POLITECNICO DI TORINO

Accelerated dynamics of spin-glasses: *A project to test the swap method*

by

Greivin A. Alfaro Miranda

Final Project

Master's Degree in Physics of Complex Systems

Supervisors & Co-supervisor:

Prof. Leticia Cugliandolo
Laboratoire de Physique Théorique et Hautes Énergies
Sorbonne Université

Prof. Marco Tarzia
Laboratoire de Physique Théorique de la Matière Condensée
Sorbonne Université

Prof. Andrea Pagnani
Department of Applied Science and Technology
Politecnico di Torino

Turin, Italy

December, 2022

Contents

Illustrations

Chapter 1

Introduction

There has been an extensive amount of work dedicated to search for more efficient ways in which one can simulate disordered systems, like spin-glasses [1–3]. The inherent slow dynamics of glasses translates into difficulties while attempting to extract quasi-equilibrium properties from Monte Carlo simulations; at low temperatures one finds relaxation times that depend on the system size, hence diverging in the thermodynamic limit. The display of out-of-equilibrium behaviour while attempting to measure observable quantities for this system seems unavoidable.

Several methods have been developed in order to get around this conundrum, such as the well established parallel tempering algorithm [4] where one modifies the acceptance procedure in the Monte Carlo simulation (whose most basic form will be described in section 3.1) to include the interchange of configurations quenched at different temperatures running in parallel. In this work we attempt to propose another candidate of a Monte Carlo algorithm that might be able to accelerate the dynamics of spin-glass systems. We argue that an algorithm that was able to accelerate the dynamics of structural glass systems, proposed by Berthier et. al [5], known as the *SWAP method*, is translatable into the context of spin-glasses and might provide an efficient way to accelerate the dynamics of the standard Monte Carlo simulation.

We want to probe the efficiency of the swap procedure for spin-glass systems, in order to do so, one needs a local degree of freedom to be interchanged between agents of the system, in our case the spins. We promote the standard Ising variables to be continuous variables and assign the *length* or *strength* of the spins as the local parameter to be affected by the SWAP procedure. This, as will be explained in later chapters, is expected to have a direct effect on the energy of the system, specifically, in overcoming the energy barriers that trap the system in meta-stable configurations that one encounters in the spin-glass problem. To have a better of understanding of the behaviour of a model with continuous spin, the mean field model of both the standard and the disordered case have been solve exactly in the first chapter, plus an introduction of the usual calculations of a mean-field disordered model (the SK model to be precise) have also been included in the theoretical framework. Although we have considered the condition that the average spin length should be centered around 1, with the aim of just adding small variations to the model without changing its overall behaviour, it is clear that the effect will not be negligible, and solving the mean-field case can provide some insight regarding the equilibrium properties of the new model. Special interest has been devoted to the dependence of the critical temperature with the change of lengths in the spins, as it is an essential property while performing the quenches during the MC simulations. We will see that promoting the spins to be continuous variables will indeed change the behaviour of the critical temperature, from this we are able to track the value of the critical temperature in order to perform the proper quench in the Monte Carlo simulation.

The second chapter is dedicated to give a small introduction of the standard MC simulation for spin-systems and comment the behaviour of the quenches and two-time observables (specifically the auto-correlation function) while performing MC simulation. We then introduce the version of the SWAP method applied to spin systems with length and present some of the results of the simulations. Although several results have been produced for several models (Sherrington-Kirkpatrick, 3D, 2D Edwards-Anderson, 3D-2D Ising models) with and without lengths, we mainly focus our discussion for the 3D Edwards-Anderson model. The finite dimensional models will always be presented in a regular square-cubic lattice, with coordination number equal to $2d$ where d is the dimension of the system.

Chapter 2

Theoretical Framework

2.1 Fully-connected Ising model with soft-spins

We will introduce a by-pass model to accelerate the relaxation dynamics of the spin-glass problem. A natural choice to probe the swap method would be to endow the spins with a akin of *length* or a *strength*, such that it will serve as the swapped degree of freedom in our system (i.e. analogous to the molecules diameter in [5]); this variation in spin-systems is commonly referred as soft-spins in the literature [6], although other less general models refer them just as continuous spins [7, 8]. We will choose the soft-spins variables (s_i) not to far from the classic Ising spins (σ_i), so they can be related via the new strength variable τ_i s.t. $s_i = \tau_i \sigma_i$. The strength degrees of freedom will be i.i.d. random variables sampled from the probability distribution $p(\tau_i)$ with positive support.
As a first approach, we will consider the model without disorder i.e. the fully-connected Ising model with soft-spins, with its Hamiltonian defined in the following way

$$H_{SS}(\{\sigma_i\},\{\tau_i\}) = -\frac{J}{2}\sum_{i\neq j}\tau_i\tau_j\sigma_i\sigma_j - \lambda_1\sum_{i=1}^{N}(\tau_i - 1) - \lambda_2\sum_{i=1}^{N}\left(\tau_i^2 - 1 - \frac{\Delta^2}{12}\right), \quad (2.1)$$

here $\sigma_i \in \{-1, 1\}$ are the classic spin variables, J will refer to the coupling constant (to be taken ferromagnetic i.e. $J > 0$) and we have included two Lagrange multipliers $\{\lambda_1, \lambda_2\}$ in order to control the fluctuations of the strength variables, specifically, we want to fixed the mean to 1 (the case of classic Ising spins) and the sample variance to be that of a uniform distribution in a box of size Δ.

In order to calculate the partition function of the model we are in need of decouple the different lattice sites, with this goal in mind we use the following identity

$$\left(\sum_{k=1}^{N} c_k\right)^2 = \sum_{k=1}^{N} c_k^2 + \sum_{l\neq k}^{N} c_l c_k. \quad (2.2)$$

Furthermore, Kac's re-scaling shall be introduced to render the energy of the long-range model extensive [9]

$$J \to \frac{J}{N}. \quad (2.3)$$

With these considerations we get

$$H_{SS}(\{\sigma_i\},\{\tau_i\}) = -\frac{J}{2N}\left(\sum_{i=1}^{N}\tau_i\sigma_i\right)^2 + \sum_{i=1}^{N}\psi_i(\tau_i), \tag{2.4}$$

where we have defined

$$\psi_i(\tau_i) = \left(\frac{J}{2N} - \lambda_2\right)\tau_i^2 - \lambda_1\tau_i + \lambda_1 + \lambda_2\left(1 + \frac{\Delta^2}{12}\right), \tag{2.5}$$

and after neglecting the terms sub-leading in N (as they will become zero in the thermodynamic limit) we are left with

$$\psi_i(\tau_i) = -\lambda_2\tau_i^2 - \lambda_1\tau_i + \lambda_1 + \lambda_2\left(1 + \frac{\Delta^2}{12}\right), \tag{2.6}$$

to be a function already decoupled of degrees of freedom. We now proceed to calculate the partition function of the model defined as $Z = \mathrm{Tr}\left[e^{-\beta H_{SS}(\{\sigma_i\},\{\tau_i\})}\right]$, here the trace operator is summing over all the degrees of freedom in the model taken to be $\{\sigma_i\}$ and $\{\tau_i\}$; in order to decouple the exponential of the first term in the Hamiltonian, we introduce the Hubbard-Stratonovich transformation, defined as

$$\exp\left(bm^2\right) = \sqrt{\frac{b}{\pi}}\int_{-\infty}^{\infty} dx \exp\left(-bx^2 + 2bxm\right), \tag{2.7}$$

this yields

$$e^{-\beta H_{SS}(\{\sigma_i\},\{\tau_i\})} = \sqrt{\frac{N\beta J}{2\pi}}\int_{-\infty}^{\infty} dx e^{-\frac{N\beta J}{2}x^2 + \beta J x\sum_{i=1}^{N}\sigma_i\tau_i - \beta\sum_{i=1}^{N}\psi_i(\tau_i)}. \tag{2.8}$$

Now we should make explicit the form of the trace operator, in the way we have defined our variables we define it as

$$\mathrm{Tr} \equiv \sum_{\{\sigma_i\}}\int\prod_{i=1}^{N} dp(\tau_i), \tag{2.9}$$

hence

$$Z(\beta) = \sqrt{\frac{N\beta J}{2\pi}}\int_{-\infty}^{\infty} dx e^{-\frac{N\beta J}{2}x^2}\sum_{\{\sigma_i\}}\int\prod_{i=1}^{N} dp(\tau_i) e^{\beta\sum_{i=1}^{N}[Jx\sigma_i\tau_i - \psi_i(\tau_i)]}, \tag{2.10}$$

that after some reordering and manipulations becomes

$$Z(\beta) = \sqrt{\frac{N\beta J}{2\pi}}\int_{-\infty}^{\infty} dx e^{-N\beta\mathcal{H}_{eff}(x)}, \tag{2.11}$$

where we have defined

$$\mathcal{H}_{\text{eff}}(x;\beta) \equiv \frac{J}{2}x^2 - \frac{1}{\beta}\log\left[2\int dp(\tau)e^{-\beta\psi(\tau)}\cosh(\beta Jx\tau)\right], \tag{2.12}$$

to be the effective Hamiltonian also known as the Landau-Ginzburg free energy. Note that the i-index has been dropped since we have fully decoupled our degrees of freedom. Now we are able to evaluate the integral in (2.11) by means of the saddle-pint method, considering $N \gg 1$ but still finite will yield

$$Z(\beta) \approx \sqrt{\frac{N\beta J}{2\pi}}e^{-N\beta \inf_x \mathcal{H}_{\text{eff}}(x;\beta)}, \tag{2.13}$$

and now we are able to evaluate the free energy density of our model (that, as can be seen in the following, coincides with the infimum of the Landau-Ginzburg free energy)

$$f(\beta) = -\frac{1}{\beta N}\log Z = \inf_x \mathcal{H}_{\text{eff}}(x;\beta). \tag{2.14}$$

We now search for the value of x that minimizes the effective Hamiltonian, hence solving for $\frac{\partial \mathcal{H}_{\text{eff}}}{\partial x}|_{x^*} = 0$ provides us with

$$x^* = \frac{\int dp(\tau)\ \tau\ e^{-\beta\psi(\tau)}\sinh(\beta Jx^*\tau)}{\int dp(\tau)\ e^{-\beta\psi(\tau)}\cosh(\beta Jx^*\tau)}, \tag{2.15}$$

value of x^* coincides precisely with the value of the order parameter of the model, hence equation 2.15 is the equation of state of the model. It is easy to show that such value is the magnetization density defined as follows

$$m = x^* = \frac{1}{N}\sum_{i=1}^{N}\tau_i\sigma_i. \tag{2.16}$$

Clearly, we can see that $x^* = 0$ is a solution, signaling the existence of a disordered phase. Moreover, we can also obtain two more equations for the constraints imposed from the Lagrange multipliers i.e. minimizing the effective Hamiltoinian w.r.t. λ_1 and λ_1 one obtains

$$\frac{\int dp(\tau)\ \tau\ e^{-\beta\psi(\tau)}\cosh(\beta Jm\tau)}{\int dp(\tau)\ e^{-\beta\psi(\tau)}\cosh(\beta Jm\tau)} = 1, \tag{2.17}$$

and

$$\frac{\int dp(\tau)\ \tau^2\ e^{-\beta\psi(\tau)}\cosh(\beta Jm\tau)}{\int dp(\tau)\ e^{-\beta\psi(\tau)}\cosh(\beta Jm\tau)} = 1 + \frac{\Delta^2}{12}. \tag{2.18}$$

