1 The Ising Spin Glass Model

Spin glass models are simplified, although still quite complex, models which are important theoretical laboratories in which the combined effects of disorder and frustration can be investigated. Indeed, they are not only of interest for the understanding of the phase diagram of materials with ferromagnetic/antiferromagnetic couplings, but their study has provided many ideas which found their applications in many different fields, ranging from biology \cite{1,2} to computer science \cite{3}.

One of the simplest models is the Ising model with random couplings. Its Hamiltonian is

\[ H = -\sum_{i,k} J_{ik} S_i S_k - \sum_{i=1}^{N} h_i S_i, \]  

(1)

where the \( N \) spins \( S_i \) take discrete values, \( S_i \in \{-1, 1\}; \) the matrix \( J_{ik} \) is called the coupling matrix and the variables \( h_i \) represent magnetic external fields. Depending on the form and the nature of the coupling matrix and of the magnetic field it is possible to obtain very different and rich physical behaviours.

According to the form of the coupling matrix we can distinguish two different situations:

- \( J_{ik} \) is different from zero for any pair of couplings; this is the so-called mean-field case.

- \( J_{ik} \) is zero if the distance between sites \( i \) and \( j \) is larger than a certain cutoff \( R \); in this case the model is defined on a given \( d \)-dimensional lattice (otherwise there is no notion of distance).
The mean-field case has been extensively studied and the phase diagram of model (1) is well understood. Much less is known for the second case, which is the only one we shall consider.

The phase diagram of model (1) depends on the nature of the coupling matrix. Its values can either be fixed or random variables distributed according to a specified probability distribution. In the standard ferromagnetic Ising model the coupling matrix is $J_{ik} = +1$ and $h_i = h$. The free energy landscape, as a function of the magnetization, changes on lowering the temperature $T$: for high values of $T$ there is only one minimum corresponding to the paramagnetic state, while below a critical temperature $T_c$, two minima appear representing two states of opposite and finite magnetization. Both the mean-field and the finite dimensional version of the model are fully under control.

The Ising spin glass model is characterized by coupling constants that can be both positive and negative. This feature leads to the so-called frustration. If frustration is large enough, the mean-field version of the Ising spin glass, the Sherrington-Kirkpatrick (SK) model [4] (with a Gaussian distribution for the coupling matrix), has a very different physical behaviour with respect to the mean-field versions of ferromagnetic models. Even if it shows a finite-temperature transition, the low-temperature phase is completely different: there is no long-range magnetic order and the order parameter is the overlap

$$q^{\alpha\beta} = \frac{1}{N} \sum_{i=1}^{N} S_i^\alpha S_i^\beta,$$

between two replicas $\alpha$ and $\beta$ obtained for the same choice of the coupling matrix. The overlap is zero at high temperatures while it shows a nontrivial distribution in the low-temperature phase, in which an exponential number of degenerate states appears, organized according to the full Replica Symmetry Breaking scheme (fRSB) [5].

In this thesis we will study the three-dimensional bimodal Ising spin glass model which is characterized by a probability distribution for the coupling constants which reads

$$P (J_{ik}) = \frac{1}{2} \left[ \delta (J_{ik} - 1) + \delta (J_{ik} + 1) \right].$$

We will also consider a modification of this distribution in order to tune the frustration of the system by multiplying for

$$P_{fr} (J_{ik}) = \exp \left[ K \sum_{\alpha} \Box_{\alpha} \right],$$

where $\Box_{\alpha}$ is given by the product of the coupling constants belonging to the $\alpha$-th plaquette [6]. By tuning the parameter $K$ we will be able to study the two limiting regimes: the low frustration one which will exhibit a paramagnetic-ferromagnetic behaviour and the fully frustrated one where the appearance of a spin glass phase is an open question.

2 Numerical Techniques

So far we described the behaviour of the Ising spin glass in the mean-field approximation. While these results are sound, and in many cases rigorously proved, much less is known
rigorously for finite dimensional systems. Hence numerical simulations are necessary to gain physical insight.

Equilibrium Montecarlo Simulations (EMCS) are difficult because of the critical slowing down the dynamics shows near and below the transition temperature. Moreover, equilibration times are widely dependent on the disorder realization. It follows that in any equilibrium simulation thermalization can only be reached for relatively small-sized systems and therefore results show large finite-size effects.

