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Computational Quantum Field Theory

9.1 Introduction

The Computational Physics Group performs basic research into classical and quantum statistical physics with special emphasis on phase transitions and critical phenomena. In the centre of interest are currently the physics of spin glasses, diluted magnets and other materials with quenched, random disorder, soft condensed matter physics with focus on fluctuating paths and interfaces, and biologically motivated problems such as protein folding, aggregation and adhesion as well as related properties of semiflexible polymers. Investigations of a geometrical approach to the statistical physics of topological defects with applications to superconductors and superfluids and research into fluctuating geometries with applications to quantum gravity (e.g., dynamical triangulations) are conducted within the EC-RTN Network "ENRAGE": *Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*. The statistical mechanics of complex networks is studied within the frame of an Institute Partnership with the Jagellonian University in Krakow, Poland, supported by the Alexander-von-Humboldt Foundation. And with the help of a Development Host grant of the European Commission, also research into the physics of anisotropic quantum magnets has been established.

The methodology is a combination of analytical and numerical techniques. The numerical tools are currently mainly Monte Carlo computer simulations and high-temperature series expansions. The computational approach to theoretical physics is expected to gain more and more importance with the future advances of computer technology, and will probably become the third basis of physics besides experiment and analytical theory. Already now it can help to bridge the gap between experiments and the often necessarily approximate calculations of analytical work. To achieve the desired high efficiency of the numerical studies we develop new algorithms, and to guarantee the flexibility required by basic research all computer codes are implemented by ourselves. The technical tools are Fortran, C, and C++ programs running under Unix or Linux operating systems and computer algebra using Maple or Mathematica. The software is developed and tested at the Institute on a cluster of PCs and workstations, where also most of the numerical analyses are performed. Large-scale simulations requiring vast amounts of computer time are car-

ried out at the Institute on a Beowulf cluster with 40 Athlon MP1800+ CPUs and an Opteron cluster with 18 processors of 64-bit architecture, at the parallel computers of the University computing center, and upon grant application at the national supercomputing centres in Jülich and München on IBM and Hitachi parallel supercomputers. This combination of various platforms gives good training opportunities for the students and offers promising job perspectives in many different fields for their future career.

Within the University, our research activities are tightly bound to the Centre for Theoretical Sciences (NTZ) of the Centre for Advanced Study (ZHS) and the recently established priority research areas ("Profilbildende Forschungsbereiche (PbF)") and Research Academy Leipzig (RAL), providing in particular the organizational frame for our cooperations with research groups in experimental physics and biochemistry. On a wider scale, they are embedded in a wide net of national and international collaborations funded by network grants of the European Commission and the European Science Foundation (ESF), and by binational research grants with scientists in Sweden, China and Poland funded by the German Academic Exchange Service (DAAD) and the Alexander-von-Humboldt Foundation. Further close contacts and collaborations are also established with research groups in Armenia, Austria, France, Great Britain, Israel, Italy, Russia, Spain, Taiwan, Turkey, Ukraine, and the United States.

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9.2 Free-Energy Landscapes and Barriers of Spin Glasses

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Spin glasses are characterized by random, competing interactions leading to "frustration" effects, i.e., no unique spin configuration is favoured by all interactions [1]. This is the reason for a rugged free energy landscape in such systems which, in Monte Carlo computer simulations, is reflected by an extremly slow (pseudo-) dynamics. To some extent this problem can be overcome by our recently proposed multi-overlap algorithm [2]. Using this algorithm in a large-scale study of the three-dimensional (3D) short-range Edwards-Anderson Ising (EAI) $\pm J$ model, we were able to determine the scaling behaviour of the barrier heights [3] and the tails of the overlap-parameter distribution [4]. In particular the barrier-height distribution was found not to agree with mean-field predictions.

This prompted us to generalize our method to long-range models [5]. By this means we investigated the finite-size scaling behaviour of free-energy barriers in the Sherrington-Kirkpatrick (SK) model. With N denoting the number of spins, here we found for the barrier-height scaling a power law N^{α} with $\alpha = 1/3$ [5], in perfect agreement with the theoretical prediction.

Since the analysis tools were precisely the same as in the previous EAI study, the central question thus is: Does the barrier-height scaling show a qualitative difference between short- and long-range models, or did we simply not yet reach the truly asymptotic region in the previous study? The latter possibility is quite conceivable because due to the technical difficulties the simulations had to be performed quite close to the freezing transition. To answer this question, we therefore further improved our multi-overlap method by combining it with parallel tempering in temperature [6]. As a result this allows us to perform meaningful simulations at much lower temperatures than before where the asymptotic limit should be reached already for much smaller lattice sizes. Still, these simulations are very demanding and require many years of CPU time on parallel supercomputers such as JUMP at Forschungszentrum Jülich. The data production is running at full pace and to date we have already completed a few hundred disorder realizations for various lattice sizes. A few more are still needed, however, before a meaningful quenched average and the final data analysis can be performed.

Along another line of this project we are investigating also the random orthogonal model (ROM), which is a generic representative for 1-step replica symmetry breaking (1SRB). Here, however, the simulations turned out to be even more intricate than in the other two models and the data production is correspondingly severely hampered.

One possible reason for the still very slow dynamics are "hidden" barriers which are not directly visible in the commonly considered quantities such as the energy, magnetization or overlap. This conjecture is born out by analogous observations for the simpler Ising model at low temperatures [7]. To underscore this possibility we have performed extensive simulations of this simpler model and studied in great detail the "hidden" barriers associated with both, the droplet-strip [8] and the evaporation/condensation [9, 10] transition [11]. Once these barriers are fully understood in the simpler Ising model, the hope is that similar ideas can be transferred to spin glasses as well.

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[1] K.H. Fischer, J.A. Hertz: *Spin Glasses* (Cambridge University Press, Cambridge 1991)
[2] B.A. Berg, W. Janke: Phys. Rev. Lett. **80**, 4771 (1998)
[3] B.A. Berg et al.: Phys. Rev. B **61**, 12 143 (2000); Physica A **321**, 49 (2003)
[4] B.A. Berg et al.: Phys. Rev. E **65**, 045 102(R) (2002); *ibid.* **66**, 046 122 (2002)
[5] E. Bittner, W. Janke: Europhys. Lett. **74**, 195 (2006)
[6] A. Nußbaumer, E. Bittner, W. Janke: in preparation.
[7] T. Neuhaus, J.S. Hager: Stat. Phys. **113**, 47 (2003)
[8] K. Leung, R.K.P. Zia: J. Phys. A Math. Gen. **23**, 4593 (1990)
[9] M. Biskup et al.: Europhys. Lett. **60**, 21 (2002)
[10] K. Binder: Physica A **319**, 99 (2003)
[11] A. Nußbaumer et al.: Europhys. Lett. **75**, 716 (2006); in: *Computer Simulation Studies in Condensed-Matter Physics XX*, ed. by D.P. Landau et al. (Springer, Berlin 2007), in print

9.3 High-Temperature Series Expansions for Potts Models: Disordered Magnets and Percolation

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Systematic series expansions for statistical physics models defined on a lattice are a well-known alternative to large-scale numerical simulations for the study of phase transitions and critical phenomena [1]. For quenched disordered systems the extension of this method [2] requires especially adapted graph theoretical and algebraic algorithms. In this project we developed a computer package based on the "star-graph" method [2, 3] which allows the generation of high-temperature series expansions for the free energy and susceptibility. We consider the class of disordered q-state Potts models on d-dimensional hypercubic lattices $\mathbb{Z}^d$ with bimodal probability distributions of quenched couplings parametrized by $P(J_{ij}) = p\delta(J_{ij} - J_0) + (1-p)\delta(J_{ij} - RJ_0)$, which includes spin glasses, diluted ferromagnets, random-bond models and transitions between them. The limiting case $p = 1$ describes the pure ferromagnetic ($J_0 > 0$) models. Even though the method is highly optimized for the problem at hand, it is extremely demanding since the number of contributing graphs grows exponentially with the order of the series and all intermediate calculations have to be performed by means of symbolic computer algebra, which we implemented ourselves in C++ since the available standard software products such as `Mathematica` or `Maple` are too slow and require far too much memory.

In a first step we considered the bond-diluted Ising model ($q = 2$) for which we used our computer package to generate high-temperature series up to order 21 in $d = 3$ dimensions [4, 5] and up to order 19 in $d = 4, 5$ [5]. Applying various analysis tools we determined the phase diagrams in the temperature-dilution plane and estimated the critical exponent γ, parametrizing the singularity of the susceptibility at criticality, $\chi \sim (T - T_c)^{-\gamma}$. Depending on the dimension, our results can be compared with field-theoretic predictions and estimates from our Monte Carlo simulations performed in another project [6]. We established the irrelevance of disorder above the critical dimension $d = 4$ and the existence of unusual logarithmic corrections at the critical dimension.

We also obtained and analysed series for the pure q-state Potts model with arbitrary parameter q [7]. The series are generated up to order 21 in $d = 3$ dimensions, order 19 in $d = 4, 5$, and order 17 for *arbitrary* dimensions, that is with d as a symbolic parameter. This allowed a throughout analysis of bond percolation (described by the $q \to 1$ limit of the Potts model) on hypercubic lattices giving new estimates of the percolation thresholds and the critical exponent of the mean cluster size.

[1] C. Domb, M.S. Green (Eds.): *Phase Transitions and Critical Phenomena*, Vol. 3 (Academic Press, New York 1974)
[2] R.R.P. Singh, S. Chakravarty: Phys. Rev. B **36**, 546 (1987)
[3] M. Hellmund, W. Janke: Cond. Matter Phys. **8**, 59 (2005)
[4] M. Hellmund, W. Janke: Comp. Phys. Comm. **147**, 435 (2002)
[5] M. Hellmund, W. Janke, Phys. Rev. B **74**, 144201 (2006)
[6] W. Janke et al.: invited plenary talk, PoS **LAT2005**, 018 (2005)
[7] M. Hellmund, W. Janke: Phys. Rev. E **74**, 051 113 (2006)

9.4 Self-Avoiding Walks on Percolation Clusters

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In close analogy to scaling laws at second-order phase transitions, the behaviour of long fexible polymer chains in a good solvent can be described by power laws in the number of monomers N. It is well established that these scaling properties are perfectly described within a model of a self-avoiding walk (SAW) on a regular lattice [1]. In particular, for the average squared end-to-end distance R and the number Z_N of SAWs with N steps, one finds in the asymptotic limit $N \to \infty$:

$$\langle R^2 \rangle \propto N^{2\nu}, \quad Z_N \propto z^N N^{\gamma-1} , \tag{9.1}$$

where ν and γ are universal critical exponents and z is the effective coordination number of the considered lattice. By exact enumerations, Monte Carlo simulations, or mapping this problem onto the $n \to 0$ limit of O(n) symmetric field theory and applying the renormalization-group approach (e.g. ϵ-expansions), the values of these exponents are very precisely known in physical dimension $D = 3$.

