COOPERATIVE BEHAVIOUR IN COMPLEX SYSTEMS

Ph.D. thesis

by

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INTRODUCTION

Cooperative phenomena is an ordinary pattern in various part of science where interacting entities attempt to satisfy some optimal conditions. Such kind of behaviour is observable in sociology, economy, biology or physics etc., where the correlative agents are defined differently but their behaviour presents universal attributes. In this sense the complexity of a system can be defined by its interconnected features arising from properties of its individual parts. Such parts could be either which govern the interactions or the dynamical rules to control the time evolution or the backgrounding structure which also can influence the system behaviour. This kind of combined effects leads to a complex system with non-trivial cooperative behaviour and brings on many interesting questions which give the motivation for advanced studies.

Correlated systems can be examined efficiently within the frame of statistical physics. The subject of this area is to study systems which depend on random variable, and describe their behaviour obtained from large number of observation using physical terminology. An interesting subject of this segment is the one of phase transitions which has been intensively studied since the beginning of the 20th century. Phase transitions occur in many part of Nature where counteractive processes compete to determine the state of the system controlled by an external parameter. The best-known examples in physics are the liquid-vapor or the ferromagnetic-paramagnetic phase transitions but similar behaviour can be observed in model systems like in different spin models, in epidemic spreading problems or in critical percolation.

The first relevant approach was the *mean field theory* which gave a phenomenological description of phase transitions and critical phenomena and is capable to describe a wide range of model systems. It was first defined by Pierre Weiss in 1907 for ferromagnetic systems where he assumed that the spins interact with another through a molecular field, proportional to the average magnetization. This *molecular field approximation* method neglects the interactions between particles and replaces them with an effective average field which enables to simplify the solution of the problem. At the same time the disadvantage of the method originates from the average molecular field also, since it neglects any kind

of fluctuations in the system. Therefore the mean field approximation is valid only in higher dimensional systems or in case of models where the fluctuations are not important.

One of the simplest and most elegant mean field speculations concerning the possible general form of a thermodynamical potential near to the critical point was introduced later by Lev. D. Landau in 1936. The *Landau theory* allows a phenomenological reproduction of continuous phase transitions based on the symmetry of the order parameter. He assumed that the free energy can be expanded as a power series of the order parameter where the only terms which contribute are the ones compatible with the symmetry of the system.

The observation that the correlation length diverges at the phase transition point and the fluctuations in the system are self-similar in every length scale, led to the recognition of scale invariant behaviour of critical systems. The first comprehensive mathematical approach of such phenomena was given by Leo Kadanoff in the 1960s. A few years later in the beginning of the 1970s based on his results, Kenneth G. Wilson gave the relevant discussion of the subject in his celebrated papers. He introduced the *renormalization group theory* which serves predictions about critical behaviour in agreement with experimental results and give a possibility to categorize critical systems into universality classes due to them singular behaviour. His investigations were awarded with a Nobel prize in 1982.

In the beginning of the 1970s another theory emerged which completed the knowledge about the universal behaviour around the criticality. The *conformal field theory* was firstly investigated by Polyakov, who capitalized that the group of conformal mappings is equivalent to the group of complex analytical functions in two dimensions. Exploiting this property and the scale invariant behaviour, the partition function of a critical system is derivable which leads to exact calculations of critical exponents. In the case of conform transformations the order parameter correlation functions can be calculated also which then enables to deduce the order parameter profiles along the system boundaries.

As a first approximation generally the investigated system is assumed to

be homogeneous, which condition simplifies its study and the physical description. However, in Nature a substance is often characterized by certain degree of inhomogeneity which could perturb its critical behaviour. Frequently stated examples of this abnormality, are the lattice defects and impurities in crystals. In theoretical description this kind of feature is introduced by the concept of disorder which is defined as random distributed values of certain properties of the investigated *disordered model*. These random properties can be the strength of interaction, a random external field or can arises by random dilution. These properties are able to modify the critical features of the system as changing the order of phase transition or shift the critical point and exponents, thus transforming the model into a new universality class.

However, inhomogeneity can arise from the geometrical structure of the backgrounding framework of materials also. Beyond solid-state physics where crystals have a regular geometry, many self-organizing media in the Nature can form random structures. Two Hungarian mathematicians, Pál Erdős and Alfréd Rényi defined the first related *random graph model* in their pioneering papers in the beginning of the 1960s which was the origin of the new science of networks. However, as the informations of real world networks became available by the emergence of large databases, a deeper view into the underlying organizing principles suggested a more complex structure. In the beginning of the 1990s Barabási, Albert and Jeong after they examined the structure of the World Wide Web found an algebraic decay of the network degree distribution. This observation made them realize the real rules which govern the evolution of such kind of *complex networks*. They defined a dynamical growing network model, *the Barabási-Albert model*, where the sites are not connected homogeneously but follow a so-called preferential attachment rule leading to a *scale-free graph* with a power-law degree distribution. This model gave a very good approximation of real complex networks and became popular after many complex systems in science and technology were found to present the same structure. This interdisciplinary behaviour which suggests universal rules behind self-organizing networks keeps this discipline to the frontline of science up to this day.