To avoid this difficulty we will perform a Nonequilibrium Relaxation (NER) \cite{7, 8} analysis of the Montecarlo (MC) dynamics for the bimodal three-dimensional Ising spin glass model. Indeed, we will analyze the relaxation part of EMCS which is usually discarded. We will use a purely relaxation dynamic which is the most common way to implement a Markovian chain in which detailed-balance is satisfied.

During the relaxation from a nonequilibrium starting configuration, the system undergoes a local thermalization for which equilibrium properties in the thermodynamic limit can be evaluated even if the system as a whole is not thermalized and its size is finite. The main requirement which has to be satisfied in order to avoid finite-size effects is that the dynamic correlation length $\xi(t)$ be much less than the linear size of the system $L$: $\xi(t) \ll L$. The dynamic correlation length estimates the linear size of a region in which the spins have become strongly correlated after an elapsed time $t$. We define the relaxation time $\tau(r)$ as the time needed for the spins in a region of linear size $r$ to correlate with each other. This quantity is defined by the relation $\xi[\tau(r)] = r$. We can thus express the requirement $\xi(t) \ll L$ with: $t \ll \tau(L)$, where $t$ is the simulation time. Of course there is also a lower bound which has to be satisfied for the results to be reliable: $\xi(t)$ must be reasonably larger than the lattice spacing leading also to a lower bound on $t$. We are interested in the asymptotic regime of the relaxation before finite-size effects show up.

Hence, the new feature of this study is the replacement of an analysis as a function of $L$ for $t_{MC} \to \infty$ (the standard finite-size scaling analysis) with an analysis in terms of finite times $t_{MC}$ in the infinite-volume limit $L \to \infty$. In such a study it is necessary to consider the dynamic exponent $z$, whose value depends on the chosen relaxation dynamic. In equilibrium this exponent relates the correlation length $\xi_{eq}$ and the relaxation time $\tau_{eq}$:

$$\tau_{eq} \sim \xi_{eq}^z.$$  \hspace{1cm} (5)

Given a nonequilibrium initial state any thermodynamic observable will relax to some equilibrium value. In the paramagnetic phase the relaxation depends exponentially on the simulation time $t$ while at the critical point of a second-order transition the dependence is algebraic (i.e. expressed by some power of $t$). As an example, it is useful to discuss the relaxation dynamic of the order parameter of the transition. We will describe both the ferromagnetic and the glassy cases in order to see how this kind of analysis works and to determine some basic, but important, differences.

2.1 NER: ferromagnetic case

The order parameter of the transition is the magnetization $m(t)$. Starting from an out-of-equilibrium state (a random configuration or an ordered one) for any $T \neq T_c$ the magnetization will exponentially decay to zero for $T > T_c$ or to a constant value for $T < T_c$. It will
relax as \( m(t) \sim t^{-\lambda_m} \) at the critical point. The dynamic exponent, \( \lambda_m \), can be linked to static exponents as well as to \( z \) at the critical point. This result is achieved considering the scaling hypothesis

\[
m(T, t, L) \sim L^{-\beta/\nu} \tilde{m} (\varepsilon L^{1/\nu}, tL^{-z}) ,
\]

where in the last equality we defined a new function in order to change the functional dependence: \( M (\varepsilon t^{1/\nu}, tL^{-z}) = (tL^{-z})^{\beta/\nu} \tilde{m} \left( \varepsilon t^{1/\nu} (tL^{-z})^{-1/\nu}, tL^{-z} \right) \). For \( \varepsilon \to 0 \) and \( L \to \infty \) we can compare this expression with the asymptotic behaviour of \( m(t) \) obtaining a relation between critical exponents

\[
\lambda_m = \frac{\beta}{z\nu}. \tag{8}
\]

It is possible to determine \( T_c \) observing the asymptotic behaviour for the relaxation of the magnetization. However a more accurate result can be obtained studying the local exponent \( \lambda_m(t) \) which is defined via the logarithmic derivative of the magnetization

\[
\lambda_m(t) = -\frac{d \log m(t)}{d \log t}. \tag{9}
\]