We are interested in finding the critical temperature of the model. We attempt an

expansion near criticality for small values of the order parameter, in doing so, it is convenient to define the following operator

$$\mathcal{E}_\tau[...] \equiv \int dp(\tau)\ e^{-\beta\psi(\tau)}[...], \tag{2.19}$$

which is clearly linear but notice that is not normalized i.e. $\mathcal{E}_\tau[1] \neq 1$. We now expand up to first order of m in the equation of state, as

$$\begin{aligned} m &= \frac{\mathcal{E}_\tau[\tau \sinh(\beta J m \tau)]}{\mathcal{E}_\tau[\cosh(\beta J m \tau)]} \\ &\approx \frac{\beta J m \mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1 + \frac{(\beta J m \tau)^2}{2}]} = \frac{\beta J m \mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1]\left(1 + \frac{(\beta J m)^2}{2}\frac{\mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1]}\right)} \\ &\approx \beta J m \frac{\mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1]}\left(1 - \frac{(\beta J m)^2}{2}\frac{\mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1]}\right) \\ &\approx \beta J m \frac{\mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1]} \end{aligned} \tag{2.20}$$

We may proceed in the same fashion with equations 2.17 and 2.18,

$$\frac{\mathcal{E}_\tau[\tau]}{\mathcal{E}_\tau[1]} \approx 1, \tag{2.21}$$

$$\frac{\mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1]} \approx 1 + \frac{\Delta^2}{12}, \tag{2.22}$$

Therefore, we are able to extract the critical temperature dependence with the parameter Δ

$$\boxed{\frac{k_B T_c}{J} = 1 + \frac{\Delta^2}{12}} \tag{2.23}$$

That we will choose it to be, as mentioned before, the size of the box centered at 1 from which we are sampling our strengths, i.e. $\tau_i \in \left[1 - \frac{\Delta}{2}, 1 + \frac{\Delta}{2}\right]$. Moreover, for the mean-field approximation we include the coordination number of a lattice with finite dimension d, this corresponds to the transformation $J \to 2dJ$ from the fully-connected model, hence

$$\frac{k_B T_c}{J} = 2d\left(1 + \frac{\Delta^2}{12}\right), \tag{2.24}$$

so that in our case of a simple cubic lattice with a box distribution of size $\Delta = 1.5$ and a natural temperature scale in which $(J/k_B = 1)$ we have $T_c = 7.125$.

The increasing quadratic behaviour of the critical temperature w.r.t. the strength

parameter Δ can also be seen from the numerical solution of equations (2.15), (2.17), (2.18) presented graphically in figure 2.1, where it can be seen that as we increase the spin-strength the low-temperature ordered phase expands its temperature domain. Notice that the critical exponent β is left unchanged w.r.t. the classical model with Ising spins, a similar behaviour will appear when we introduce disorder in this model at section 2.2.2.

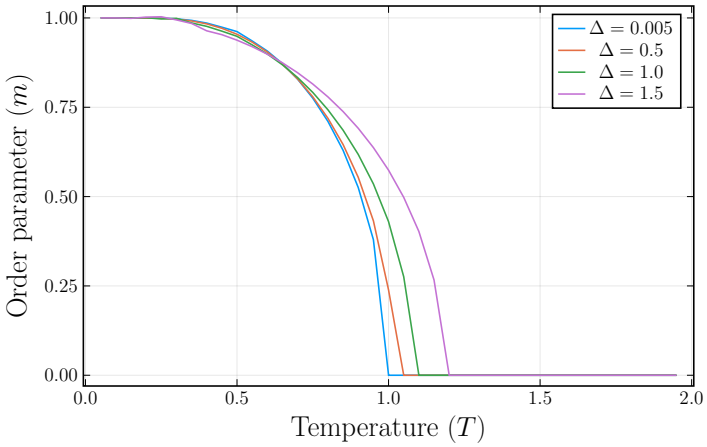

Figure 2.1 : Magnetization density (m) dependency with temperature (T) for several values of the strenght parameter (Δ). The increasing quadratic behaviour of the critical temperature is confirmed.

2.2 Disordered models

The spin-glass phase arises when we take into account disordered interactions within our model. In such cases the computation of the partition function develops further difficulties that are dealt with by introducing the notion of *replicas* [10]. we then introduce the simplest model bearing a spin-glass phase: the Sherrington-Kirkpatrick model, basically, a fully-connected Ising model with random couplings. known as the Sherrington-Kirkpatrick model [11].

2.2.1 Sherrington-Kirkpatrick (SK) Model

We defined the Hamiltonian of the disordered model with spins of fixed length i.e. we are dealing with standard Ising variables where $\sigma_i \in \{-1, +1\}$

$$H_{SK}(\{\sigma_i\}) = -\frac{1}{2}\sum_{i \neq j} J_{ij}\sigma_i\sigma_j, \tag{2.25}$$

and we are considering the case where no external field is present. Note that we have introduced the disordered nature of the system through the couplings (J_{ij}), by taking them to be independent and identically distributed (*i.i.d.*) Gaussian random variables

$$p(J_{ij}) = \frac{1}{\sqrt{2\pi J^2}} \exp\left[-\frac{(J_{ij} - J_0)^2}{2J^2} \right], \tag{2.26}$$

with $\overline{J_{ij}} = J_0$, $J^2 = \overline{J_{ij}^2} - \overline{J_{ij}}^2$ *.

For any quantity Q, our notation implies that $\overline{Q}$ will be used to denote an average *over the disorder* (accordingly, in this context, a Gaussian average). Nevertheless, we want to consider just the symmetric case i.e. where $J_0 = 0$ hence, as we shall soon confirm, the case where no ordered ferromagnetic phase is present. Moreover, a proper Kac's re-scaling shall be taken into account, in this case just to the couplings' variance.

$$J^2 \to \frac{J^2}{N} \tag{2.27}$$

2.2.1.1 Free Energy Calculation

As in the preceding section, our goal is to obtain the free energy of the system, specifically, as we are dealing with a disordered system, we proceed to calculate the disorder-averaged free energy, from it we are able to derive most of the typical properties of the model [12].

$$\overline{F_J} = -\frac{1}{\beta} \int dJ_{ij} p(J_{ij}) \log Z_J = -\frac{1}{\beta} \overline{\log Z_J} \tag{2.28}$$

The sub-index J stresses out the explicit dependence of the partition function on the specific disorder realization of the couplings, hence the couplings are said to be *quenched* variables, i.e. they remain "frozen" within the scales where the d.o.f. vary†. This problem translates into a difficult evaluation of the free energy that is simplified by using the identity

$$\log Z_J = \lim_{n \to 0} \frac{Z_J^n - 1}{n}, \tag{2.29}$$

here we relax the nature of n for it to be a natural number, representing the number of copies of our system called *replicas*. It has been shown that the analytic continuation while evaluating the limit yield the exact results [10]; therefore, we may write

$$\overline{F_J} = -\frac{1}{\beta} \lim_{n \to 0} \frac{1}{n} \left(\overline{Z_J^n} - 1 \right). \tag{2.30}$$

From now onwards we concern ourselves with the evaluation of $\overline{Z_J^n}$. The n copies of the partition function are calculated as follows

*Note that here J is no longer the coupling constant in this section, but the variance of the random couplings

†Note that the previous calculation (the one with soft-spins) represented a case of annealed disorder, as the random strengths vary on the timescale of the other degrees of freedom

$$Z_J^n = \sum_{\{\sigma_i^1\}} e^{-\beta H_{SK}(\{\sigma_i^1\})} \sum_{\{\sigma_i^2\}} e^{-\beta H_{SK}(\{\sigma_i^2\})} ... \sum_{\{\sigma_i^n\}} e^{-\beta H_{SK}(\{\sigma_i^n\})}, \tag{2.31}$$

we define a new index a running through the replicas ($a = 1, ..., n$) and denote the sum over all d.o.f. as a trace operator Tr. We then re-write the equation above as

$$Z_J^n = \mathrm{Tr}\, e^{-\beta \sum_{a=1}^n H_{SK}(\{\sigma_i^a\})}, \tag{2.32}$$

at this point the usefulness of the replica trick becomes evident; as we attempt to compute the disorder-average of the partition function, we can now exchange the trace and the Gaussian average, i.e. the couplings and the spins have become temporarily **annealed** variables that vary together. Thence

$$\overline{Z_J^n} = \overline{\mathrm{Tr}\, e^{-\beta \sum_{a=1}^n H_{SK}(\{\sigma_i^a\})}} = \mathrm{Tr}\, \overline{e^{-\beta \sum_{a=1}^n H_{SK}(\{\sigma_i^a\})}}, \tag{2.33}$$

with the couplings as our random variables, we compute the Gaussian expected value of the quantity above

$$\overline{Z_J^n} = \mathrm{Tr}\, \overline{e^{\beta \sum_{a=1}^n \sum_{i>j} J_{ij}\sigma_i\sigma_j}} = \mathrm{Tr} \exp\left[\frac{\beta^2 J^2}{2N} \sum_{i>j} \left(\sum_a \sigma_i^a \sigma_j^a\right)^2\right]. \tag{2.34}$$

We now are confronted again with the task of decoupling variables interactions, but this time is between the replica indices, we will use again the identity

$$\left(\sum_{k=1}^N c_k\right)^2 = \sum_{k=1}^N c_k^2 + 2\sum_{l>k}^N c_l c_k = \sum_{k=1}^N c_k^2 + \sum_{l\neq k}^N c_l c_k, \tag{2.35}$$

that in our case yields

$$\frac{\beta^2 J^2}{2N} \sum_{i>j} \left(\sum_a \sigma_i^a \sigma_j^a\right)^2 = \frac{n\beta^2 J^2}{4}(N-1) + \frac{\beta^2 J^2}{N} \sum_{a>b} \sum_{i>j} \sigma_i^a \sigma_i^b \sigma_j^a \sigma_j^b. \tag{2.36}$$

Using (2.35) again to expand the $i > j$ sum on the right-hand side of the equation we arrive at

$$\frac{\beta^2 J^2}{N} \sum_{a>b} \sum_{i>j} \sigma_i^a \sigma_i^b \sigma_j^a \sigma_j^b = \frac{\beta^2 J^2}{2N} \sum_{a>b} \left(\sum_{i=1}^N \sigma_i^a \sigma_i^b\right)^2 - \frac{n\beta^2 J^2}{4}(n-1), \tag{2.37}$$

as we take the thermodynamic limit $N \to \infty$ we can consider $N - 1 \approx N$ in the first term of equation (2.36), and neglect the last term in equation (2.37) (as it just produces a constant factor that will go to zero when the $n \to 0$ limit is taken), hence

$$\overline{Z_J^n} = \mathrm{Tr}\exp\left[\frac{nN\beta^2J^2}{4} + \frac{N\beta^2J^2}{2}\sum_{a>b}\left(\frac{1}{N}\sum_{i=1}^{N}\sigma_i^a\sigma_i^b\right)^2\right]. \tag{2.38}$$

Once again, a form similar to (2.4) has been reached, where a suitable decoupling of the different lattice-site variables is required; this is achieved by means of (2.7). In this case the conjugated variable will be a matrix of the replica indices, set to be q_{ab}, with this consideration the equation above yields

$$\overline{Z_J^n} = e^{\frac{\beta^2J^2}{4}nN}\int\prod_{a>b}dq_{ab}e^{-\frac{N\beta^2J^2}{2}\sum_{a>b}q_{ab}^2}\,\mathrm{Tr}\,e^{\beta^2J^2\sum_{a>b}q_{ab}\sum_{i=1}^{N}\sigma_i^a\sigma_i^b}. \tag{2.39}$$

Finally, we are able to extract a factor of N from the sum over the lattice-sites, that are now *i.i.d.* random variables by virtue of the H-S transformation. We are now able to drop the i index so that the remaining spin variables will depend solely on the replica indices a and b. We then define the function[‡]

$$\mathcal{L}(\{\sigma^a\}) \equiv \beta^2J^2\sum_{a>b}q_{ab}\sigma^a\sigma^b, \tag{2.40}$$

so the exponential term affected by the trace in equation (2.39) can be re-expressed as

$$Tre^{\beta^2J^2\sum_{a>b}q_{ab}\sum_{i=1}^{N}\sigma_i^a\sigma_i^b} = e^{\log\mathrm{Tr}\exp[N\mathcal{L}(\{\sigma^a\})]}, \tag{2.41}$$

thereof transforming equation (2.39) into

$$\overline{Z_J^n} = \exp\left(\frac{nN\beta^2J^2}{4}\right)\int\mathcal{D}q_{ab}\exp\left[-\frac{N\beta^2J^2}{2}\sum_{a>b}q_{ab}^2 + N\log\mathrm{Tr}\,e^{\mathcal{L}(\{\sigma^a\})}\right]. \tag{2.42}$$

