Fractal Geometries and their Nonequillibrium Behaviour in Two Dimensional Ising Magnets

Ph. D. Theses

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Szeged, 2008.

Abstract

In my Ph. D. thesis I was conducting statical and dynamical investigations with models based on the two dimensional Ising model. I studied the phases of the Random Field Ising Model (RFIM) analyzing geometric properties of macroscopic clusters at zero temperature. I also quested for nonequillibrium dynamic properties of the two dimensional Ising model, when the initial states are prepared specificly.

The two-state spins of the RFIM sit on sites of a square lattice. Beside the homogene first-neighbour pair-wise interaction of energy J, there is also a local magnetic field of random strength and direction with average strength of H and spread of Δ. In this parameter field of J-T-H-D there is a phase, where domains with fractal properties appear. I studied systems at zero temperature and with no external field ($H = 0$), residing at the ground state. The specific samples were generated and analyzed with a computer. For each sample I generated external fields using pseudo random number generators, and then obtained the matching ground state using methods of combinatorical optimization. I pointed out, that domains in this model and domains emerging in the critical standard percolation are geometrically similar. I also demonstrated that the domain size distribution and the geometric correlation scale well, as well as the later is also conform invariant.

The dynamics of the Ising model is realized by the Glauber model. For each unit of time every single spin has one opportunity on average to change, according to local energy ambience and temperature. In equillibrium processes the value of the order parameter converges to the equillibrium value in a monotonic way. Under critical temperature, this process becomes time scale free, and magnetization decays with a polynomial function with an exponent z, that is called the (equillibrium) dynamic exponent. If the system is started from high temperature with small positive magnetization, and then quenched to the critical point, magnetization starts to increase with the (nonequillibrium) exponent θ for a specific time scale, which can become macroscopic for a small enough starting value. I was curious, if specifically preparing the initial state would influence the nonequillibrium, or even the equillibrium process.

I prepared the necessary initial states, and conducted the dynamic simulations using computer software. I implemented the Heat Bath algorythm to simulate

the relaxation. The initial states were chosen from samples in critical state of two dimensional models. I used ground states from the Random Fiels Ising model with percolating clusters, as well as critical states from Baxter-Wu (three-spin interaction on a triangle graph) and Turban models (two spin in one, and three or four spin interaction in the other direction of the square lattice). Nonequillibrium behaviour was triggered by sudden change in the interaction and temperature. I observed, that depending on the universality class of the model, critical behaviour can change. Starting from the ground states of the RFIM also introduces a reentering type change in the course of the magnetization.

Geometrical clusters of the RFIM

The Lenz-Ising model is probably the oldest and most simple non-trivial model for cooperative behaviour which shows spontaneous symmetry breaking. Most homogene systems can be treated in an algebraic manner, however real-list systems scarcely include translation invariance even on local scale. The two simplest models to rule out this symmetry is the Random Bond Ising Ferromagnet Model (RBIFM), where neighbours have bonds of random energy, and the Random Fiels Ising Model (RFIM), where a random local field is introduced to each spin.

Some physical examples on the later, the one I will be invesstigating. The $Fe_xZn_{1-x}F_2$ is a dilluted antiferromagnet. Its model can be mapped exactly onto the RFIM, however. A more direct example is the $Rb_2Co_xMg1-xF_4$, that is described by the two dimensional RFIM. Interactions in this material is highly anisotropic: it consists of parallel layers. Interaction within these layers are strong, however in between there are far weaker. Here, it can also be observed, how the random field dims the phase transition of the two dimensional Ising system.

Since its seminal discussion by Imry and Ma [5] in 1975, this model is under intensive investigation both experimentally and theoretically. The frustration caused by the random field can be observed even at lower temperatures. The direction of the random field is incidental, neighbouring spins cannot decide wether to stay parallel, or to adjust to the field. In lower dimensions this effect is so decisive, that any small randomness in the field will break the ferromagnetic order even at zero temperature. In three dimensions the ferromagnetic phase is present, however the order of phase transition depends on the type of the distribution of the random field. Small fluctuations in the random field are always relevant in this

system.

According to investigations conducted by Seppälä and Alava, in the two dimensional Randon Fiels Ising model there are two phases in the parameter field assigned by the external field, H, and the random field strength spread Δ[6]. For small values of Δ, there are percolating clusters present in the system, whos linear size matches that of the system, however their mass is effectively zero. For Δ being large enough, clusters shrink to a finite size. The percolating boundary separating the two phases is symmetric on the sign of the external field.

For finite system sizes and values of Δ small enough, the sample can become homogene. The critical system size, where the ferromagnetic order is broken, is called break-up length. For fixed random field strength spread, the corresponding break-up length scale is always present in the system.

