Universiteit Utrecht

Master Thesis
Master of Theoretical Physics

Memory Effects in Spin Glasses

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Abstract

It has been a while since Edwards and Anderson started investigating spin glasses through introducing random bonds in the Ising Model in 1975. The resulting Random Bond Ising Model (RBIM) has since been the focus point of much study, but it is still far from being fully understood. For my thesis, I investigated the dynamics of the RBIM when simulated using the Metropolis algorithm.

Contents

1 Introduction

Glass (vitreous SiO_2) is an interesting substance. It is characterised by two specific properties:

1. **Disorder**: typically, glass structures do not show long-ranged order. If liquid glass is cooled, it gets trapped into non-equilibrium structures with local order (each silicon atom is connected to four oxygens, and each oxygen to two silicon atoms; and the O-Si-O angles between the bonds are close to tetrahedral), but there is no translational or rotational symmetry of the entire sample.

2. **Frustration**: glass gets stuck into non-equilibrium samples, in which tiny ordered regions can be identified, that do not match to each other. The slower the rate of cooling, the lower the energy at which the sample gets stuck. There is a crystalline ground state, but it is only accessible if the cooling rate is very low. Once the temperature is low, the viscosity is very high and the ground state is generally not reachable by waiting very long.

If you cool glass, the viscosity may increase by as much as 17 orders of magnitude, causing it to become virtually solid. However, there are no manifest changes in the structure of the glass. This rapid increase in the viscosity is called the glass transition. Part of this glass transition is also a significant increase in the correlation time and the correlation length.

This divergence of the correlation time makes it impractical to do experiments on the dynamical properties of real glass at temperatures well below the glass transition. Various computer simulations of real glasses have been carried out, but the used models have a high computational complexity.

There is a wide variety of systems that have these same two characterising properties and exhibit similar behaviour. A class of glassy systems are the spin glasses. In a spin glass the frustration and disorder are in the magnetic state of the system, as opposed to the real glass where the frustration and disorder are of a structural nature. The frustration and disorder in spin glasses arise from the simultaneous presence of ferromagnetic and antiferromagnetic interactions. A typical material spin glass is an alloy of a nonmagnetic metal with a diluted magnetic metal, for example AuFe.[1]

1.1 Random bond Ising Model

The system that we investigated is a model that also has frustration and disorder in its magnetic state and that therefore also is a spin glass. It is called the Random Bond Ising Model (RBIM) and it was first introduced in 1975 by Edwards and Anderson [2]. It consists of $N = L^3$ spins on a cubic lattice. The spins can be either plus one or minus one. The Hamiltonian of the system is defined to be

$$H = -\sum_{\langle ij \rangle} J_{ij} S_i S_j, \tag{1}$$

where the sum $\langle ij \rangle$ is taken over all pairs of nearest neighbours. $J_{ij} = \pm J$ is the bond between the spin at position i and the spin at position j. The values of J_{ij}

[1] A more detailed plea on the significance of the research of spin glasses can be read in [1].

