The interactions between the spins are randomly ferromagnetic or anti-ferromagnetic, so it can happen, as in this case, that it is impossible to satisfy all constraints. It is clear that in a very large system finding the configuration of spins that satisfies the most number of constraints is a very hard task.

![Figure 1.1: A toy model which shows frustration. If the interaction on the bond is a “+”, the spins want to be parallel and if it is a “-” they want to be anti-parallel. The model is frustrated because it is impossible to satisfy all the conditions simultaneously. In a spin lattice any loop of spins, in which the product of the interactions is negative, is frustrated.](image)

The first spin glass model was presented in 1975 by S.F. Edwards and P.W. Anderson [9] to modelize a dilute solution of Mn in Cu, in which the interactions between particles can be ferromagnetic or anti-ferromagnetic depending on their mutual distance.

In the Edwards-Anderson (EA) model the spins are placed in fixed positions in a $D$-dimensional regular lattice. This is because the typical
1.1 Defining a spin glass model

time scales of the movement of the particles is overwhelmingly greater, and non-trivial interesting effects can be seen on a regular lattice. The model’s Hamiltonian is

\[ H = - \sum_{\langle \vec{x}\vec{y} \rangle} J_{xy} \vec{s}_x \cdot \vec{s}_y, \quad (1.1) \]

where the brackets \( \langle \cdot \rangle \) indicate that the sum is performed only over the nearest neighbours. The spins \( \vec{s}_x \) are \( m \)-dimensional vectors with \( ||\vec{s}_x|| = 1 \). The type of spins has a different name depending on \( m \)’s value:

- \( m = 1 \): Ising spins
- \( m = 2 \): XY spins
- \( m = 3 \): Heisenberg spins.

It is clear that the choice of \( m \) depends strictly on the anisotropy of the material we want to study. The couplings \( J_{xy} \) are random variables with zero mean to avoid any bias towards ferromagnetism or antiferromagnetism, and their standard deviation has to be finite. If we call \([\cdot]\) the average over the different realizations over the disorder these conditions express as

\[ [J_{xy}] = 0, \quad [J^2_{xy}]^{1/2} = J (= 1). \quad (1.2) \]

The most used probability distribution functions for the \( J_{xy}’s \) are the bimodal and the Gaussian distribution. We stress that in these systems disorder is not only due, like in most models, to thermal fluctuations, but it also appears explicitly in the Hamiltonian, giving two levels of disorder. We decided to write the averages over the different realizations of the couplings with square brackets \([\cdot]\), and the thermal averages will be written in angular brackets \( \langle \cdot \rangle \).

Experimentally we can find spin glasses in many different systems:
• Metals: Magnetic alloys in which we have atoms with strong mutual interactions diluted in a non-magnetic metal such as Mn in Cu have two-site interactions

\[ J_{xy} \sim \frac{\cos(2k||\vec{x} - \vec{y}||)}{||\vec{x} - \vec{y}||^3} \]  

which depend on the distance and evidently yield the possibility of having both ferromagnetic and anti-ferromagnetic interactions.

• Insulators: An example is Fe\(_{0.5}\)Mn\(_{0.5}\)TiO\(_3\), which comprises hexagonal layers. The spins align perpendicular to the layers. Within a layer the spins in pure FeTiO\(_3\) are ferromagnetically coupled while spins in MnTiO\(_3\) are antiferromagnetically coupled. Hence the mixture gives an Ising spin glass with short range interactions.

• Non-conventional spin glasses: Spin glass theory has been used to study a numerous amount of problems outside the condensed matter domain, such as:

  − Optimization problems in computer science
  − Protein folding
  − Polymer glasses, foams...

1.2 Order Parameters

A phase transition presents often a spontaneous symmetry breaking in the system. The order parameter is the observable to whom we impute the breaking of the symmetry. It usually transforms, under the symmetry changes, in a homogeneous non-trivial way, so that, when it is zero, symmetry is preserved and, when it is non-zero, it is broken.

It is now assumed, after consistent experimental, theoretical and numerical work, that EA spin glasses have two thermodynamic phases: the paramagnetic phase and the spin glass phase. This issue has been quite
1.2 Order Parameters

controversial for years, because the static aspect of a configuration in the spin glass phase was not easily distinguishable from a paramagnetic one. As a matter of fact the order parameter of a spin glass is not a trivial object, and it deserves particular attention.

1.2.1 Ising Spins

To make the order parameter definition easier we rely on the comparison with the order parameters in the non-disordered counterparts of our models. Thus, for Ising spins we will show how the order parameter is defined in the Ising model, and see how to extend this definition to the EA Ising model.

Symmetries and Order Parameter in the Ising Model

The Ising model’s Hamiltonian is

\[ H = - \sum_{<\vec{x},\vec{y}>} s_\vec{x}s_\vec{y}, \]  

(1.4)

with \( s_\vec{x} = \pm 1 \).

It is immediate to see that its symmetry group is \( Z_2 \), since making the symmetry transformation

\[ Z_2 : \{ s_\vec{x} \} \rightarrow \{-s_\vec{x}\} \]  

(1.5)

the Hamiltonian and the functional integration measure are invariant. The order parameter is the magnetization

\[ m = \frac{1}{N} \sum_\vec{x} s_\vec{x} \]  

(1.6)

which is not invariant under our \( Z_2 \) symmetry

\[ Z_2 : \, m \rightarrow -m \]  

(1.7)

so in the disordered phase, for \( T > T_c \), we have \( m = 0 \), and for \( T < T_c \), in the ordered phase, we have \( m \neq 0 \). Unfortunately the symmetry breaking, hence the phase transition, occurs only in the thermodynamic limit.
$L \to \infty$ because in finite systems the average magnetization is zero also in the ordered phase, since the energy barriers that cause the ergodicity breaking are infinite only in an infinitely large system. Therefore, if we want to extract infinite-size properties from a finite-size system, as it is done in numerical simulations, we should better study invariant quantities that are not negatively influenced by the absence of phase transition.

The correlation function

$$G(\vec{x}, \vec{y}) = \langle s_{\vec{x}} s_{\vec{y}} \rangle$$

is clearly invariant under our symmetry transformation

$$Z_2 : \quad s_{\vec{x}} s_{\vec{y}} \to (-s_{\vec{x}})(-s_{\vec{y}}) = s_{\vec{x}} s_{\vec{y}}$$

The correlation function is strictly bound to the order parameter, since

$$\langle m^2 \rangle = \langle \frac{1}{N} \sum_{\vec{x}} s_{\vec{x}} \rangle \langle \frac{1}{N} \sum_{\vec{y}} s_{\vec{y}} \rangle = \frac{1}{N^2} \sum_{\vec{x}} \sum_{\vec{y}} \langle s_{\vec{x}} s_{\vec{y}} \rangle .$$

If the system has periodic boundary conditions the correlation function is also translationally invariant so $G(\vec{x}, \vec{y}) = G(\vec{x} - \vec{y})$, hence

$$\langle m^2 \rangle = \frac{1}{N} \sum_{\vec{r}} \langle s_0 s_{\vec{r}} \rangle = \frac{1}{N} \sum_{\vec{r}} G(\vec{r}) = \frac{1}{N} \hat{G}(\vec{k} = \vec{0})$$

where the hat indicates the function’s Fourier transform. We see then that the correlation function contains a lot of interesting information over the thermodynamic system.

**Symmetries and Order Parameter in the EA Ising Model**

Introducing disorder in the Ising model we have

$$H = - \sum_{<\vec{x}\vec{y}>} J_{\vec{x}\vec{y}} s_{\vec{x}} s_{\vec{y}}$$

which, as we said in section 1.1, puts us in the position to have to define two levels of disorder. We have two types of symmetry now. One is
1.2 Order Parameters

the global $Z_2$ related to the positions of the spins belonging to a single sample of which we just talked. The second is a local symmetry (gauge symmetry) related to the realizations of the disorder. Speaking more clearly if we associate to each site $\vec{x}$ a variable $\eta_{\vec{x}} = \pm 1$ it is clear that the transformation

\begin{align*}
J_{xy} & \rightarrow J'_{xy} = \eta_x J_{xy} \eta_y \\
\eta_x & \rightarrow \eta'_{x} = \eta_x \eta_x
\end{align*}

keeps invariant the relevant magnitudes $H$ and $Z$. Notice that the probability distribution function of the $J$’s does not change with the gauge transformation.

While the global invariance is verified only in the thermodynamic limit, the local symmetry is always true. Let’s see how it is possible to study a finite size system.

Since we want to study the properties of the system no matter the disorder realization, we can no longer use $s_x s_y$ as observable for its investigation because it is not gauge-invariant.

To construct a gauge-invariant observable that preserves all the symmetries that we need, we resort to a simple trick, redefining the Hamiltonian in a harmless way, in order for it to represent two replicas $(a)$ and $(b)$ of the same realization of the disorder:

$$H^{(2)} = - \sum_{<x,y>} J_{xy} (s_x^{(a)} s_y^{(a)} + s_x^{(b)} s_y^{(b)})$$

The local symmetry remains the same, while the global symmetry group changes then to $Z_2 \otimes Z_2$ because the invariance holds also if we flip all the spins of only one of the two replicas.

We can now construct a gauge-invariant object

$$q_x = s_x^{(a)} s_x^{(b)}$$
that is not invariant under the global symmetry. If we define the Edwards-Anderson parameter as
\[ q = \frac{1}{N} \sum_x q_x \] (1.18)
we see that it is a good order parameter since under the global symmetry \( q \to \pm q \).

As we did before we relate the square order parameter with the correlation function, which in presence of quenched disorder and translation invariance is
\[ G_J(x, y; J_{xy}) = \langle q_x q_y \rangle = G_J(x - y; J_{xy}), \] (1.19)
so
\[ \langle q^2 \rangle = \left( \frac{1}{N^2} \sum_x \sum_y \langle q_x q_y \rangle \right) = \frac{1}{N} \sum_r G(r) = \frac{1}{N} \chi. \] (1.20)

### 1.2.2 Heisenberg Spins

We have seen how to define the order parameter in the EA Ising model and how it is related to some other useful observable. Is there a great difference when we pass from \( m = 1 \) spin dimensions to \( m = 3 \)?

Indeed we know that the universality class will not be the same, so critical exponents and scaling functions will not be the same. Nevertheless those are not the only important differences between the two models. It will be in the next chapter that we will focus on the recent results that stress the diversity implied by \( m = 3 \).

Here we will concentrate on the symmetries implied by 3-dimensional spins, showing how it is possible to identify a new order parameter that possibly changes the whole physics of the EA model.

### Symmetries and Order parameter in the Heisenberg Model

In the Heisenberg model the Hamiltonian is slightly modified
\[ H = - \sum_{<x,y>} \mathbf{s}_x \cdot \mathbf{s}_y \] (1.21)
where now the spins $\vec{s}_x$ are 3-dimensional vectors with the constraint $s^2 = 1$. A Heisenberg system is invariant under the rotation or inversion of all the spins, so its global symmetry group is

$$O(3) : \vec{s}_x \rightarrow T\vec{s}_x, \quad TT^t = I \quad (1.22)$$

and the order parameter

$$\vec{m} = \frac{1}{N} \sum_x \vec{s}_x \quad (1.23)$$

is vectorial. As in the Ising case, for a finite system $<\vec{m}> = \vec{0}$ at all temperatures, so there is no point in computing it, and we have to find a non trivial quantity in finite volumes, as the correlation function

$$G(x,y) = <\vec{s}_x \cdot \vec{s}_y> \quad (1.24)$$

that is related to the order parameter in the usual way

$$<\vec{m}^2> = \frac{1}{N} \sum_r G(r) \quad (1.25)$$

### Symmetries and Order parameter in the EA Heisenberg Model

Knowing already the consequences of the presence of disorder we apply directly the trick seen in section 1.2.1 and we write the two-replica Hamiltonian

$$H = - \sum_{<x,y>} J_{xy} (s_x^{(a)} \cdot s_y^{(a)} + s_x^{(b)} \cdot s_y^{(b)}) \quad (1.26)$$

that makes us possible to get the Edwards-Anderson parameter. The symmetries are

- Disorder: $Z_2$ (local)
- Thermal: $O(3) \otimes O(3)$ (global)
1.2 Order Parameters

Our gauge invariant this time is a tensor that we call spin-glass site overlap

\[ \tau_{\alpha\beta}(\vec{x}) = \vec{s}_{\vec{x},\alpha} \cdot \vec{s}_{\vec{x},\beta}, \]  

(1.27)

where \( \alpha, \beta = 1, 2, 3 \) are the components of the spin vectors, thus the Edwards-Anderson parameter in the EA Heisenberg model is

\[ Q_{\alpha\beta} = \sum_{\vec{x}} \tau_{\alpha\beta}(\vec{x}), \]  

(1.28)

that is related with the correlation function

\[ G(x, y) = \langle \text{tr}(\tau(\vec{x})\tau^\dagger(\vec{y})) \rangle \]  

(1.29)

in the usual way

\[ \langle \text{tr}(QQ^\dagger) \rangle = \frac{1}{N} \sum_{\vec{r}} G(\vec{r}) = \frac{1}{N} \sum_{\vec{r}} \hat{G}(\vec{k} = 0) = \frac{1}{N} \chi \]  

(1.30)

**Chirality**  The order parameter scenario in the EA Heisenberg model even more interesting than what we have just exposed. In fact one can admit the possibility of breaking the global symmetry \( Z_2 \) keeping intact the \( SO(3) \) symmetry [10].