A question of great current interest is the influence of structural disorder on the universal properties of a SAW, namely: does the scaling law holds with new exponents ν_p and γ_p when a SAW resides on a structurally disordered (diluted) lattice? The question of how linear polymers behave in disordered media is not only of academic interest, rather it is also of relevance for understanding transport properties of polymer chains in porous media, such as enhanced oil recovery, gel electrophoresis, gel permeation chromatography, etc. [2].

Currently, the behaviour of SAWs in disordered media is still a subject where many principal questions are unsettled. In this project, we focus on the special case where the disordered lattice is taken as a percolation cluster exactly at threshold. Both, SAWs and percolation clusters are among the most frequently encountered examples of fractals in condensed matter physics. As it has become clear by now, higher-order correlations of a fractal object living on another fractal lead to multifractality, so that a SAW on a percolation cluster is thus a good candidate for observing multifractal behaviour.

Flory like theories predict that [3]

$$\nu_p = \frac{3}{2 + d_f} , \tag{9.2}$$

where d_f is the fractal dimension of the percolation cluster, leading in three dimensions to $\nu_p = 0.662$, in fairly good agreement with Monte Carlo simulations [3], while recent ϵ-expansions yield $\nu_p = 0.678$ [4]. In higher dimensions, up to the so-called upper critical dimension $d_u = 6$ (where mean-field behaviour sets in), much less is known. In our ongoing numerical study we employ chain growth methods with population control, in particular the Pruned-Enriched Rosenbluth-Rosenbluth Method (PERM) [5], relying on our experience with similar simulations of lattice proteins [6].

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[1] J. des Cloizeaux, G. Jannink: *Polymers in Solution* (Clarendon Press, Oxford 1990); P.-G. de Gennes: *Scaling Concepts in Polymer Physics* (Cornell University Press, Ithaca and London 1979)
[2] K. Barat, B.K. Chakrabarti: Phys. Rep. **258**, 378 (1995)
[3] K. Kremer: Z. Phys. B **45**, 149 (1981)
[4] V. Blavatska et al.: Phys. Rev. E **70**, 035 104(R) (2004)
[5] P. Grassberger: Phys. Rev. E **56**, 3682 (1997); H.-P. Hsu et al.: J. Chem. Phys. **118**, 444 (2003)
[6] M. Bachmann, W. Janke: Phys. Rev. Lett. **91**, 208 105 (2003); J. Chem. Phys. **120**, 6779 (2004)

9.5 Percolation of Vortex Networks in the $U(1)$ Lattice Higgs Model

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Simple field theories in three dimensions like the complex ϕ^4 theory coupled to an electromagnetic field (gauge field) play an important role as effective theories describing phase transitions in the field of superconductivity and QCD. These transitions occur upon a change of (coupling) parameters like the self-coupling λ of the ϕ field and the parameter κ which couples the ϕ and gauge field.

Recently, we analysed the compact lattice version of such a field theory, the $U(1)$ lattice Higgs model, via Monte Carlo simulations [1] and argued that despite the non-existence of an ordinary phase transition the phase diagram is clearly separated into two phases which can be identified by the existence of monopoles or vortex lines. The latter are objects much like the vortex lines found in superconducting liquids. Our central thesis [2] was therefore, that the phase separation line can be interpreted as a Kertész line [3] on which a vanishing line tension leads to a proliferation of vortices. Although no divergences (phase transition) in the (free) energy can be seen we should find weak singularities in so-called cluster or droplet observables as a consequence. One such quantity is for instance the size of clusters formed by vortices. Our most recent simulations focused on these cluster quantities directly and give strong support for our previous findings. Figure 9.1 shows that we find the expected scaling behaviour of the maximal cluster size. As a second result we find that the critical exponents describing this phenomena are just the ordinary percolation exponents [4].

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[1] S. Wenzel: Master Thesis, Universität Leipzig 2004
[2] S. Wenzel et al.: Phys. Rev. Lett. **95**, 051 601 (2005)
[3] J. Kertesz: Physica A **161**, 58 (1989)
[4] D. Stauffer, A. Aharony: *Introduction to Percolation Theory* (Taylor and Francis, London 1994)

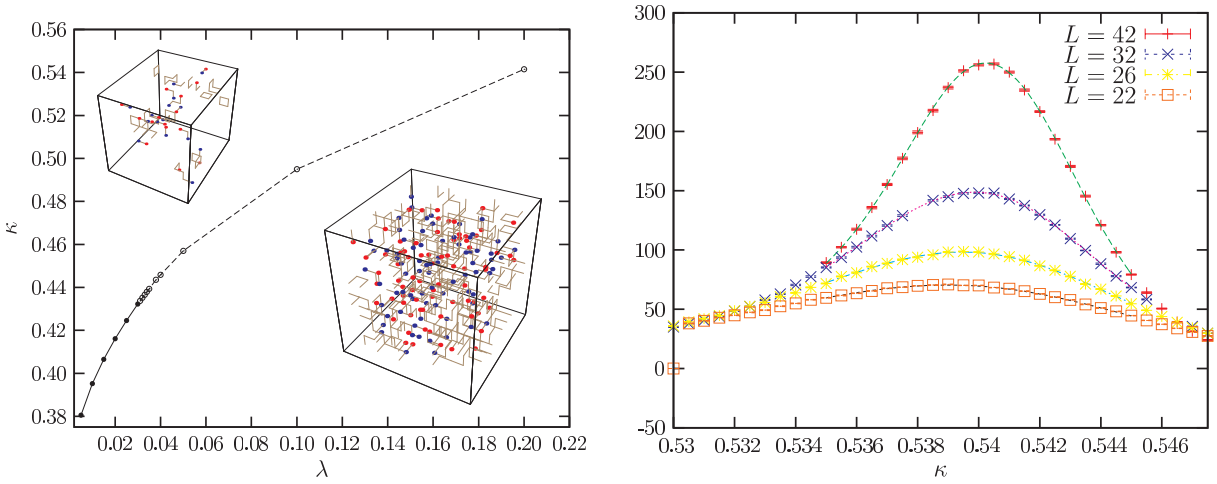

Figure 9.1: *Left:* Phase diagram of the $U(1)$ lattice Higgs model in dependence on two coupling constants. While for small λ the type of the transition line is of first order (*black dots*), the line continues as a Kertész line (*open dots*) with no thermal phase transition. The *insets* show typical configurations of the vortex network in the two phases. *Right:* Diverging susceptibility of the maximal cluster size at the Kertész line $\lambda = 0.20$.

9.6 Geometric and Stochastic Clusters: Fractal Dimensions and Critical Exponents in Regular and Gravitating Potts Models

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The relation between the percolation problem and thermal phase transitions of lattice spin systems has been a question of intense research for at least three decades. Clusters of even spins are natural objects occurring in the analysis of phase ordering processes and nucleation [1], and a theory of critical phenomena in terms of purely geometrical objects appears appealing. In this context, it had long been surmised that a continuous phase transition of a spin system might be accompanied (or, in fact, caused) by a percolation transition of the clusters of like spins (*geometric clusters*), the appearance of a percolating cluster sustaining the onset of a non-zero magnetisation. While for the special case of the Potts model in two dimensions it turned out that, indeed, the thermal phase transition point coincides with the percolation transition of the spin clusters, this behaviour is not generic and does not occur in three-dimensional systems [2]. Also, the critical exponents associated to the percolation of geometric clusters are not directly related to the thermal exponents of the spin model. However, a close relation between the percolation and thermal phase transitions can be established by considering *stochastically* defined clusters (or droplets) as they occur in the Fortuin–Kasteleyn (FK) representation of the Potts model, and it can be shown that, in fact, the Potts model is equivalent to a site-bond correlated percolation problem [3] such that the corresponding critical exponents agree. This

identification of the proper cluster objects (*FK clusters*) percolating at the thermal phase transition subsequently also allowed for the design of *cluster algorithms* for the efficient simulation of Potts models in the vicinity of the ordering transition [4], beating the observed critical slowing down of local update algorithms. Similarly, relations of continuous-spin models to percolation problems could be established and corresponding cluster algorithms formulated [5], such that the continuous phase transitions of many standard models of statistical mechanics are by now understood in terms of the percolation properties of some suitably defined ensemble of stochastic clusters.

Although not sharing the critical exponents of the thermal phase transition, the clusters of like spins or geometric clusters still undergo a percolation transition in the course of thermal phase ordering. This transition is in general not equivalent to ordinary (site or bond) percolation and it remains an interesting open question to determine the general critical behaviour of clusters of aligned spins. For the case of the two-dimensional Ising model, it has been conjectured and numerically verified that the geometric clusters are described by the $q = 1$ tricritical Potts model; this correspondence can be understood from a direct construction starting from the dilute Potts model [6] and the fact that both models are characterized by the same central charge c. Subsequently, analogous conjectures for the $2 < q \leq 4$ Potts models were made and some of them substantiated by numerical simulations [7]. Analytical calculations concerning clusters occurring in systems of statistical physics and their boundaries, traditionally based on methods of conformal field theory and the Coulomb gas [8], have recently seen major advances from the insight that fractal random curves can be described in a framework dubbed *stochastic Loewner evolution* (SLE) [9]. Collecting these observations, a more systematic analysis of the relation between the critical and tricritical branches of the Potts model and their connection to the FK and geometric clusters has been performed, resulting in the identification of exact values for the different cluster fractal dimensions and their numerical verification [10, 11].