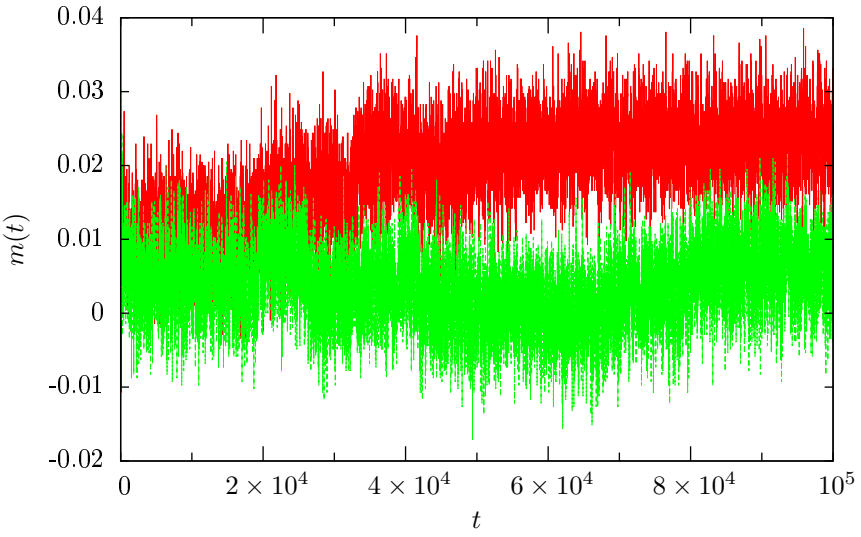

Figure 1: Plot of the average magnetisation per spin as a function of time. The two lines were obtained with with two different runs with the same configuration of random bonds, however, the startconfigurations of the spins were two different, random, uncorrelated spinconfigurations. The runs were carried out with the Metropolis Algorithm on a threedimensional cubic lattice of size 16^3.

– plus J or minus J –, are randomly assigned at the beginning of the experiment and usually[2] remain the same during the entire experiment. If $J_{ij} = +J$ we call the bond ferromagnetic because then the state of lowest energy is the state in which the spins are aligned (i.e. have the same sign). If $J_{ij} = -J$ the bond is antiferromagnetic.

To see that the RBIM indeed contains frustration, we consider a square of four spins. If three of the four bonds in the square are ferromagnetic and the fourth is antiferromagnetic, there is no spin configuration in which all four bonds are satisfied. The disorder in the RBIM is obvious, although its nature is slightly different from that of the disorder in glass. Where the disorder in glass is influenced by the configuration of the neighbouring atoms and evolves in time, the disorder in the RBIM is preset and is not dependent on the state of the system. This kind of disorder is called quenched disorder.

In figure 1 we have plotted the evolution of the average magnetisation in the RBIM. In the plot we plotted two lines from two different runs with the same configuration of random bonds, but with different initial configurations of the spins. In the ferromagnetic Ising Model, there would be a preferred value of the magnetisation and if we were to make the same plot for the ferromagnetic Ising Model, we would see that independent on the initial configuration, the magnetisation would quickly converge to that value. But here we see that the magnetisation does not have a clear attractor and moves in a seemingly random way. We also see that – although this system is relatively small – the evolution

[2]We actually did experiments where after the thermalisation we flipped a plane of bonds and then looked how the added energy dispersed over time.

of the magnetisation shows long and slow movements; which indicates that the system does have memory effects.

1.2 The Metropolis Algorithm

When you investigate a typical phase transition you are interested in equilibrium quantities and the algorithm you use to investigate your system is less important, as long as you make sure that your algorithm samples the partition sum in a reliable way, i.e. satisfying detailed balance and ergodicity. However, when you look at memory effects, it is the dynamics that matters and in Monte Carlo simulations it is the used algorithm that determines the dynamics of your system.

We used the Metropolis Algorithm [3][3]. In the Metropolis Algorithm a step consists of randomly picking a site i. The spin at that site is then flipped $s_i \to -s_i$ with a probability

$$P = \begin{cases} 1 & \text{if } \Delta E \leq 0, \\ e^{-\beta \Delta E} & \text{if } \Delta E > 0, \end{cases} \tag{2}$$

where ΔE is the amount with which the total energy of the system would be changed if the spin were flipped.

To make sure that time remains an intensive property, we choose as unit of time one Monte Carlo sweep: N attempted spin flips. In that way, after one unit of time, every site will on average be picked once.

1.3 This thesis

This thesis will start by explaining how we increased the efficiency of the simulations using a multispin scheme. Then we will describe the dynamics of the ferromagnetic Ising Model at the critical temperature and explain why we expect memory effects. In the last section, we will present and describe the data we gathered using the before-mentioned implementation of the Metropolis Algorithm, both for the ferromagnetic and for the random bond Ising Model.