As $N \gg 1$, we can evaluate the integral above using the saddle-point method

$$\overline{Z_J^n} \approx \exp\left[\frac{nN\beta^2J^2}{4} - \frac{N\beta^2J^2}{2}\sum_{a>b}\left(q_{ab}^*\right)^2 + N\log\mathrm{Tr}\,e^{\mathcal{L}^*(\{\sigma^a\})}\right], \tag{2.43}$$

where $*$ denotes we have evaluated q_{ab} in its saddle-node value, q_{ab}^*. We now extract a factor nN and consider the limit $n \to 0$ while keeping N large but still finite, so we can expand the exponential as a series. Keeping just the first order term, yields

$$\overline{Z_J^n} \approx 1 + nN\left[\frac{\beta^2J^2}{4} - \frac{\beta^2J^2}{2n}\sum_{a>b}\left(q_{ab}^*\right)^2 + \frac{1}{n}\log\mathrm{Tr}\,e^{\mathcal{L}^*(\{\sigma^a\})}\right], \tag{2.44}$$

we may now extract a factor of N to work with the free energy density ($f_J = F_J/N$),

[‡]whose convenience shall become apparent when dealing with the soft-spins case

then inserting this in (2.29) we arrive at

$$\beta\overline{f_J} = \lim_{n\to 0}\left[-\frac{\beta^2 J^2}{4} + \frac{\beta^2 J^2}{2n}\sum_{a>b}(q^*_{ab})^2 - \frac{1}{n}\log \mathrm{Tr}\, e^{\mathcal{L}^*(\{\sigma^a\})}\right]. \tag{2.45}$$

2.2.1.2 Replica-symmetric solution

In order to evaluate the limit (2.45), we consider the simplest case, that of replica symmetry i.e. the fact that

$$q^*_{ab} = q \text{ for } a \neq b, \tag{2.46}$$

even-though we are neglecting the vast richness of the free-energy landscape inside the spin-glass phase with this assumption, the result provides a first approximation to the equilibrium and critical properties of the spin-glass phase, although testing the stability through the Replica Symmetry Breaking solution should attempt in future work; for the time being we will our analysis to the replica-symmetric scenario. Inserting explicitly this assumption into equation (2.45) yields

$$\beta\overline{f_J} = -\frac{1}{4}\beta^2 J^2 q^2 - \lim_{n\to 0}\frac{1}{n}\log \mathrm{Tr}\, e^{\mathcal{L}^*(\{\sigma^a\})}, \tag{2.47}$$

where we have neglected the constant term in (2.47). Making explicit the form of the $\mathcal{L}^*$ function in order to take the limit of vanishing replicas, equation (2.40) with condition (2.46) takes the form

$$\mathcal{L}(\{\sigma^a_i\}) = \beta^2 J^2 q \sum_{a>b}\sigma^a\sigma^b, \tag{2.48}$$

this in turn can be expanded using (2.35) again. Upon exponentiation of the function above, we subsequently use a H-S transformation in the arising squared-sum term, arriving at

$$e^{\mathcal{L}^*(\{\sigma^a_i\})} = \sqrt{\frac{\beta^2 J^2 q}{2\pi}}\int_{-\infty}^{\infty} dx \exp\left(-\frac{\beta^2 J^2 q}{2}x^2 + \beta^2 J^2 q x\sum_a \sigma^a - \frac{n}{2}\beta^2 J^2\ q\right), \tag{2.49}$$

after computing the trace of the expression above the only affected term will be the second term inside the exponential, that can be evaluated as

$$\mathrm{Tr}\exp\left(\beta^2 J^2\ qx\sum_a \sigma^a\right) = \prod_a\sum_{\{\sigma^a\}}\exp\left(\beta^2 J^2\ qx\sigma^a\right) = 2^n\cosh^n(\beta^2 J^2 qx), \tag{2.50}$$

all together can be written as

$$\mathrm{Tr}\, e^{\mathcal{L}^*(\{\sigma_i^a\})} = \int \mathcal{D}z \exp\Big[-\frac{n}{2}\beta^2 J^2 q + n\log(2\cosh(\beta J\sqrt{q}z))\Big], \tag{2.51}$$

where we have simplified our original expressing by using the change of variables

$$z = \beta J\sqrt{q}x, \tag{2.52}$$

and defined the Gaussian measure

$$\int \mathcal{D}z = \int_{-\infty}^{\infty} \frac{dz}{\sqrt{2\pi}} e^{-\frac{z^2}{2}}. \tag{2.53}$$

Returning to (2.45) we can now evaluate the $n \to 0$ limit by extracting a factor of n, then expanding the exponential for small n values and subsequently using the identity

$$\lim_{n\to 0} \frac{1}{n}\ln(1 + n\alpha) = \alpha; \tag{2.54}$$

all in all, we get

$$\beta\overline{f_J} = -\frac{\beta^2 J^2}{4}(1-q)^2 - \int \mathcal{D}z \log[2\cosh(\beta J\sqrt{q}z)], \tag{2.55}$$

after the several transformations introduced, we have arrived at the Landau-like free energy density of our model, depending on q, the corresponding order parameter.

2.2.1.3 Phase Transition

The extremum of the thermodynamic free energy w.r.t. its order parameter defines an equilibrium phase; i.e. as seen in the previous sections by extremizing the free energy we get the respective equation of state for the model. Usually we regard such extremum as a minimum, however, due to the nature of the limit $n \to 0$, this is not longer the case. The limit induces a change of sign, such that second order coefficient in the free energy becomes negative for $T > T_{sg}$; hence the paramagnetic solution ($q = 0$) corresponds to a maximum instead [13]. Therefore, extremizing w. r. t. q

$$\beta\frac{\partial\overline{f_J}}{\partial q} = \frac{\beta^2 J^2}{2}(q-1) + \int \mathcal{D}z\ \frac{\beta J}{2\sqrt{q}} z\ \tanh(\beta J\sqrt{q}z) = 0, \tag{2.56}$$

and after integrating by parts

$$q = \int \mathcal{D}z \tanh^2(\beta J\sqrt{q}z). \tag{2.57}$$

It is straight-forward to see that the equation of state (2.57) fulfills the paramagnetic solution ($q = 0$), while at low temperatures $q \neq 0$ and it corresponds to the spin-glass phase, thence q plays the role of the order parameter for our model.

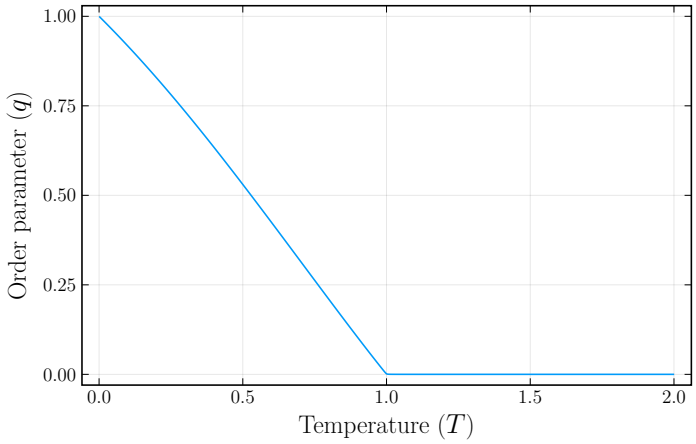

Figure 2.2 : Edwards-Anderson order parameter for the standard Sherrington-Kirkpatrick model, here the temperature scale is set such that $J/k_B = 1$.

We may expand equation (2.57) near criticality to obtain the critical temperature, by doing so we arrive at

$$q = \int \mathcal{D}z(\beta J\sqrt{q}z)^2, \tag{2.58}$$

solving for the critical temperature, T_{sg}, yields

$$\boxed{\beta_{sg}^2 = \frac{1}{J^2} \Rightarrow T_{sg} = \frac{J}{k_B}} \tag{2.59}$$

by setting the temperature scale $J/k_B = 1$, we are able to compare the above result with the numerical solution of equation (2.57), shown in Figure 2.2.

2.2.2 SK model with soft-spins

After examining in detail the two prior models, we are now able to merge both considerations in the present section: search for the critical temperature for a 1) soft-spin 2) disordered system; i.e. we will consider the soft version of the SK model. This will serve as the by-pass model to probe the accelerating dynamics of the swap algorithm with continuous spins, as will be discussed in later sections.

The Hamiltonian of the model is defined as

$$H_{SKSS}(\{\sigma_i\},\{\tau_i\}) = -\sum_{i>j} J_{ij}\tau_i\tau_j\sigma_i\sigma_j - \lambda_1\sum_{i=1}^{N}(\tau_i - 1) - \lambda_2\sum_{i=1}^{N}\left(\tau_i^2 - 1 - \frac{\Delta^2}{12}\right), \tag{2.60}$$

here the only difference w.r.t. (2.1) is that now as in (2.25) the couplings (J_{ij}) are now deemed *i.i.d.* random variables. Again, the $\{\tau_i\}$ variables are the *strength* or *length* of the spins, also a random variable sampled from some distribution $p(\{\tau_i\})$

for which we are setting the mean equal to 1 and its sample variance as $\Delta^2/12$ and, once again, σ_i is the standard Ising variable taking discrete values ± 1.

2.2.2.1 Free energy calculation for soft-spins

Here, we proceed in a similar fashion as in the SK-model. This time inside the partition function (Z_J) we should also take into account the distribution of spin-strengths, hence, equation (2.31) acquires the following form:

$$Z_J^n = \int \prod_i \mathcal{D}\left[s_i^{(1)}\right] e^{-\beta H_{SKSS}\left(\{s_i^{(1)}\}\right)} \dots \prod_i \mathcal{D}\left[s_i^{(n)}\right] e^{-\beta H_{SKSS}\left(\{s_i^{(n)}\}\right)}, \tag{2.61}$$

where we have set $s_i = \sigma_i \tau_i$. Repeating the procedure of the previous section, we can define the index a running over the replicas and the trace operator, so we will have the same expressions as (2.32) and (2.33) but with the change $H_{SK}\left(\{\sigma_i^{(1)}\}\right) \to H_{SKSS}\left(\{s_i^{(1)}\}\right)$. Moreover, the trace operator is redefined, as the degrees of freedom are no longer just standard Ising variables

$$\mathrm{Tr} \equiv \int \prod_{i,a} \mathcal{D}\left[s_i^{(a)}\right] = \sum_{\{\sigma_i^a\}} \int \prod_{i,a} dp(\tau_i^a), \tag{2.62}$$

where $dp(\tau_i^a)$ is just the probability measure that as in 2.1 we will just restrict it to have positive support.