Recently we considered the fractal dimensions of critical clusters occurring in configurations of a q-state Potts model coupled to the planar random graphs of the dynamical triangulations formulation of Euclidean quantum gravity in two dimensions which, from a statistical mechanics point of view, may be regarded as a particular type of annealed connectivity disorder. We applied the KPZ formalism [12] to derive exact theoretical predictions for the fractal dimensions of both FK and geometric clusters in the case of Potts models and employed numerical simulation methods to succesfully confirm them for the Ising case $q = 2$ [13].

[1] K. Binder et al.: Phys. Rev. B **12**, 5261 (1976); A.J. Bray: Adv. Phys. **43**, 357 (1994)
[2] A. Coniglio et al.: J. Phys. A **10**, 205 (1977)
[3] C.M. Fortuin, P.W. Kasteleyn: Physica **57**, 536 (1972); A. Coniglio, W. Klein: J. Phys. A **13**, 2775 (1980)
[4] R.H. Swendsen, J.-S. Wang: Phys. Rev. Lett. **58**, 86 (1987); U. Wolff: Phys. Rev. Lett. **62**, 361 (1989)
[5] P. Blanchard et al.: J. Phys. A **33**, 8603 (2000)
[6] C. Vanderzande, A.L. Stella: J. Phys. A **22**, L445 (1989); A.L. Stella, C. Vanderzande: Phys. Rev. Lett. **62**, 1067 (1989)

[7] B. Duplantier, H. Saleur: Phys. Rev. Lett. **63**, 2536 (1989); C. Vanderzande: J. Phys. A **25**, L75 (1992)
[8] B. Duplantier: J. Stat. Phys. **110**, 691 (2003)
[9] O. Schramm: Israel J. Math. **118**, 221 (2000); M. Bauer, D. Bernard: arXiv:math-ph/0602049
[10] Y.J. Deng et al.: Phys. Rev. E **69**, 026 114 (2004)
[11] W. Janke, A.M.J. Schakel: Nucl. Phys. B **700**, 385 (2004); Phys. Rev. E **71**, 036 703 (2005); Braz. J. Phys. **36**, 708 (2006)
[12] V.G. Knizhnik et al.: Mod. Phys. Lett. A **3**, 819 (1988)
[13] W. Janke, M. Weigel: Phys. Lett. B **639**, 373 (2006)

9.7 Statistical Mechanics of Complex Networks

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Complex networks are present in many systems, having either natural or artificial origin [1]. For example, the Internet is built up of computers linked by various physical or wireless links. The World Wide Web is a large complex of webpages connected by hyperlinks. The living cell can be described as a set of chemicals and appropriate chemical reactions. Also the social contacts between people form a network with high level of complexity, which allows for spreading ideas as well as diseases. The above systems are only a few examples of a rapidly developing interdisciplinary field of research often called the "science of complex networks", joining many different areas of human activity. The subject of interest of biologists, chemists, sociologists, computer scientists and others is to find general laws governing the creation and growth of complex networks. Despite an enormous variety of networks and big differences in their physical structure it is possible to form such general laws. This situation still motivates researchers to study basic mechanisms underlying many properties of observed networks.

The main objective of this project is to investigate the influence of coupled matter fields on the geometry and topology of complex networks. Similar problems have been addressed in the context of quantum simplicial gravity or string theory but have not yet been thoroughly studied in the context of complex networks. Only the opposite problem has been investigated so far, namely how geometrical and topological properties of the underlying network influence the behaviour of matter fields. In a broad sense, one can understand by matter field any set of dynamical degrees of freedom living on the nodes or links of a network. This type of questions plays an important role in studies of complex systems whose architecture is represented by a network resulting from the interactions of entities forming the system. In our investigations we try to adapt methods of statistical mechanics developed earlier in the different applications mentioned above, employing both numerical Monte Carlo simulations as well as analytic calculations.

More specifically, we consider so-called zero-range processes [2], where particles move through the sites of a network according to some ultra-local rules. The main objective is to understand how geometrical and topological properties of networks and the dynamics of the particles are interrelated [3]. This is an example of interaction between "matter" and "geometry".

Similar problems appear in the dynamical triangulation approach to quantum gravity [4, 5], where one studies an ensemble of graphs of a special kind, preserving Lorenzian or Euclidean symmetry. There one tries to understand how the space-time geometry represented by those graphs changes when it interacts with matter fields [6]. For example the Ising model on dynamical triangulation corresponds to a fermionic field coupled to two-dimensional quantum gravity [7]. At the critical point, the appearance of long-range correlations of the Ising spins strongly influences the geometrical properties of the dynamical triangulations on which the "matter" model is defined. This is a clear signal of the back-reaction of geometry to the changes in the matter sector.

Part of the project is devoted to studies of non-equilibrium processes. In particular, the zero-range process mentioned above, when studied on a network can be used as a model for the dynamics of backgammon or "balls-in-boxes" condensation [8]. The statistical properties of this condensation have already been well established, but the issue of how the equilibrium of the condensate is reached, has not yet been studied thoroughly. The condensation of backgammon-type is a state of the system represented by a distribution of balls on the nodes such that one of the nodes collects a finite fraction of balls proportional to the total number in the system, similar to Bose-Einstein condensation, but here in real space. One can think of the links of the network as channels along which balls can flow between the nodes. The question of interest for non-equilibrium physics is how the condensate is produced in time and how much time it takes to produce it [9].

This type of problem can be a prototype for a wide class of problems concentrating on the back-reaction of the architecture of a complex system on internal matter flows and distributions and can be of interest for transportation, telecommunication, sociology and biology, where the systems automatically adjust to the changing situation.

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[1] R. Albert, A.-L. Barabási: Rev. Mod. Phys. **74**, 47 (2002)
[2] C. Godreche, J.M. Luck, J. Phys. A **38**, 7215 (2005)
[3] L. Bogacz et al.: arXiv:cond-mat/0701553, Chaos (in print)
[4] J. Ambjorn et al.: Phys. Rev. D **72**, 064 014 (2005)
[5] J. Ambjorn et al.: Phys. Rev. D **48**, 3695 (1993)
[6] W. Janke et al.: Cond. Matter Phys. **9**, 263 (2006)
[7] D.V. Boulatov, V.A. Kazakov: Phys. Lett. B **186**, 379 (1987)
[8] P. Bialas et al.: Nucl. Phys. B **493**, 505 (1997)
[9] B. Wacław et al.: arXiv:cond-mat/0703243, submitted to Phys. Rev. E.

9.8 Microcanonical Analyses of Peptide Aggregation Processes

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Thermodynamic phase transitions in macroscopic, infinitely large systems are typically analysed in the thermodynamic limit of a canonical ensemble, i.e., the temperature is treated as an intensive external control parameter adjusted by a heat bath, and the total system energy is distributed according to the Boltzmann-Gibbs statistics. Since the microcanonical entropy is typically a concave function of energy, the microcanonical specific heat is positive. The specific heat can only become negative in an energetic regime, where the entropy is convex. In this region, the caloric temperature, i.e., the temperature as a function of energy, bends back, i.e., the system becomes colder with increasing total energy and the temperature is no appropriate control parameter [1]. It is a surprising fact that the backbending effect is indeed observed in transitions with phase separation. Although this phenomenon has already been known for a long time from astrophysical systems [2], it has been widely ignored since then as somehow "exotic" effect. Recently, however, experimental evidence was also found from melting studies of sodium clusters [3], nuclei fragmentation [4], spin models [5], and a large number of other isolated finite model systems for evaporation and melting effects [6].

We could show that the aggregation transition of peptides (small proteins) is also a phase separation process, where the loss of entropy due to the existence of the phase boundary results in negative specific heat [7, 8]. This effect is guided by changes of the interfacial entropy as a result of surface effects. Since peptides and proteins, like the exemplified model heteropolymers used in our study, are *necessarily* systems of *finite* length, a thermodynamic limit cannot be defined and, therefore, the effect does not vanish. For this reason, standard canonical formalisms are not suitable for the interpretation of conformational pseudophase transitions with phase separation, as the temperature is not a unique control parameter and the total system energy is not an extensive, separable quantity. In such cases, microcanonical thermodynamics with the energy itself as the external control parameter provides a more favorable basis for the study of first-order-like transitions. The interesting phenomenon of the negativity of the microcanonical specific heat in peptide aggregation should motivate an experimental verification which is still pending.

[1] D.H.E. Gross: *Microcanonical Thermodynamics* (World Scientific, Singapore 2001)
[2] W. Thirring: Z. Physik **235**, 339 (1970)
[3] M. Schmidt et al.: Phys. Rev. Lett. **86**, 1191 (2001)
[4] O. Lopez et al.: Phys. Rev. Lett. **95**, 242 701 (2005)
[5] W. Janke: Nucl. Phys. B Proc. Suppl. **63A-C**, 631 (1998); H. Behringer, M. Pleimling: Phys. Rev. E **74**, 011 108 (2006)
[6] S. Hilbert, J. Dunkel: Phys. Rev. E **74**, 011 120 (2006)
[7] C. Junghans et al.: Phys. Rev. Lett. **97**, 218 103 (2006)
[8] C. Junghans, M. Bachmann, W. Janke: Mainz/Lund/Leipzig preprint (2007)

9.9 Structural Cooperativity in Collapse, Crystallization, and Folding Transitions of Polymers and Proteins

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In general, phase transitions of many-particle systems are due to a complex interplay between a large number of system constituents, called cooperativity. In single-molecule systems, structure formation results from competing covalent and noncovalent interactions between atoms or, on a coarse-grained level, between mesoscopic parts of the molecule. For flexible homopolymers, which are in the focus of our interest, the situation *seems* to be plausible. At the critical temperature, a polymer of infinite length collapses from random-coil to globular conformations. This transition is expected to be continuous. But, as the upper critical dimension is $d = 3$, field theory predicts logarithmic corrections to the scaling – which have, however, neither been confirmed in experiments nor in computer simulations over more than three decades. In our chain-growth studies of lattice polymers with up to 32000 monomers [1], we also find rather mean-field-like behaviour which might be reasoned by the chain lengths which are still too short. A second transition homopolymers experience, is the crystallization transition, where globular ("fluid") conformations go over into metastable, glass-like structures. In a recent study of a specially parametrized bond-fluctuation model, it was shown that in the thermodynamic limit, collapse and crystallization can happen at the same temperature [2]. We have found that this is not a universal, model-independent phenomenon as there are strong indications in our lattice studies that both transitions will remain separated in the thermodynamic limit.