2 Multispin coding

A way to increase the accuracy of the obtained results is to generate more data. Since Monte Carlo simulations are intrinsically computer intensive, it is wise to put some effort into optimising your implementation of the algorithm, either to reduce the computational effort needed to generate a given amount of data or to increase the amount of data that is generated with a given amount of computational effort. Since our model consists of two-state spins, it is natural to exploit this fact and code the spins as bits. The CPU's of most computers operate on words of q bits (usually q is 32 or 64) instead of single bits. Therefore, it is equally expensive to do an operation on q spins as it is to do the same operation on 1 spin. The easiest way to deal with this is to simultaneously simulate q realisations of the RBIM; this is called multispin coding.

[3]For a more detailed discussion of the Metropolis algorithm, the reader is referred to [4].

A	B	$A \wedge B$	$A \vee B$	$A \oplus B$	$\overline{A}$
1	1	1	1	0	0
1	0	0	1	1	0
0	1	0	1	1	1
0	0	0	0	0	1

Table 1: Truth table of bitwise operators.

2.1 Bitwise operators

A drawback of multispin coding is that every statement in the program has to be translated to a bitwise operation. There are 4 bitwise operators: and ($\wedge$), inclusive or ($\vee$), exclusive or ($\oplus$) and negation ($\overline{\ }$). The truth table of these operators is displayed in Table 1. These bitwise operators are bitwise, which means that they operate per bit, i.e. if you operate them on two bitstrings, the bits of the resulting bitstring are obtained by operating the operator on the corresponding bits.

The idea now is to create bitstrings s_i where i signifies the place in the lattice and the position of a bit in s_i signifies in which one of the q realisations it is.[4] If we would be able to create a bitstring f that has a 1 if we want to flip the corresponding spin and a 0 if we don't, we could simultaneously flip all spins in bitstring s_i we want to flip, with the simple statement

$$s_i := s_i \oplus f. \tag{3}$$

If we were to define bitstrings J_{ij} that code the coupling constants and have a zero for ferromagnetic bonds and a one for antiferromagnetic bonds we could calculate a variable a that has a zero if the energy of the bond between two neighbouring sites s_i and s_j is negative and a one if it is positive, with

$$a := s_i \oplus s_j \oplus J_{ij}. \tag{4}$$

The main step in the Metropolis Algorithm is to pick a site s_i and to determine whether to flip it or not. We start by calculating a_n with $n = 1...6$: the signs of the energies of the bonds with the six neighbouring sites. If three or more of the a_n have a one, the spin has to be flipped whatsoever. If only two of the a_n have a one, four have a zero and the sum of the energies of the bonds is $-2J$. If we then flip the spin, the sum of the energies of the bonds will become $+2J$ and will thus be increased by $4J$. Hence, in this case we want to flip with a probability $e^{-4\beta J}$. In the same way, in the case where only one of the a_n has a zero we want to flip with probability $e^{-8\beta J}$ and in the case of no zero's at all we want to flip with probability $e^{-12\beta J}$.

We will now try and demonstrate a way to achieve this. We will use three random bitstrings r_1, r_2 and r_3 that are generated in such a way that in every one of them every bit has a probability $e^{-4\beta J}$ to be one. Next we define three variables P_1, P_2 and P_3 that count the number of ones in a_1, a_2 and a_3: P_1 has a one if at least one of the three a's has a one, P_2 has a one if at least two

[4] To encode spins as bits, one has to change from the spins having values $s = \pm 1$ to spins with values 0 or 1. If you then want to calculate physical quantities like the magnetisation M you have to reverse this translation: $M \to 2M - 1$.

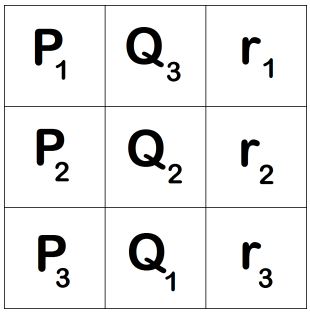

Figure 2: This array can be used to visualise equation (5); for f to have a one, in every row at least one entry has to have a one.