The present percolation transition can be approached by different manners. You can vary the external field, H, while keeping random field strength Δ constant, or you can vary Δ, while keeping the external field off. The first case has been thoroughly investigated, I was performing my studies with $H = 0$.

Actual investigations were realized with computer programs, in two steps. First, samples with specific linear size L, and random field strength spread Δ, and no external field were calculated at zero temperature, minimising energy. For each sample the specified random field was generated from pseudo random numbers. The minimum energy ground state was calculated utilizing the maximum flow - minimum cut algorythm, a well known tool in combinatorical optimization[7]. I generated and analyzed 10000 independent samples for every pair of L and Δ. Lack of computational resources limited the maximum system size to 256. The second step, analyzing the samples, was separated, as the generation of samples was highly demanding in computation time. Generator programs created files for each parameter sets, that contained generated samples. Analyzing programs read and processed these files.

In a certain regime of Δ, the largest clusters emerging are fractals. I scryed their properties measuring the domain size distribution, $R(m, L)$, and geometric correlation function, $G(r, L)$. $R(m, L)$ measures the fraction of clusters having a mass (number of spins) m in a system of linear size L, as for $G(r, L)$ measures the probability of two spins r cells apart belonging to the same cluster in a system of linear size L. I also verified the conformal properties of the geometric correlation

function with the logarythmic transformation mapping onto a periodic strip.

In this work I have reached the following results [1]:

$\mathcal{I}/a$ In the percolation phase the largest clusters are fractals. The fractal dimension of $d_f = 1.89(2)$ is consistent with $d_f = 91/48$ of standard percolation. So the percolating clusters of the two dimensional random fiels Ising model and the clusters evolving in two dimensional percolations are similar in geometry.

$\mathcal{I}/b$ In the percolating phase the cluster-mass distribution function scales as $R(m, L) = m^{-\tau}\bar{R}(m/L^{d_f})$, where $\tau = 2/d_f$. For smaller clusters ($m \ll L^{d_f}$) the scaling function is constant, $\bar{R}(m/L^{d_f}) \sim \mathcal{O}(1)$, and there is a sudden cutoff at $m \to L^{d_f}$. The largest clusters of size L^{d_f} are fractals of dimension $d_f = 1.89(2)$. This is in good agreement with the extracted values of $\tau = 1.055(3)$.

$\mathcal{I}/c$ I studied the geometric properties of clusters using the geometric correlation function. It shows an algebraic decay, $G(r) \sim r^{\eta}$ in the percolating phase, with an exponent $\eta = 2(d - d_f) = 5/24$. There is a finite size scaling, $G(r, L) = r^{\eta}\tilde{G}(r, L)$, where $\tilde{G}(r, L) \sim \mathcal{O}(1)$, for $1 \ll r \ll L$. This region fits an polynomial decay with the exponent $\eta = 5/24$. I also studied the probability of the farthest spins belonging to the same cluster, $G(L) \equiv G(L/2, L)$. In the percolating phase $G(L)$ scales as $G(L) = L^{-\eta}\hat{G}(L/\xi)$, having $\hat{G}(L/\xi) \sim \exp[-L/2\xi]$. Using the extracted values of $\xi(\Delta)$ I was able to determine, that the correlation length diverges at a certain value of the random field strength spread, $\Delta_c = 1.65$. In the vicinity of Δ_c the correlation length, ξ, diverges as $\sim |\Delta - \Delta_c|^{-\nu}$, with the exponent $\nu = 1.98(5)$. I argued that the correlation length depends on the critical external field of percolation, H_p, as $\xi \sim H_p^{-\tilde{\nu}}$. Here the governing exponent has a value of $\tilde{\nu} = 0.97(5)$. This value coincides with the second thermal exponent of tricritical percolation.

$\mathcal{I}/d$ I investigated the conform properties of the geometric correlation function, so I studied its behaviour in the strip geometry obtained with logarithmic transformation. I concluded, that the finite correlation length, ξ, and the strip width, L_w, is connected by the formula $\xi = L_w/\pi\eta$, where η is the exponent of the decay of the original geometric correlation function. Herewith I proved the conform invariance of the geometric correlation.

Nonequillibrium processes

Understanding cooperative behaviour in far from equillibrium processes is one of the most intriguing challenges in present research. We can even discover such systems in our every day life, like living biological organisms, or the meteorology of the atmosphere are examples, where local behaviour, random fluctuations, or more complicated microprocesses keep the system in a far from equillibrium state. The most widely known physical example is the glass, which if cooled suddenly below certain critical temperature, crystallisation process slows down in such an immerse way, that traps the material in a far from equillibrium state[8]. The fluid properties of the liquid surface in a scope of centuries. This ageing is reversible opposed to biological ageing.