Conformational transitions are also of essential importance in biological systems, mainly for stabilizing the functional network of biomolecules keeping cells alive. A major fraction of these functional molecules are proteins, and the unraveling of their folding characteristics into stable "native" conformations is one of the major keys to the understanding of the biophysical mechanisms behind a large number of epidemic diseases, such as Alzheimer's disease or bovine spongiform encephalopathy (BSE). Due to the large number of possible amino acid sequences building up proteins and the evolutional factor which is hardly understood, systematic experimental or computational analyses of the relations between sequence, native fold, and folding characteristics are extremely difficult. Employing a simple mesoscopic hydrophobic-polar protein model [3], we could show that typical tertiary protein folding processes such as two-state folding, folding through weakly stable intermediate structures, as well as folding into metastable structures do not necessarily depend of atomic details as it is widely believed. Figure 9.2 shows folding channels and free-energy landscapes of three different hydrophobic-polar sequences with the same content of hydrophobic and polar residues: Fig. 9.2a two-state folding with a single free-energy barrier that separates folded (N) from unfolded, denatured (D) states; Fig. 9.2b an example with two barriers, i.e., the folding pathway involves an intermediate macrostate (I); Fig. 9.2c bifurcation of the folding channel into two separate degenerate, metastable macrostates (M_1 and M_2) [4, 5]. These results shed new light on an old story: Tertiary protein folding depends

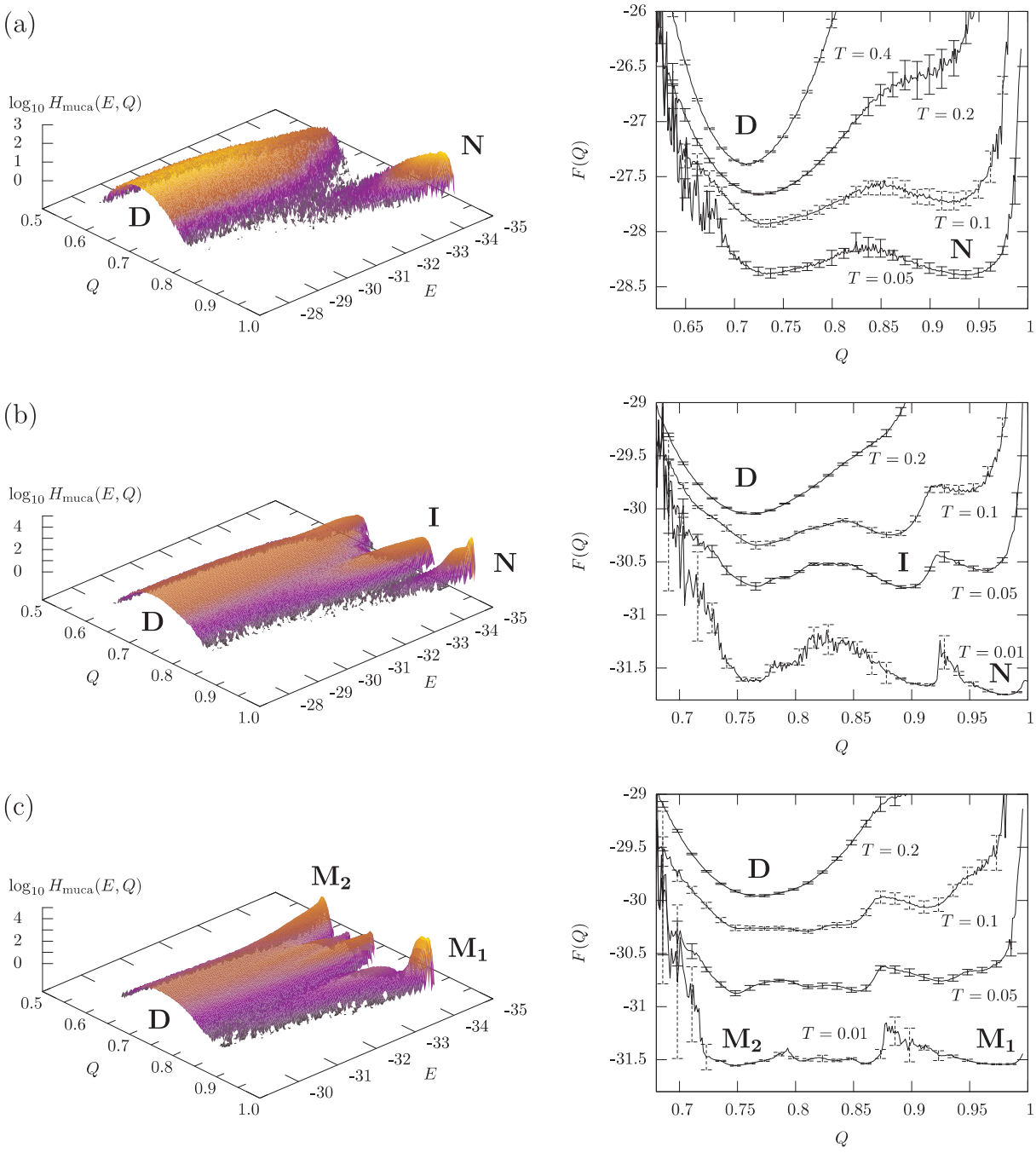

Figure 9.2: Folding channels (*left*) and free energies as a function of a suitable order parameter, parametrized by temperature (*right*) for three different protein-like hydrophobic-polar heteropolymers with different sequences.

on *general intrinsic* properties of polymeric objects at a mesoscopic scale in combination with the nonnegligible hydrophobic interaction, and these intrinsic properties are probably responsible for the "native" folds to be the only possible thermodynamically stable geometries.

[1] T. Vogel, M. Bachmann, W. Janke: Leipzig/Lund preprint (2007)
[2] F. Rampf et al.: Europhys. Lett. **70**, 628 (2005)
[3] F.H. Stillinger et al.: Phys. Rev. E **48**, 1469 (1993); F.H. Stillinger, T. Head-Gordon: Phys. Rev. E **52**, 2872 (1995)
[4] S. Schnabel et al.: Phys. Rev. Lett. **98**, 048 103 (2007)
[5] S. Schnabel et al.: J. Chem. Phys. **126**, 105 102 (2007)

9.10 Adsorption and Solution Behaviour of Semiconductor-Binding Synthetic Peptides

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In recent experimental and theoretical works [1–4], it could be shown that peptide binding to solid substrates, in particular, semiconductor surfaces, is specific to crystallographic (e.g., atomic pattern of the surface net plane) and physicochemical properties (e.g., hydrophobicity) of the substrate and solvent (pH value, temperature). The understanding of these adsorption processes is not only of particular importance for biosensory and nanoelectronic applications, but it is also a great theoretical challenge as a computationally tractable realistic hybrid model for the interaction between soft *and* solid matter is still simply lacking.

For this reason, we have first performed computer simulations to analyze solvent properties (without substrate) of four synthetic peptides used in the experiments. In these experiments [1], three of these sequences exhibited good binding properties to (100) GaAs and poor adhesion to (100) Si surfaces, whereas the (100) Si binding strength of the fourth sequence was comparatively quite good. We employed two different implicit-solvent models, one being based on the ECEPP forcefield with all atomic details [5], the other one with a reduced set of atomic parameters and simplified energetic contributions [6]. The big advantage of the latter model is that it is capable to predict realistic transition temperatures [7]. The shortness of the peptide sequences with 12 residues each is responsible for the expected behaviour that under physiological conditions the peptides are widely unstructured in solution. This result confirms the experimental observation from analyzing corresponding CD spectra [1]. Nonetheless, decreasing the temperature, the computer simulations revealed the remarkable result displayed in Fig. 9.3: Three peptides showed tendency to fold into α helical conformations, whereas the fourth formed a β sheet. The latter sequence was exactly the one with the improved Si binding properties. A first analysis showed that the position of proline, one of the amino acids in all sequences, is responsible for the different folding behaviour. To what extent this will be the reason for the different adsorption qualities is still unclear and is subject of ongoing computational studies of the hybrid system.

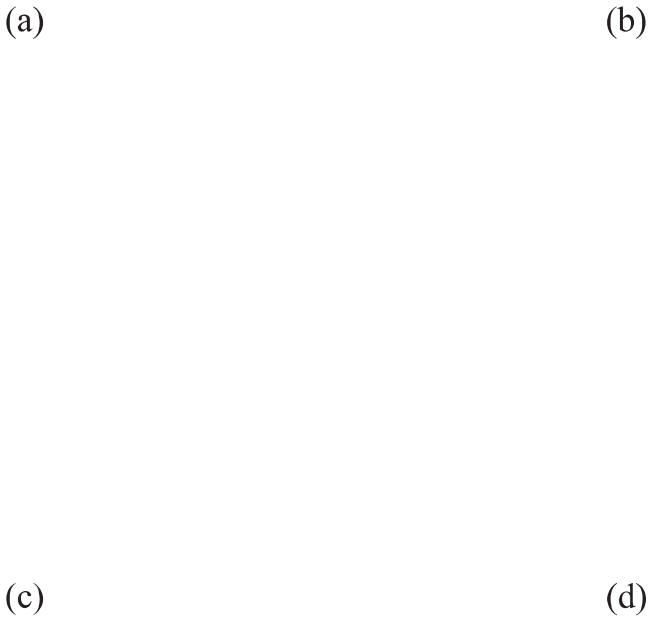

Figure 9.3: Typical low-energy conformations for the peptide sequences (**a**) AQNPSDNNTHTH, (**b**) AQNPSDNNTATA, (**c**) TNHDHSNAPTNQ, and (**d**) AQAPSDAATHTH, where (**b**) is a double His → Ala mutant of (**a**), (**c**) a random permutation of (**a**), and (**d**) a triple Asn → Ala mutant of (**a**). These structures had the lowest energy in ten simulated annealing runs for each sequence, starting from random conformations. The three sequences (**a**), (**b**), and (**d**) exhibit α helical conformations, whereas sequence (**c**) forms a β sheet.