Once again we compute the disorder-averaged partition function, concerning ourselves first with the n power of the function after introducing the replica trick

$$\begin{aligned} \overline{Z_J^n} &= \mathrm{Tr}\left\{ \overline{e^{\beta \sum_{a=1}^n \sum_{i>j} J_{ij} s_i s_j}} e^{\beta \sum_a \sum_i \left[\lambda_1(\tau_{i,a}-1)+\lambda_2\left(\tau_{i,a}^2-1-\frac{\Delta^2}{12}\right)\right]} \right\} \\ &= \mathrm{Tr}\, e^{\frac{\beta^2 J^2}{2N} \sum_{i>j}\left(\sum_a s_i^a s_j^a\right)^2 + \beta \sum_a \sum_i \left[\lambda_1(\tau_{i,a}-1)+\lambda_2\left(\tau_{i,a}^2-1-\frac{\Delta^2}{12}\right)\right]}, \end{aligned} \tag{2.63}$$

note that the second exponential factor (dependent on the lagrange multipliers) is unaffected by the disorder-average. Moreover, these coincide again with the definition in (2.6), with the modification of adding the replica index a

$$\psi_i^a(\tau_{i,a}) = -\lambda_2 \tau_{i,a}^2 - \lambda_1 \tau_{i,a} + \lambda_1 + \lambda_2 \left(1 + \frac{\Delta^2}{12}\right), \tag{2.64}$$

we now proceed then by using (2.35) only to the first exponential term to produce

$$\mathrm{Tr}\, e^{\frac{\beta^2 J^2}{2N}\left[\sum_{a>b}\left(\sum_i \tau_i^a \tau_i^b \sigma_i^a \sigma_i^b\right)^2 - \sum_{a>b}\sum_i (\tau_i^a \tau_i^b)^2 + \sum_a \sum_{i>j} (\tau_i^a \tau_j^a)^2\right]}, \tag{2.65}$$

where we have made explicit the form of the soft-spin variable s_i. Notice that the last two sums in the exponential will depend solely on $\{\tau_i^a\}$. Again, using a rearrangement of (2.35)

$$\sum_{i>j}\tau_{i,a}^2\tau_{j,a}^2=\frac{1}{2}\left(\sum_i\tau_{i,a}^2\right)^2-\frac{1}{2}\sum_i\tau_{i,a}^4, \tag{2.66}$$

and after neglecting the terms[§] sub-leading in N (as their contribution to the free energy will vanish in the thermodynamic limit) we obtain

$$\overline{Z_J^n}=\mathrm{Tr}\,e^{\frac{1}{2}NJ^2\beta^2\left[\sum_{a>b}\left(\frac{1}{N}\sum_i\tau_i^a\tau_i^b\sigma_i^a\sigma_i^b\right)^2+\frac{1}{2}\sum_a\left(\frac{1}{N}\sum_i(\tau_i^a)^2\right)^2\right]-\beta\sum_{i,a}\psi_i^a(\tau_{i,a})}, \tag{2.67}$$

and we may now use the H-S transformation to each of the two terms in (2.67)

$$\exp\left[\frac{1}{2}NJ^2\beta^2\sum_{a>b}\left(\frac{1}{N}\sum_i\tau_i^a\tau_i^b\sigma_i^a\sigma_i^b\right)^2\right]$$
$$=\prod_{a>b}\sqrt{\frac{NJ^2\beta^2}{2\pi}}\int_{-\infty}^{\infty}dq_{ab}\exp\left(-\frac{N}{2}J^2\beta^2q_{ab}^2+J^2\beta^2q_{ab}\sum_i\tau_i^a\tau_i^b\sigma_i^a\sigma_i^b\right) \tag{2.68}$$

$$\exp\left[\frac{1}{4}NJ^2\beta^2\sum_a\left(\frac{1}{N}\sum_i\tau_{i,a}^2\right)^2\right]$$
$$=\prod_a\sqrt{\frac{NJ^2\beta^2}{4\pi}}\int_{-\infty}^{\infty}d\phi_a\exp\left(-\frac{N}{4}J^2\beta^2\phi_a^2+\frac{1}{2}J^2\beta^2\phi_a\sum_i(\tau_i^a)^2\right) \tag{2.69}$$

dropping the constant factors and re-inserting the products into the integrals (by defining $\mathcal{D}[\phi_a,q_{ab}]=\prod_a d\phi_a\prod_{a>b}dq_{ab}$) we get

$$\overline{Z_J^n}=\int\mathcal{D}[\phi_a,q_{ab}]\exp\left[-\frac{N}{2}J^2\beta^2\left(\sum_{a>b}q_{ab}^2+\frac{1}{2}\sum_a\phi_a^2\right)\right]\mathrm{Tr}\,e^{\mathcal{L}'(\{t_i^a,\sigma_i^a\})}, \tag{2.70}$$

here

$$\mathcal{L}'(\{t_i^a,\sigma_i^a\})=\beta^2J^2\sum_{a>b}q_{ab}\sum_i\tau_i^a\sigma_i^a\tau_i^b\sigma_i^b+\frac{1}{2}\beta^2J^2\sum_{i,a}\phi_a\tau_{i,a}^2-\beta\sum_{i,a}\psi_i^a(\tau_{i,a}); \tag{2.71}$$

moreover, we have fully decoupled the spin site variables within this last expression, and we are now able to extract the sum over i as a product outside the exponential. We safely drop the index i as we include a factor of N, and now, as with the standard

[§]those terms being: $-\frac{1}{N^2}\sum_i\sum_{a>b}(\tau_i^a\tau_i^b)^2$ and $-\frac{1}{2N^2}\sum_a\sum_i\tau_{i,a}^4$

calculation, we can re-define the trace term as

$$\mathrm{Tr}\exp[\mathcal{L}'(\{\tau_i^a,\sigma_i^a\})] = \exp\left[N\log\mathrm{Tr}\, e^{\mathcal{L}(\{\tau_a,\sigma_a\})}\right], \tag{2.72}$$

where

$$\mathcal{L}(\{t_a,\sigma_a\}) = \beta^2 J^2 \sum_{a>b} q_{ab}\tau_a\tau_b\sigma_a\sigma_b + \frac{1}{2}\beta^2 J^2 \sum_a \phi_a\tau_a^2 - \beta\sum_a \psi_a(\tau_a), \tag{2.73}$$

hence

$$\overline{Z_J^n} = \int \mathcal{D}[\phi_a, q_{ab}] \exp\left[-\frac{N}{2}J^2\beta^2\left(\sum_{a>b} q_{ab}^2 + \frac{1}{2}\sum_a \phi_a^2\right) + N\log\mathrm{Tr}\, e^{\mathcal{L}(\{\tau_a,\sigma_a\})}\right]. \tag{2.74}$$

Once again, we use the saddle-point method to solve the integral above, under the proper considerations

$$\overline{Z_J^n} \approx \exp\left\{-\frac{N}{2}J^2\beta^2\left[\sum_{a>b}(q_{ab}^*)^2 + \frac{1}{2}\sum_a(\phi_a^*)^2\right] + N\log\mathrm{Tr}\, e^{\mathcal{L}^*(\{\tau_a,\sigma_a\})}\right\}, \tag{2.75}$$

by extracting the factor nN and consider the limit $n\to 0$ while keeping N large but still finite, so we expand the first order term in the exponential

$$\overline{Z_J^n} \;\approx\; 1 - nN\left\{\frac{1}{2n}\beta^2 J^2\left[\sum_{a>b}(q_{ab}^*)^2 + \frac{1}{2}\sum_a(\phi_a^*)^2\right] - \frac{1}{n}\log\mathrm{Tr}\, e^{\mathcal{L}^*(\{\tau_a,\sigma_a\})}\right\}. \tag{2.76}$$

Finally, evaluating for the free energy density ($f = F/N$) we get

$$\beta\overline{f_J} = \lim_{n\to 0}\left\{\frac{1}{2n}J^2\beta^2\left[\sum_{a>b}(q_{ab}^*)^2 + \frac{1}{2}\sum_a(\phi_a^*)^2\right] - \frac{1}{n}\log\mathrm{Tr}\, e^{\mathcal{L}^*(\{\tau_a,\sigma_a\})}\right\} \tag{2.77}$$

2.2.2.2 Replica-symmetric solution

Once again we probe the replica-symmetric solution of the model, we consider the usual condition (2.46), plus a new one for the other variable depending on the replica label

$$\phi_a^* = \phi, \tag{2.78}$$

inserting both assumptions into (2.77)

$$\beta\overline{f_J} = -\frac{1}{4}J^2\beta^2q^2 + \frac{1}{4}J^2\beta^2\phi^2 - \lim_{n\to 0}\frac{1}{n}\log \mathrm{Tr}\, e^{\mathcal{L}(\{\tau_a,\sigma_a\})} \tag{2.79}$$

with

$$\begin{aligned}\mathcal{L}(\{\tau_a,\sigma_a\}) = &\frac{1}{2}\beta^2J^2q\left(\sum_a \tau_a\sigma_a\right)^2 - \frac{1}{2}\beta^2J^2q\sum_a\tau_a^2 \\ &+ \sum_a\left[\left(\frac{1}{2}\beta^2J^2\phi + \beta\lambda_2\right)\tau_a^2 + \beta\lambda_1\tau_a - \beta\lambda_1 - \beta\lambda_2\left(1+\frac{\Delta^2}{12}\right)\right],\end{aligned} \tag{2.80}$$

that for reasons that will become apparent in following calculations, it is convenient to define the last term as

$$\Psi_a(\tau_a;\phi,\lambda_1,\lambda_2) = \left(\frac{1}{2}\beta^2J^2\phi + \beta\lambda_2\right)\tau_a^2 + \beta\lambda_1\tau_a - \beta\lambda_1 - \beta\lambda_2\left(1+\frac{\Delta^2}{12}\right), \tag{2.81}$$

both last terms are already decoupled terms of the replicas, so we proceed with a H-S transformation for the remaining one

$$e^{\frac{1}{2}\beta^2J^2q\left(\sum_a\tau_a\sigma_a\right)^2} = \sqrt{\frac{\beta^2J^2q}{2\pi}}\int_{-\infty}^{\infty}dx\exp\left(-\frac{1}{2}\beta^2J^2qx^2 + \beta^2J^2qx\sum_a\tau_a\sigma_a\right), \tag{2.82}$$

the first term inside the integral of (2.82) is unaffected by the trace operator, while the remaining term plus the two untouched terms of (2.80) are. Thence, we are able to take the trace operator as

$$\begin{aligned}\mathrm{Tr}\, e^{\sum_a\left[-\frac{1}{2}\beta^2J^2q(\tau_a^2-2x\tau_a\sigma_a)+\Psi_a(\tau_a;\phi,\lambda_1,\lambda_2)\right]} &= \sum_{\{\sigma_a\}}\prod_a\int dp(\tau_a)e^{-\frac{1}{2}\beta^2J^2q(\tau_a^2-2x\tau_a\sigma_a)+\Psi_a(\tau_a;\phi,\lambda_1,\lambda_2)} \\ &= \left[\int dp(\tau)2e^{-\frac{1}{2}\beta^2J^2q\tau^2+\Psi(\tau;\phi,\lambda_1,\lambda_2)}\cosh\left(\beta^2J^2qx\tau\right)\right]^n,\end{aligned}$$

thence arriving at a new form of the exponential term (now independent of $\{\sigma_a,\,\tau_a\}$)

$$\mathrm{Tr}\, e^{\mathcal{L}} = \sqrt{\frac{\beta^2J^2q}{2\pi}}\int_{-\infty}^{\infty}dxe^{-\frac{1}{2}\beta^2J^2qx^2}\left[\int dp(\tau)2e^{-\frac{1}{2}\beta^2J^2q\tau^2+\Psi(\tau;\phi,\lambda_1,\lambda_2)}\cosh\left(\beta^2J^2qx\tau\right)\right]^n,$$

in order to isolate the q and ϕ dependence as much as possible, the equation above can be recast by using (2.52), and introducing (2.53) while denoting the integral inside the square parenthesis above as $I(z;q,\phi,\lambda_1,\lambda_2)$

$$\mathrm{Tr}\, e^{\mathcal{L}} = \int \mathcal{D}z[I(z;q,\phi,\lambda_1,\lambda_2)]^n, \tag{2.83}$$

then setting $[I(z;q,\phi,\lambda_1,\lambda_2)]^n = e^{\log[I(z;q,\phi,\lambda_1,\lambda_2)]^n} = e^{n\log I(z;q,\phi,\lambda_1,\lambda_2)}$ and expand for $n \ll 1$

$$\mathrm{Tr}\, e^{\mathcal{L}} = 1 + n \int \mathcal{D}z \;\; \log I(z;q,\phi,\lambda_1,\lambda_2), \tag{2.84}$$

and we are now able to take the limit of the replicas going to zero by using the identity (2.54). Finally, the disorder-averaged free energy acquires the form

$$\beta\overline{f_J} = -\frac{1}{4}\beta^2 J^2(q^2-\phi^2) - \int \mathcal{D}z \log I(z;q,\phi,\lambda_1,\lambda_2), \tag{2.85}$$

stressing out again that we have defined

$$I(z;q,\phi,\lambda_1,\lambda_2) = \int dp(\tau) 2e^{-\frac{1}{2}\beta^2 J^2 q\tau^2 + \Psi(\tau;\phi,\lambda_1,\lambda_2)} \cosh(\beta J\sqrt{q}z\tau). \tag{2.86}$$