The general method to observe nonequillibrium behaviour of the Ising model is to suddenly cool the system from high temperature to the Curie point. This method is called *quench*[9]. Issuing the quench to a ferromagnetic ordered state will dissolve the ordering, and geometries characteristic to the critical temperature will appear in time. The magnetization as order parameter will change monotonicly. In this case we can speak of an equillibrium process. However for macroscopic system this is a slow process: correlations decay in a polynomial manner. This phenomen is called critical slowdown. The exponent of the decaying polynom is the critical exponent characterizing the equillibrium process.

Quenching from high temperature will start local ordering. The total magnetization is zero, however its value can vary greatly in small subsystems due to local fluctuations, so pair interactions will cause ordering on an increasing length scale, forming clusters, which are units consisting of neighbourghing parallel spins. This coarsening continues up to macroscopic length scales, which is followed by the equillibrium process. If there is a small, positive magnetization present in the initial state, its value will increase for the duration of the nonequillibrium regime at a scale free slope determined by an independent exponent, θ, that is called nonequillibrium exponent.

Studying nonequillibrium properties you seek the change in the corresponding exponents. Starting from disordered state, and quenching to the Curie temperature the course of the magnetization is described by $M(t) \simeq M_i t^{\theta}$, where t is the time elapsed, M_i is the initial magnetization, and θ is the independent nonequillibrium exponent. One time step is considered L^2 number of spin flips, that is each

particle has the chance to flip once per time step on average. Non equillibrium coarsening is limited by the equillibrium processes taking place inside the evolving clusters within a limited time frame, t_0. This time scale scales with the initial magnetization (t_0 $simM_i^{-z/xi}$, where $x_i = \theta z + \beta/\nu$ is the anomal dimension of the magnetization).

Besides magnetization I also measured the autocorrelation function. I checked, how the initial state correlates to later states. This function decayes as $A(s,t) \simeq (t/s)^{-\lambda/z}$ after the quench. The critical exponent λ can be expressed using θ: $\lambda = 2 - \theta z$, where 2 is the actual dimension. It is to be noted, that you can only see clear nonequillibrium effects in the autocorrelation, if the initial magnetization is zero.

Nonequillibrium relaxation starting from the RFIM ground state

It is still an open question, how the initial state can influence nonequillibrium relaxation. RFIM ground states with very small or very large random field strength spread are similar to equillibrium samples of the original Ising model at low and high temperatures. So adjusting the random field strength, we can observe a transition from the nonequillibrium to the equillibrium process. There are also ground states with the largest clusters being fractals, so we can also check, if these kind of long range correlations do alter dynamic behaviour.

I issued the nonequillibrium studies as follows. RFIM ground states were generated, as described in the previous section (they were already present). For each pair of linear size, L and random field strength spread, Δ 10000 independent samples were analyzed, each one ran 20 times with different random seed to improve statistics.

During measurements regarding magnetization, domain borders of the initial states were adjusted in the sample to include a small initial magnetization. This adjustment was introduced randomly and spin by spin. The non equillibrium process was implemented using Heat Bath algorythm. In the corresponding time scale of one Monte Carlo step, L^2 spins were chosen randomly one after the other, independently. For each chosen spin I calculated the energies corresponding to the up and down state of the spin, that determined transition probabilities each

way, based on what I chose the next spin state randomly.

As described above, I studied the Glauber type dynamic process of the two dimensional Ising model on critical temperature, initialized by specific ground states of the two dimensional Random Fiels Ising model with no external field. During the process I measured the magnetization $M(t)$, and the autocorrelation, $A(t) \equiv A(s = 0, t)$, introducing az initial magnetization of $M_i = 0.04$ in the first case. I wondered if fractal structures present in the initial state around Δ_c affect critical dynamic behaviour.

The results can be summarized as following [2, 3]:

$\mathcal{II}/a$ I studied the magnetization $M(t)$ on the nonequilibrium time regime $t \ll t_0$. For $\Delta_b < \Delta <\leq 2.0$, the magnetization was decreasing initially up to t_{min}. I realized, that this value depends on Δ in the vicinity of the critical point like $\ln t_{min} \sim 1/\Delta^2$ I concluded, that in this regime compact regions of linear size L_b present in the RFIM ground states are dissolving.

$\mathcal{II}/b$ I investigated the impact of fractal structures analyzing the nonequilibrium critical exponent θ. So I studied the time evolution of the magnetization, $M(t)$, in the asymptotic regime $t_{min} \ll t \ll t_0$. The measured value of this exponent is $\theta_{RFIM} = 0.184(1)$, that does not depend on the random field strength spread Δ. This result is in good agreement with the original value of $\theta = 0.183(1)$ for random initial state and $M_i = 0.04$ initial magnetization. I concluded, that regarding the exponent θ, long range correlations in the RFIM ground states do not influence nonequilibrium behaviour.