APPLIED NUMERICAL METHODS

Analyzing a complex many body system was difficult earlier since generally these systems have large degrees of freedom and those could be in many possible states. However, by the improvement of computational engines new possibilities appeared and high precision numerical methods were developed to examine the relevant models. It was the base of the new discipline of numerical physics which then became the third pillar of the science beyond the experiments and theory. By using numerical calculations, the statistical description of many body systems became available which then led to a renaissance of the statistical physics. This relation induced the evaluation of *Monte Carlo methods* which provided special computational technics for statistical physics simulations.

One of the first and most frequently used method which is capable to simulate interacting spin systems is the *Metropolis algorithm*, introduced in 1953. This so-called single spin flip algorithm evaluate the system through a Markov chain where the system energy change depends on local configurations. However, some other algorithms of *Swendsen-Wang* and *Wolff* provided more efficient methods where instead of one-by-one spin flips, complete domains are turned in one step and evaluate the system faster toward its equilibrium.

Beyond that, many other kind of statistical methods were developed in order to calculate some thermodynamical function using mathematical considerations. A recent algorithm which capitalize *combinatorial optimization* is capable to calculate exactly the free energy for models where the free energy function can be recognized as a *submodular function*. This iterative method which provided results in strongly polynomial time was applied frequently in course of my work.

MOTIVATIONS AND NEW SCIENTIFIC RESULTS

My motivation during my PhD studies was to examine cooperative behaviour in complex systems using the previously mentioned methods of statistical and computational physics. The aim of my work was to study the critical behaviour of interacting many-body systems during their phase

transitions and describe their universal features analytically and by means of numerical calculations. In order to do so I completed studies in four different subjects which are presented in the dissertation as follows:

I. Non-equilibrium phase transitions and finite-size scaling in weighted scale-free networks

My first investigated subject was a study of non-equilibrium phase transitions in weighted scale-free networks where I introduced edge weights and rescaled each of them by a power of the connectivities, thus a phase transition could be realized even in realistic networks having a degree exponent $\gamma \leq 3$ [1]. The investigated non-equilibrium system was the contact process which is a reaction-diffusion model belonging to the universality class of directed percolation. This epidemic spreading model presents a phase transition between an infected and a recovered state ordered by the ration of the recovering and infecting probability.

I/a: First I gave the dynamical mean-field solution of the model in scale-free networks and I located the previously known three critical regimes. The first regime is the one where the mean-field behaviour is conventional. Then this solution becomes unconventional since critical properties are γ dependent. In the third regime, the system is always in an active phase.

I/b: I also made some theoretical considerations to generalize recent field-theoretical results about finite-size scaling which are expected to be valid above the upper critical dimension i.e. in the conventional mean-field regime. I introduced in a simple way the volume of the network into the scaling functions that I derivate for two cases, where the infection was initiated from a typical connected site or from the most connected vertex of the network.

I/c: I executed high performance numerical simulations in order to simulate the contact process in the conventional mean-field regime. I located the phase transition point and I calculated the finite-size scaling exponents for typical and maximally connected site that I found to be in good agreement with the field-theoretical predictions. I also determined the correlated volume exponent which was found equal in the two cases

and compatible with the theoretical expectations. Finally I analyzed the dynamical scaling of the system at the critical point for the two above mentioned cases. Through extrapolations I considered the related exponents to be different in the case of typical and maximally connected sites but compatible with the mean-field and finite-size scaling predictions.

II: Rounding of first-order phase transitions and optimal cooperation in scale-free networks

The second problem I investigated was the ferromagnetic random bond Potts model with large values of q on evolving scale-free networks [2]. This problem is equivalent to an optimal cooperation problem, where the agents try to find an optimal situation where the benefits of pair cooperation (here the Potts couplings) and total sum of the support, which is the same for all projects (introduced here as the temperature), is maximized. A phase transition occurs in the system between a state when each agents are correlated and a high temperature disordered state. I examined this model using a combinatorial optimization algorithm on scale-free Barabási-Albert networks with homogeneous couplings and when the edge weights were independent random values following a quasi-continuous distribution with different strength of disorder.

II/a: As a first point I gave the exact solution of the system for a wide class of evolving networks with homogeneous couplings. The phase transition was found to be strictly first-order and the critical point was determined through simple theoretical considerations.

II/b: By numerical calculations I examined the magnetization curve for different strength of disorder and found the theoretically predicted first-order phase transition in the pure case. However, the phase transition softened to a continuous one for any strength of disorder larger than zero. I examined the structure of the optimal set and I found out its structural behaviour was altered by the temperature.

II/c: I studied also the critical properties of the system and I calculated the distribution of the finite-size critical temperatures for different sizes in case of maximal disorder. I deduced by iterative calculations the critical

magnetization exponent and I located the critical temperature using two independent methods. The scaling of the finite-size transition points distribution was characterized by two distinct exponents, that I located and used to consider a scaling collapse of the distribution curves.