It is straightforward to see that for $dp(\tau) = \delta(t-1)dt$, i.e. the case where the spin-strengths are fixed to 1, $\phi = 1$ i.e. the self-overlap for classic Ising variables [14], and the constraints are lifted ($\lambda_1 = 0, \lambda_2 = 0$) the standard SK-model is recovered

$$\Psi(\tau;\phi=1,\lambda_1=0,\lambda_2=0) = \frac{1}{2}\beta^2 J^2\tau^2 \tag{2.87}$$

$$\begin{aligned} I(z;q,\phi,\lambda_1,\lambda_2) &= \int_0^\infty d\tau\delta(\tau-1)\exp\left[-\frac{1}{2}\beta^2J^2(q-1)\tau^2\right]\cosh(\beta J\sqrt{q}z\tau) \\ &= \exp\left[-\frac{1}{2}\beta^2J^2(q-1)\right]\cosh(\beta J\sqrt{q}z), \end{aligned} \tag{2.88}$$

yields

$$\beta\overline{f_J} = -\frac{\beta^2J^2}{4}(1-q)^2 - \int \mathcal{D}z \log[2\cosh(\beta Jz\sqrt{q})], \tag{2.89}$$

that coincides with equation (2.55).

2.2.2.3 Equations of state

As we discussed before, we search for an extremum of the free energy as the equilibrium condition. However, we now have three new parameters to extremize: the new defined self-overlap (now different from 1) and both Lagrange multipliers, for the first and second moments of the distribution.
For he self-overlap we have

$$\beta\frac{\partial\overline{f_J}}{\partial\phi} = 0, \tag{2.90}$$

$$\phi = \int \mathcal{D}z \left[\frac{\int dp(\tau)\tau^2 \cosh\left(\beta J\sqrt{q}z\tau\right) e^{-\frac{1}{2}\beta^2 J^2 q\tau^2 + \Psi(\tau;\phi,\lambda_1,\lambda_2)}}{\int dp(\tau) \cosh\left(\beta J\sqrt{q}z\tau\right) e^{-\frac{1}{2}\beta^2 J^2 q\tau^2 + \Psi(\tau;\phi,\lambda_1,\lambda_2)}} \right], \tag{2.91}$$

for the replica overlap

$$\beta \frac{\partial \overline{f_J}}{\partial q} = 0, \tag{2.92}$$

$$q = \phi - \frac{1}{\beta J\sqrt{q}} \int \mathcal{D}z \left[\frac{\int dp(\tau) z\tau \sinh\left(\beta J\sqrt{q}z\tau\right) e^{-\frac{1}{2}\beta^2 J^2 q\tau^2 + \Psi(\tau;\phi,\lambda_1,\lambda_2)}}{\int dp(\tau) \cosh\left(\beta J\sqrt{q}z\tau\right) e^{-\frac{1}{2}\beta^2 J^2 q\tau^2 + \Psi(\tau;\phi,\lambda_1,\lambda_2)}} \right], \tag{2.93}$$

and for the Lagrange multipliers

$$\beta \frac{\partial \overline{f_J}}{\partial \lambda_1} = 0, \qquad \beta \frac{\partial \overline{f_J}}{\partial \lambda_2} = 0, \tag{2.94}$$

$$\int \mathcal{D}z \left[\frac{\int dp(\tau)\tau \cosh\left(\beta J\sqrt{q}z\tau\right) e^{-\frac{1}{2}\beta^2 J^2 q\tau^2 + \Psi(\tau;\phi,\lambda_1,\lambda_2)}}{\int dp(\tau) \cosh\left(\beta J\sqrt{q}z\tau\right) e^{-\frac{1}{2}\beta^2 J^2 q\tau^2 + \Psi(\tau;\phi,\lambda_1,\lambda_2)}} \right] = 1, \tag{2.95}$$

$$\int \mathcal{D}z \left[\frac{\int dp(\tau)\tau^2 \cosh\left(\beta J\sqrt{q}z\tau\right) e^{-\frac{1}{2}\beta^2 J^2 q\tau^2 + \Psi(\tau;\phi,\lambda_1,\lambda_2)}}{\int dp(\tau) \cosh\left(\beta J\sqrt{q}z\tau\right) e^{-\frac{1}{2}\beta^2 J^2 q\tau^2 + \Psi(\tau;\phi,\lambda_1,\lambda_2)}} \right] = 1 + \frac{\Delta^2}{12}. \tag{2.96}$$

Investigating the equations above at the high temperature limit ($\beta \to 0$), we see that $\Psi \to 0$ and find the equations

$$\begin{aligned} q &= 0 \\ \phi &= \int dp(\tau)\tau^2, \end{aligned} \tag{2.97}$$

confirming the vanishing order parameter in the disordered high-temperature phase. Moreover, is clear that ϕ, is indeed a parameter controlling the fluctuations of the spin-strengths (the second moment for our chosen distribution $p(\tau)$).

We can now proceed in a similar fashion to what we did in 2.1 to find the critical temperature of the model. In this case we shall defined the new operator

$$\mathcal{E}_\tau[...] \equiv \int dp(\tau) e^{\Psi(\tau;\phi,\lambda_1,\lambda_2)}[...], \tag{2.98}$$

where one should stress out that this operator still depends implicitly of ϕ, λ_1 and λ_2. We proceed to expand the functions dependent on q up to $\mathcal{O}(q)$. First we take into account the common denominator

$$\begin{aligned}\mathcal{E}_\tau[\cosh(\beta J\sqrt{q}z\tau)e^{-\frac{1}{2}\beta^2J^2q\tau^2}] &\approx \mathcal{E}_\tau\left[\left(1-\frac{1}{2}\beta^2J^2q\tau^2\right)\left(1+\frac{1}{2}\beta^2J^2qz^2\tau^2\right)\right]\\ &= \mathcal{E}_\tau\left[1-\frac{1}{2}\beta^2J^2q\tau^2(1-z^2)+\mathcal{O}(q^2)\right]\\ &\approx \mathcal{E}_\tau[1]-\frac{1}{2}\beta^2J^2q(1-z^2)\mathcal{E}_\tau[\tau^2],\end{aligned} \tag{2.99}$$

where again notice that $\mathcal{E}_\tau[1] \neq 1$ as the operator is not normalized.
Now, for the numerators of each equation, starting with the ϕ variable

$$\begin{aligned}\mathcal{E}_\tau[\tau^2\cosh(\beta J\sqrt{q}z\tau)e^{-\frac{1}{2}\beta^2J^2q\tau^2}] &\approx \mathcal{E}_\tau\left[\tau^2\left(1-\frac{1}{2}\beta^2J^2q\tau^2\right)\left(1+\frac{1}{2}\beta^2J^2qz^2\tau^2\right)\right]\\ &= \mathcal{E}_\tau\left[\tau^2-\frac{1}{2}\beta^2J^2q\tau^4(1-z^2)+\mathcal{O}(q^2)\right]\\ &\approx \mathcal{E}_\tau[\tau^2]-\frac{1}{2}\beta^2J^2q(1-z^2)\mathcal{E}_\tau[\tau^4],\end{aligned} \tag{2.100}$$

that is actually the same for the second multiplier λ_2 and the first multiplier has just one less power of τ, so it yields

$$\mathcal{E}_\tau[\tau\cosh(\beta J\sqrt{q}z\tau)e^{-\frac{1}{2}\beta^2J^2q\tau^2}] \approx \mathcal{E}_\tau[\tau]-\frac{1}{2}\beta^2J^2q(1-z^2)\mathcal{E}_\tau[\tau^3], \tag{2.101}$$

finally, for the numerator of the order parameter q

$$\begin{aligned}&\mathcal{E}_\tau\left[\frac{z\tau}{\beta J\sqrt{q}}\sinh(\beta J\sqrt{q}z\tau)e^{-\frac{1}{2}\beta^2J^2q\tau^2}\right]\\ &\approx \mathcal{E}_\tau\left[\left(\frac{z\tau}{\beta J\sqrt{q}}-\frac{z\tau}{2}\beta J\sqrt{q}\tau^2\right)\left(\beta J\sqrt{q}z\tau+\frac{1}{6}\left[\beta^2J^2qz^2\tau^2\right]^{3/2}\right)\right]\\ &= \mathcal{E}_\tau\left[z^2\tau^2+\frac{1}{6}\beta^2J^2z^4\tau^4q-\frac{1}{2}\beta^2J^2z^2\tau^4q+\mathcal{O}(q^2)\right]\\ &\approx z^2\mathcal{E}_\tau\left[\tau^2\right]+\beta^2J^2q\left(\frac{z^4}{6}-\frac{z^2}{2}\right)\mathcal{E}_\tau\left[\tau^4\right].\end{aligned} \tag{2.102}$$

All together, we expand again the denominator as a binomial series of the form

$$\begin{aligned}&\mathcal{E}_\tau[1]\left(1-\frac{1}{2}\beta^2J^2q(1-z^2)\frac{\mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1]}\right)^{-1}\\ &\qquad= \mathcal{E}_\tau^{-1}[1]\left(1+\frac{1}{2}\beta^2J^2q(1-z^2)\frac{\mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1]}+\mathcal{O}(q^2)\right),\end{aligned} \tag{2.103}$$

then joining all numerators and denominators for each equation on ϕ, q, λ_1 and λ_2 respectively, we get

$$\begin{aligned}\phi &\approx \int \mathcal{D}z\mathcal{E}_\tau^{-1}[1]\left(1+\frac{1}{2}\beta^2J^2q(1-z^2)\frac{\mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1]}\right)\left(\mathcal{E}_\tau[\tau^2]-\frac{1}{2}\beta^2J^2q(1-z^2)\mathcal{E}_\tau[\tau^4]\right)\\ &= \int \mathcal{D}z\left(\frac{\mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1]}-\frac{1}{2}\beta^2J^2q(1-z^2)\frac{\mathcal{E}_\tau[\tau^4]}{\mathcal{E}_\tau[1]}+\frac{1}{2}\beta^2J^2q(1-z^2)\frac{\mathcal{E}_\tau^2[\tau^2]}{\mathcal{E}_\tau^2[1]}+\mathcal{O}(q^2)\right)\\ &\approx \frac{\mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1]}\end{aligned} \tag{2.104}$$

$$\begin{aligned}q &\approx \phi-\int \mathcal{D}z\mathcal{E}_\tau^{-1}[1]\left(1+\frac{1}{2}\beta^2J^2q(1-z^2)\frac{\mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1]}\right)\left(z^2\mathcal{E}_\tau\left[\tau^2\right]+\beta^2J^2q\left(\frac{z^4}{6}-\frac{z^2}{2}\right)\mathcal{E}_\tau\left[\tau^4\right]\right)\\ &= \phi-\int \mathcal{D}z\left(z^2\frac{\mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1]}+\beta^2J^2q\left(\frac{z^4}{6}-\frac{z^2}{2}\right)\frac{\mathcal{E}_\tau\left[\tau^4\right]}{\mathcal{E}_\tau[1]}+\frac{1}{2}\beta^2J^2qz^2(1-z^2)\frac{\mathcal{E}_\tau^2[\tau^2]}{\mathcal{E}_\tau^2[1]}+\mathcal{O}(q^2)\right)\\ &\approx \phi-\frac{\mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1]}+\beta^2J^2q\frac{\mathcal{E}_\tau^2[\tau^2]}{\mathcal{E}_\tau^2[1]}=\beta^2J^2q\frac{\mathcal{E}_\tau^2[\tau^2]}{\mathcal{E}_\tau^2[1]}\end{aligned} \tag{2.105}$$