[1] K. Goede et al.: Langmuir **22**, 8104 (2006)
[2] K. Goede et al.: *Specific Adhesion of Peptides on Semiconductor Surfaces in Experiment and Simulation*, to appear in: Proc. 28th Int. Conf. Physics of Semiconductors, Vienna, 24. – 28. July 2006
[3] M. Bachmann, W. Janke: Phys. Rev. E **73**, 020 901(R) (2006)
[4] M. Bachmann, W. Janke: Phys. Rev. E **73**, 041 802 (2006)
[5] G. Gökoğlu et al.: Phys. Rev. E **74**, 041 802 (2006)
[6] S. Mitternacht et al.: J. Phys. Chem. B **111**, 4355 (2007)
[7] A. Irbäck et al.: Biophys. J. **85**, 1466 (2003)

9.11 Quantum Critical Phenomena: Dimerized Spin Systems and (Heisenberg) Spin Chains

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Understanding quantum critical phenomena in low-dimensional quantum spin systems becomes ever more important since experimentalists succeed more and more in fabricating such materials in laboratories. One example are the well known cuprate-superconductors which are well described by quantum anti-ferromagnets. In our work we are thus interested in such systems which can be effectively described by a quantum Heisenberg model.

Our focus in the first subproject lies on studying the phase transitions that non-equivalent nearest neighbour couplings can trigger there. Changing the ratio J_1/J_2 of those couplings can drive the system from an ordered (Néel) state to disorder. Figure 9.4 (left) shows an example of this model class. Since analytical quantum many-body calculations pose an extreme challenge we use Quantum Monte Carlo methods to characterize the phase transition. Such methods have recently seen a surge of improvements. Among these is the so called Stochastic Series Expansion (SSE) [1, 2] which we have implemented and customized for our needs. Using this method we are able to determine the quantum critical point of the model in Fig. 9.4 by looking at quantities like the spin stiffness or correlation lengths. These quantities have (close to) universal features and curves at different system sizes meet in the quantum critical point. Taking into account finite-size corrections we can give the quantum critical point to be $J_1/J_2 = 2.521(1)$

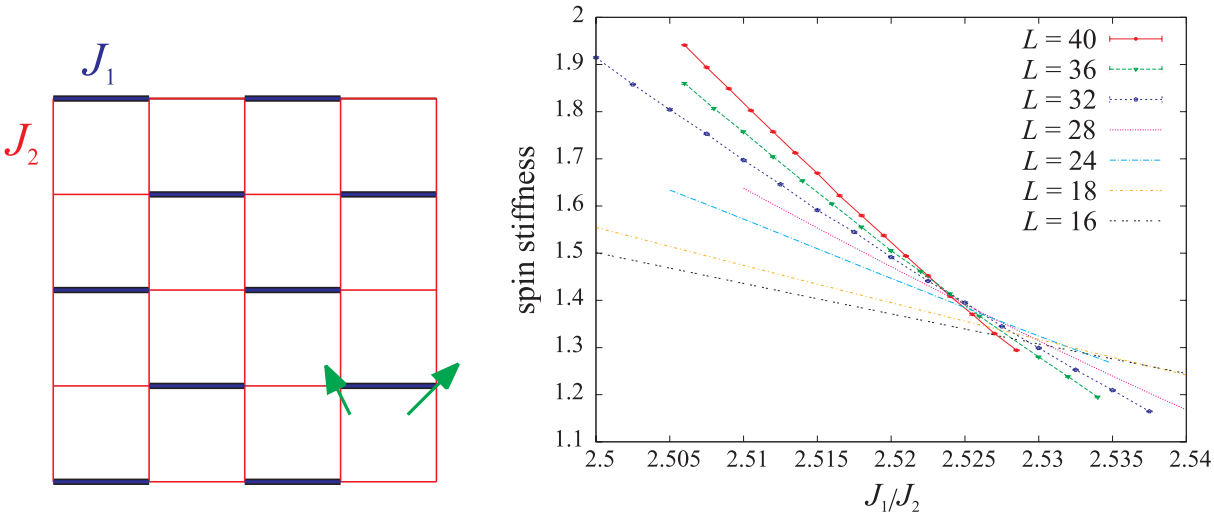

Figure 9.4: *Left:* An example for the class of models we consider here. The green quantum spins ($S = 1/2$) live on a square lattice with different nearest-neighbour couplings (*red* and *blue*). *Right:* The spin stiffness allows extraction of the quantum critical value for J_1/J_2. Note that there are large corrections which can be accounted for by finite-size scaling.

which is a considerable improvement to best previously known values. Secondly, we can show that the phase transition lies in the 3D Heisenberg universality class.

In the second subproject we have investigated quantum chains of mixed spins [3, 4]. The low temperature properties of quantum spin chains (1D Heisenberg model) depend significantly on the size of spins involved. Uniform chains of half-odd integer spins have no energy gap between ground state and first excited states (i.e. they are quantum critical), whereas chains with integer spins do show this gap [5]. However, even integer spin chains can be driven to quantum criticality by tuning the bond alternation of the coupling strength.

By means of quantum Monte Carlo simulations (continuous imaginary time loop-cluster algorithm) at low temperatures, the quantum phase transitions in antiferromagnetic Heisenberg spin chains consisting of two different kinds of spin, S_a and S_b, that appear alternatingly in pairs, have been studied for the cases $S_\mathrm{a} = 1/2$ and $S_\mathrm{b} = 1$, $S_\mathrm{a} = 1/2$ and $S_\mathrm{b} = 3/2$ as well as $S_\mathrm{a} = 1$ and $S_\mathrm{b} = 3/2$. In particular, the so-called twist order parameter as well as spatial and imaginary temporal correlation lengths have been measured in order to analyse quantum critical points that separate regions with qualitatively different ground states (quantum phases).

The twist order parameter showed a temperture dependent formation of a plateau, which could be directly linked to the width of the quantum critical region at non-zero temperatures. This feature will be, among certain extensions of the model, subject of future studies.

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[1] A.W. Sandvik, J. Kurkijärvi: Phys. Rev. B **43**, 5950 (1991)
[2] O.F. Syljuasen, A.W. Sandvik: Phys. Rev. E **66**, 046 701 (2002)
[3] K. Takano: Phys. Rev. Lett. **82**, 5124 (1999); Phys. Rev. B **61**, 8863 (2000)
[4] Z. Xu et al.: Phys. Rev. B **67**, 214 426 (2003)
[5] F.D.M. Haldane: Phys. Rev. Lett **50**, 1153 (1983)

9.12 Interface Tension of the Square Lattice Ising Model with Next-Nearest-Neighbour Interactions

A. Nußbaumer, E. Bittner, W. Janke

In a recent letter [1], Zandvliet presented a simple derivation of an analytical expression for the interface free energy in the (10) direction of the Ising model on a square lattice with nearest- *and* next-nearest-neighbour couplings having a Hamiltonian of the form

$$\mathcal{H} = -J_x \sum_{\langle i,j \rangle} \sigma_i \sigma_j - J_y \sum_{\langle i,j \rangle} \sigma_i \sigma_j - J_\mathrm{d} \sum_{(i,j)} \sigma_i \sigma_j \,, \tag{9.3}$$

where J_x, J_y are the nearest-neighbour couplings, J_d the next-nearest-neighbour couplings and $\sigma_i = \pm 1$ classical Ising spins. For the special case of only nearest-neighbour

interactions ($J_d = 0$) Zandvliet's expression reproduces the famous exact Onsager formula [2]

$$\sigma_0 = 2J_y + k_B T \ln \tanh (J_x/k_B T) \ , \tag{9.4}$$

where σ_0 is the interface free energy. By comparing the resulting transition temperatures, determined as the point where the interface tension vanishes ($\sigma_0 = 0$), with previous numerical results in the literature, support for the validity of the new analytical formula in the general case was claimed. Guided by the fact that Zandvliet's simple, but rather heuristic derivation neglects overhang configurations and bubble excitations completely, we show that his approach is equivalent to the classic solid-on-solid (SOS) approximation [3] which is known [4] to reproduce accidentally the exact interface tension along one of the two main axes in the case of only nearest-neighbour interactions [5]. In the limiting situation where only next-nearest-neighbour interactions are considered ($J_x = J_y = 0$), we prove analytically that such a coincidence no longer holds.

To assess the accuracy of Zandvliet's formula for the general model we have performed a careful computer simulation study using multicanonical Monte Carlo techniques combined with finite-size scaling analyses. Figure 9.5 shows a typical scaling plot of the maximum-to-minimum ratio of the magnetisation distribution at a temperature close to the critical temperature. The extrapolation of the fit gives an estimate of the interface tension of the infinite system ($L \to \infty$) which is clearly off the value predicted by Zandvliet.

Our results for the hitherto unknown interface tension and the transition temperatures show that the analytical formula yields fairly good approximations but, in general, is not exact.

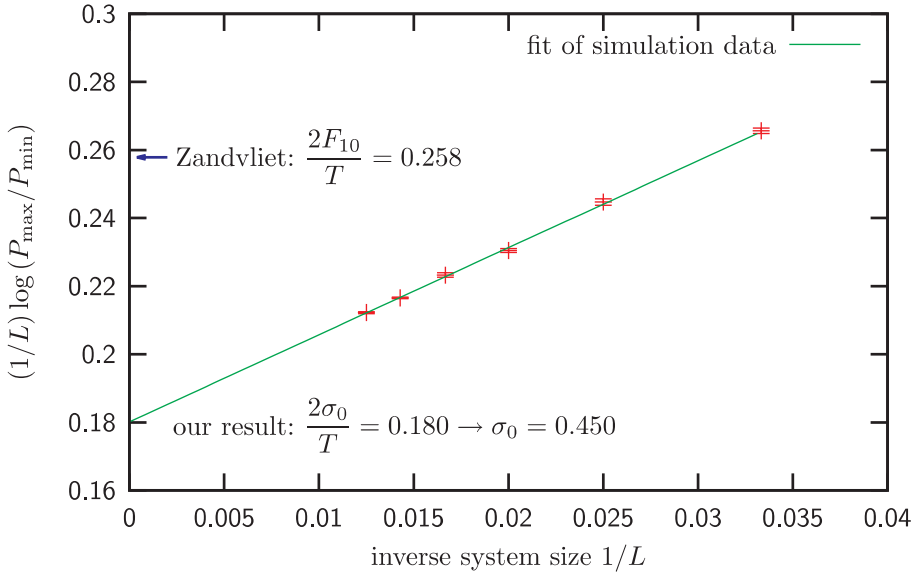

Figure 9.5: Scaling of the interface-tension estimates from the histogram method for $J_x = J_y = J_d = 1.0$, temperature $T = 5.0$ and system sizes $L = 30, 40, 50, 60, 70$, and 80. The straight line shows the fit of the ratio $\ln(P^{(L)}_{\max}/P^{(L)}_{\min})$ with goodness-of-fit parameter $Q = 0.42$, yielding an interface tension estimate of $\sigma_0 = 0.4504 \pm 0.0014$. The *arrow* on the y axis points to the analytical result of Zandvliet [1].