II/d: I also deduced the critical magnetization exponent by two-point fits using the average size of the critical cluster. I obtained compatible values with previous results within the error of the calculations.

III: Density of critical clusters in strips of strongly a disordered system

The third examined problem was related to the large-q sate random bond Potts model also. Here I examined the critical density of clusters which touched a certain border of a perpendicular strip like geometry [3]. Following from conformal prediction I expected the same density behavior as it was exactly derived for critical percolation in infinite strips. I calculated averages by the above mentioned effective combinatorial optimization algorithm and I compared the numerical means to the expected theoretical curves.

III/a: During my study I used a bimodal form of disorder for the random couplings, which intensity influenced the breaking-up length of the critical clusters. I allocate an appropriate value of the strength of the disorder which set the breaking up length large enough for relevant measurements but small enough to keep away from the percolation limit.

III/b: First, I examined the critical densities of spanning clusters which touch both boundaries along the strip geometry. I found a good agreement between the predicted conformal values and the calculated averages of different linear size. I checked the validity of a combination of the bulk and surface magnetization exponents coming from scaling predictions through the study of the density behaviour close to the boundaries and I found reasonable accordance. I also applied a correction close to the boundaries in order to obtain a better fit between the calculated and predicted curves.

III/c: Second, I considered the density of the clusters which are touching one boundary of the strip. This density is analogous to the order parameter profile in the system with fixed-free boundary conditions. This profile close to the fixed boundary was strongly perturbed by surface effects, which are due to the presence of the finite breaking up length. However, at the free boundaries the density curves approached a scaling curve which sat on the predicted conformal function. Close to the fixed boundary I estimated the asymptotic behaviour of the scaling curve through extrapolation and I obtained values in agreement with the conformal results.

III/d: Finally I considered the density of points in clusters that are touching one of the boundaries or both. This density is analogous to the order parameter profile with parallel fixed spin boundary conditions. This density profile was found to be strongly perturbed by the breaking-up length at both boundaries thus I studied another density which was defined on crossing clusters only. However, it was supposed to be related to the same operator profile and expected to present the same scaling form. I performed the same calculation for percolation also and I found that the numerical and analytical results for this type of density profile were in good agreement in both cases.

IV: Non-equilibrium dynamics of triangular antiferromagnetic Ising model at T=0

The last investigated problem was the antiferromagnetic Ising model on two-dimensional triangular lattice at zero temperature in the absence of external field [4]. This model was intensively studied during the last few decades, since it shows exotic features in equilibrium due to its geometrical frustration. However contradictory explanations were published in the literature about its non-equilibrium dynamical behaviour as it was characterized by a diffusive growth with logarithmic correction or by a sub-diffusive dynamics with effective exponents. My aim was to find independent evidences for one of the explanation and examine the dynamical behavior in the aging regime.

IV/a: To study the non-equilibrium behaviour of the system I introduced a new quantity, the non-equilibrium relaxation time t_r, which depends only

on the dynamics and that is capable to determine directly the true value of the dynamical exponent z. The analysis of the distribution provided a strong proof for the dynamics in the aging regime to be governed by an exponent $z=2$ with logarithmic correction as it was found in related problems like the two-dimensional XY model and the fully frustrated Ising model.

IV/b: Following some recent published methods [30] I also studied numerically the two-time autocorrelation function in the equilibrium regime with different waiting times, after the system was relaxed into an equilibrated state. Here I found the expected time-translational invariant behaviour of the autocorrelation function and I located the same dynamical exponent value as above through some exponent combination.

IV/c: Finally I considered the scaling of the autocorrelation function of different waiting times in the aging regime where I used two kind of scaling variables. The one without logarithmic correction did not show a good scaling collapse which suggested that this variable choice was inconvenient. However the scaling with a logarithmically corrected variable presented an asymptotically good scaling collapse which proved the validity of the logarithmic corrections during the non-equilibrium dynamics in agreement with the previous considerations.

Related publications:

[1] **Karsai, M.**; Juhász, R. and Iglói, F.: *Non-equilibrium phase transitions and finite-size scaling in weighted scale-free networks.*
Physical Review E, **73**, 036116 (2006)

[2] **Karsai, M.**; Anglès d'Auriac, J-Ch. and Iglói, F.: *Rounding of first-order phase transitions and optimal cooperation in scale-free networks.*
Physical Review E, **76**, 041107 (2007)

[3] **Karsai, M.**; Kovács, I. A.; Anglès d'Auriac, J-Ch. and Iglói, F.: *Density of critical clusters in strips of strongly disordered systems.*
Physical Review E, **78**, 061109 (2008)

[4] **Karsai, M.**; Anglès d'Auriac, J-Ch. and Iglói, F.: *Non-equilibrium dynamics of triangular antiferromagnetic Ising model at T=0.*
publication in progress (2009)