We define chirality of a site along the direction \( \mu = 1, 2, 3 \) as

\[ \kappa^\mu(\vec{x}) = \vec{s}_{\vec{x} - \hat{e}_\mu} \cdot (\vec{s}_{\vec{x}} \times \vec{s}_{\vec{x} + \hat{e}_\mu}) \]  

(1.31)

where \( \hat{e}_\mu \) is the unit vector in the direction \( \mu \). If we make a mirror exchange of all the particles respect to a plane the chirality of the sites remains the same except for the spins on the plane. A ferromagnetic system would not feel the reflection because the system is homogeneous and non zero chirality is generated only by thermal fluctuations, and not by the energy landscape, so it would not be a good observable. On the other side spin glasses are not homogeneous, and the in the ground states the spins are not aligned, so they are not invariant under this transformation.
In compliance with what we did above, we define our chiral gauge invariant
\[ \epsilon^\mu(\vec{x}) = \kappa^{(a)}(\vec{x})\epsilon^{(b)}(\vec{x}), \] (1.32)
from which descends the chiral-glass (CG) overlap in the direction \( \mu \), which is our order parameter,
\[ E^\mu = \frac{1}{N} \sum \epsilon^\mu(\vec{x}), \] (1.33)
and we remark its connection with the symmetrized correlation function
\[ C^{CG}_{\mu \nu}(\vec{x}\vec{y}) = \frac{<\epsilon^\mu(\vec{x})\epsilon^\nu(\vec{y})> + <\epsilon^\nu(\vec{x})\epsilon^\mu(\vec{y})>}{2} \] (1.34)
through the usual relation
\[ [<E_\mu E_\nu>] = \frac{1}{N} \sum r C^{CG}_{\mu \nu}(r) = \frac{1}{N} \chi^{CG} \] (1.35)

**Overlaps** A very handy feature of disordered systems is the overlap, a magnitude that tells us how similar two configurations are, being equal to zero if there is no resemblance, and far from zero in the opposite case. There are numerous ways to define an overlap, but all of them are not invariant under the global symmetries of a Heisenberg spin glass. This could be a problem in numerical simulations, because we could think that two identical replicas, who differ only by a rotation, have very different configurations. Solutions to this would be very computationally expensive, so a symmetry-invariant definition of the overlap would be very useful.

For the chirality the solution is direct, since it is a scalar object and it is always invariant, so we can use the chiral glass overlap \( E^\mu \) introduced just above.

For the spin-glass (SG) overlap, for example we could use the Edwards-Anderson parameter, but it is not \( O(3) \) invariant. If we look at the previous paragraphs we can remark that the square overlap
\[ Q^2 = tr(\tau(x)\tau^\dagger(x)) \] (1.36)
1.2 Order Parameters

not only is an invariant, but it also gives an idea of the similarity between two configurations. It is zero for completely different replicas, and about 1/3 when we compute it for a replica with itself and its spins are isotropically distributed (in presence of anisotropy it tends to 1).
Chapter 2

Update on developments in spin glasses

Contents

2.1 Ising vs Heisenberg .......................... 22
  2.1.1 Ising ordering in zero field ............... 22
  2.1.2 Heisenberg ordering in zero field and chirality
       scenario .................................. 23
2.2 Dynamics ..................................... 26
  2.2.1 Energy Landscape Scenario ............... 26
2.1 Ising vs Heisenberg

The original version of the EA model was proposed for Heisenberg spins, as it is expected that they represent a good approximation for most of the spin glass material, in particular those who posses weak magnetic anisotropy. In fact Heisenberg spins are much more present in nature than Ising spins, so it is logical to be more interested in them. Nevertheless Ising spins have been studied far more because of their greater simplicity. It has been argued, in the initial studies of the EA Ising model, that their weak magnetic anisotropy present in real magnets causes a crossover from the isotropic behavior to the anisotropic, shifting the universality class of the systems, so that Ising spins, corresponding to the strong anisotropy limit would describe also the behavior of magnets with weak anisotropy [11].

2.1.1 Ising ordering in zero field

It hasn’t been clear whether the three dimensional EA Ising model presented a finite-temperature spin-glass transition until in 1985 Monte Carlo simulations from Ogielski, Bhatt and Young [12, 13] found solid evidence of a finite $T_{SG}$. Later investigations on the critical exponents found values that were difficult to compare with an experimental realization of the Ising spin glass because at present we know of only one type of Ising spin glass really existing in nature that we can study in laboratory, an insulating spin glass magnet of Fe$_{0.5}$Mn$_{0.5}$TiO$_3$ that we have already mentioned in section 1.1. We stress that when estimates of the critical exponents started to be found the argument mentioned above, that Ising spins may fairly represent a weakly anisotropic Heisenberg spin glass, collapsed immediately, since they were very far from being compatible.

A point that raises a lot of controversies is the nature of the SG ordered state. There are two dominant visions: the “droplet picture”
that claims that EA spin glasses are disguised ferromagnets without a spontaneous Replica Symmetry Breaking (RSB) and only two ordered states [14], and the “hierarchical RSB picture”, inspired on Parisi’s exact solution of the mean field model, which claims that the ordered state is accompanied with a hierarchical RSB [15]. In figure 2.1 we show the distribution of the order parameter in one case and in the other.

![Figure 2.1: The overlap distribution $P(q)$ in the thermodynamic limit for a finite-range spin glass. In figure (a) we show the droplet picture: the spin glass is a disguised ferromagnet and has only two ordered states, represented with two delta functions at $\pm q_{EA}$. In figure (b) we see how with hierarchical RSB $P(q)$ possesses an additional plateau connecting the two delta-function peaks.](image)

2.1.2 Heisenberg ordering in zero field and chirality scenario

Early numerical simulations individuated in common agreement that the EA Heisenberg model had only a zero temperature phase transition, in evident contrast with experiments, which clearly showed a finite $T_{SG}$. The scientific community used to explain this inconsistency invoking the weak magnetic anisotropy present in real spin glasses, that wasn’t reproduced in numerical simulations, that caused a shift to the Ising behavior of the real materials. Nevertheless, this explanation wasn’t
at all satisfactory, since the critical exponents found in the experiments were completely different from the Ising ones. In 1992 an elegant theory was proposed by H.Kawamura, who suggested that a finite-temperature phase transition took place in the chiral sector. This scenario kept also after more modern simulation stated that the model has $T_{SG} > 0$. It consists in two steps:

1. Spin-Chirality decoupling
   (for a completely isotropic system, as the simulated ones)

2. Spin-Chirality recoupling
   (for a weakly anisotropic system, as the experimental ones)

The first part claims that the ordering is not simultaneous for both the order parameters (chiral and spin glass overlap). When we decrease temperature from the paramagnetic phase we first meet at $T_{CG}$ the spontaneous breaking of the discrete $Z_2$ symmetry with the preservation of the continuous $SO(3)$ symmetry, and only at lower temperature $T_{SG} < T_{CG}$ the whole $O(3)$ symmetry is broken. The higher transition, in which only the $Z_2$ symmetry is broken is called the “chiral glass transition”, and the phase between $T_{CG}$ and $T_{SG}$, in which only the chiralities are ordered, is called the “chiral glass state”.

In the second part of this scenario this result in adapted to a real spin glass, with inevitable weak magnetic anisotropy, which reduces the Hamiltonian’s symmetry from $SO(3) \times Z_2$ to only $Z_2$, mixing the chirality to the spin sector. So of the two transitions that take place in an isotropic system, it would be the chiral glass transition to dominate the real spin glasses’ phase transition.

The chirality decoupling scenario explains in a natural way questions on the experimental phase transition like the origin of the non-Ising critical exponents experimentally observed in canonical spin glasses, and it gave a very elegant explanation of what could be occurring when the early
numerical simulations estimated $T_{SG} = 0$. Yet, specially now that it is accepted that $T_{SG} = 0$ was a problem of finite size system, or interpolations too far from the critical temperature, it is not a dominant scenario in the scientific community, since although there are recent works that would confirm it [16], there are others that give evidence of a simultaneous spin and chirality transition [17].

For what concerns the type of ordering, while for the SG order parameter the nature of the glassy phase is debated not differently than with Ising spins, in the chiral sector there has been some evidence (figure 2.2) of a one-step RSB [7], so the $P(q)$ in the thermodynamic limit would be represented by two delta-function peaks at $\pm q_{EA}$ and one at $q = 0$.

Figure 2.2: The overlap distribution at $T = 0.15$ for the chirality of the 3D Heisenberg spin glass with $\pm J$ couplings from [7, Kawamura (2005)]. This plot suggests that there may be a one-step RSB for the chirality.

**Mean Field Analysis** Evaluating the help that the mean field resolution gives to the understanding of the finite-range interaction model is a troublesome issue. Table 2.1, which compares the mean field critical temperature $T^{MF}_{SG} = \frac{\sqrt{z}}{m}$, where $z$ is the coordination number ($z = 6$ in our case), with the estimates of the finite-range $T_{SG}$, shows us how increasing
2.2 Dynamics

$m$ it becomes always less reliable. What happens is that the fluctuations neglected with the mean field approximation are more important the larger $m$ is, so the mean field results with Heisenberg spins are even less reliable than those obtained with Ising spins. We remark also how the data in the table suggests that $T_{SG} = 0$ for $m \to \infty$. Unfortunately no mean field solution exists in the chiral sector because it is impossible to define chirality in a non metric space.

| $m$ | Model  | $T_{SG}^{MF}$ | $T_{SG}$ | $T_{SG}/T_{SG}^{MF}$ |
|-----|--------|---------------|----------|----------------------|
| 1   | Ising  | 2.45          | 0.97     | 0.40                 |
| 2   | XY     | 1.22          | 0.34     | 0.28                 |
| 3   | Heisenberg | 0.82    | 0.12     | 0.15                 |

Table 2.1: Comparison of the critical temperature, between mean field approximation and numerical evaluation, varying the number of components of the order parameter. We see that $T_{SG}/T_{SG}^{MF}$ is small and decreases with $m$. Physically this means that fluctuations get larger increasing $m$. Data suggests that $T_{SG} \rightarrow 0$, and evidence has been found for this conjecture being true [20].

2.2 Dynamics

At low temperature the dynamics in spin glasses become very slow, such that below the critical temperature the system is always out of equilibrium. There are many out of equilibrium effects in the dynamics of spin glasses that still haven’t been well understood as aging, rejuvenation and temperature cycles. Yet, in the present work we want to concentrate in another aspect that attracted our curiosity, that is the possibility of a straightforward analogy between the dynamics of spin and structural glasses.

2.2.1 Energy Landscape Scenario

Although out of equilibrium dynamics is proper of the spin glass phase, an interesting feature could be revealed if we notice that works
that look for the critical temperature with dynamical criteria tend to overestimate it. This could suggest an analogy with structural glasses, in which Mode Coupling Theory predicts a power law divergence of the correlation time at $T = T_{MC} > T_c$. This divergence doesn’t take place because when we get close to $T_{MC}$ different effects come in play, but it could be what is being observed in those works. Goldstein’s scenario [21], which by now is widely accepted, says that the dynamics at low temperature are completely different from those at high temperature.

When $T$ is low a supercooled liquid explores the phase space mainly by activated jumps between the local minima of the free energy. The characteristic time $\tau$ to jump from one minimum to another is, in agreement with the Arrhenius law $\tau \propto \exp^{-\beta \Delta V}$, proportional to the exponential of the energy gap. On the contrary at higher temperatures the typical configurations are not local minima with a positive definite hessian, but saddles with negative directions, so the dynamics is much faster. The characteristic time does not represent any more how much it takes for the thermal agitation to cause the barrier jump, but how much it takes to the system to individuate the negative directions in the hessian. We understand, in this scenario, how the decrease of negative directions in lowering the temperature may increase the relaxation time making it apparently diverge, just until it becomes of the order of $\tau \propto \exp^{-\beta \Delta V}$.

Our main aim in this work was to find evidence of the influence of the energy landscape in the dynamics of a spin glass, to give a basis for constructing a solid connection with the theory of the dynamics of structural glasses. In this perspective we did a deep investigation of the magnitudes that concern dynamics, such as time correlation functions, and tried to connect them to the energy landscape, by making a massive research of inherent structures (local energy minima).
Chapter 3

Numerical Techniques

Contents

3.1 Thermalization Dynamics .......................... 30
  3.1.1 Metropolis ................................. 30
  3.1.2 Heat Bath .................................. 31
  3.1.3 Over Relaxation ............................ 32

3.2 Minimizing the Energy ............................ 32
  3.2.1 Gauss-Seidel ................................. 33
  3.2.2 Genetic Algorithms .......................... 35
  3.2.3 Successive Over Relaxation .................. 36

3.3 Computing Observables ............................ 38
  3.3.1 Energy ...................................... 39
  3.3.2 Overlaps .................................... 39
  3.3.3 Correlation Lengths and Functions .......... 41
  3.3.4 Magnetic Susceptibility ...................... 44
  3.3.5 Binder’s Cumulants .......................... 45
  3.3.6 Self-correlation Times and Functions ....... 46
3.1 Thermalization Dynamics

Monte Carlo (MC) is the most used technique for spin glass computer simulations. It is a stochastic Markov Chain method that aims not to sample the whole configuration space, but only its most significant parts (importance sampling) in order to extract a fine estimate of the observables.