of the three a's have a one and P_3 has a one if all of the three a's have a one. We define Q_1, Q_2 and Q_3 in the same way based on a_4, a_5 and a_6. We now construct the bitstring f that determines whether we flip the spins with

$$\begin{aligned} f \quad := \quad & (P_1 \vee Q_3 \vee r_1) \\ & \wedge (P_2 \vee Q_2 \vee r_2) \\ & \wedge (P_3 \vee Q_1 \vee r_3) \end{aligned} \tag{5}$$

To understand why this works, we can visualise the previous expression with a 3×3-array as in figure 2. For f to have a one, every row of the array has to have at least one one. So in every row where neither the P nor the Q has a one, the r has to have a one. So for example in the case where in two rows neither P nor Q has a one, two r's have to have a one, which has a probability $(e^{-4\beta J})^2 = e^{-8\beta J}$. To verify that this works, we constructed table with all possible cases (table 2).

The way the random bitstrings r are generated is the following. We make 100000 bitstrings and calculate how many ones should be in them at the temperature at which the current simulation is supposed to be running. Then we place that number of ones at random places in the bitstrings. During the simulation, as soon as the 100000 bitstrings have all been used, we do something that we call "reshuffling": we put the bitstrings in a random order and also cyclically bitshift every bitstring by a random amount.

2.2 Performance

Using the scheme (5) to determine which spins are to be flipped means a great improvement upon the most straightforward implementation – determine what spins have $N_S = 0, 1, 2, \geq 3$ and then flipping them with the corresponding probabilities. After the determination of a_n, the former needs only 21 bitwise operations to determine f, whereas the latter needs 40.

Using a single thread on a dual quadcore 2.4 GHz AMD 2378 processor, we observed the program to need 245 seconds for 10^9 repetitions, including initialization and reshuffling of the random bitstrings. That is 3.8 ns per attempted spin flip.

N_P	N_Q	N_S	symbol	N_r	P
0	0	0		3	$e^{-12\beta J}$
0	1	1		2	$e^{-8\beta J}$
0	2	2		1	$e^{-4\beta J}$
0	3	3		0	1
1	0	1		2	$e^{-8\beta J}$
1	1	2		1	$e^{-4\beta J}$
1	2	3		0	1
1	3	4		0	1
2	0	2		1	$e^{-4\beta J}$
2	1	3		0	1
2	2	4		0	1
2	3	5		0	1
3	0	3		0	1
3	1	4		0	1
3	2	5		0	1
3	3	6		0	1

Table 2: In this table, the various possible cases are listed. Here N_P and N_Q are the numbers of 1's in the two subsets of a_n, N_S their sum. The symbol is a visualisation, it is constructed by taking the array from figure 2 and making a square P_i or Q_i black if the corresponding value is 1. A square r_i is then coloured red if that r_i needs to be 1 to have a spin flip. N_r is the number of r's that need to be 1 to have a spinflip and P is the probability of these r's being one.

3 Memory effects in the ferromagnetic Ising Model

We will now turn to the original, ferromagnetic Ising Model. It is defined in the same way as the RBIM (1), but now $J_{ij} = +J$ for all i, j. With this Hamiltonian, neighbouring spins with the same sign will be favoured, resulting in a two-fold degenerate ground state: the state in which all spins are plus one and the state in which all spins are minus one. The system exhibits a second order phase transition in the absolute magnetisation $\langle |M| \rangle$, from 0 above the critical temperature to nonzero at temperatures below the critical temperature.

We will analyse the dynamics of the ferromagnetic Ising Model at the critical temperature.

3.1 Dynamics

To analyse the dynamics of a system, various quantities could be defined. The magnetisation autocorrelation function

$$\chi_M(t) = \langle M(0) \cdot M(t) \rangle \tag{6}$$

and the mean square deviation (MSD) of the magnetisation[5]

$$h(t) = \Big\langle \big(M(t) - M(0)\big)^2 \Big\rangle \tag{7}$$

measure changes in the total magnetisation $M = \sum_i s_i$, whereas the spin-spin autocorrelation function

$$\chi_S(t) = \langle S(0) \cdot S(t) \rangle = \Big\langle \sum_i s_i(0) \cdot s_i(t) \Big\rangle \tag{8}$$

measures changes in the total spin configuration. In all definitions, $\langle \cdots \rangle$ denotes a time average, for example in (6), we actually mean

$$\chi_M(t) = \frac{1}{T} \int_0^T dt'\, M(t') \cdot M(t + t'). \tag{9}$$

The magnetisation autocorrelation function and the magnetisation MSD are closely related.