$$\begin{aligned}&\int \mathcal{D}z\mathcal{E}_\tau^{-1}[1]\left(1+\frac{1}{2}\beta^2J^2q(1-z^2)\frac{\mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1]}\right)\left(\mathcal{E}_\tau[\tau]-\frac{1}{2}\beta^2J^2q(1-z^2)\mathcal{E}_\tau[\tau^3]\right)\\ &\quad= \int \mathcal{D}z\left(\frac{\mathcal{E}_\tau[\tau]}{\mathcal{E}_\tau[1]}-\frac{1}{2}\beta^2J^2q(1-z^2)\frac{\mathcal{E}_\tau[\tau^3]}{\mathcal{E}_\tau[1]}+\frac{1}{2}\beta^2J^2q(1-z^2)\frac{\mathcal{E}_\tau[\tau^2]\mathcal{E}_\tau[\tau]}{\mathcal{E}_\tau^2[1]}+\mathcal{O}(q^2)\right)\\ &\quad= \frac{\mathcal{E}_\tau[\tau]}{\mathcal{E}_\tau[1]}\approx 1\end{aligned} \tag{2.106}$$

as the equation for λ_2 is exactly the same as for ϕ, we conclude

$$\phi \approx \frac{\mathcal{E}_\tau[\tau^2]}{\mathcal{E}_\tau[1]} \approx 1+\frac{\Delta^2}{12} \tag{2.107}$$

hence finding the closed form of the critical temperature as a function of Δ

$$\frac{k_BT_{sg}}{J} \approx 1+\frac{\Delta^2}{12}. \tag{2.108}$$

Note that the form of the critical temperatures for the disorder-less case is conserved. The only remaining difference comes with the explicit form of the operator $\mathcal{E}_\tau[...]$, this just complicates further the numerical solution of the equations of state although the increasing quadratic behaviour of the critical temperature remains.

Chapter 3

Numerical Simulations

3.1 Single-Spin-Flip Dynamics with Metropolis' rates

The simplest approach to model the evolution of spin-systems is by means of a Monte-Carlo (MC) simulation. Several versions of the algorithm have been explored in the past [15], we restrict ourselves to the simplest case of a Markov Chain Monte Carlo with Glauber kinetics. The procedure consists of

1. Starting with some randomly generated spin configuration $\mathbf{S}_0$*
2. A new trial configuration is proposed, which differs from the previous one by just a single spin flip (Glauber), $\mathbf{S}^{tr}_{i+1}$
3. The trial configuration is accepted as the one following $\mathbf{S}_i$ with some acceptance probability $w(\mathbf{S}^{tr}_{i+1}|\mathbf{S}_i)$. If rejected, the next configuration in the Markov chain will correspond to the previous one $\mathbf{S}_i$.

We require the acceptance probability defined above to be such that, after several iterations of the procedure, it properly samples spin configurations in agreement with the Boltzmann distribution, i.e. $w(\mathbf{S}^{tr}_{i+1}|\mathbf{S}_i)$ should fulfill *detailed balance*. This condition, for two spin configurations $\mathbf{S}$ and $\mathbf{S}'$ with a differing spin flip between each other, is expressed as

$$w(\mathbf{S}|\mathbf{S}')P_{eq}(\mathbf{S}') = w(\mathbf{S}'|\mathbf{S})P_{eq}(\mathbf{S}), \tag{3.1}$$

where the equilibrium probabilities P_{eq} are precisely Boltzmann distributions.

There are several ways of choosing the acceptance probabilities for the condition above to be fulfilled, during the present work we consider the standard Metropolis' choice

$$w(\mathbf{S}'|\mathbf{S}) = \min\{1, \exp[-\beta(E(\mathbf{S}) - E(\mathbf{S}'))]\}, \tag{3.2}$$

although others are possible, such as heat-bath acceptance rates [16]. Moreover, we will adopt the convention of defining our MC steps system-size independent i.e. defining the time unit as the MC step per site, so for a system of size N a MC time-step will refer to N attempted moves of flipping a random spin in the lattice, with every spin having probability $1/N$ of being selected. The pseudo-code for the implementation of the Metropolis' step can be seen in **Algorithm 1**.

*This configuration, of each spin pointing in either direction with a probability 1/2 is the typical configuration of a sample at $T = \infty$, while the completely ordered phase, that of every spin pointing parallel to each other, hence $T = 0$, is another possible choice of the initial condition. However, during the present work, we will always choose $T = \infty$, unless otherwise stated.

Algorithm 1 Metropolis rule for Monte-Carlo step

procedure MCSTEP(**S**, **J**)
  Initialize **S** randomly
  for $k \in \{1, 2, ..., N\}$ **do**
    $\Delta E = 2 \sum_{i(\neq k)}^{N} J_{ik} S_i S_k$
    $P_{acc} = \exp(-\beta \Delta E)$
    if $P_{acc} > rand() \in [0, 1)$ **then**
      $S_k \leftarrow -S_k$
    end if
  end for
end procedure

We have chosen this procedure to be our benchmark case when measuring the performance of the SWAP algorithm, yet to be defined in the following chapters. With it, we are able to measure several quantities such as energy, magnetization and, the auto-correlation functions (ACF), among others. We will devote our attention in the last of this quantities as it provides us with rich information regarding the evolution dynamics of the system[†]. We have also set periodic boundary conditions to diminish the finite size effects.

3.2 Quench dynamics & the ACF

Before diving deeper into the subtleties and details of the simulations, we need to understand the underlying dynamics of any system that can be separated into two equilibrium phases; an ordered phase below some critical temperature T_c and a disordered one above it. As stated before, we start with some initial condition in one of the extremes of the critical line, say at $T = \infty$, and perform a rapid quench to a desired temperature T_F. This will correspond, in our computational setting, of passing the configurations through the algorithm described in the previous section, but any possible choice of suitable dynamics should produce the same behaviour.

Take $T_F > T_c$, the system is obliged to pass from a configuration with vanishing correlation length ($\xi = 0$) towards one with a finite one ($0 < \xi(T_F) < \infty$) this leads to a finite relaxation time (t_{eq}). Nevertheless, for $T_F \leq T_c$, the correlation length diverges in the thermodynamic limit and, as the correlation length scales as a power law [17], we are deemed to have ever-increasing relaxation times with system size, this is known as *aging phenomena*. While studying these quenches, since t_{eq} is infinite, the only relevant time scale we are able to probe is that of "the age of the sample" t_w, that we will call the *waiting time*, and compared it to the observational time t[‡]; this is achieved by the auto-correlation function, defined in our model as

[†]As it is also the case with other two-time observables, like the auto-response function $R(t, t_w)$, that however, we will not discuss during the present work.

[‡]Actually $t - t_w$ as we are considering in the following t to span the entire evolution of the dynamics.

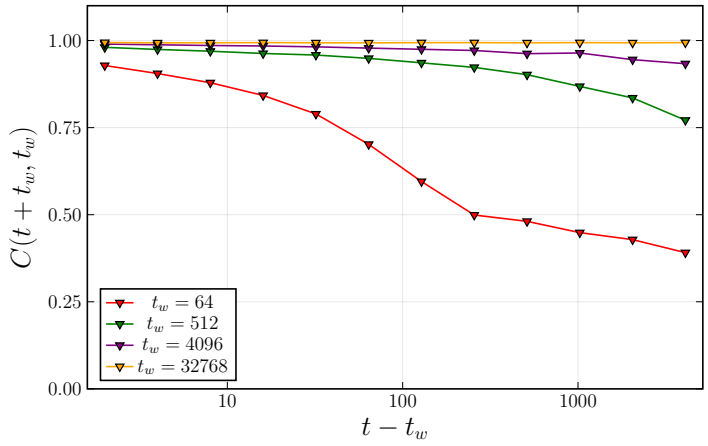

Figure 3.1 : ACF for 2D Ising model ($L = 40$, $T_F = 0.53T_c$). The quasi-equilibrium regime is evident for $t_w = 32769$ while for $t_w = 512, 4096$ aging manifests. The lowest waiting time $t_w = 64$ doesn't even reach the same plateau, we can conclude that t_w is not large enough to have a separation of time scales and we are just witnessing the decay due to the thermal fluctuations inside the domains.

$$C(t_w, t_w + t) = \frac{1}{N}\sum_{i=1}^{N}\langle S_i(t_w)S_i(t_w + t)\rangle \tag{3.3}$$

where $\langle ...\rangle$ is the standard thermal average, and both times will be measured in units of MC steps. Given a large enough t_w is possible to observe a separation of timescales. At the short timescale, $t - t_w \ll t_w$, we are in a quasi-equilibrium regime where the system appears to have relaxed to equilibrium at the quenched temperature T_F and the auto-correlation function becomes time-translation-invariant

$$C(t_w, t_w + t) = C_{eq}(t - t_w, T_F), \tag{3.4}$$

we then say the system is ageless and it has apparently reached a plateau, in the ACF as seen in Figure 3.1, where we have computed the ACF for an Ising 2d model, for several ages of the system. In terms of domain growth this would correspond to a relaxation of the thermal fluctuations inside big domains of parallel spins, while the domains themselves remain frozen. As we reach $t - t_w \sim t_w$ the system "realizes" it is not in equilibrium and its purely out-of-equilibrium behaviour becomes apparent; again, under the domain growth view, this is associated to the motion of the domain walls composing the system. This last behaviour defines the start of the second timescale, the large timescale where $t - t_w \gg t_w$, this is the aging regime where ACFs start decaying.

The exact functional form of the aging regime is unknown and depends on the model of consideration, within a model of simple aging one can express it as the product of a power law of t_w with a scaling function also dependent of both observational and waiting times. In a more general way, one can define the ACF as

$$C(t, t_w) = C_{eq}(t - t_w, T_F) + C_{ag}\left(\frac{h(t + t_w)}{h(t_w)}\right), \tag{3.5}$$

where $h(t)$ is an unknown increasing function with time, and C_{ag} is a scaling function. It is worth noting that this behaviour breaks at criticality (i.e. when the quenched temperature is $T_F = T_c$), and the functional form of ACF should be separated as a product of the quasi-equilibrium and aging regimes [18].

Notice that, for large enough systems ($L \to \infty$), the plateau at the quasi-equilibrium regime defines the Edwards-Anderson order parameter,

$$q_{EA} = \lim_{t\to\infty} \lim_{t_w\to\infty} C(t_w, t_w + t), \tag{3.6}$$

that in the disorder-less coincides with the magnetization squared; as can be seen that for a quench performed at higher-temperatures t_{eq} is finite and the system becomes age-less, decaying towards zero for several t_w, hence yielding the value of zero for the limit above (i.e. $M = 0$, as it should be for the disordered paramagnetic phase). Recall hence that $q_{EA} = q_{EA}(T)$ and for $q_{EA}(T = 0) = 1$, that coincides with the equilibrium value of the magnetization density. However, this apparent equilibrium can always be broken for a finite t_w, as we go deeper into larger observation times the system is always able to escape far from the initial configuration reached at t_w; leading to weak-ergodicity breaking [19], for which the commutativity of the limits in (3.6) breaks down

$$\lim_{t\to\infty} \lim_{t_w\to\infty} C(t_w, t_w + t) = 0. \tag{3.7}$$

A system undergoing strong-ergodicity breaking for infinite times lacks definite stable states in the phase phase, for which the system can relax to, while for the weak case the dynamic behaviour of the states depend in the initial conditions. See that a relaxation is possible for a quench from $T = \infty$ to $T_F > T_c$, this condition is symmetric for a quench on the other extreme of the critical line, the relaxation time is still finite for a quench from $T = 0$ towards $T_F < T_c$; for initial conditions close (not crossing T_c) to the equilibrium state there's a fast relaxation process and aging is not present.