For Ising spins there exist numerous MC variants that one can easily obtain imposing detailed balance to be satisfied, such as [22] the most famous Metropolis-Hastings, local sampling methods, perfect sampling and heat bath. All those consist in flipping sequentially the spins with the constraint of preserving the detailed balance.

For multi-dimensional spins the deal is similar. We will now show the extension of a couple of those methods to Heisenberg spins.

3.1.1 Metropolis

The fingerprint of a Metropolis updating scheme is that new configurations are accepted with a probability $\min[1, e^{-\beta \Delta E}]$. We generate new configurations by modifying the orientation of a single spin in the following way:

A $3-D$ random vector $\vec{r}$ in the sphere of radius $\delta$ is extracted.

The new spin proposal is

$$\vec{s}_x^{\text{new}} = \frac{s_x^{\text{old}} + \vec{r}}{||s_x^{\text{old}} + \vec{r}||}. \quad (3.1)$$

The new spin is accepted with probability $P = \min[1, e^{-\beta \Delta E}]$ and rejected with probability $1 - P$.

We see that the probability of proposing $s_x^{\text{old}} \rightarrow s_x^{\text{new}}$ is the same of proposing $s_x^{\text{new}} \rightarrow s_x^{\text{old}}$. The choice of $\delta$ must be sufficiently accurate to give an acceptance rate of $40\% \sim 60\%$, because a too small $\delta$ (hence a
3.1 Thermalization Dynamics

too small rejection rate) would make the dynamics too slow, while a too large rejection rate would keep the system still.

3.1.2 Heat Bath

The Heat Bath (HB) updating scheme has the main advantage of reducing to zero the rejection rate, and for this reason for Heisenberg spins it is much more performing than Metropolis. The main idea is that, chosen a site, the new spin proposal does not depend by the old spin, but it is chosen according to its probability distribution.

For a given site the local field is known, so the conditional probability for the spin’s orientation is

$$dP(\vec{s}|\vec{h}) = d\vec{s} \frac{e^{\beta J(\vec{s} \cdot \vec{h})}}{\int d\vec{s} e^{\beta J(\vec{s} \cdot \vec{h})}}. \quad (3.2)$$

We can make a wise reference change to coordinates \((x', y', z')\) with \(z' \parallel \vec{h}\) to get trivial scalar products, and then pass to polar coordinates, with \(s = (\cos \theta' \cos \phi', \sin \theta' \cos \phi', \sin \phi' = z'):\n
$$dP(\vec{s}|\vec{h}) = d\phi d\theta e^{\beta Jh} \sin \theta \sin \theta \int d\phi d\theta e^{\beta Jh} \sin \theta \sin \theta. \quad (3.3)$$

This way we get a factorized probability distribution function

$$dP(\vec{s}|\vec{h}) = \frac{d\phi}{2\pi} \times dz' e^{\beta Jhz'} \int dz' e^{\beta Jhz'} \quad (3.4)$$

where \(h = ||\vec{h}||\). Since the angle \(0 < \phi' < 2\pi\) is uniformly distributed it’s easy to get its pseudo-random value. For \(z'\) we use \(u = e^{\beta Jhz'}\) that is uniformly distributed in the interval \(e^{-\beta Jh} < u < e^{\beta Jh}\).

At this point we have to come back to our original frame with minimum computational effort. To do so we remark that our spin is

$$\vec{s} = z' \frac{\vec{h}}{h} + \sqrt{1 - z'^2} \vec{R}_\perp \quad (3.5)$$

where \(\vec{R}_\perp\) is a unitary random vector, orthogonal to the local field \(\vec{h}\), that we can obtain by extracting a random unitary vector, peeling its component parallel to \(\vec{h}\), and renormalizing it.
3.2 Minimizing the Energy

3.1.3 Over Relaxation

The present is a deterministic, very computationally-fast, microcanonical simulation scheme. Although its dynamics are not physical, it helps when we want to sweep quickly the configuration space. Performing 1 HB sweep every $L$ Over Relaxation (OR) sweeps we generate in the lattice an iso-energetic spin wave after each energy change. Of course it cannot reproduce real dynamics, but it is very useful to generate thermalized configurations of the system.

The algorithm proposes the maximum spin change that leaves the energy invariant so the new spin will always be accepted (see the Metropolis acceptance rate in section 3.1.1). The new spin is so binded the condition

$$\vec{s}^{\text{new}} \cdot \vec{h} = \vec{s}^{\text{old}} \cdot \vec{h}$$

and we obtain the maximal change by reversing the spin’s component that is perpendicular to the local field $\vec{h}$:

$$\vec{s}^{\text{new}} = 2\vec{h} \frac{\vec{h} \cdot \vec{s}_x}{\vec{h}_x^2} - \vec{s}_x$$

3.2 Minimizing the Energy

Obtaining spin glass low energy configurations is computationally hard[23], and this makes our objective of finding inherent structures a real challenge. While for Ising spins there exists a whole literature of numerical methods used to minimize the energy such as simulated annealing [24], cluster algorithms [25], genetic algorithms[26, 27], and combinations of those methods[28, 29], almost nothing exists for Heisenberg spin glasses.

We will now give a review of the small amount of methods used for Heisenberg spin glasses, and present our choice, which is not applicable to Ising spins and is new for HSG.
3.2 Minimizing the Energy

3.2.1 Gauss-Seidel

The most trivial and common way to find low-energy states is performing a quench.

It is easy to see that the energy of a single site

\[ e_x = -\vec{s}_x \cdot \vec{h}_x \] (3.8)

is minimized if the spin \( \vec{s}_x \) is parallel to the local field \( \vec{h}_x \). This observation can suggest us a quite brutal way to lower the energy, i.e. aligning sequentially the spins to the local field, i.e. making the substitution

\[ \vec{s}_x \rightarrow \frac{\vec{h}_x}{||\vec{h}_x||} \] (3.9)

This type of method is much older than the mere existence of spin glass models. In fact we will see that it is exactly the application to our model of the Gauss-Seidel method, used to solve systems of linear equations[30]. In fact the problem solving the linear system \( A\phi = f \), where \( A \) is a given symmetric positive-definite matrix and \( f \) is a given vector, is equivalent to the one of minimizing the Hamiltonian

\[ H(\phi) = \frac{1}{2}(\phi, A\phi) - (f, \phi). \] (3.10)

Given the Hamiltonian in equation 3.10, the Gauss-Seidel Algorithm consists in sweeping through the sites \( i \), and at each step replacing \( \phi_i \) by that new value \( \phi_i' \) which minimizes \( H \) when the other fields \( \{\phi_j\}_{j \neq i} \) are held fixed at their current values[30]. In other words, if we write

\[ H(\phi_i, \phi_j \neq i) = \frac{1}{2}A_{ii}(\phi_i - b_i)^2 + c_i \] (3.11)

the Gauss-Seidel algorithm consists in simply replacing \( \phi_i \) with \( b_i \). This is exactly what we do with the quench routine when we substitute \( \vec{s}_x \) with \( \frac{\vec{h}_x}{||\vec{h}_x||} \), so if we show that the EA-Heisenberg Hamiltonian is reducible to the same form, we can state immediately this algorithm’s main property:
it’s ineffectiveness, and seek for a better solution. As a matter of fact this algorithm has an extremely slow rate of convergence [31]. For example for \( A = \Delta + m^2 \) the convergence time grows as \( m^{-2} \).

**Reduction of the EA Heisenberg Hamiltonian to a quadratic form**  Let’s show how, when we are close to a local minimum, our Hamiltonian can be reduced to a quadratic form in chiral perturbation theory.

If we call \( \{ s^0 \} \) a generic inherent structure configuration, i.e. with all the spins aligned to the local field, any spin is expressible as

\[
\vec{s}_x = s^0 \sqrt{1 - \vec{\pi}_x^2 + \vec{\pi}_x}
\]

with the condition

\[
\vec{h}_x \cdot \vec{\pi}_x = s^0_x \vec{\pi}_x = 0.
\]

\( \vec{\pi} \) is the component of the spin perpendicular to the local field, and we call it pion. If \( |\vec{\pi}| \) is small, i.e. we are close to the local minimum, we can develop the Hamiltonian to the second order in \( \vec{\pi} \), keeping in mind condition 3.13, in order to obtain

\[
H(\{ \vec{s} \}) = H(\{ s^0 \}) + \frac{1}{2} \sum_x (\vec{h}_x \cdot \vec{s}^0_x) \vec{\pi}_x^2 + \sum_x \vec{\pi}_x \cdot \left( \sum_{||x-y||=1} J_{xy} \vec{\pi}_y \right). \tag{3.14}
\]

This way the variation \( \Delta H \) can be written as a quadratic form in an \( N \)-dimensional space:

\[
\Delta H = H(\{ \vec{s} \}) - H(\{ s^0 \}) = -\frac{1}{2} \{ \vec{\pi} \}, M \{ \vec{\pi} \} + o(\vec{\pi}^3) \tag{3.15}
\]

with

\[
M_{xy} = \delta_{xy} - D \sum_{\mu = \pm 1} \delta_{x+\mu y} J_{xy}, \tag{3.16}
\]

so finding an inherent structure is actually equivalent to minimizing a quadratic form when we’re in the limit of small pions.
3.2 Minimizing the Energy

3.2.2 Genetic Algorithms

Other than brutally applying the Gauss-Seidel method, very little has been done for Heisenberg spin glasses. Nevertheless, in a recent article [32] from Y. Iyama and F. Matsubara we can see an attempt to extend the genetic algorithm thought up by Pál [28] for Ising spins, to Heisenberg spins, with the intention of finding ground states. Since this is the only other kind of energy-minimizing routine we found in literature we will explain the ideas on which it is based.

The basic idea of a genetic algorithm is to find a low energy state mixing in a smart way the parts of a selection parent configurations (from analogy with reproduction the name genetic, since it is as if the configurations pass to their heirs their genetic code). Clearly the initial choice of the parent configurations is a crucial step.

Pál’s suggestion [28] is to use a hybrid algorithm which alternates the genetic algorithm steps with a generic non-genetic minimization algorithm, and this is what is done by Iyama and Matsubara in [32], who chose to alternate quenches (Gauss-Seidel) to the genetic steps.

It appears, from their work, that a very big computational effort is necessary to find low energy configurations with their algorithm, since they study very small lattices \((L \leq 13)\), and the number of samples studied is not high (500 samples for \(L = 13\)).

Later in this paper we will refer to this work since it is the only example in literature of search of ground states in Heisenberg spin glasses (although they study \(\pm J\) bonds, while ours have a Gaussian distribution), and they give the only existing (to now) estimate of the ground state energies. In a brief study of \(\pm 1\) bonds we will show how results comparable to theirs are achievable with much smaller computational effort.
3.2 Minimizing the Energy

3.2.3 Successive Over Relaxation

It is common sense that greedy algorithms such as Gauss-Seidel are not very effective, especially compared to ungreedier versions of their selves. Taking advantage of this precious advice we can improve this scheme in a simple and effective way. Instead of choosing the $\phi_i$ that minimizes the Hamiltonian we can make an apparent non-optimal choice that lowers the energy, but less. On the long run the convergence time is definitely quicker (for $A = \Delta + m^2$ the convergence time grows as $m^{-1}$ instead of $m^{-2}$ with the best choice of the parameters).

In our problem, if we call
\[
\vec{s}_{\text{GS}} = \frac{\vec{h}_x}{||\vec{h}_x||} \quad \text{(3.17)}
\]
the new spin that minimizes the local Hamiltonian, and
\[
\vec{s}_{\text{OR}} = 2\vec{h}_x \cdot \frac{\vec{s}_{\text{GS}}}{\vec{h}_x^2} - \vec{s}_{\text{GS}} \quad \text{(3.18)}
\]
the spin deriving from the Over Relaxation algorithm described in section 3.1.3, the Successive Over Relaxation is expressed by choosing the new spin as
\[
\vec{s}_{\text{SOR}} = \frac{\vec{s}_{\text{GS}} + \lambda \vec{s}_{\text{OR}}}{||\vec{s}_{\text{GS}} + \lambda \vec{s}_{\text{OR}}||} \quad \text{(3.19)}
\]
where $\lambda > 0$ is the parameter that determines how ungreedy the routine is. This way we are choosing our new spin damping the maximum energy minimization with the iso-energetic change that most varies the Hamiltonian.

Figure 3.1 shows how the energy decrease is initially lower with higher $\lambda$’s, but there is a time after which the ungreedier routine (greater $\lambda$) becomes more efficient.