This work was partially supported by the Deutsche Forschungsgemeinschaft (DFG) under grant No. JA483/22-1.

[1] H.J.W. Zandvliet: Europhys. Lett. **73**, 747 (2006)
[2] L. Onsager: Phys. Rev. **65**, 117 (1944)
[3] W.K. Burton et al.: Phil. Trans. Roy. Soc. (London) A **243**, 299 (1951)
[4] F. Calheiros et al.: J. Phys. A **20**, 5991 (1987)
[5] A. Nußbaumer et al.: Europhys. Lett. **78**, 16 004 (2007)

9.13 Football Fever: Goal Distributions and Non-Gaussian Statistics

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In recent years, the generic properties of socially interacting systems have followed economic and biological systems in exciting the interest of statistical physicists [1]. In this context, it is hoped that the experience with simplification and model building gathered from the investigation of interacting physical systems might add a new perspective to the much more detailed investigations performed in the social sciences and humanities on the same subjects.

In this context, we investigated motivation and demotivation effects occurring in ball sports such as football, reflected in the probability distributions of the total number of goals scored by a team in a single match [2, 3]. It is assumed that, considering averages over the matches played in a league season or cup, scoring is a random process where, however, the scoring probability might depend on parameters that can change in the course of a match. Previous studies [4–6] have effectively considered goals scored as statistically independent events, leading to descriptions with Poissonian, negative binomial or extremal value distributions. Although satisfactory descriptions of the score data for a number of football leagues can be obtained in this way, each of these distributions seems to describe at most a certain number of cases while failing in others. What is more, there appear to be no plausible microscopic stochastic processes explaining the occurrence of these distributions. We argue that the crucial ingredient missed in these descriptions are the *correlations* between subsequent scoring events, leading to a feedback effect where each goal motivates or enables a team to score more likely subsequently. This leads to simple feedback models involving an initial scoring probability and a motivation parameter describing the "football fever", which can be solved exactly from a Pascal type recurrence relation, and precise closed-form approximations are derived from a saddle-point calculation [3]. The corresponding increase of the average scoring probability over the course of a match has been explicitly observed previously [7].

We consider football score data from many European leagues and, in particular, the premier leagues of the East and West in the divided Germany as well as the subsequently united league, the German women's premier league, and the qualification stage of the FIFA World Cup series. We find that at least one of the considered feedback

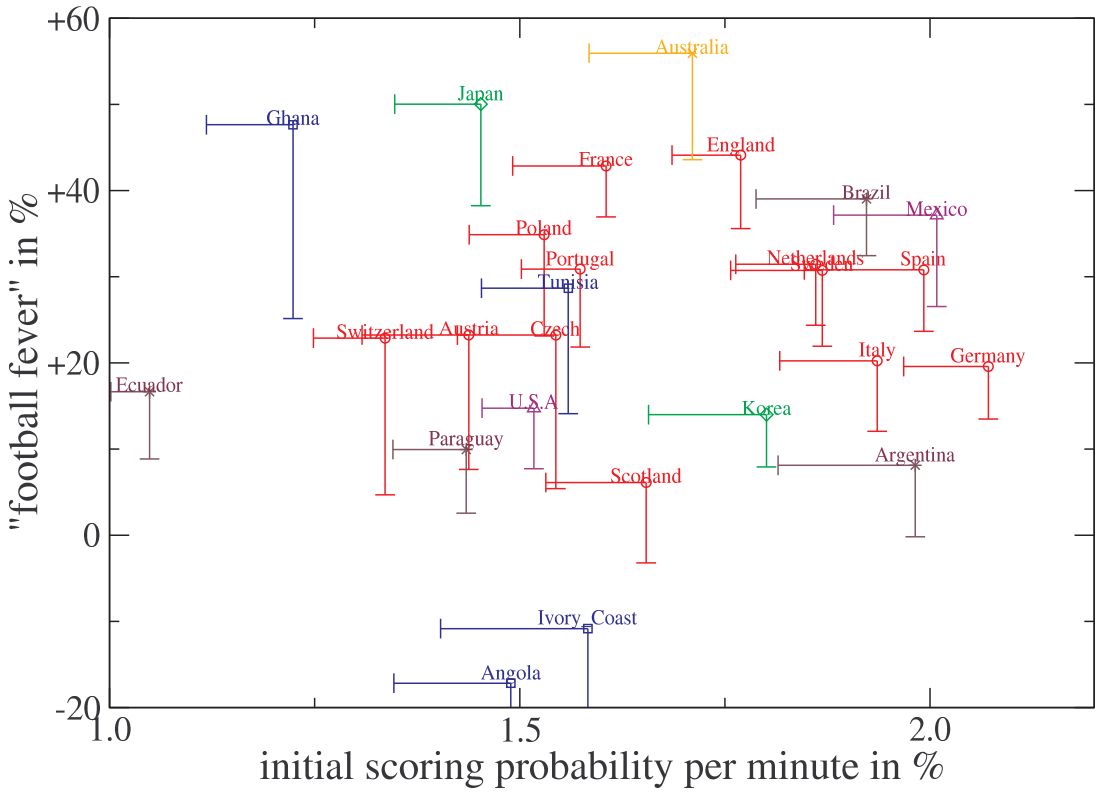

Figure 9.6: Initial scoring probability and self-affirmation parameter ("football fever") of the national teams as estimated from the past world cup qualifications.

models describes *all* of the considered data well, providing a unified description of the problem of scoring in football with a plausible model of microscopical correlations. In terms of the self-affirmation parameter of the model, we find some significant differences between the considered data sets, with the less professionalized women's and East German men's premier leagues apparently being more seriously infected with the football fever. A team-specific analysis of the world cup data allows to extract estimates for the self-affirmation parameters of the nations participating in the qualification as depicted in Fig. 9.6, to be compared with everyone's favorite prejudices about national characteristics in the football world.

Work partially supported by the DFG under grant Nos. JA483/22-1 & 23-1, the EC RTN-Network "ENRAGE" under grant No. MRTN-CT-2004-005616, and the EC MC-EIF programme under contract No. MEIF-CT-2004-501422.

[1] D. Stauffer: Physica A **336**, 1 (2004)
[2] E. Bittner et al.: *Self-affirmation model for football goal distributions*, Eur. Phys. Lett. (in print)
[3] E. Bittner et al.: arXiv:physics/0606016
[4] M.J. Moroney: *Facts from Figures*, 3rd Ed. (Penguin, London 1956)
[5] C. Reep et al.: J. Roy. Stat. Soc. A **134**, 623 (1971)
[6] J. Greenhough et al.: Physica A **316**, 615 (2002)
[7] M.J. Dixon, M.E. Robinson: Statistician **47**, 523 (1998)

9.14 Wang–Landau/Multibondic Cluster Algorithm for Simulations of Second-Order Phase Transitions

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Equilibrium properties of statistical physics systems are often estimated by Markov chain Monte Carlo (MCMC) simulations [1]. In many cases one is interested in calculating expectation values for a range of temperatures with respect to the Gibbs canonical ensemble. It has turned out that instead of performing simulations of the canonical ensemble at distinct temperatures it is often advantageous to combine them into one simulation of a "generalized" ensemble [2–5]; for reviews see [6–8].

While the power of generalized ensembles is well documented for first-order phase transitions and complex systems such as spin glasses and peptides (small proteins), this is not the case for second-order phase transitions. In the latter case the critical energy range of interest is often larger than the energy range covered by a canonical Monte Carlo simulation close to the critical temperature. Such an extended energy range can, in principle, be covered by performing a Wang–Landau recursion [5] for the spectral density followed by a multicanonical simulation [3] with fixed weights. However, in the conventional approach one loses the advantage of cluster algorithms [9], which can reduce critical slowing down dramatically. The goal of this project was therefore to develop a cluster version of the Wang–Landau recursion and to combine it with a subsequent multibondic simulation [10]. Our present implementation of this idea improves for 2D and 3D Ising models the efficiency of the conventional Wang–Landau/multicanonical approach by power laws in the lattice size [11]. In our simulations real gains in CPU time reach two orders of magnitude.

[1] J. Gubernatis (Ed.): *The Monte Carlo Method in Physical Sciences*, AIP Conf. Proc., Vol. 690 (AIP, Melville 2003)
[2] G.M. Torrie, J.P. Valleau: J. Comp. Phys. **23**, 187 (1977)
[3] B.A. Berg, T. Neuhaus: Phys. Rev. Lett. **68**, 9 (1992)
[4] A.P. Lyubartsev et al.: J. Chem. Phys. **96**, 1776 (1992); E. Marinari, G. Parisi: Europhys. Lett. **19**, 451 (1992)
[5] F. Wang, D.P. Landau: Phys. Rev. Lett. **86**, 2050 (2001)
[6] U.H. Hansmann, Y. Okamoto: Ann. Rev. Comp. Phys. **6**, 120 (1999)
[7] B.A. Berg: *Markov Chain Monte Carlo Simulations and Their Statistical Analysis* (World Scientific, Singapore 2004)
[8] W. Janke: in *Computer Simulations of Surfaces and Interfaces*, NATO Science Series, II. Mathematics, Physics and Chemistry – Vol. **114**, ed. by B. Dünweg et al. (Kluwer, Dordrecht 2003) p 137
[9] R.H. Swendsen, J.-S. Wang: Phys. Rev. Lett. **58**, 86 (1987); U. Wolff: Phys. Rev. Lett. **62**, 361 (1989)
[10] W. Janke, S. Kappler: Phys. Rev. Lett. **74**, 212 (1995); M.S. Carroll, W. Janke, S. Kappler: J. Stat. Phys. **90**, 1277 (1998)
[11] B.A. Berg, W. Janke: Phys. Rev. Lett. **98**, 040 602 (2007)

9.15 Scaling Relations for Logarithmic Corrections at Second-Order Phase Transitions

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The conventional leading scaling behaviour at a second-order phase transition are power-laws in the reduced temperature $t = 1 - T/T_c$ and field h. With $h = 0$, the correlation length, specific heat and susceptibility behave as $\xi_\infty(t) \sim |t|^{-\nu}$, $C_\infty(t) \sim |t|^{-\alpha}$ and $\chi_\infty(t) \sim |t|^{-\gamma}$, while the magnetization in the broken phase has $m_\infty(t) \sim |t|^{\beta}$. Here the subscript indicates the assumed infinite extent of the system. At $t = 0$ the magnetization scales as $m_\infty(h) \sim h^{1/\delta}$ while the anomalous dimension η characterizes the correlation function at criticality. In the 1960's, it was shown that these six critical exponents are related via four scaling relations, which are now firmly established and fundamentally important in the theory of critical phenomena [1].