$$\begin{aligned} h(t) &= \langle M(t)^2 + M(0)^2 - 2M(0) \cdot M(t) \rangle \\ &= \langle M(t)^2 \rangle + \langle M(0)^2 \rangle - 2\langle M(0) \cdot M(t) \rangle, \end{aligned} \tag{10}$$

and since $\langle \cdots \rangle$ signifies a time average, $\langle M(0)^2 \rangle = \langle M(t)^2 \rangle \equiv \langle M^2 \rangle$; hence we find

$$\frac{\chi_M(t)}{\langle M^2 \rangle} = 1 - \frac{h(t)}{2\langle M^2 \rangle}. \tag{11}$$

Now, using a Taylor expansion, we know that

$$\log(1 - x) = -x - \frac{1}{2}x^2 - ..., \tag{12}$$

[5] At other places in this thesis, we will also use a normalised version that uses the average magnetisation: $\tilde{h}(t) = \Big\langle \big(m(t) - m(0)\big)^2 \Big\rangle = \frac{h(t)}{N^2}$.

and hence, if $\frac{h(t)}{2\langle M^2\rangle} \ll 1$,

$$\log(\frac{\chi_M(t)}{\langle M^2\rangle}) \approx -\frac{h(t)}{2\langle M^2\rangle}. \tag{13}$$

Specifically, if the MSD behaves like a power law, $h(t) \propto t^\alpha$, the autocorrelation function will behave like a stretched exponential, $\chi_M(t) \propto e^{-t^\alpha}$.

In the following, we will focus on the magnetisation MSD, because that function is much easier to measure, since it is less prone to noise. We will now analyse how it looks at the critical temperature in the threedimensional cubical ferromagnetic Ising model.[6]

For t small, roughly smaller than 1,[7] the spin flips will be sparse and hence uncorrelated, so $h(t) \propto L^d t$ where the proportionality factor is the acceptance ratio, the average probability that a spin, after it has been selected, is flipped.

At times that are far apart, the correlation between states becomes very small, so for t large,[8] $\chi_M(t) \to 0$. So from (10), $h(t) \approx 2\langle M^2\rangle$. Now, at the critical temperature, the magnetic susceptibility, $\chi \equiv \frac{\beta}{N}\langle M^2\rangle$, diverges like $\chi \propto L^{\gamma/\nu}$, so since $N = L^d$, $\langle M^2\rangle \propto L^{d+\gamma/\nu}$, so

$$h(t) \propto L^{d+\gamma/\nu}. \tag{14}$$

So we now have

$$h(t) \propto \begin{cases} L^d t & \text{if } t \lesssim 1, \\ L^{d+\gamma/\nu} & \text{if } t \gtrsim L^{z_c}. \end{cases} \tag{15}$$

Since $h(t)$ should be a continuous function, it should go from $h(t \approx 1) \approx L^d$ to $h(t \approx L^{z_c}) \approx L^{d+\gamma/\nu}$. A good guess is that it will behave like a power law. Assuming power law behaviour, we find

$$h(t) \propto t^{\gamma/(\nu z)}. \tag{16}$$

[6] The following is based upon calculations in [6].

[7] Remember that we measure time in Monte Carlo sweeps, so at $t = 1$, on average, every site has been visited once and has either or not been flipped. At time t, there have been $Nt = L^d t$ attempted spinflips where d is the dimension of the system, in our case it is 3.

[8] Specifically for $t > \tau$, where τ is the correlation time, defined to be the time that is needed between two states for their correlation to decrease by an order of magnitude. For finite systems, the correlation time is reported to scale with the system size as a power law, $\tau \propto L^{z_c}$. The value of the dynamical critical exponent z_c is reported to be $z_c = 2.03 \pm 0.04$ [5].