We remark the two trivial limits in $\lambda$ for this algorithm:
\[
\lim_{\lambda \to 0} s_{\lambda}^{\text{SOR}} = s_{\text{GS}} \quad \text{(3.20)}
\]
\[
\lim_{\lambda \to \infty} s_{\lambda}^{\text{SOR}} = s_{\text{OR}} \quad \text{(3.21)}
\]
3.2 Minimizing the Energy

Figure 3.1: Successive Over Relaxation in a $L=100$ after having performed $t^*=0$ Gauss-Seidel steps before starting with SOR. With small $\lambda$ the dynamics is similar to a quench: the system dives into a valley of the free energy without selection, and it stays there a lot of time before converging, as we know that with the Gauss-Seidel method convergence is a bad issue. On the other side dynamics with very large $\lambda$ spend a lot of time at high energy: they select better the valley where to get inside, so they reach lower energies (it will be more evident in the zoomed figure 4.2) and once they’re in a valley they converge faster. We can remark the too greedy routines, which converge too slowly because they spend too much time at low energies, and the too greedy ones, that stay too much time at high energies.

It is clear that $\lambda$ has to be chosen with care, because a small one risks to be too greedy, hence too similar to a brutal quench, while a too big one may be too ungreedy, having a too long plateau, and never converge.
Variants If we want our routine to be more site-dependent we can slightly modify it as follows:

\[
\vec{s}_{\lambda, x}^{\text{new}} = \frac{\vec{h}_x + \lambda \vec{s}_x^{\text{OR}}}{||\vec{h}_x + \lambda \vec{s}_x^{\text{OR}}||},
\]

(3.22)

This way the dynamics will be less damped in the sites where the local field is strong, and more where it is weak. This is the variant we used throughout our investigation.

Another idea could be to alternate \(aL\) \((a = 1, 2)\) Over Relaxation steps with one quench steps instead of updating the spins with always in the same ungreedy way. This would mean that before lowering the energy we sweep the system with an iso-energetic wave of spins. We tested this method both alternating GS and OR, and SOR and OR. The result was more satisfying than pure Gauss-Seidel, but the convergence time resulted being less convenient with respect to Successive Over Relaxation.

### 3.3 Computing Observables

A main advantage of simulations is that we can know the exactly properties of each single particle of the system, while in real experiments only some (global) observables can be found by analysing the reaction to determinate stimuli. The possibility of computing observables directly represents a great advantage and it pays off the problem of small sizes.

The observables that we computed in our simulations were:

- Energy
- Overlaps
- Correlation Lengths and Functions
- Magnetic Susceptibility
- Energy-Overlap Correlation
3.3 Computing Observables

- Binder Cumulants
- Correlation Times and Functions

Let’s analyse them one by one.

### 3.3.1 Energy

The energy is the most intuitive and basic observable to look for in a simulation, and it represents one of the great challenges of SG systems, since due to the frustration it is very hard to find low energy configurations, and in fact this is what we’re going for.

It can be found very trivially, as it is defined by the model’s Hamiltonian:

\[
H = \frac{1}{2} \sum_{\vec{x}} \vec{s}_{\vec{x}} \cdot \vec{h}_{\vec{x}}
\]  

(3.23)

It simply requires a sweep over all the spins summing the energy per site:

\[
e_{\vec{x}} = \frac{1}{2} \vec{s}_{\vec{x}} \cdot \vec{h}_{\vec{x}}
\]  

(3.24)

### 3.3.2 Overlaps

There are two types of overlap to compute, the CG overlap, and the SG. We used the overlap definitions anticipated in chapter 1. The CG overlap was the scalar quantity

\[
E_{CG} = \frac{1}{3} \sum_{\mu=1}^{3} E^{\mu} = \frac{1}{3N} \sum_{\mu=1}^{3} \sum_{\vec{x}} e^{\mu}(\vec{x}),
\]  

(3.25)

while for the SG overlap we used a slightly more complicated object, also introduced in chapter 1, that guarantees rotational invariance. As a matter of fact it is not an overlap, but a square overlap:

\[
q^2 = \frac{1}{N^2} tr(Q Q^\dagger).
\]  

(3.26)
3.3 Computing Observables

**Properties of $q^2$** Let’s see the typical values of $q^2$. We remind that the tensors $Q_{\alpha\beta}$ are defined as

$$Q_{\alpha\beta} = \sum_{\vec{x}} \tau_{\alpha\beta}(\vec{x}) = \sum_{\vec{x}} s_{\vec{x},\alpha}^{(a)} s_{\vec{x},\beta}^{(b)}, \quad (3.27)$$

so, by substituting this definition and rearranging the sums we get, with trivial calculation,

$$tr(QQ^\dagger) = \sum_{\vec{x}} \sum_{\vec{y}} (s_{\vec{x}}^{(a)} \cdot s_{\vec{y}}^{(a)})(s_{\vec{x}}^{(b)} \cdot s_{\vec{y}}^{(b)}), \quad (3.28)$$

that may be easily bounded thanks to the Cauchy-Schwarz inequality, that guarantees us that $s_{\vec{x}} s_{\vec{y}} \leq \sqrt{s_{\vec{x}}^2 s_{\vec{y}}^2} = 1$, so

$$tr(QQ^\dagger) \leq N^2, \quad (3.29)$$

and the square overlap, with the normalization that we chose, gets the bound

$$q^2 = \leq 1 \quad (3.30)$$

**SG Self-overlap** We want to show the typical value of the SG self-overlap for a random configuration. To evaluate it we impose $(a) = (b)$ in eq. 3.28, and obtain

$$tr(Q_{\text{self}} Q_{\text{self}}^\dagger) = \sum_{\vec{x}} \sum_{\vec{y}} (s_{\vec{x}} \cdot s_{\vec{y}})^2 \quad (3.31)$$

$$= \sum_{\vec{x}} s_{\vec{x}}^4 + \sum_{\vec{x} \neq \vec{y}} (s_{\vec{x}} \cdot s_{\vec{y}})^2. \quad (3.32)$$

To estimate the average of the product $(s_{\vec{x}} \cdot s_{\vec{y}})^2$ we can put ourselves in a reference frame $(\hat{x}, \hat{y}, \hat{z})$ with $s_{\vec{x}}//\hat{z}$. The value of the scalar product is then given by the third component of $s_{\vec{y}}, s_{\vec{y},z}$. This way

$$(s_{\vec{x}} \cdot s_{\vec{y}})^2 = s_{\vec{y},z}^2 \quad (3.33)$$

is a uniformly distributed random variable whose mean value is $1/3$, since our system is completely isotropic.
3.3 Computing Observables

We can now determine the average self-overlap

\[<q_{\text{self}}^2> = \frac{1}{N^2}(N + \sum_{\vec{x} \neq \vec{y}} <(\vec{s}_{\vec{x}} \cdot \vec{s}_{\vec{y}})^2>) \]  (3.34)

\[= \frac{1}{N} + \frac{1}{3} - \frac{1}{3N} \xrightarrow{N \to \infty} \frac{1}{3} \]  (3.35)

3.3.3 Correlation Lengths and Functions

An extremely important quantity for our simulations was the correlation length, because not only it gives information regarding the properties of a state (e.g. it is zero at infinite temperature while it diverges at the phase transition), but since it estimates until which distance two spins can be considered correlated, it indicates us if we can consider the system in thermodynamic limit or not. For the latter check we can also see if the correlation functions go to zero within half lattice size\(^1\).

The correlation function relative to a generic observable \(\phi\) is defined as:

\[G(\vec{r}) = \sum_{\vec{x}} \phi_{\vec{x}} \phi_{\vec{x}+\vec{r}} \]  (3.36)

As it is shown in appendix A.1, together with a computationally smart way to write it, a way to compute the correlation length \(\xi\) involves the correlation function’s Fourier transform \(\hat{G}(\vec{k})\):

\[\xi_F^2 = \frac{1}{4 \sin^2(\frac{\pi}{L})} \left[ \frac{\hat{G}(\vec{0})}{\hat{G}(\vec{k}_{\text{min}})} - 1 \right] = \frac{1}{4 \sin^2(\frac{\pi}{L})} \left[ \frac{\chi}{F} - 1 \right] \]  (3.37)

where we stressed that the magnetic susceptibility \(\chi\) is the \(\vec{k} = 0\) Fourier transform of the correlation function:

\[\chi = \hat{G}(\vec{0}) \]  (3.38)

\[F = \hat{G}(\vec{k}_{\text{min}}) \]  (3.39)

and due to the periodic boundary conditions \(\vec{k}_{\text{min}} = (\frac{2\pi}{L}, 0, 0)\).

\(^1\)Since the boundary conditions are periodic the maximum distance between two points is \(L/2\), not \(L\).
3.3 Computing Observables

**Integral Estimators** If we define an integral estimator \( I_k \) as:

\[
I_k = \int_0^L d\vec{r} r^k G(\vec{r})
\]  

(3.40)

we can readily see that (appendix A.2) in the thermodynamic limit we can define two more ways to find the correlation length in a \( D \)-dimensional system:

\[
\xi^{(02)} = \sqrt{\frac{I_{D+1}}{I_{D-1}}} \simeq \xi
\]  

(3.41)

\[
\xi_{k,k+1} = \frac{I_{k+1}}{I_k} \propto \xi
\]  

(3.42)

All these definitions suffer from systematic errors because they are derived from the long distance decay of \( G \):

\[
G(\vec{r}) \sim \frac{1}{r^a} \exp\left(-\frac{r}{\xi}\right)
\]  

(3.43)

that is only an asymptotic formula for large values of \( r \). The systematic errors in these definitions can be reduced by considering a large value of \( k \) (since the \( r^k \) factor would suppress the deviations at short distances). However, there is also the issue of statistical errors to consider. As it can be seen in figure 3.2, borrowed from reference [33], a large value of \( k \) pushes the maximum of \( r^k G(\vec{r}) \) towards a zone where the statistical error becomes too big. Therefore it is necessary to find a compromise \( k \).

**Plane to plane correlation functions** We can define three types of plane to plane correlation functions, one for each direction. To avoid making notation heavy we write it explicitly for a given direction:

\[
C^{x}(r) = \frac{1}{N} \sum_{x=0}^{L-1} P(x)P(x + r)
\]  

(3.44)

\[
P(x) = \sum_{y,z} \phi_{xyz}
\]  

(3.45)
3.3 Computing Observables

Figure 3.2: Comparison between $\vec{r}_2 G(r)$ and $\vec{r}_4 G(r)$ from simulations of an $L = 80$ Ising spin lattices at three different temperatures. In the first case the significant data is clearly out of the noise-dominated region, while in the second the maximum is pushed rightwards giving plenty of noise to the calculation of $I_4$. Figure borrowed from [33].

where $\phi_{xyz}$ is any observable with which a correlation function has sense. Since the space is perfectly isotropic we can reduce the error by calculating

$$C(r) = \frac{1}{3}(C^x(r) + C^y(r) + C^z(r)). \quad (3.46)$$

Plane to plane correlation functions represent a fine way to have more precise estimates of the correlation length $\xi$, since beyond being a natural choice for square lattices, in which we can easily average it on the euclidean directions, and they decay far more slowly than the point to point correlation functions.

In fact if we define the plane to plane integral estimators:

$$J_k = \int_0^{L/2} drr^k C(r) \quad (3.47)$$

where we called $C(r)$ the mean of the plane to plane correlation functions in all the directions, it is immediate to see that since the space is homogeneous and isotropic

$$J_k \sim 4\pi I_{k+2} \quad (3.48)$$

$$\chi = 2J_0 - C(0) - C(L/2) \quad (3.49)$$
3.3 Computing Observables

so for the same integral estimator we need to use lower powers of \( r \) if we’re using the \( J_k \)’s. This means that \( r^k C(r) \) will have sense in a larger span of distances, so the amount of data without signal will drastically decrease.

**Truncating data** Another thing that can be done to reduce consistently the statistical error, in favor of a small bias, is to do as proposed by Martín-Mayor, Marinari et al. in [33], i.e. to use a self-consistent integration cut-off as it has always been done with the study of correlated time series [34].

What we do is to decide *a posteriori* a critical distance \( r_c \) beyond which collecting data has no sense because the measure is dominated by the statistical error. This distance was chosen to be the first one at which the error became greater than one third of the correlation function:

\[
I_k = \sum_{0}^{r_c} r^k G(\vec{r}) \rightarrow \tilde{I}_k = \sum_{0}^{r_c} r^k G(\vec{r})
\]

\[
r_c \equiv \{ \text{first } r : C(r+1) < 3\sigma(r+1) \}\]

A truncation of this type in our work has reduced the error of several orders of magnitude, giving a quite small bias [33] (one or two percents), that could be seen from the change of the value of the magnetic susceptibility \( \chi \).

### 3.3.4 Magnetic Susceptibility

In theoretical physics, the magnetic susceptibility is defined as the zero-moment Fourier transform of the correlation function

\[
\chi = \hat{C}(k = 0) = \sum_{r} C(r) \tag{3.52}
\]

The magnetic susceptibility that we calculate in our simulations is what in the experimental jargon is called the non-linear susceptibility. If
we put a spin glass under a uniform magnetic field $h$, the magnetization $m$ can be written as a series of $h$

$$m(h) = \chi_L h + \chi_{NL} h^3 + ...$$  \hspace{1cm} (3.53)

The term $\chi_L$ is the linear magnetic susceptibility $\frac{\partial m}{\partial h}$ that does not diverge at $T_{SG}$. What diverges is the non-linear magnetic susceptibility $\chi_{NL}$ and that’s what makes it a more interesting observable.