Multiplicative logarithmic corrections to scaling are frequently encountered in the critical behaviour of certain statistical-mechanical systems, e.g., at their upper critical dimension d_u from which on mean-field behaviour (which is independent of d) prevails [2]. In our work [3], a Lee–Yang zero approach is used to systematically analyse the exponents of such logarithms and to propose new scaling relations between them.

In a second step [4], by considering also Fisher zeros, the theory has been extended to account for circumstances which often occur when the leading specific-heat critical exponent vanishes such as, e.g., for the two-dimensional Ising model. Furthermore the theory could be widened to encompass also the correlation function.

These proposed scaling relations among the exponents of logarithmic corrections were then successfully confronted with a variety of results from the literature and some new predictions for logarithmic corrections in certain models could be made which are still subject to numerical or experimental verification.

[1] M.E. Fisher: Rev. Mod. Phys. **70**, 653 (1998); D.A. Lavis, G.M. Bell: *Statistical Mechanics of Lattice Systems 2* (Springer, Berlin 1999)
[2] F.J. Wegner: in *Phase Transitions and Critical Phenomena VI*, ed. by C. Domb, M.S. Green (Academic Press, London 1976) p 8
[3] R. Kenna et al.: Phys. Rev. Lett. **96**, 115 701 (2006)
[4] R. Kenna et al.: Phys. Rev. Lett. **97**, 155 702 (2006)

9.16 Funding

Random Geometry and Random Matrices: From Quantum Gravity to Econophysics
W. Janke
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Dynamik und Statik von Spingläsern
W. Janke
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Investigation of Thermodynamic Properties of Lattice and Off-Lattice Models for Proteins and Polymers
M. Bachmann, W. Janke
Deutsche Forschungsgemeinschaft (DFG), Grant No. JA483/24-1/2

Phasenübergänge in Systemen mit einschränkender Geometrie
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Two-Dimensional Magnetic Systems with Anisotropy
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A. Irbäck, W. Janke
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Quantum Monte Carlo Studies of Valence Bond Solid Transitions
W. Janke, B. Zheng
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Statistical Mechanics of Complex Networks
W. Janke, Z. Burda
Alexander-von-Humboldt Foundation "Institutspartnerschaft" with the Jagellonian University, Krakow, Poland

Monte Carlo Simulations of Self-Avoiding Walks on the Percolation Cluster
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B. Wacław (Jagellonian University, Krakow, Poland)
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Quantum Monte Carlo Simulations
W. Janke
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9.17 Organizational Duties

E. Bittner

- Scientific Secretary of the Workshop *CompPhys06 – 7. NTZ-Workshop on Computational Physics*, ITP, Universität Leipzig, 30. November – 02. December 2006

W. Janke

- Director of the Naturwissenschaftlich-Theoretisches Zentrum (NTZ) at the Zentrum für Höhere Studien (ZHS), Universität Leipzig
- Chairperson of the Programme Committee "Scientific Computing" of Forschungszentrum Jülich
- Member of the Scientific-Technical-Council of the Supervisory Board ("Aufsichtsrat") of the Forschungszentrum Jülich GmbH
- Editor: "Computational Physics", Central European Journal of Physics
- Member of Editorial Board: Cond. Matter Phys.
- Permanent Member of "International Advisory Board" of the *Conference of the Middle European Cooperation in Statistical Physics (MECO)*
- Member of the "Advisory Committee" of the International Workshop *COVLAT06 – 16. Workshop on Lattice Field Theory*, Coventry, England, UK, 29. June – 01. July 2006
- Member of the "Local Organizing Committee" of the International Conference *MG11 – 11th Marcel Grossmann Meeting*, FU Berlin, 23. – 29. July 2006
- Member of the "International Program Committee" of the International Conference *Mathematical Modeling and Computational Physics 2006*, High Tatra Mountains, Slovakia, 28. August – 01. September 2006
- Organizer of the Workshop *CompPhys06 – 7. NTZ-Workshop on Computational Physics*, ITP, Universität Leipzig, 30. November – 02. December 2006
- Organizer of the Symposium *Finite-Size Effects at Phase Transitions* within the German Physics Spring Meeting ("Physiker-Tagung") 2007, Universität Regensburg, 27. – 28. March 2007 (with Prof. Dr. Walter Selke, RWTH Aachen)
- Organizer of the 9th International Conference *Path Integrals – New Trends and Perspectives*, Max Planck-Institut für Physik komplexer Systeme (MPI-PKS), Dresden, 23. – 28. September 2007 (with PD Dr. Axel Pelster, Universität Duisburg-Essen)
- Organizer of the Workshop *Statistical Mechanics of Complex Networks*, Jagellonian University, Krakow, Poland, 11. – 13. October 2007 (with Prof. Dr. Zdzisław Burda, Jagellonian University, Krakow, Poland)
- Editor of *Rugged Free Energy Landscapes: Common Computational Approaches in Spin Glasses, Structural Glasses and Biological Macromolecules*, Proceedings of CECAM Workshop, to appear in Lecture Notes in Physics (Springer, Berlin 2007) (in print)
- External Reviewer: Humboldt-Stiftung; Studienstiftung des deutschen Volkes; "Jeffress Memorial Trust", Bank of America, Virginia, USA; "Fond zur Förderung der wissenschaftlichen Forschung (FWF)", Österreich; "The Royal Society", UK; "Engineering and Physical Sciences Research Council (EPSRC)", UK; The University of Warwick, UK; Coventry University, UK; CECAM, Lyon, France
- Referee: Phys. Rev. Lett., Phys. Rev. B, Phys. Rev. E, J. Chem. Phys., Europhys. Lett.,

Phys. Lett. A, Phys. Lett. B, Eur. Phys. J. B, Physica A, Proc. Royal Phys. Soc., J. Phys. A, Comp. Phys. Comm., J. Stat. Mech.-Theory E., New J. Phys., Int. J. Mod. Phys. C

9.18 External Cooperations

Academic

- EU RTN-Network "ENRAGE" – *Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*
  research collaboration with 13 teams throughout Europe
- Department of Physics, Florida State University, Tallahassee, USA
  Prof. Dr. Bernd A. Berg
- CEA/Saclay, Service de Physique Théorique, France
  Dr. Alain Billoire
- Laboratoire de Physique des Matériaux (UMR CNRS No 7556), Université Henri Poincaré, Nancy, France
  Prof. Dr. Bertrand Berche, Dr. Christophe Chatelain
- Groupe de Physique des Matériaux (UMR CNRS No 6634), Université de Rouen, France
  Dr. Pierre-Emmanuel Berche
- School of Mathematical and Computer Sciences, Heriot-Watt University, Edinburgh, UK
  Prof. Dr. Desmond A. Johnston, Dr. Martin Weigel
- School of Mathematical and Information Sciences, Coventry University, UK
  Dr. Ralph Kenna
- Department of Physics, Hacettepe University, Ankara, Turkey
  Prof. Dr. Tarik Çelik, Dr. Handan Arkin, Gökhan Gökoğlu
- Institute for Condensed Matter Physics, National Academy of Sciences, Lviv, Ukraine
  Prof. Dr. Yurij Holovatch
- Complex Systems Division, Department of Theoretical Physics, Lund University, Sweden
  Prof. Dr. Anders Irbäck, Simon Mitternacht
- NIC, Forschungszentrum Jülich
  Prof. Dr. Ulrich Hansmann, Prof. Dr. Peter Grassberger, PD Dr. Thomas Neuhaus
- Institut für Physik, Universität Mainz
  Prof. Dr. Kurt Binder, Dr. Hsiao-Ping Hsu
- Atominstitut, TU Wien, Austria
  Prof. Dr. Harald Markum, Dr. Rainer Pullirsch
- Brunel University of West London, UK
  Dr. Gernot Akemann
- Institut für Theoretische Physik, FU Berlin
  Prof. Dr. Hagen Kleinert, Dr. Adriaan M.J. Schakel

- IAC-1, Universität Stuttgart
  PD Dr. Rudolf Hilfer
- Institut für Theoretische Physik, Universität Bielefeld
  PD Dr. Thomas Neuhaus
- Institute of Physics, Jagellonian University, Kraków, Poland
  Prof. Dr. Zdzisław Burda
- Landau Institute for Theoretical Physics, Chernogolovka, Russia
  Prof. Dr. Lev N. Shchur
- Yerevan Physics Institute, Yerevan, Armenia
  Prof. Dr. David B. Saakian
- University of Sri Jayewardenepura, Sri Lanka
  Dr. Ranasinghe P.K.C. Malmini
- Department of Physics, Sri Venkateswara College, University of Delhi, New Delhi, India
  Dr. Bibudhananda Biswal
- Department of Mechanical Engineering and Intelligent Systems, Tokyo University of Electro-communications, Chofu, Tokyo, Japan
  Prof. Dr. Hans-Georg Mattutis
- Zhejiang Institute of Modern Physics, Zhejiang University, Hangzhou, PR China
  Prof. Dr. He-Ping Ying, Prof. Dr. Bo Zheng

9.19 Publications

Journals

M. Bachmann, W. Janke: *Substrate Adhesion of a Nongrafted Polymer in a Cavity*, Phys. Rev. E **73**, 041 802 (2006)

M. Bachmann, W. Janke: *Substrate Specificity of Peptide Adsorption: A Model Study*, Phys. Rev. E **73**, 020 901(R) (2006)