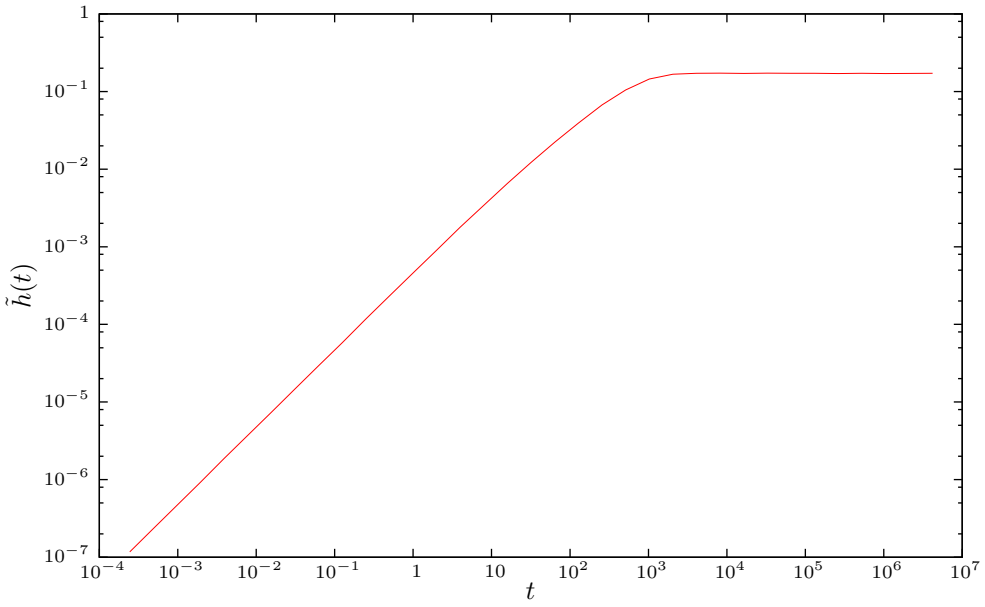

Figure 3: Double logarithmic plot of $\tilde{h}(t)$ for a ferromagnetic Ising Model on a threedimensional cubic lattice with 16^3 spins. The presented data are an average over 128 different realisations; in each realisation, for each t in $\{2^{-12}, 2^{-11}, \ldots, 2^{23}\}$, $\tilde{h}(t)$ was measured 300 times and averaged.

4 Results

Using the implementation described earlier, we carried out measurements of the magnetisation MSD, both for the RBIM as for the ferromagnetic Ising Model. All simulations were carried out on a threedimensional cubic lattice with 16^3 spins.

4.1 Ferromagnetic Ising Model

The critical temperature of the threedimensional ferromagnetic Ising Model on a cubic lattice is reported to be [7]

$$\beta_c J = 0.221655(5), \tag{17}$$

so that is also the temperature at which we have done the simulations. The results are shown in figure 3. We see that the expected behaviour for small t is indeed observed: we see a straight line with slope one, so that $\tilde{h}(t)$ is indeed proportional to t. After $t \approx 1$ the slope gradually decreases. However, from this plot it remains unclear whether it transitions to another constant slope – supporting our hypothesis of memory effects – or if the decrease of the slope is just part of the gradual transition to the constant value that we predicted for large t. For the threedimensional case this is indeed extremely hard to find out, because using $\gamma = 1.2372$, $\nu = 0.6301$ and $z = 2.02$ [8], $\gamma/(\nu z) = 0.972$ which is almost 1, so there is only a very slight change in the slope.