### 3.3.5 Binder’s Cumulants

Binder’s cumulants are ratios of cumulants of the order parameter that give us a good comprehension of the finite-size effects. They are often used to individuate phase transitions because at $T_c$ they are size-invariant. In our case we used them to have a check of how close to the thermodynamic limit we were throughout our work.

Due to the presence of two order parameter, we can define two Binder Cumulants. The chiral-glass Binder Cumulant is

$$B^CG_L = \frac{<E^2_{CG}>^2}{<E^4_{CG}>}$$ \hspace{1cm} (3.54)

while the spin glass cumulant is

$$B^SG_L = \frac{<tr(QQ^\dagger)>^2}{<tr(QQ^\dagger)^2>} = \frac{<q^2>^2}{<q^4>}. \hspace{1cm} (3.55)$$

It is possible to show that the asymptotic values of these cumulants for systems at infinite temperature in the thermodynamical limit are

- $B^SG_\infty = 11/9$
- $B^CG_\infty = 3$

The interested reader can refer to appendix A.3 for the calculation of $B^SG_\infty$. 

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45
3.3 Computing Observables

3.3.6 Self-correlation Times and Functions

The self-correlation time \( \tau \) represents the amount of time in which a system loses all the memory of its initial configuration. It is calculated from the time-correlation functions \( C(t) \), that give us an idea of how much the system at time \( t \) is correlated with itself at time 0. The time-correlation functions measure how much a particular observable changes during time, so it is evident that it is possible to define a whole set of self-correlation times and functions, and that the most important of the times is the greatest, since it is the characteristic time after which all the observables have no correlation with their initial values.

In our work these quantities have been used both to know how much we needed to wait for the thermalization of the system, and to measure the scaling of the \( \tau \) in the paramagnetic phase.

We used three self-correlation functions:

- **Scalar Correlation function**
  \[
  C_{\text{Scalar}}(t) = \langle \vec{s}_x(0) \cdot \vec{s}_x(t) \rangle = \frac{1}{N} \sum_x \vec{s}_x(0) \cdot \vec{s}_x(t)
  \] (3.56)

- **Tensorial Correlation function**
  \[
  C_{\text{Tensorial}}(t) = \frac{1}{N^2} \text{tr}(Q_{0,t} Q_{0,t}^\dagger)
  \] (3.57)

  where \( Q_{0,t} \) is the overlap calculated between configurations of the same replica at times 0 and \( t \).

- **CG Correlation function**
  \[
  C_{\text{Scalar}}(t) = \frac{1}{3N} \sum_{\mu} \sum_x \kappa_{x\mu}(0) \kappa_{x\mu}(t)
  \] (3.58)

And calculated the correlation times:
3.3 Computing Observables

\[ \tau_{Scalar} = \int_0^\infty C_{Scalar}(t)dt \quad (3.59) \]

\[ \tau_{CG} = \int_0^\infty C_{CG}(t)dt \quad (3.60) \]

Just as in the case of the spatial correlation times, we truncated the data when \( C(t) \) was smaller than 3 times its error bar. We did not calculate \( \tau_{Tensorial} \) because the square overlap does not go to zero for uncorrelated samples, but to \( 1/N \), so the data would be biased and not \( L \)-independent, especially when truncating data.

**Aging** It looks obvious that if one measures the self-correlation function starting not from an initial time \( 0 \), but from a time \( t_0 \), nothing should change. Nevertheless, in spin glasses this time-translational invariance is not so obvious. In fact what happens is that while this symmetry is verified at high temperatures, below \( T_{SG} \) the value of the self-correlation function depends on the amount of time we wait before starting our measures. This phenomenon, called aging, obliges us to redefine the correlation functions as \( C(t_w, t) \), where \( t_w \) is the time we wait before starting to collect data.

We measured self-correlation functions from many \( t_w \), to verify that we did not have aging. Indeed the data was independent from \( t_w \) as we can see from the collapse of the data in figures 3.3 where we plotted \( C(t; t_w) \) for many \( t_w \). It is because \( C(t_w, t) = C(t - t_w) \) that in this report we refer to it as \( C(t) \).
3.3 Computing Observables

Figure 3.3: The scalar and chiral-glass time-correlation function $C_{\text{scalar}}(t_w, t)$ and $C_{\text{CG}}(t_w, t)$ in an $L = 64$ lattice at $T = 0.3$. As we can see there is no aging in the paramagnetic phase, since data for different $t_w$’s collapse perfectly.
Chapter 4

Results

Contents

4.1 Using Gauss-Seidel .................................... 50
4.2 Using Successive Over Relaxation ................. 51
  4.2.1 Parameter choice .................................. 51
4.3 A comparison with genetic algorithms ............. 56
  4.3.1 Inherent structures at infinite temperature .. 58
4.4 Inherent structures at finite temperature ......... 62
4.5 Dynamics .............................................. 71
4.6 Extrapolations ......................................... 72
  4.6.1 An Estimate of $T_{SG}$ ............................ 73
  4.6.2 An Estimate of the Exponent $\nu$ ............... 74
  4.6.3 Self-correlation times .............................. 75
  4.6.4 A Lower Bound for the Dynamic Exponent $z$ 77
4.7 Minima or Saddles? ................................... 78

49
4.1 Using Gauss-Seidel

Although we showed in chapter 3.2.1 that the Gauss-Seidel algorithm is not effective for our problem, a complete analysis should start from the simplest cases to be able to make comparisons which make us understand if different routines really do improve the dynamics or not.

In this perspective we investigated the convergence of the Gauss-Seidel algorithm in quite large lattices, and as it is shown in figure 4.1 the convergence rate is with a power law, which is far too slow for our needs.

![Figure 4.1: Evolution of the energy density during a quench in a L = 100 lattice. The plot shows 20 quenches from random configurations (red lines), i.e. from T = ∞ configurations, which were stopped when the energy gain after a sweep was less than 10^{-10}. The green line is the mean with error bars, which was performed only in the points where all the data was present, since the duration of the runs was not even. The dashed blue line is a fit in the linear regime t^{-1} < 0.0005, which yields a good χ^2 test.]

At the beginning of our work our convergence criterion has been checking the energy gain in the last sweep, but we readily realized that
4.2 Using Successive Over Relaxation

A disadvantage of Successive Over Relaxation respect to classical quenches is that it depends from the parameter $\lambda$, therefore it’s performance is not univocally determined, and it is necessary to do some preliminary studies to choose the optimal one. We demand a good algorithm the capability of converging to low energies in an affordable amount of time.

Since at the beginning of a simulation a greedy routine such as Gauss-Seidel descends in energy much faster than an ungreedy one such as Successive Over Relaxation, one could argue that to increase the convergence speed it could be convenient to start with the Successive Over Relaxation only after having performed $t^*$ quench steps. This increases the number of non-physical parameters of our routine to two: $\lambda$ and $t^*$.

4.2.1 Parameter choice

To decide how to choose $t^*$ and $\lambda$ we ran simulations on a large lattice seeking for the best performances.

We start by stressing the properties of $t^*$. Figure 4.2 shows how the convergence time does not depend from this variable, but completely on $\lambda$. We can also see (figure 4.3) that, as intuition suggests, more Gauss-Seidel steps we perform before starting with $\lambda \neq 0$ less we will be able to descend in energy: it is impossible for the Successive Over Relaxation to recover the “unwise” greedy quench steps.

So if making a number of quench steps before does not decrease the convergence time, and it entails an increase in the final energy, there is absolutely no point in keeping $t^* \neq 0$. 

a more solid one was to see the maximum pion in the lattice, since in an inherent structure the pion field is zero.
4.2 Using Successive Over Relaxation

Figure 4.2: The evolution of the energy for 3 different λ’s, and t*’s in a L = 100 lattice. Each λ has an associated color. The runs stopped when the maximum spin component perpendicular to the local field was smaller than 10^{-10}. It is possible to see the point t* = 100 where the Gauss-Seidel routine stops in favor of the SOR. Depending on λ, after this point, the evolution at this point is faster or slower than the quench. The most ungreedy λ on the long run reaches a lower energy, but at the cost of a much longer convergence time. What appears clear is that the convergence time depends exclusively on λ, and also that the greater the quantity of quench steps before turning to SOR, the higher are the energies achieved. Hence, there is no point on having t* > 0.

The situation is more delicate when we proceed to select an optimal λ. In this case the choice is not univocal, since it depends on which criteria we consider dominant.

Looking at the raw data one could be attracted by the possibility of a pretty scaling law for λ such as, for example,

\[ e^{(IS)}(\lambda) = e^{(IS)} + A\lambda^{-\lambda}, \]  

from where it would be easy to extrapolate the energy of the inherent
4.2 Using Successive Over Relaxation

Figure 4.3: The final energies one obtains with different \( t^\star \)'s in a \( L = 100 \) lattice. Each color indicates a different \( \lambda \). Definitely the energy of the inherent structure is higher the greater \( t^\star \) is, no matter \( \lambda \).

structure. Unfortunately it is not so direct to state the existence of a similar scaling law (fig 4.4), and also if it exists, it is not as simple as the one described in eq. 4.1. Since the objective of this work is not to find all the characteristics of our minimizing routine we did not linger in finding a scaling law.

The other criterion to keep in mind when choosing our \( \lambda \) is the convergence time, which is absolutely not negligible. In fact although for small \( \lambda \) the Successive Over Relaxation makes the convergence faster, there is a \( \lambda \) around 100 (see fig. 4.5) in which the algorithm becomes too ungreedy, and the convergence times start growing. Indeed it is true that any \( \lambda < 10^5 \) represents an objective gain respect to the quench, since it yields lower energies in less time.
4.2 Using Successive Over Relaxation

Figure 4.4: The energy of the inherent structures in a $L = 100$ lattice (except the point at $\lambda = 300$ that comes from an $L = 64$ lattice). We can ideally divide the plot in two sectors. In the left sector we have large $\lambda$'s: the dynamics takes place mainly at high energies and the system takes its time to choose the valley in which it wants to lay down. In the right sector, for smaller $\lambda$, the system dives quickly in a minimum, losing the choice of a lower valley. Mind that the dependency of $e^{(IS)}$ on the system size $L$ is studied in Fig. 4.7, below. With our statistical accuracy, the results seem $L$-independent from $L = 32$.

Nevertheless we ought to choose only one single $\lambda$ between the infinity available. Since we did not believe that our algorithm could cross the phase transition for a specifically big $\lambda^1$, and start finding sub-exponentially numerous low energy configurations, and since the definition of inherent structure is intrinsically related to the minimizing routine

---

$^1$If the algorithm were to cross the phase transition, the correlation lengths would depend strictly on the system size for any $L$, since at the phase transition $\xi$ becomes infinite. On the contrary, we see that the correlation functions collapse perfectly once the system is large enough (figures 4.8 and 4.13), giving an $L$-independent correlation length $\xi$. 

54
4.2 Using Successive Over Relaxation

Figure 4.5: Convergence times for different $\lambda$. Here, as in figure 4.4, it is possible to identify the two regimes. For small $\lambda$ the system drops quickly into a minimum, but it takes it a long time to converge once in the valley. For large $\lambda$ it stays plenty of time at high energies. We see that from the pure Gauss-Seidel the convergence time decreases linearly with $\lambda$, because it becomes more and more effective once in a valley. On the other side, if we increase $\lambda$ too much the algorithm becomes too ungreedy, loses too much time at high energies, and the convergence time starts growing with $\lambda$. All the points come from $L = 100$ systems, except $\lambda = 300$ that is extracted from $L = 64$.

used, we had no problem choosing the $\lambda$ which made our simulations the fastest, for the rest of the investigation, except in the next section, where we wanted to remark the differences (other than the energy) between configurations achieved with different $\lambda$’s or where we explicitly needed to achieve a very low energy. Another good reason for having chosen $\lambda = 100$ is that a greater one would have yielded inherent structures with too long correlation lengths, preventing us from being able to calcu-
late inherent structures at the finite temperature we were interested in. For those reasons we made our investigation with $\lambda = 100$, comparing it with $\lambda = 300$ to see if there is some physical difference between the regime in which the system passes most of the time at low energies and the one where it delays at high energies.

## 4.3 A comparison with genetic algorithms

A nice check for our new algorithm is comparison with different methods for finding low energy configurations. The only work of this type that we found in literature is [32], which uses a hybrid genetic algorithm to find ground states in EA Heisenberg spin glasses with $\pm J$ couplings. In spite of those two differences, we thought that it might be interesting to make a comparison with their results, so we made a little parenthesis in our work and studied the $\pm J$ model, since the maximum lattice size analysed by them has been $L = 13$ and this allowed us to not spend too much CPU time in this intent.

We made a series of simulations with growing $\lambda$ to see how close we could get to what they claimed to be the ground state energy (we will call it $e_{GS}^{(GA)}$). As the reader can see in figure 4.6 although we never reached $e_{GS}^{(GA)}$, the gap between our lowest energy and theirs is of the order of a standard deviation.