This aging behaviour becomes ubiquitous in disordered systems like spin-glasses. The relaxation times at low temperatures in spin-glass systems becomes exceedingly large, as there are a plethora of meta-stable configurations within the frustrated system that lead to extremely slow dynamics. Therefore, the waiting times required to assess the quasi-equilibrium plateau in the ACF will become increasingly large with system size at low temperatures. This can be seen in Figure 3.2 where we have recreated the results of Takayama et al [20] for the case of the SK model.
As we decrease the temperature of the system the number of overlapping curves for different waiting times decrease, clearly revealing the presence of aging behaviour.

In the following we have performed simulations for several systems, with our main interest being the 3D Edwards-Anderson model, basically, a 3D Ising model with couplings $\{J_{ij}\}$ promoted to random variables taken from some distribution, as the SK-model, but with just nearest-neighbor interactions. This system has been studied

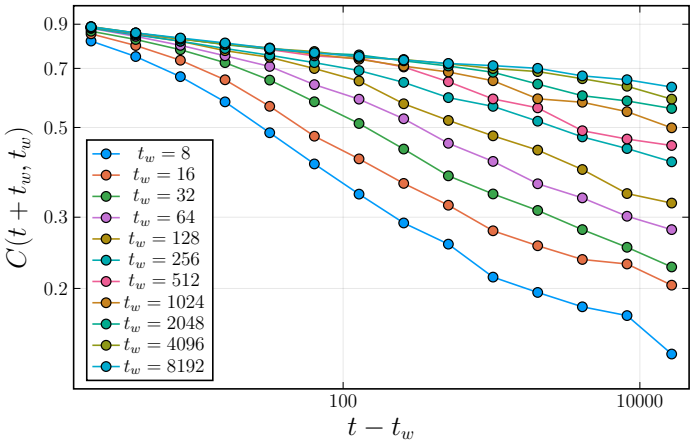

Figure 3.2 : SK-model ($N = 512$, $T = 0.4$ and $J_{ij} \sim \mathcal{N}\left(0, \frac{1}{N}\right)$). Aging behaviour in the auto-correlation function. As we increase t_w the quasi-equilibrium starts to become visible while the aging regime is lost deeper in larger observation times.

extensively through numerical simulations, and the knowledge of its main properties may be verified from several works [21–23]. In the present work we have chosen the probability distribution of the $\{J_{ij}\}$ to be bimodal

$$p(\{J_{ij}\}) = \frac{1}{2}\delta(J_{ij} - J) + \frac{1}{2}\delta(J_{ij} + J), \tag{3.8}$$

as it preserves the frustrated properties of the system and in turn, decreases the computational cost of the simulation. One can refer to several works, as that pointed out by [3], where the numerical value of the critical temperature for these distribution of the couplings is found to be around 1.1, with natural units of temperature ($J/k_B = 1$). Furthermore, as shown in the theoretical framework, by endowing our spin variables with a length between the range $[1 - \Delta/2, 1 + \Delta/2]$, the critical temperature scales as a quadratic function of Δ. Although we are not simulating the mean-field case, we expect this increasing dependence to be preserved, even if the exact quadratic form requires some higher-order corrections we expect that the shift on the critical temperature to be small thence tractable when performing simulations and let us distinguish between temperature quenches above and below the critical point.

3.3 The SWAP method

As discussed in the introduction, the goal of the project is to probe if the mapping of the SWAP algorithm, originally designed by Berthier et al. in [5], to the context of spin-glass systems accelerates their dynamics. In the original work, an implementation of an hybrid Molecular-Dynamics (MD)/Monte-Carlo simulation was performed; the standard MD evolution is periodically interrupted by MC-step, in it, the proposed configuration in the MC-step is one with some molecules interchanged w.r.t. the precedent configuration of molecules. Being a poly-disperse mixture, some configurations where the energy is minimized will correspond to the case where molecules

of larger diameter size are interchanged with smaller ones. A pictorial representation of the physical system is shown in Figure 3.3. Here one can distinguish between large diameter particles (blue) and the small ones (red); the green particles denote the proposed ones to be exchanged. Notice that if such exchange takes place there will be a local acceleration in the highlighted orange region and the small particles inside it are free to wander when the MD evolution is reinstated.

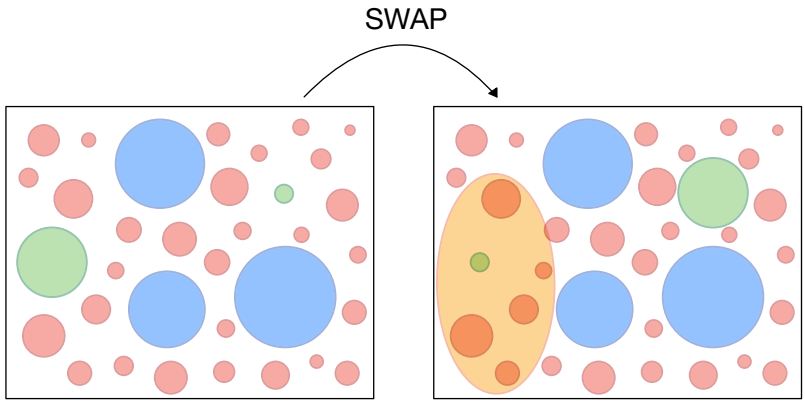

Figure 3.3 : SWAP MC-step for polydisperse mixture.

In terms of the energy of the system, the SWAP procedure basically performs a jump out of the energy barriers surrounding the trap configuration in which the system was frozen, after overcoming those barriers the system is able to explore other possible (meta)-stable configurations. In general, this is achieved by exchanging some local degree of freedom that directly affects the energy of the system, in this case the diameter of the molecules plays the role of this local degree of freedom that affects the in the inter-molecular forces via some potential energy.

We argue that by endowing the system with lengths we are setting up a feasible local degree of freedom to can serve as the exchange parameter during the simulation, and producing also the escape from the local barriers of energy that enclose the configuration in the trapped state, this would lead to an accelerated dynamics towards equilibrium, as seen in the structural case. This effect can be visualized in the spin analog from the pictorial representation (with bimodal couplings) shown in Figure 3.4 where we have 3 possible spin length values $s_+ = +1/2$, $S_+ = +2$ and $S_- = -2$. One can see that while attempting to flip the central spin in the first plaquette in the upper-left side, the Metropolis' acceptance using standard single-spin-flip dynamics fails to access this new configuration the flipped spin ($\Delta E = 20 > 0$), while the attempt of interchanging the spins highlighted in green through the swap method is accepted ($\Delta E = -9/4 < 0$).

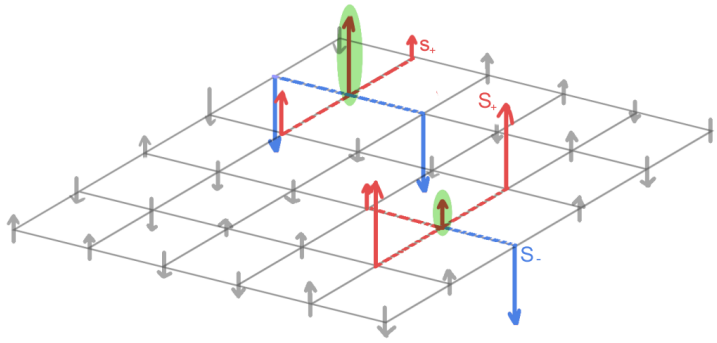

Figure 3.4 : SWAP method for soft-spins in a regular grid.

However, this situation is uncommon, as it has been stated that the acceptance rates for the swap method are low [24]; nevertheless, it seems that when it occurs it produces a measurable impact on the dynamics for a suitable choice of the parameters, at least in the structural case. All in all, the SWAP algorithm for the spin case is defined as presented in **Algorithm 2**.
Notice that it can also be interpreted as a sort-of non-local Kawasaki dynamics inserted in the single-spin-flip evolution.

We have defined n_{swap} as the frequency probability of performing a SWAP move i.e. $n_{swap} = 1$ means every move in our MC simulation will be spin-exchanges while $n_{swap} = 0$ reduces to the standard single-spin-flip dynamics.
We have implemented this algorithm for the 3D Edwards-Anderson model, and measure the auto-correlation function[§] for several values of n_{swap}, here the case of $n_{swap} = 0.5$ is shown in Figure 3.5 below. One can see a quicker decay of the auto-correlation function for every waiting time considered, so both timescales of the ACF seem to be accelerated.

Here, one needs to remember that as we are dealing with continuous spins, the zero temperature Edwards-Anderson order parameter is no longer 1, but $1 + \Delta^2/12$, the value of the spin length variance. Moreover, we can measure the characteristic time of decay, that in which the ACF has decay to $1/e$ of its original value. As we don't have access to the EA order parameter for this specific temperature, we used as a reference the value $q_{EA}(T = 0) = 1+\Delta^2/12$. This characteristic time (τ) for several temperatures is shown below in Figure 3.6, one can observe from it an improvement of the performance for low temperatures, while the expected convergence of both methods at high-temperatures becomes apparent. The proper q_{EA} needs to be assess in order to have a good measure of the characteristic time, this can be extracted from the replica distribution $P_J(q)$, this is currently being performed, however the times to access these spin-glass configurations are large and are not yet available by the time

[§]One needs to remember that, as we are dealing with a disordered system, one needs to include an average over the disorder in the definition of the correlation function shown in 3.3

Algorithm 2 Metropolis rule for Monte-Carlo step with swap

procedure MCSTEP($\boldsymbol{S}$, $\boldsymbol{J}$, n_{swap})
  Initialize **S** randomly
  for $k \in \{1, 2, ..., N\}$ **do**
    $x = 1$, with probability n_{swap} and $x = 0$ with probability $1 - n_{swap}$
    if $x = 0$ **then**
      $\Delta E = 2 \sum_{j \in nn(k)} J_{jk} S_j S_k$
      $P_{acc} = \exp(-\beta \Delta E)$
      if $P_{acc} > rand() \in [0, 1)$ **then**
        $S_k \leftarrow -S_k$
      end if
    else
      $\Delta E = (S_\mu - S_\nu) \left(\sum_{j \in nn(\mu)} J_{\mu j} S_j - \sum_{j \in nn(\nu)} J_{\nu j} S_j \right)$
      $P_{acc} = \exp(-\beta \Delta E)$
      if $P_{acc} > rand() \in [0, 1)$ **then**
        $S_\mu, S_\nu \leftarrow S_\nu, S_\mu$
      end if
    end if
  end for
end procedure

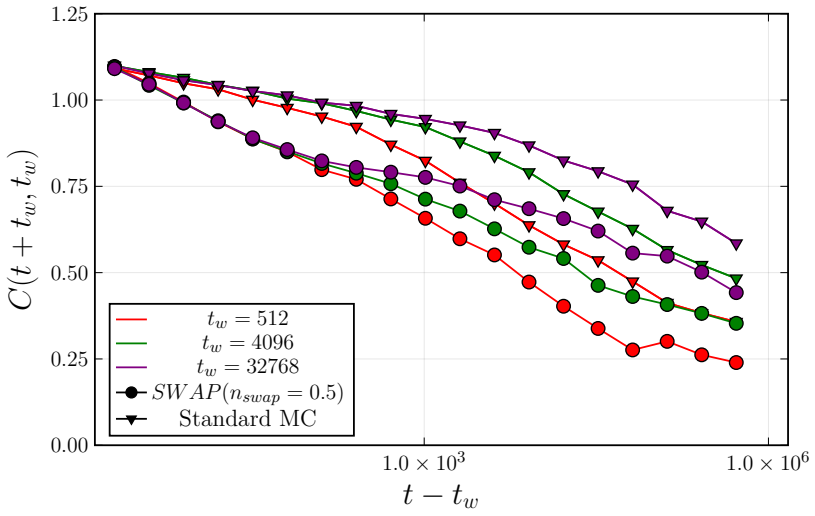

Figure 3.5 : 3D Edwards-Anderson model ($L = 8$, $\Delta = 1.5$, $T \approx 0.80\ T_{sg}$). Apparent acceleration of the dynamics.

of the writing of this work.