$\mathcal{II}/c$ I also studied the nonequilibrium exponent λ/z utilizing the correlation function $A(t)$. This exponent also becomes independent of the random field strength spread, Δ, in the asymptotic regime. Also the extracted value of $\lambda_{RFIM}/z = 0.73(1)$ corresponds with $\lambda/z = 0.737(1)$ of the original process. These results are in good agreement with the previous results of relaxation.

Nonequillibrium relaxation from correlated initial state

Starting from the RFIM ground states, nonequillibrium exponent values match that of the original relaxation starting from high temperatures. There are more

models, where initial state does not affect long time behaviour[10]. However, there are several examples showing the contrary, like the XY model, where the corresponding anomal dimension depends on both starting and ending temperature of the quench[11]. In the d dimensional spherical model time evolution depends on the dimension, and the exponent of the initial correlation as well[12].

In order to change critical behaviour, I tried changing the type of interactions within the system. I selected three models with multispin bonds. The Baxter-Wu model is defined on the triangle lattice, the energy of the bonding depends on all three spins sitting on the vertices of a single triangle. It is proportional to the product of the three spin values: all spins up, or two spins down will form a stable triplet. While altering the interaction type, edges along one direction of the lattice are also deleted, so the relaxation happens on a square lattice. The Turban model is one kind of a multispin extention to the Ising model on the two dimensional square lattice. While in one direction all interaction are 2-spin, in the other direction $n(> 2)$ neighbouring spins affect each other, and the bond energy is proportional to the product of the spins. I utilized the Turban model with $n = 3$ and $n = 4$.

On critical temperature states of threespin-interaction models consist of a mix of four type of clusters, which is based on the four stable spin triplet. The total magnetization of the system is fluctuating between the two favoured values of 1 and $-1/3$. In rare cases, the total magnetization is eventually 0, when quarter part of the system consists of clusters type $\uparrow\uparrow\uparrow$, and three quarter part of type $\downarrow\uparrow\downarrow$. The sudden interaction change will induce a sharp change in the order parameter within the second typs of clusters, which results in sudden transformation in the beginning of the relaxation.

Phase transition is of the first order in the case of the $n = 4$ Turban model. At the critical temperature the ordered and disordered phases coexist[13]. The order parameter is not necessarily zero, or even small, so I studied its properties as initial state issueing only autocorrelation measurements.

Initial states were generated beforehand for several linear sizes, up to a scale of 240×240. For each system size, 1000 independent samples were chosen at critical temperature with the Monte Carlo method using importance sampling. No further change was necessary, i.e. no initial magnetization was needed. Each independent sample was measured 20 times using different random number seeds.

I can summarize the following results [4]:

$\mathcal{III}/a$ I studied nonequilibrium properties using the exponent θ. I analyzed the evolution of magnetization, $M(t)$, after changing the types of interactions of the equilibrium states in the second order transition point of the Baxter-Wu and $n = 3$ Turban models. In both cases two regimes can be separated after the initial transient. For the first regime both models exhibit the same exponent value $\theta_1 = 0.13(1)$. As well for the second regime $\theta_{BW} = \theta_{3T} = 0.18(1)$, that coincides with the value $\theta = 0.187(3)$ for $M_i = 0.0$ of the classical nonequilibrium process. This concludes, that the change in the interaction type can have an effect on the nonequilibrium behaviour.

$\mathcal{III}/b$ I also studied the nonequilibrium exponent, λ/z using the autocorrelation function, $A(t)$. This function scales as $A(t) \sim t^{-\lambda/z} \exp[-t/t_L]$, as long as $t \gg 1$. I obtained the values $\lambda_{BW}/z = 0.18(1)$ for the Baxter-Wu model, and $\lambda_{3T}/z = 0.165(10)$ for the $n = 3$ Turban model. Both of them is substantially smaller than $\lambda/z = 0.732(3)$, measured for the process with random initial state. These results agree with the previous findings.

$\mathcal{III}/c$ I considered investigating the change in interaction in a critical system residing in a first order transition point. So I used equilibrium critical states of the $n = 4$ Turban model as initial states for the 2D Ising relaxation. I studied its behaviour with the exponent λ/z extracted from the autocorrelation function $A(t)$. This function scales as $A(t) \sim t^{-\lambda/z} \exp[-t/t_L]$ as well. The obtained value of $\lambda_{4T}/z = 0.475(10)$ differs from the classical value of $\lambda/z = 0.732(3)$ significantly. The calculated value of $\lambda_{4T} \simeq 1 = d/2$ can be argued with fluctuations in the volume of the evolving clusters.

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