We also tried to reach lower temperatures by thermalizing the system at low temperatures and starting SOR from these configurations. Although they were slightly lower, they still were not in the error bar of $e_{GS}^{(GA)}$:

1. $e_{\pm J}(T = 0.14, \lambda = 10^5; L = 13) = -2.0394 \pm 0.0002$
2. $e_{\pm J}(T = 0.12, \lambda = 10^5; L = 13) = -2.0396 \pm 0.0001$
3. $e_{GS}^{(GA)} = -2.0403 \pm 0.0003$
4.3 A comparison with genetic algorithms

Figure 4.6: Inherent structures in the ±J Heisenberg model for $L = 13$. The energy density is normalized in conformity with ref. 4.6, i.e. without dividing by the number of dimensions. The blue points represent the average energies of the inherent structures we found for each $\lambda$. The continuous black line represents $e^{(GA)}_{GS}$ obtained in ref. 4.6 with a hybrid genetic algorithm, and the dotted lines its uncertainty. The difference between the energies achieved by their protocol and ours is fairly small, and they can’t cope with system sizes greater than $L = 13$, where finite-size effects are dramatic, so to our scope their algorithm would not be as useful as SOR, that converges quickly and permits us to study very large lattice, keeping our measures in the thermodynamic limit.

It is to be noted that the correlation lengths of the inherent structures found after having thermalized at $T < \infty$ were appreciably different from those from $T = \infty$. This means that the situation is not so simple as it may appear, and a state cannot be characterized by the only energy.

We know that our relaxation routine is definitely not going under the phase transition, since the correlation lengths stay constant when we increase the size of the lattice.
4.3 A comparison with genetic algorithms

If $e_{GS}^{(GA)}$ is really the ground state energy this means that the energy gap between the topological transition and the ground states is very small and the topological transition does not have the importance one would like to give it. Nevertheless this would demonstrate that the energy landscape is quite trivial until very close to the ground state, and a simple relaxation algorithm as SOR is enough to almost reach it.

It could also be, on the contrary, that $e_{GS}^{(GA)}$ does not indicate the ground state energy, but it is only a different estimate of the energy at the topological transition. In this scenario the energy landscape would be quite non-trivial, proving that neither a hybrid genetic algorithm can easily pass the topological transition.

Unfortunately in [32] the only physical magnitude reported is the energy, so this does not allow us to get to any conclusion. We can only say that SOR has revealed quite satisfying, since it yielded, with a competitive CPU effort, energies at two standard deviations from what are claimed to be ground states.

4.3.1 Inherent structures at infinite temperature

The first physically relevant survey to do is the investigation of the inherent structures of the typical states of infinite temperature, doing SOR from random configurations, since at $T = \infty$ all the configurations are equally probable. We stress immediately that, no matter the system size, for different $\lambda$’s not only the energy of the states is distinct (figure 4.7), but also the correlation functions, consequently the correlation lengths and the magnetic susceptibilities, are different. This follows physical intuition, since a lower achieved energy corresponds to greater ordering. It is then clear how the concept of inherent structure is strictly binded to the routine we use to descend in energy.

Table 4.1 shows the typical values of the correlation lengths and magnetic susceptibilities one could extract from correlation functions such as
4.3 A comparison with genetic algorithms

Figure 4.7: The energy of the inherent structures for different system sizes. Already from $L = 16$ this magnitude seems to become quite stable. Nevertheless we're far from the thermodynamic limit, since we'll see that other quantities need bigger lattices.

the ones in figure 4.8, for four different $\lambda$'s. As we just argued, it is not surprising that the correlation lengths increase monotonically with $\lambda$.

Regarding the size of the system, from figure 4.7 we see that already from $L = 16$ the energy seems to be stable, so for $T = \infty$ we could consider ourselves in the thermodynamic limit from $L = 32$. Nevertheless we need to be careful, since energy is a quickly converging quantity. In fact from figure 4.8 we see that for small $L$’s the correlation functions do not go to zero.

This fact is confirmed by the binder cumulants, which only for larger sizes are compatible with their asymptotic values, as it is shown in table 4.2, where we compare inherent structures at infinite temperature for
4.3 A comparison with genetic algorithms

Figure 4.8: Normalized SG plane to plane correlation functions of the Inherent Structures for many $\lambda$'s and $L$'s at $T = \infty$. The data was truncated when it became smaller than three times its error, since at that point it was dominated by the statistic noise. It appears clear from here that the configurations obtained depend strictly $\lambda$ since we can appreciate three different trends, one for each $\lambda$. Moreover, this plot shows the strong finite-size effects for smaller lattices, since many correlation functions do not converge to zero. Notice how greater $\lambda$’s require larger lattices.

$\lambda = 100$ for different system sizes.
4.3 A comparison with genetic algorithms

Table 4.1: ξ and χ from $T = \infty$, for different $\lambda$’s.

| $\lambda$ | $\xi_{SG}$ | $\xi_{CG}$ | $\chi_{SG}$ | $\chi_{CG}$ |
|-----------|------------|------------|-------------|-------------|
| 10        | 2.79 ± 0.05| 0.93 ± 0.03| 178 ± 3     | 0.0992 ± 0.0011 |
| 100       | 3.06 ± 0.04| 1.06 ± 0.02| 205.3 ± 1.4 | 0.1106 ± 0.0010 |
| 1000      | 4.49 ± 0.07| 1.57 ± 0.05| 443 ± 6     | 0.213 ± 0.003  |
| 10000     | 5.90 ± 0.13| 2.48 ± 0.10| 927 ± 22    | 0.432 ± 0.021  |

Table 4.1: Growth of the correlation lengths and the magnetic susceptibilities of the Inherent Structures from $T = \infty$ for increasing $\lambda$. Higher $\lambda$’s yield lower energies which correspond to more correlated configurations, as the data shows. All of the data comes from $L = 128$ lattices, except the one for $\lambda = 10000$ that has $L = 64$. Of course it suffers fair finite-size effects, since we see from figure 4.8 that $L = 64$ isn’t enough also for $\lambda = 1000$.

Table 4.2: Binder Cumulants for $\lambda = 100$ and $T = \infty$.

| $L$ | $B_{CG}^L$ | $B_{SG}^L$ |
|-----|------------|------------|
| 8   | 3.58 ± 0.07| 1.071 ± 0.002 |
| 16  | 3.34 ± 0.09| 1.179 ± 0.004 |
| 32  | 2.97 ± 0.06| 1.215 ± 0.004 |
| 64  | 3.05 ± 0.06| 1.232 ± 0.004 |
| 128 | 2.80 ± 0.22| 1.213 ± 0.015 |
| $\infty$ | 3 | 1.2 |

Table 4.2: The binder cumulants reflect the conclusions on the finite-size effects that we took when looking at the scaling of the energy with $L$. They tell us that from $L = 32$ we are already in the thermodynamic limit, since they are compatible with their infinite limit. The uncertainty for $L = 128$ is greater because we took less measures than with the other sizes, since there was no point in spending too much CPU time in data we did not really need for our investigation.
4.4 Inherent structures at finite temperature

To find inherent structures at finite temperature it was necessary to thermalize the system and only then go down in energy. Our ambition was to be always in the thermodynamic limit, so that thermalization could become a very time-expensive task for low temperatures. We chose temperatures from $T = 0.19$ and greater because a previous article based on dynamical studies [8, M.Picco and F.Ritort (2004)] affirmed that at that temperature a phase transition was taking place. Also, we wanted our investigation to be in the thermodynamic limit, so we could not descend too much in temperature because the closer to $T_{SG}$ we are, the longer the correlation lengths are.

To get to know the thermalization time of the system we have waited until the energy became stationary and the three time-correlation functions described in section 3.3.6 went to zero.

It turned out that although the thermalization time was not fast, it was not either prohibitive, so we have been able to thermalize 1000 samples for each chosen temperature. For $T > 0.23$ a $L = 64$ lattice was enough, while for lower temperatures the correlations grew too much and it was imperative to use $L = 128$.

Trend of the Inherent Structure Energy Figure 4.9 shows how $e^{(IS)}$ varies with the inverse temperature $\beta = 1/T$. It is almost constant from $T = \infty$ to $T = 0.5$, as the error bars of those two points overlap, and it starts descending appreciably around $T = 0.3$ ($\beta = 3.3$). This is the same qualitative scenario we encounter in structural glasses [35], where $e^{(IS)}$ is temperature independent for high $T$’s, and it starts decreasing significantly only from some certain temperature.
4.4 Inherent structures at finite temperature

Figure 4.9: Energies of the inherent structures in function of the inverse temperature $\beta = 1/T$ for two different $\lambda$’s. We plotted in function of $\beta$ to be able to show the infinite-temperature limit. The trend is qualitatively the same we encounter in supercooled liquids and structural glasses, where the energy of the inherent structure is almost independent from $T$ at high temperatures, and it descends steeply at lower temperatures. Keep in mind that being in function of $\beta$ the energy descent at low temperature looks less steep than what it would with $T$ on the $x$-axis. Nevertheless this lets us appreciate the extremely small variation between $T = \infty$ ($\beta = 0$) and $T = 0.50$ ($\beta = 2$), since their error bars cross, in contrast with the appreciable descent for lower temperatures (higher $\beta$). Notice how the difference between the two protocols decreases with decreasing temperature, so the choice of $\lambda$ becomes less relevant the lower $T$ is. The three points at lowest temperature (highest $\beta$) have less uncertainty than the others because the low-temperature data requested using $L = 128$ while for the other we used $L = 64$.

Anharmonic Energy Term  From the equipartition theorem we can divide the average energy at a given temperature in many contributions. There is a term given from the topology of the energy landscape, a harmonic term, proportional to $T$, that represents the thermal agitation...
4.4 Inherent structures at finite temperature

Figure 4.10: The anharmonic contribution to the energy. The red points refer to the left y-axis, and give the absolute value of the anharmonic term of the energy. The other lines refer to the right y-axis. The blue points indicate the relative weight of the anharmonic contribution. The value 1 indicates that it has no weight, and that is why there is a horizontal line indicating it. From the blue points we understand that the anharmonic term is no larger than the 12% at $T = 0.5$, which is way over the critical temperature. At lower temperatures, though always in the deep paramagnetic phase, the anharmonic contribution is less than half. This gives space to an interpretation of the energy of a state as principally an inherent structure plus harmonic thermal fluctuations.

around a minimum, and an anharmonic term that permits the movement through different valleys, which is more relevant the higher $T$ is. The relation is

$$e(T) \simeq e^{(IS)}(T) + \frac{T}{3} + e^{(anh)}(T)$$

(4.2)

where $e^{(anh)}(T)$ is the anharmonic contribution to the energy and the factors $1/3$ derive from the energy normalization we chose. We can compute
the anharmonic contribution to the total energy by reversing equation 4.2, and compute

$$\epsilon^{(anh)}(T) = \epsilon(T) - \epsilon^{(IS)}(T) - \frac{T}{3}$$  \hspace{1cm} (4.3)

that alone does not mean a lot to us, so we can understand its relative weight by looking at the quantity

$$\frac{\epsilon(T) - \epsilon^{(IS)}(T)}{T/3} = 1 + \frac{\epsilon^{(anh)}(T)}{T/3}.$$  \hspace{1cm} (4.4)

Figure 4.10 shows the absolute anharmonic term of the energy on the $y_1$-axis, and it shows its relative weight on the $y_2$-axis, where $y_2 = 1$ marks the absence of an anharmonic contribution. We see that its weight does not exceed 12% even when the temperature is quite high, since $T = 0.5 \approx 5T_{SG}$; hence it represents a non-primary effect. This fact lets us figure out that the energy of a configuration is almost completely determined by the shape of the energy landscape plus harmonic thermal fluctuations over it. The small, but yet absolutely not negligible, anharmonic effects are those that make us find different energies when we change the algorithm of energy descent, since they’re the cause of its movement from one valley to the other.

**Correlation lengths**  We also want to show (figures 4.11 and 4.12) how correlation lengths vary with temperature. From these trends we made extrapolations that we will show in a further section. By now we can appreciate the apparent divergence that both present around $T \sim 0.15$.

A more interesting fact that the correlation lengths can remark to us is that more we go down in temperature, more important the role of the energy landscape becomes. In fact we can see in figure 4.12 that as we descend in energy the correlation length of a thermalized configuration becomes more and more dominated by the one of its inherent structure. We can guess that the divergence of the correlation length at the criti-
4.4 Inherent structures at finite temperature

Figure 4.11: The longitudinal and transversal Chiral Glass correlation lengths of the Inherent Structures in function of the inverse temperature $\beta = 1/T$. The trend is the same for both, specially when going towards lower temperatures and the derivative starts growing consistently. According to the most recent works $\beta_{SG} = 1/T_{SG} \simeq 7.75$.

The finite-size effects for the $L = 64$ samples, since it is quite clear that the correlation lengths do not go to zero.