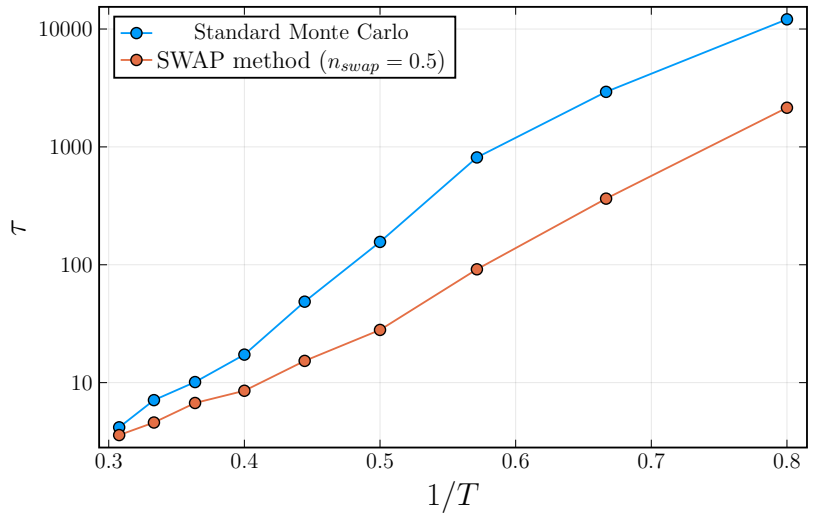

Figure 3.6 : 3D Edwards-Anderson model ($L = 8$, $\Delta = 1.5$). Characteristic time of decay for the auto-correlation function for several temperatures.

Moreover, we are interest in probing the dependency of the method with the parameter n_{swap}, as optimized in the original work. We measure the characteristic time τ for increasing values of n_{swap}, as shown in Figure 3.7 where again, one observes an acceleration of the dynamics for the several t_w, although no clear pattern for the optimization of the method is observed, at least w.r.t. the n_{swap}; as soon as one introduces a swap step, the characteristic time decreases, irrespective of the frequency. This plot was performed for several values of the temperature where one can see that as we increase it, all the different curves start to collide from the large t_w towards the lower one, again indicating the entrance of the system to the disordered phase where both methods are equivalent.

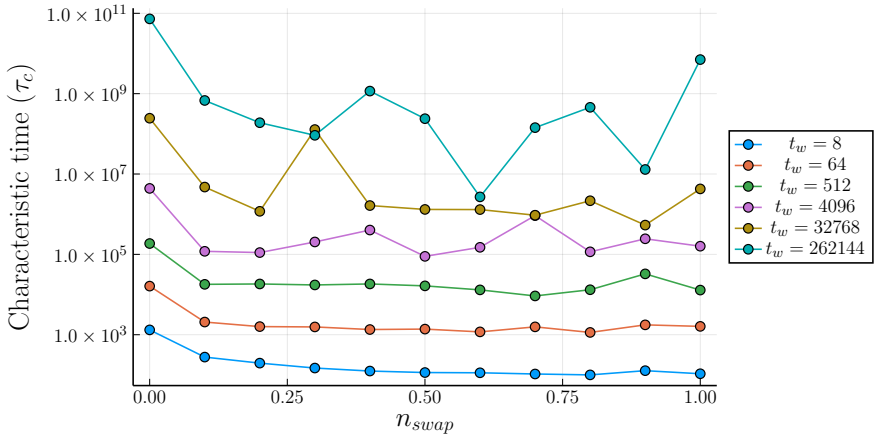

Figure 3.7 : 3D Edwards-Anderson model ($L = 8$, $\Delta = 1.5$, $T \approx 0.80\ T_{sg}$). Characteristic time of decay for the ACF for several values of the frequency probabilty n_{swap}.

Chapter 4

Conclusions and further work

At first glance, the swap method appears to be improving the characteristic times of decay of the ACF, although for more waiting time values need to be considered to clearly point out any difference between the possible acceleration on the quasi-equilibrium regime and the aging one. Along the same lines, a strange behaviour seems to be happening for the quasi-equilibrium regime, this becomes clearer when one studies the disorder-less model (i.e. the standard Ising model with continuous spins), where the quasi-equilibrium regime seems to be yielding different values between the two methods, this is not possible as the equilibrium properties of the models should remain the same independent of the dynamics. Moreover, this behaviour is not present in the models with $\Delta = 0$ (i.e. the standard Ising models for 2D and 3D) i.e. the correct equilibrium behaviour is display for both methods within the auto-correlation function. One argument for what could be happening with the soft-spin model is that endowing the spins with lengths introduces akin of "glassiness" into the system without disorder, in the form of a proliferation of meta-stable states that may stuck the dynamics for one of the two methods hence longer sampling times are required to extract the correct quasi-equilibrium behaviour.

Furthermore, the behaviour around criticality has been probed just for the replica-symmetric solution in the disordered case of soft-spins, the stability of this solution needs to be tested at least with the 1-step Replica Symmetry Breaking (1RSB) solution. Furthermore, although it seems that one is able to reconstruct the correct increasing behaviour for the critical temperature with the parameter (Δ) this calculation is barely a guide, as it just contemplates the mean-field case, and more precise and quantitatively analysis should be performed to understand the short-ranged model. The precise critical temperature should be found (both in the disorder and disorder-less case) with a proper scaling of the binder cumulant to assess the finite size effects of the simulations.

Finally, after overcoming the difficulties mentioned above, more systematic simulations ought to be performed, varying the other parameters such as Δ and larger system sizes, this might provide us with a proper quantitative measure of the efficiency of the swap method; if the results seem to be promising compared to the standard MC as the benchmark case, more confrontations may be deemed necessary to measure further the possible application of the SWAP for this kind of systems.

Bibliography

[1] Billoire A and Marinari E 2001 *J. Phys. A: Math. Gen.* **34** L727–L734 ISSN 0305-4470, 1361-6447 arXiv:cond-mat/0101177 URL http://arxiv.org/abs/cond-mat/0101177

[2] Billoire A 2008 Some Aspects of Infinite-Range Models of Spin Glasses: Theory and Numerical Simulations *Rugged Free Energy Landscapes: Common Computational Approaches to Spin Glasses, Structural Glasses and Biological Macromolecules* Lecture Notes in Physics ed Janke W (Berlin, Heidelberg: Springer) pp 11–46 ISBN 978-3-540-74029-2 URL https://doi.org/10.1007/978-3-540-74029-2_2

[3] Katzgraber H G, Körner M and Young A P 2006 *Phys. Rev. B* **73** 224432 ISSN 1098-0121, 1550-235X URL https://link.aps.org/doi/10.1103/PhysRevB.73.224432

[4] Marinari E and Parisi G 1992 *Europhys. Lett.* **19** 451–458 ISSN 0295-5075, 1286-4854 arXiv:hep-lat/9205018 URL http://arxiv.org/abs/hep-lat/9205018

[5] Berthier L, Flenner E, Fullerton C J, Scalliet C and Singh M 2019 *J. Stat. Mech.* **2019** 064004 ISSN 1742-5468 URL https://iopscience.iop.org/article/10.1088/1742-5468/ab1910

[6] Sompolinsky H and Zippelius A 1982 *Phys. Rev. B* **25** 6860–6875 ISSN 0163-1829 URL https://link.aps.org/doi/10.1103/PhysRevB.25.6860

[7] Krasnytska M, Berche B, Holovatch Y and Kenna R 2020 *J. Phys. Complex.* **1** 035008 ISSN 2632-072X arXiv:2004.05134 [cond-mat, physics:physics] URL http://arxiv.org/abs/2004.05134

[8] Bialas P, Blanchard P, Fortunato S, Gandolfo D and Satz H 2000 *Nuclear Physics B* **583** 368–378 ISSN 05503213 arXiv:hep-lat/0003014 URL http://arxiv.org/abs/hep-lat/0003014

[9] Campa A, Dauxois T, Fanelli D and Ruffo S 2014 *Physics of Long-Range Interacting Systems* (Oxford University Press) ISBN 978-0-19-958193-1 URL https://oxford.universitypressscholarship.com/view/10.1093/acprof:oso/9780199581931.001.0001/acprof-9780199581931

[10] Mezard M, Parisi G and Virasoro M 1986 *Spin Glass Theory and Beyond: An Introduction to the Replica Method and Its Applications* (*World Scientific Lecture Notes in Physics* vol 9) (WORLD SCIENTIFIC) ISBN 978-9971-5-0116-7 978-981-279-937-1 URL https://www.worldscientific.com/worldscibooks/10.1142/0271

[11] Sherrington D and Kirkpatrick S 1975 *Phys. Rev. Lett.* **35** 1792–1796 ISSN 0031-9007 URL https://link.aps.org/doi/10.1103/PhysRevLett.35.1792

[12] Brout R 1959 *Phys. Rev.* **115** 824–835 ISSN 0031-899X URL https://link.aps.org/doi/10.1103/PhysRev.115.824

[13] Nishimori H 2001 *Statistical Physics of Spin Glasses and Information Processing* (Oxford University Press) ISBN 978-0-19-850941-7 URL https://oxford.universitypressscholarship.com/view/10.1093/acprof:oso/9780198509417.001.0001/acprof-9780198509417

[14] Castellani T and Cavagna A 2005 *J. Stat. Mech.* **2005** P05012 ISSN 1742-5468 URL https://iopscience.iop.org/article/10.1088/1742-5468/2005/05/P05012

[15] Newman M E J and Barkema G T 2010 *Monte Carlo methods in statistical physics* reprinted (with corr.) ed (Oxford: Clarendon Press [u.a.]) ISBN 978-0-19-851796-2 978-0-19-851797-9

[16] Puri S (ed) 2009 *Kinetics of phase transitions* Chemistry (Boca Raton, Fla.: CRS Press) ISBN 978-0-8493-9065-4

[17] Bray A 1994 *Advances in Physics* **43** 357–459 ISSN 0001-8732, 1460-6976 URL http://www.tandfonline.com/doi/abs/10.1080/00018739400101505

[18] Berthier L and Young A P 2004 *Phys. Rev. B* **69** 184423 ISSN 1098-0121, 1550-235X URL https://link.aps.org/doi/10.1103/PhysRevB.69.184423

[19] Bouchaud J P, Cugliandolo L F, Kurchan J and Mezard M 1997 Out of equilibrium dynamics in spin-glasses and other glassy systems arXiv:cond-mat/9702070 URL http://arxiv.org/abs/cond-mat/9702070

[20] Takayama H, Yoshino H and Hukushima K 1996 Aging Processes within One 'Pure State' of the SK Model number: arXiv:cond-mat/9612071 arXiv:cond-mat/9612071 URL http://arxiv.org/abs/cond-mat/9612071

[21] Andersson J O, Mattsson J and Svedlindh P 1992 *Phys. Rev. B* **46** 8297–8304 publisher: American Physical Society URL https://link.aps.org/doi/10.1103/PhysRevB.46.8297

[22] Mártin D A and Iguain J L 2017 *J. Stat. Mech.* **2017** 113302 ISSN 1742-5468 arXiv:1609.09860 [cond-mat] URL http://arxiv.org/abs/1609.09860

[23] Katzgraber H G, Palassini M and Young A P 2001 *Phys. Rev. B* **63** 184422 ISSN 0163-1829, 1095-3795 arXiv:cond-mat/0007113 URL http://arxiv.org/abs/cond-mat/0007113

[24] Berthier L and Reichman D R 2022 Modern computational studies of the glass transition arXiv:2208.02206 [cond-mat] URL http://arxiv.org/abs/2208.02206