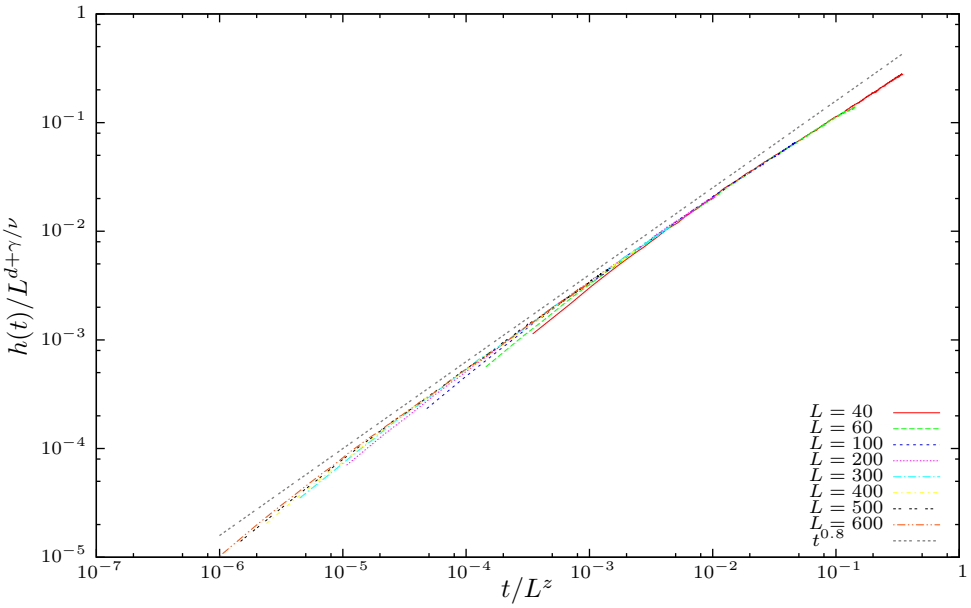

Figure 4: Double logarithmic plot of $h(t)/L^{d+\gamma/\nu}$ versus t/L^z in the *twodimensional* ferromagnetic Ising model for various lattice sizes. The used values for the critical exponents are $\gamma = 1.75$, $\nu = 1$ and $z = 2.17$, and the experiments were carried out at the critical temperature $\beta_c = \frac{1}{2}\ln(1+\sqrt{2}) \approx 0.441$. The used data are a courtesy of Gerard Barkema.

Gerard Barkema did the same experiment for the twodimensional ferromagnetic Ising Model at the critical temperature; the results are shown in figure 4. Using the critical exponents for the twodimensional Ising model $\gamma = \frac{7}{4}$, $\nu = 1$ and $z = 2.17$ [9], we find $\gamma/(\nu z) = 0.81$, which is in accordance with the presented data.

4.2 Random bond Ising Model

The results for $\tilde{h}(t)$ in the RBIM are presented in figure 5. We see that there is a part of all lines – roughly up to $t = 10^{-1}$ – where they are all straight and perpendicular with slope 1. The reason is that for such small times, the spin flips are completely uncorrelated: there is a certain acceptance rate P that the spin that is chosen is flipped, that acceptance rate is temperature dependent, but that is all there is to it. So in that regime, $\tilde{h}(t) = \frac{4}{N}Pt$,[9] and in a double logarithmic plot it will show up as a straight line with slope 1.

For $\beta = 0$, the acceptance rate will be $P = 1$, so then $\tilde{h}(t) = \frac{4}{N}t$ and that is exactly what is measured. For lower temperatures, the acceptance rate will be composed of freeflipping spins for which the change in energy upon flip is $\Delta E \leq 0$ and the thermal flipping of spins for which the energy increases upon flip. In the limit $T \to 0$, only the part of the freeflipping spins will be left.

[9] In the factor $\frac{4}{N}$, the N is because the function $\tilde{h}(t)$ has been normalised by a factor N^2 where the time has only been normalised by one factor of N. The factor $4 = 2^2$ is because the flip of one spin means a change of 2 in M.