In figure 4.13 we show the spin glass correlation function for the states thermalized at $T = 0.19$, and the same magnitude for their inherent structures. The correlation lengths are indeed very similar since the difference between them is indiscernible by eye. We can also appreciate the finite-size effects for the $L = 64$ samples, since it is quite clear that the correlation lengths do not go to zero.
Figure 4.12: The Spin Glass correlation length versus the inverse temperature $\beta = 1/T$. There are both the correlation lengths of the inherent structures reached with two different protocols, and of the thermal states. We see that although at infinite temperature ($\beta = 0$) they are consistently different, when $\beta$ grows they become more and more similar, up to the point that one could argue that the divergence is due exclusively to the shape of the energy landscape. We see also how, lowering the temperature, the correlation lengths of the inherent structures depend less and less from the $\lambda$ used.

**Variety of the Inherent Structures and CG self-overlaps** By comparing the energies obtained with SOR from $T = \infty$ with a very high $\lambda$, with the ones obtained having first thermalized at finite temperature, but with a lower $\lambda$, one could notice that it is possible to obtain the same energies in different ways. A naive thought could be that these are simply two different ways to achieve the same result. This assertion would be incorrect because the energy is not the only relevant observable, and as we already said in section 4.3, it does not characterize univocally...
4.4 Inherent structures at finite temperature

Figure 4.13: The correlation functions of the thermal state and its inherent structure at $T = 0.19$. The similarity between the correlation lengths is quite evident, as also the exponential trend. We see that at $T = 0.19$ the lattice size $L = 64$ is not enough since the correlation function does not go to zero (it is always far from being compatible with zero), while $L = 128$ is enough because the last ten distances are compatible with zero.

a state. As a matter of fact magnetic susceptibilities, correlation lengths (fig. 4.14) and CG self-overlaps (fig. 4.16) may be very different for inherent structures with the same energy, hence there is a whole variety of inherent structures for each energy.

The CG self-overlaps deserve a separate discussion. It is commonly known that in Ising spin glasses there is no visual difference between a minimum and a random configuration, so that visual inspection can not discern one from the other. On the contrary, we noticed that this is not true in Heisenberg Spin Glasses. In fact, as one can see in figure 4.15,
4.4 Inherent structures at finite temperature

Figure 4.14: The correlation lengths of the inherent structures, associated to their energy. The dashed lines represent inherent structures from $\lambda = 100, 300$ protocol, starting from states thermalized at different temperatures. The solid line instead describes inherent structures from infinite temperature, with different $\lambda$’s. If the energy were enough to characterize an Inherent Structure, each energy would have associated only one correlation length. On the contrary we see that same energies reached with different protocols have different $\xi$, so we can’t sample all the inherent structure population only performing SOR with different $\lambda$’s from one temperature, neither can we conforming ourselves to a single $\lambda$ from different temperatures. All the data comes from $L = 128$ lattices, except the points for $\lambda = 100, 300$ at $T = 0.25, 0.30, 0.50$, which can be recognized because of their lower correlation length, and the point for $\lambda = 10000$ and $T = \infty$, whose study was so slow that we had to limit ourselves to few samples, which were obtained from $L = 64$ lattices.

the CG self-overlaps are very different between thermal configurations and relative Inherent Structures. More specifically, we see that the CG self-overlaps are considerably smaller in the Inherent Structures, which have greater alignment properties.
Figure 4.15: The Chiral Glass self-overlaps of the inherent structures compared with the ones of the thermal states. The Inherent Structures have remarkable spin aligning properties, so, differently from Ising spin glasses, one could say whether a configuration can be a ground state or not, by simple visual inspection.

Although it might seem, from figure 4.15, that the Inherent Structures’ self-overlap is constant with temperature, one can correctly guess from figure 4.16 that those too descend appreciably with $T$. Consequently we can characterize an Inherent Structure also with its Chiral Glass self-overlap, and see, as it is well shown in that same figure, that this is another feature, other than the energy and the correlation length, that distinguishes different kinds of Inherent Structure.
4.5 Dynamics

Figure 4.16: The CG self-overlap for Inherent Structures obtained with two different protocols. It appears clear that Inherent Structures with the same energy have different self-overlaps, therefore the energy does not individuate univocally the Inherent Structures. The error bars are greater in six of the points because they represent data coming from $L = 64$ lattices, differently from the others that come from $L = 128$ (we had to use $L = 128$ for lower $T$’s due to finite-size effects). Notice that lower $T$’s yield lower energies, so the same plot as a function of $T$ would look similar. For this reason the reader can notice that the self-overlap of the inherent structure decreases with $T$, and is not constant as it may appear from figure 4.15.

4.5 Dynamics

The self-correlation times (figure 4.17) yield more or less the same result obtained in ref. [8]. They diverge at a temperature significantly greater than $T_{SG}$ (or $T_{CG}$), justifying the analogy with structural glasses. Also in this case we postpone the interpolations to the next section. In any case the divergence seems quite predictable also qualitatively, to a
$T > T_{SG} \simeq 0.12$. Notice how the Spin Glass signal is sensibly stronger than the Chiral Glass.

![Figure 4.17: The two relaxation times $\tau_{\text{Scalar}}$ and $\tau_{\text{CG}}$. The chiral sector carries information for much less time.](image)

4.6 Extrapolations

Since most of the critical exponents of the 3-dimensional Heisenberg model are not known yet, we made some extrapolations that were possible with the data we collected. We have been able to estimate the critical exponents $\nu$ and $z$, the exponent of the divergence predicted by Mode Coupling Theory (MCT), and we also wanted to give some estimates of $T_{SG}$ by making extrapolations from far from $T_{SG}$, to show how large lattices far from the critical temperature are effective as small lattices.
close to it, to make understand how it was possible to underestimate it so much to think it zero, and specially to remark that the nature of the overestimation of $T_c$ with the $\tau$'s is not a trivial misestimation effect due to being far from $T_{SG}$, since that effect would result in an underestimation.

### 4.6.1 An Estimate of $T_{SG}$

We tried to estimate, the spin glass critical temperature by means of the divergence of the Inherent Structures’ correlation length. The scaling behavior near $T_{SG}$ should be

$$\xi^{-1/\nu} \sim (T - T_{SG}), \quad (4.5)$$

so if we plot $\xi^{-1/\nu}$ versus $(T - T_{SG})$, and impose $\nu$ to be the best estimate found until now, given in [17], i.e. $\nu = 1.5$, we can find $T_{SG}$ from the linear fit’s intercept (figure 4.18). Except for the point at $T = 0.5$ the data fits quite well, but yet we find $T_{SG}^{(fit)} = 0.095(2)$, 20% lower than $T_{SG} = 0.129$ reported in [17]. This result was expected, since we are estimating $T_{SG}$ with tools that are valid only near it, while our data are very far from it. Intuition leads to think that the data would assume curvature if we got closer to $T_{SG}$, until reaching a stable slope, so probably the real value of $\nu$ greater than 1.5.

Of course it is fairly reasonable that our estimate for $T_{SG}$ didn’t reproduce the results obtained in works who focused on the phase transition. This because the scaling laws are valid only close to $T_{SG}$, so for this aim it is worth to get some finite-size effects and work at smaller temperatures, around $T_{SG}$.
4.6 Extrapolations

The point at highest temperature has been excluded from the fit since it didn’t respect the linear trend, and the scaling law is valid only close to $T_{SG}$. The intersect gives us $T_{SG} = 0.95(2)$, that underestimates it considerably. We see how using very large systems is not effective if we look for critical quantities. It is quite better to work closer to $T_{SG}$ in spite of the finite effects, since the scaling laws are valid only very close to $T_{SG}$.

4.6.2 An Estimate of the Exponent $\nu$

From the same data set of figure 4.18 we can try to deduce the exponent $\nu$, by fixing $T_{SG} = 0.129$ as reported in [17], and fitting on $\nu$. We plot $\xi^{-1}$ versus $T - T_{SG}$ and expect a trend of the form

$$\xi^{-1} \propto (T - T_{SG})^\nu,$$

and obtain $\nu = 1.146 \pm 0.009$ as it is shown in figure 4.19. If we compare it with the results in [17] we see that they get $\nu(L = 8) =$
4.6 Extrapolations

Figure 4.19: Imposing the $T_{SG}$ as the one evaluated in reference [17] ($T_{SG} = 0.129$), we calculate the critical exponent $\nu$ with a fit. The result $\nu = 1.146(9)$ is compatible with the one obtained in [17] with smaller lattices, but closer to $T_{SG}$. They obtain $\nu = 1.01$ in a $L = 8$, and $\nu = 1.35$ with $L = 12$.

$1.01 \pm 0.02$ and $\nu(L = 12) = 1.35 \pm 0.05$. Already $L = 12$ with measures taken close to $T_{SG}$ gives a better estimate than ours. It appears clear how investigating the critical properties far from $T_{SG}$ is equivalent to going very close to the phase transition with very small lattices, so are data is only good for an investigation of the pure paramagnetic phase.

4.6.3 Self-correlation times

This the most significant fit we present in this section, as it represents one of the objectives of the present work. What we want to see is if the analogy with structural glasses holds and we can individualize a Mode Coupling transition, which predicts a power law diverging trend of the
relaxation times in the disordered phase, which is stopped, at lower temperatures, when we get in the region where activation leads the dynamics. The trend predicted by MCT is

$$\tau \propto (T - T_c)^{-\zeta}. \quad (4.7)$$

Figure 4.20: Power law fit of the scaling of the scalar relaxation times $\tau_{Scalar}$ in the paramagnetic phase. We encounter the same scaling, for 3–4 orders of magnitude, in supercooled liquids. The scaling individuates the divergence of the $\tau_{Scalar}$'s at $T = 0.1489(8)$, which far in the paramagnetic phase, just as predicted by Mode Couping Theory for supercooled liquids.

In figure 4.20 we can see how this prediction fits perfectly also for the EA Heisenberg model. We get a $T_c > T_{SG}$ that overestimates the phase transition, just as MCT requests, and a perfect power law with exponent $B = 3.33(2)$ which is of the same order of the those found by Kob in [36] ($B = 2.5, 2.6$). We find $T_c = 0.1489(8)$, that is lower than the one found in [8] ($T'_c = 0.19(2)$), but only two standard deviations away. We
stress that this $T_c$ shows itself as completely different from $T_{SG}$. In fact
if it were different from $T_{SG}$ just for the fact that we’re very far from
it, our result would at least be consistent with the one of the previous
paragraph, underestimating $T_{SG}$, while we find $T_c >> T_{SG} >> T_{SG}^{(fit)}$.

This result gives strong support to the possibility of a strong analogy
between short-range interaction HSG and structural glasses.

4.6.4 A Lower Bound for the Dynamic Exponent $z$

Having data both for $\tau$ and for $\xi$ we can think of trying to estimate
the exponent $z$, that relates them through

$$\tau(\xi) = A\xi^z (1 + B\xi^{-\omega} + ...)$$

(4.8)

Unfortunately $\tau(\xi)$ has strong scale corrections, since we only have
$\xi \leq 8$, so we only feel to give a lower bound for $\xi$. As we show in figure
4.21 we can be reasonably sure that $z > 4$. but we cannot say how much
it will grow.
4.7 Minima or Saddles?

To complete the frame that should indicate us if the analogy between the 3-dimensional EA Heisenberg model and structural glasses is too hasty we need to do a study of the density of negative directions in the hessian. In fact Mode Coupling Theory claims that the typical configurations should be saddles until the temperature at which we have the topological transition. We need so to find if the typical configurations are closer to a minimum or to a saddle point.

Figure 4.21: The relation between relaxation time $\tau_{\text{Scalar}}$ and correlation length $\xi_{\text{Scalar}}$ follows a power law with exponent $z$ close to the critical point. Since our data was far from the critical point it was not linear enough (in the logarithmic scale) to permit a decent fit, we limited ourselves to giving a lower bound for this exponent. The points connected by a solid line represent our measures, and the dashed line is the function $f(\xi) = A\xi^4$. It is clear how this function gives a loose lower bound of $z \geq 4$. 

4.7 Minima or Saddles?

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To this sake the algorithms we talked about until now are useless, since they are conceived to find minima of the potential energy and they would not make us perceive the presence of saddles. We need to find a new routine that returns us the stationary configurations mindless of if they are stable (minima) or unstable (saddles).

The stationary configurations in our model are those for whom each spin $\vec{s}_x$ is parallel to the local field $\vec{h}_x = \sum_{y, ||\vec{x}-\vec{y}||=1} J_{xy} \vec{s}_y$. The problem of looking for both minima and saddle points then is equivalent to minimizing the spins’ component perpendicular to $\vec{h}$, or maximizing the modulus of the parallel component. This way we could apply the algorithms we already used, to the energy functional

$$H^{(\text{saddle})} = -\sum_{\vec{x}} (\vec{h}_x \cdot \vec{s}_x)^2$$

and analyse the configurations out coming from this routine.
Conclusions

We have made a systematic investigation of the behavior of the 3-dimensional EA Heisenberg model in the paramagnetic phase in the thermodynamic limit, to see if we could remark features in common with structural glasses. Mode Coupling Theory predicts that the dynamics of structural glasses is dominated by the underlying structure of the energy landscape, so we made a deep study of the inherent structures of the model.