For this system \( \lambda_m(t) \to \infty \) in the paramagnetic phase, \( \lambda_m(t) \to 0 \) in the ferromagnetic phase and finally \( \lambda_m(t) \to \lambda_m \) at the critical point. It is possible to approximate the critical temperature from above and below observing the convergence to zero or the divergence of the local exponent in narrow temperature ranges. The narrower the range the better the approximation. Moreover this measure does not suffer systematic errors because the error is simply given by half the amplitude of the temperature range in which we recognize two different phases. Of course accurate measures require long simulations, hence very large values of \( L \), because approaching the critical temperature leads to relaxations which need more time to diverge from the critical behaviour. Another important feature of this kind of analysis is that if the thermodynamic limit requirement \( t \ll \tau(L) \) holds then the error on one sample for \( m(t) \) is of order \( N^{-1/2} \) (in our case \( N = L^3 \)) and the error on the average among \( N_{\text{hist}} \) histories is then of order \( (N \times N_{\text{hist}})^{-1/2} \). This is an important feature in the case of limited computational time because one could reach a good statistic with few runs over big samples (for which the thermodynamic limit requirement holds for long times) rather than more runs over little ones.

\subsection{NER: glassy case}

The NER for spin glasses interestingly reproduces the experimental framework in which measurements on this kind of system are performed: the observation time is always shorter
than the equilibration time. For glassy systems, whose dynamics is critically slowed down near the transition, the NER analysis seems to be a suitable choice in order to extrapolate properties in the thermodynamic limit.

Nevertheless some problems arise such as the difficulty of finding a good nonequilibrium initial state for the low $T$ phase (as the all-aligned state we mentioned in the ferromagnetic case where we used its characteristic long range magnetic order) and the definition of a good dynamical order parameter. One of the characteristic features of the glassy phase is that measurements depend on the time elapsed since the preparation of the sample: the waiting time $t_w$. Choosing as a dynamical order parameter the two times overlap

$$q_{\alpha\beta}(t_w,t) = \frac{1}{N} \sum_{i=1}^{N} S_{\alpha}^{\alpha}(t + t_w) S_{\beta}^{\beta}(t + t_w),$$  

(10)

where the upper line indicates the average over the disorder, one finds an exponential decay in the paramagnetic phase which is function of the waiting time and the thermalization time $\tau_{th}$ which is the characteristic time of the decay. Near the transition temperature a power-law decay is observed: two different regimes can be distinguished for $t \ll t_w$ and $t \gg t_w$. The main difference with the ferromagnetic case is that below the transition temperature the behaviour of the dynamical order parameter is always a power law even if with different scaling properties: hence the transition temperature can be estimated only from above with this method. In fact the local exponent does not seem to converge to zero for $T < T_g$.

3 GPUs

In order to study the NER dynamics of the Ising spin glass model we will simulate cubic systems of variable sizes $L$ on cubic lattice. We will use random configurations of the spins as initial configurations and we will measure the NER of invariant ratios constructed in terms of powers of the overlap.

Simulations will be performed on a cluster of NVIDIA GPUs using a multispin Metropolis algorithm. Multispin coding is very convenient since it allows us to exploit the whole length of a word to store spins and couplings value and it significantly speeds up simulations. Even though it is possible nowadays to obtain high performances multicore clusters based on commercial CPUs some years ago a renewed interest of the High Performance Computing (HPC) community towards GPUs arithmetic capabilities spread out. In fact these units, which were designed in order to sustain high requiring graphical calculations, offer a highly specialized solution for scientific computing. This happens because GPUs offer several cores which can evaluate arithmetical expressions in parallel. As an example the GeForce GTX 580 has 512 cores which can perform both integer and floating point operations. However the algorithm implementation must be specialized on the particular architecture adopted in order to obtain the best performances. Furthermore NVIDIA offers through the CUDA development toolkit an easy way to program in C and C++ languages.

A first work [9] evaluating the advantages of a GTX 480 GPU against a commercial CPU (Intel I7 @ 2.93 GHz) shows that a microcanonical algorithm runs almost 10 times faster on a GPU. A detailed study [10] of the Wolff single-cluster algorithm shows that for the 2D
Ising model with $L = 4096$ at the critical temperature the GPU (GTX 285) computational speed is 5.60 times as fast as the CPU (Intel Xeon W3520 @ 2.67GHz) computational speed. For 3D Ising model for $L = 256$ the improvement factor is 7.9.

4 Aims

The aims of this thesis are to study in the most accurate way:

- a) the nature of the paramagnetic-glassy transition, using the three-dimensional bimodal Ising spin glass model and the same model modified by the frustration tuning term;
- b) the nature of the low-temperature phase;
- c) the role of a magnetic field and the Almeida-Thouless transition.

References