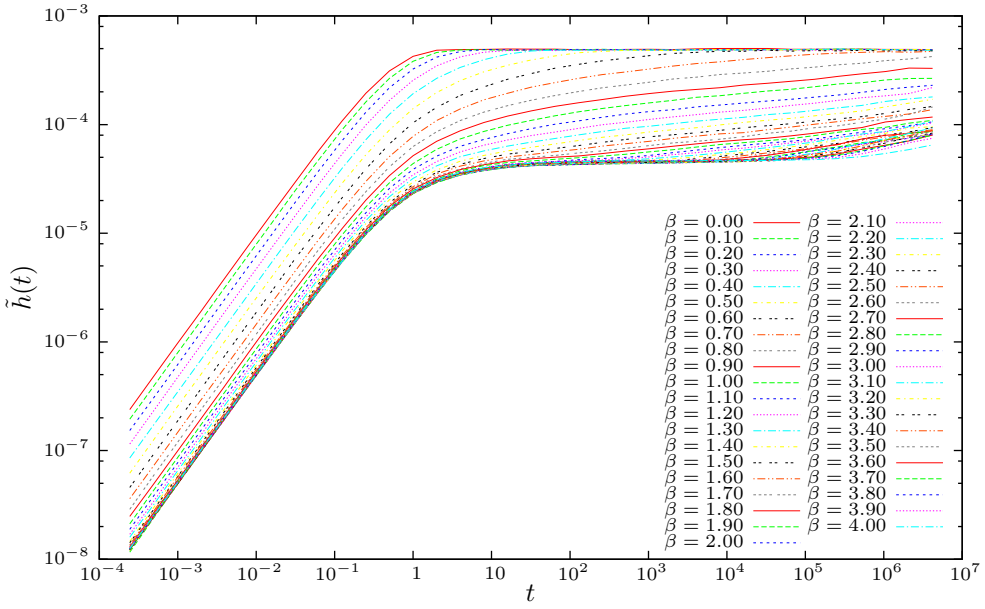

Figure 5: Double logarithmic plot of $\tilde{h}(t)$ for the RBIM on a threedimensional cubic lattice with 16^3 spins. Runs were carried out for different values of β. The upper line corresponds with $\beta = 0$ (infinite temperature) and the lower lines are for ever increasing β.
The presented data are an average over 128 different realisations of the RBIM; in each realisation, for each t in $\{2^{-12}, 2^{-11}, \ldots, 2^{23}\}$, $\tilde{h}(t)$ was measured 300 times and averaged. For each temperature, a new set of runs was carried out, but the runs for all temperatures were carried out using the same set of bond configurations.

For long times we see that the line $\beta = 0$ goes to a constant value of $\frac{2}{N}$. This ceiling corresponds to completely uncorrelated states. At lower temperatures, theoretically, $\tilde{h}(t)$ also goes to the ceiling at long times, but we see that already at $\beta = 0.80$ the ceiling is not reached within the timescale at which we did the experiments.

Then for these lower temperatures (somewhere in the range $\beta = 0.8$ to $\beta = 1.6$), the lines show a bend at $t \approx 1$, and then still seem to go to the ceiling at a distinctly slower rate. The lines seem to have a straight part for several decades after the bend, but on further analysis we were not able to put a definite exponent to it. Considering the forms of the lines at lower and higher temperatures it seems probable that their seeming straightness can be attributed to a convex and a concave bend that when added result in seemingly straight line.

The most striking feature of the plot is that at even lower temperatures the bend at $t \approx 1$ bends to something that looks like a plateau. Then after staying at the plateau during some time that depends on the temperature – longer at lower temperatures – the line bends up again. The plateau is not a real plateau because it tilts a little bit upwards, but one could expect that this is caused by the finite size of the system. The plateau is roughly a factor 10 below the

ceiling.

5 Conclusion

Through the existence of memory effects in the ferromagnetic Ising model, we argued that there should also be memory effects in the random bond Ising model. We did simulations on the threedimensional random bond Ising model using a multispin implementation of the Metropolis algorithm. From the resulting data we calculated the mean square deviation of the magnetisation as a function of time. There we see that already above $\beta \approx 0.8$, the system does not become fully uncorrelated on measurable timescales. At even lower temperatures, $h(t)$ seems to stay at a plateau for some time, after which it bends up again. These observations form clear evidence for the presence of memory effects in the threedimensional random bond Ising model.

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