For this sake the algorithms already used in literature were not enough effective, so we adapted the Successive Over Relaxation method to our problem and obtained a very performing routine. This algorithm depended on a parameter $\lambda$, whose modification influenced highly its convergence time and the properties of the obtained inherent structures. We chose $\lambda$ who made our routine very fast, although it did not yield the lowest energies. This because we did not believe that the properties of the configurations we found were intrinsically different from the others, and also because this choice permitted us to maintain ourselves in the thermodynamic limit since lower energies were related to longer correlation lengths. We noticed also that the energy is not enough to identify univocally an inherent structure, since same energies found with different routines lead to configurations with completely different correlation lengths.
We analysed the dependence of the energy of the inherent structures from temperature, and remarked a trend that was qualitatively similar, with almost no dependence at high temperatures, and a sudden decrease of their energies at lower temperature. Furthermore, we noticed that lowering the temperature the correlation lengths of thermal configurations and inherent structures converge, so the divergence of the correlation length could be due exclusively to the energy landscape. An analysis of the anharmonic term of the energy showed that its contribution is fairly small up to pretty high temperatures, so it is not so crazy to schematize the energy of a thermal state as harmonic agitation over a local minimum.

We also noticed that the Inherent Structures of the Heisenberg Spin Glasses have particular alignment properties. In fact their Chiral Glass self-overlap is consistently lower than the one of the thermal states, and decreases with the energy of the Inherent Structure. This feature would be very helpful to recognize a Ground State, since it implies that, differently from Ising Spin Glasses, the minima of the energy are qualitatively different from random configurations.

Moreover, the data we had collected permitted us to make estimates for the critical exponents $\nu$ and $z$ of the model. Although they are not very reliable, since they come from states far from the critical temperature, where the scaling does not apply, they were useful to give some bounds that can be useful for further reference, since in literature there still are very few attempts of evaluating the critical exponents of the EA Heisenberg model. We focused on how working far from the phase transition with very large lattices is equivalent to using small systems close to the phase transition, giving a measure of $T_{SG}$ that underestimated it consistently, just as it happened when this study was approached using too small lattices.

Later on we passed to the dynamic behavior of the model, since we wanted to see if we could observe the power law divergence of the relax-
ation time in proximity of the dynamic transition, deep in the paramagnetic phase. Also this test had a positive feedback, since we observed the apparent divergence of the relaxation time for 4 decades just as in structural glasses, the temperature at which the characteristic times would diverge was clearly greater than $T_{SG}$ and the scaling exponents of the same order of those obtained for supercooled liquids.

All this data is consistent with the identification of the EA Heisenberg model as a possible lattice model with the same universality class of structural glasses. If this were true it would be very useful to study in an alternative way structural glasses. Further studies to make more solid this impression, would refer to the investigation of the configurational entropy of the model, and, work that is already in progress, a detailed analysis of the density of negative directions in the hessian matrix, to see if we can individuate the topological transition as its vanishing, with the arising of an activated dynamics. If those tests too will give a positive result it will be then enough evidence to start considering a rigorous, more engaged, theory of our conjectures.
A.1 Fourier Correlation length

We show how to get to the formula 3.37 for the correlation length, and show a computationally efficient way to calculate its terms.

Given a generic field $\phi(\vec{x})^1$ the action for a free Hamiltonian is

$$S = \frac{1}{2} \int d^3x \{(\nabla \phi(x))^2 + \bar{m}^2 \phi(x)^2\},$$

(A.1)

from which descends the propagator

$$\hat{G}(\vec{k}) = \frac{Z(\bar{m}^2)}{k^2 + \bar{m}^2}, \quad k^2 = 4D \sum_{\mu=1}^{\bar{m}} \sin^2 \left(\frac{k_{\mu}}{2}\right)$$

(A.2)

where $Z(\bar{m}^2)$ is an unknown function of the mass $\bar{m}$. We know that the propagator $\hat{G}$ is the Fourier Transform of the correlation function

$$G(\vec{r}) = \frac{1}{N} \sum_{\vec{x}} <\phi(\vec{x})\phi(\vec{x}+\vec{r})>.$$  

(A.3)

We can obtain the correlation length $\xi^2 = 1/m^2$ by making the ratio between the $\hat{G}$ calculated for two different impulses $k$. This way we would get rid of the factor $Z(m^2)$. To this sake we use $\vec{k} = 0$ and

$^1$For the purpose of our work $\phi$ can represent both the Chiral Glass overlap $e^\mu$ and the Spin Glass overlap $\tau_{\alpha\beta}$. 

85
\( \tilde{k}_{\text{min}} = (2\pi/L, 0, 0) \), that is the minimum impulse with periodic boundary conditions, and we consider the ratio between

\[
F = \hat{G}(\tilde{k}_{\text{min}}) = \frac{Z(\bar{m}^2)}{4 \sin^2 \left( \frac{\pi}{L} \right) + \bar{m}^2}
\]  

(A.4)

and the magnetic susceptibility

\[
\chi = \hat{G}(0) = \frac{Z(\bar{m}^2)}{\bar{m}^2}
\]  

(A.5)

that yields directly

\[
\xi_F^2 = \frac{1}{4 \sin^2 \left( \frac{\pi}{L} \right)} \left[ \chi - 1 \right].
\]  

(A.6)

Just to stay connected with the literature, we stress that with a finite differences approximation the correlation length in eq. A.6, can be written in differential form, since

\[
\xi_F^2 = \frac{1}{\tilde{k}_{\text{min}}^2} \left[ \hat{G}(0) - \hat{G}(\tilde{k}_{\text{min}}) \right] = - \frac{1}{\hat{G}(\tilde{k}_{\text{min}})} \frac{dG}{d\tilde{k}^2} \bigg|_{\tilde{k}=0}
\]  

(A.7)

**Calculating \( F \) and \( \chi \)** An operative way of calculating \( F \) and \( \chi \) is made very simple thanks to the convolution theorem. Infact we see from equation A.3 that the correlation function is a convolution product of the field \( \phi \) with itself, hence its Fourier Transform \( \hat{G} \) is equal to

\[
\hat{G}(\tilde{k}) = \frac{1}{N} |\hat{\phi}(\tilde{k})|^2,
\]  

(A.8)

where \( \hat{\phi}(\tilde{k}) \) is the Fourier Transform of the field \( \phi(\tilde{x}) \). Remembering that we’re only interested in its value at \( \tilde{k} = 0, \tilde{k}_{\text{min}} \), we can use an explicitly computable form for \( \hat{\phi}(\tilde{k}) \) for \( F \) and \( \chi \), helped by the fact that \( \tilde{k}_{\text{min}} \) is parallel to the \( x \)-axis

\[
\hat{\phi}(\tilde{k}_{\text{min}}) = \sum_{n_x} e^{i 2\pi n_x/L} \sum_{n_y, n_z} \phi(n_x, n_y, n_z) = \sum_{n_x} e^{i 2\pi n_x/L} P(\tilde{x})
\]  

(A.9)

where \( n_x, n_y \) and \( n_z \) are the components of the position vector \( \tilde{x} \), and we recognize the plane variables \( P(\tilde{x}) \) defined in section 3.3.3.
We now have a numerically simple way to express $F$, from which the one for $\chi$ descends trivially,

$$\chi = \frac{1}{N} \left( \sum_{\vec{x}} \phi(\vec{x}) \right)^2$$  \hfill (A.10)

$$F = \frac{1}{N} \left( \sum_{n_x} e^{i 2\pi n_x / L} \sum_{n_y, n_z} \phi((n_x, n_y, n_z)) \right)^2.$$  \hfill (A.11)

## A.2 Integral Estimators

We want to show that in the thermodynamic limit the integral estimators $\xi^{(02)}$ are exactly equal to the correlation length $\xi_F$. We remind its definition

$$\xi^{(02)} = \sqrt{\frac{J_2}{\chi}}, \quad J_2 = \sum_{r=1}^{L/2} r^2 C(r)$$  \hfill (A.12)

The minimum impulse propagator, keeping in mind that we work with periodic boundary conditions, can be rewritten as

$$F = C(0) + C(\frac{L}{2}) + \sum_{r=1}^{L/2-1} C(r) \cos(\frac{2\pi r}{L})$$  \hfill (A.13)

where the sum on the sines disappears because we’re summing an odd function over a symmetric interval. If we pass to the large $L$ limit, in which we want to demonstrate the identity, we can develop the cosine for small angles and neglect the term $C(\frac{L}{2})$, since $C(r)$ vanishes at long distance. Hence

$$F = C(0) + 2 \sum_{r=1}^{L/2-1} C(r) \left[ 1 - \frac{2\pi^2 r^2}{L^2} + o\left(\frac{r^4}{L^4}\right) \right] =$$  \hfill (A.14)  

$$= \chi - \left(\frac{2\pi}{L}\right)^2 J_2 + o\left(\frac{J_4}{L^4}\right).$$  \hfill (A.15)

We can insert this expression in the formula for $\xi_F$ getting

$$\xi_F^2 = \frac{1}{4 \sin^2\left(\frac{\pi}{L}\right)} \left[ 1 - \left(\frac{2\pi}{L}\right)^2 J_2 \frac{1}{\chi} + o\left(\frac{J_4}{L^4\chi}\right) - 1 \right],$$  \hfill (A.16)
from which if we develop another time for large \( L \), keeping in mind that for small \( x \) we have \( \frac{1}{1-x} \approx 1 + x \), and take the limit \( L \to \infty \) we obtain finally

\[
\lim_{L \to \infty} \xi_F = \sqrt{\frac{J_2}{\chi}} \equiv \xi^{(02)}.
\] (A.17)

Figure A.1 shows how the correlation lengths \( \xi_F \) and \( \xi^{(02)} \), that differ quite much for small system size, converge as the system approaches the thermodynamic limit.

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**Figure A.1:** Correlation lengths of configurations obtained with 3 different protocols \( (\lambda = 10, 100, 1000) \). We see how in small lattices, far from the thermodynamic limit, \( \xi_F \) and \( \xi^{(02)} \) belonging to the same type of configuration are very different, since their equality is valid only in the thermodynamic limit. With growing system sizes the two correlation lengths start converging considerably. The convergence of these two correlation functions can be used as index to establish if the thermodynamic limit is valid or not.
A.3 Asymptotic values of Binder’s Cumulants

We show how to extract the asymptotic value $B_{SG}^{\infty}$ of the SG Binder Cumulant $B_{SG}^{L}$ defined in section 3.3.5 in the case of configurations at infinite temperature (random configurations). The calculation of $B_{CG}^{\infty}$ is analogous so it won’t be shown. We remind the definition

$$B_{SG}^{L} = \frac{<trag(QQ^\dagger)>^2}{<trag(QQ^\dagger)^2>} = \frac{<q^2>^2}{<q^4>^2}$$

and proceed calculating separately numerator and denominator for spins with $m$ components. We start with the numerator

$$<trag(QQ^\dagger)> = \sum_{\alpha,\beta} Q_{\alpha\beta} Q_{\alpha\beta}^\dagger =$$

$$= \sum_{\alpha,\beta} \sum_{x,y} <s_{x,\alpha}^{(a)} s_{x,\beta}^{(b)} s_{y,\alpha}^{(a)} s_{y,\beta}^{(b)} > =$$

$$= \sum_{x,y} <s_{x}^{(a)} \cdot s_{y}^{(a)} > <s_{x}^{(b)} \cdot s_{y}^{(b)} > =$$

$$= \sum_{x,y} \delta_{xy} =$$

$$= N$$

and proceed with the denominator, where due to the square we have two more position indexes

$$<trag(QQ^\dagger)^2> = \sum_{x,y,z,t} <(s_{x}^{(a)} \cdot s_{y}^{(a)})(s_{z}^{(b)} \cdot s_{t}^{(b)})(s_{x}^{(a)} \cdot s_{t}^{(a)})(s_{z}^{(b)} \cdot s_{t}^{(b)})> =$$

$$= \sum_{x} <s_{x}^{(a)} s_{x}^{(b)4} > +$$

$$+ \sum_{x,z} <s_{x}^{(a)2} s_{z}^{(b)2} s_{x}^{(a)2} s_{z}^{(b)2} > +$$

$$+ 2 \sum_{x,y} <(s_{x}^{(a)} \cdot s_{y}^{(a)})^2 > <(s_{x}^{(b)} \cdot s_{y}^{(b)})^2 >.$$

We compute the average $<(s_{x}^{(a)} \cdot s_{y}^{(a)})^2 >$ by putting ourselves in the reference frame of $s_{x}$, aligning to it our first axis. This way the scalar product
asymptotic values of Binder’s Cumulants

is equal to the first component of $\vec{s}_y$. Hence

$$< (\vec{s}_x \cdot \vec{s}_y)^2 > = s_{y,1}^2 = \frac{1}{m}$$

since $\sum_{\alpha=1}^m s_{y,\alpha}^2 = 1$ and there is no preferential direction. Therefore, summing up all terms we have

$$< tr(QQ^\dagger)^2 >= N + N(N-1) + \frac{2}{m^2}N(N-1). \quad (A.18)$$

Recomposing the cumulant and performing the thermodynamic limit we get

$$B_{SG}^{N \to \infty} \xrightarrow{N \to \infty} 1 + \frac{2}{m^2} \quad (A.19)$$

So in our case $m = 3$ we have $B_{SG}^{\infty} = \frac{11}{3} = 1.\bar{2}$. 

90
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