B.A. Berg, W. Janke: *Wang–Landau Multibondic Cluster Simulations for Second-Order Phase Transitions*, Phys. Rev. Lett. **98**, 040 602 (2007)

E. Bittner, W. Janke: *Free-Energy Barriers in the Sherrington-Kirkpatrick Model*, Europhys. Lett. **74**, 195 (2006)

G. Gökoğlu, M. Bachmann, T. Çelik, W. Janke: *Structural Properties of Small Semiconductor-Binding Synthetic Peptides*, Phys. Rev. E **74**, 041 802 (2006)

M. Hellmund, W. Janke: *High-Temperature Series Expansions for the q-State Potts Model on a Hypercubic Lattice and Critical Properties of Percolation*, Phys. Rev. E **74**, 051 113 (2006)

M. Hellmund, W. Janke: *High-Temperature Series for the Bond-Diluted Ising Model in 3, 4 and 5 Dimensions*, Phys. Rev. B **74**, 144 201 (2006)

W. Janke: *Der Faktor Zeit – Theoretische Physiker interessieren sich für alternde Materialien*, Universität Leipzig Journal **4/2006**, 25 (2006)

W. Janke, D.A. Johnston, R. Kenna: *Properties of Higher-Order Phase Transitions*, Nucl. Phys. B **736**, 319 (2006)

W. Janke, D.A. Johnston, M. Weigel: *Two-Dimensional Quantum Gravity – A Laboratory for Fluctuating Graphs and Quenched Connectivity Disorder*, Cond. Matter Phys. **9**, 263 (2006)

W. Janke, A.M.J. Schakel: *Two-Dimensional Critical Potts and its Tricritical Shadow*, Braz. J. Phys. **36**, 708 (2006)

W. Janke, M. Weigel: *Geometric and Stochastic Clusters of Gravitating Potts Models*, Phys. Lett. B **639**, 373 (2006)

C. Junghans, M. Bachmann, W. Janke: *Microcanonical Analyses of Peptide Aggregation Processes*, Phys. Rev. Lett. **97**, 218 103 (2006)

R. Kenna, D.A. Johnston, W. Janke: *Scaling Relations for Logarithmic Corrections*, Phys. Rev. Lett. **96**, 115 701 (2006)

R. Kenna, D.A. Johnston, W. Janke: *Self-Consistent Scaling Theory for Logarithmic Correction Exponents*, Phys. Rev. Lett. **97**, 155 702 (2006)

E. Lorenz, W. Janke: *Numerical Tests of Local Scale Invariance in Ageing q-State Potts Models*, Europhys. Lett. **77**, 10 003 (2007)

S. Mitternacht, S. Schnabel, M. Bachmann, W. Janke, A. Irbäck: *Differences in Solution Behavior Between Four Semiconductor-Binding Peptides*, J. Phys. Chem. B **111**, 4355 (2007)

A. Nußbaumer, E. Bittner, W. Janke: *Interface Tension of the Square Lattice Ising Model with Next-Nearest-Neighbour Interactions*, Europhys. Lett. **78**, 16 004 (2007)

A. Nußbaumer, E. Bittner, T. Neuhaus, W. Janke: *Monte Carlo Study of the Evaporation/Condensation Transition of Ising Droplets*, Europhys. Lett. **75**, 716 (2006)

S. Schnabel, M. Bachmann, W. Janke: *Identification of Characteristic Protein Folding Channels in a Coarse-Grained Hydrophobic-Polar Peptide Model*, J. Chem. Phys. **126**, 105 102 (2007)

S. Schnabel, M. Bachmann, W. Janke: *Two-State Folding, Folding Through Intermediates, and Metastability in a Minimalistic Hydrophobic-Polar Model for Proteins*, Phys. Rev. Lett. **98**, 048 103 (2007)

Books

M. Bachmann, W. Janke: *Adsorption Phenomena at Organic-Inorganic Interfaces*, in: *From Computational Biophysics to Systems Biology 2006*, Proc. NIC Workshop, Jülich, 06. – 09. June 2006, ed. by U.H.E. Hansmann, J. Meinke, S. Mohanty, O. Zimmermann, NIC Series, Vol. **34** (John von Neumann Institute for Computing, Jülich 2006) p 95

M. Bachmann, W. Janke: *Chain-Growth Simulations of Lattice-Peptide Adsorption to Attractive Substrates*, in: *NIC Symposium 2006 Proceedings*, ed. by G. Münster, D. Wolf, M. Kremer, NIC Series, Vol. **32**, (John von Neumann Institute for Computing, Jülich 2006) p 245

M. Bachmann, W. Janke: *Reduction to the Simplest – The Complexity of Minimalistic Heteropolymer Models*, in: *From Computational Biophysics to Systems Biology 2006*, Proc. NIC Workshop, Jülich, 06. – 09. June 2006, ed. by U.H.E. Hansmann, J. Meinke, S. Mohanty, O. Zimmermann, NIC Series, Vol. **34** (John von Neumann Institute for Computing, Jülich 2006) p 59

W. Janke: *Introduction to Simulation Techniques* in: *Ageing and the Glass Transition*, ed. by M. Henkel, M. Pleimling, R. Sanctuary, Lecture Notes in Physics **716** (Springer, Berlin 2007) p 207

W. Janke (Ed.): *Rugged Free Energy Landscapes: Common Computational Approaches in Spin Glasses, Structural Glasses and Biological Macromolecules*, Lecture Notes in Physics (Springer, Berlin 2007) in press

W. Janke, E. Bittner: *Phase Transitions in a Generalized $|\psi|^4$ Model*, in: *Proc. 8th Int. Conf. Path Integrals from Quantum Information to Cosmology*, Prague, Czech Republic, 06. – 10. June 2005, ed. by Č. Burdik, O. Navrátil, S. Pošta (JINR Press, Dubna 2006) p 1 [electronically available at www.jinr.ru/publish/Proceedings/Burdik-2005/index.html]

in press

M. Bachmann, W. Janke: *Minimalistic Hybrid Models for the Adsorption of Polymers and Peptides to Substrates*, Proc. Conf. Mathematical Modeling and Computational Physics 2006, High Tatra Mountains, Slovakia, 28. August – 1. September, 2006

M. Bachmann, W. Janke: *Thermodynamics of Protein Folding from Coarse-Grained Models' Perspectives*, in: *Rugged Free Energy Landscapes: Common Computational Approaches in Spin Glasses, Structural Glasses and Biological Macromolecules*, ed. by W. Janke, Lecture Notes in Physics (Springer, Berlin 2007)

E. Bittner, A. Nußbaumer, W. Janke, M. Weigel: *Self-Affirmation Model for Football Goal Distributions*, Europhys. Lett.

L. Bogacz, Z. Burda, W. Janke, B. Wacław: *Balls-in-Boxes Condensation on Networks*, Chaos

K. Goede, M. Bachmann, W. Janke, M. Grundmann: *Specific Adhesion of Peptides on Semiconductor Surfaces in Experiment and Simulation*, Proc. 28th Int. Conf. Physics of Semiconductors (ICPS-28)

W. Janke, A.M.J. Schakel: *Spacetime Approach to Phase Transitions*, in: *Order, Disorder and Criticality: Advanced Problems of Phase Transition Theory*, Vol. 2, ed. by Y. Holovatch (World Scientific, Singapore 2007)

Talks

M. Bachmann: *Adsorption Phenomena at Hybrid Organic-Inorganic Interfaces*, Workshop *Statistical Physics and Low-Dimensional Systems*, Nancy, France, 17. – 19. May

M. Bachmann: *Adsorption Phenomena at Hybrid Organic-Inorganic Interfaces*, Workshop *Self-Assembly of Complex Nanostructures*, Leipzig, 25. – 26. September

M. Bachmann: *Complex Conformational-Phase Diagrams of Simple Hybrid Polymer–Substrate Models*, Workshop *Recognition and Adsorption Processes of Biomolecules*, Bielefeld, 06. – 07. March

M. Bachmann: *Complex Conformational-Phase Diagrams of Simple Hybrid Polymer–Substrate Models*, 31th Conf. of the Middle European Cooperation in Statistical Physics MECO31, Primošten, Croatia, 23. – 26. April

M. Bachmann: *Folding and Aggregation of Protein-Like Heteropolymers at Mesoscopic Scales*, Seminar talk, Computational Biology & Biological Physics Group, Lunds Universitet, Lund, Sweden, 30. October

M. Bachmann: *Mesoscopic Modeling of Protein Folding and Aggregation*, 7th NTZ Workshop Computational Physics, Leipzig, 30. November – 02. December

M. Bachmann: *Minimalistic Hybrid Models for the Adsorption of Polymers and Peptides to Solid Substrates*, Conf. Mathematical Modeling and Computational Physics (MMCP 2006), High Tatra Mountains, Štrba (Slovakia), 28. August – 01. September

M. Bachmann: *Minimalistic Models for Polymer and Peptide Adhesion to Solid Substrates*, Seminar talk, Institut für Physik, Johannes Gutenberg-Universität Mainz, 17. January

M. Bachmann: *Molekulare Strukturbildung bei Faltungs-, Aggregations- und Adsorptionsprozessen von weicher Materie*, Colloquium talk, Universität Dortmund, 18. December

M. Bachmann: *Polymer and Peptide Adsorption to Attractive Substrates*, Spring Meeting of the German Physical Society, Dresden, 27. – 31. March

M. Bachmann: *Proteinfaltung – Interdisziplinäre Herausforderung für die Physik*, Colloquium talk, Technische Universität Ilmenau, 18. April

M. Bachmann: *Reduction to the Simplest – The Complexity of Minimal Heteropolymer Models*, Workshop "From Computational Biophysics to Systems Biology", Jülich, 06. – 09. June

E. Bittner: *Droplet Condensation/Evaporation Transition*, *Workshop on Computational Physics* CompPhys06, Leipzig, 30. November – 02. December

E. Bittner: *Free-Energy Barriers in a Mean-Field Spin*, Spring Meeting of the German Physical Society, Dresden, 27. – 31. March

E. Bittner: *Free-Energy Barriers in the Sherrington-Kirkpatrick Model*, Les Houches Meeting 2006, Les Houches, France, 20. – 24. February

E. Bittner: *Football Fever: Goal Distributions and Non-Gaussian Statistics*, invited talk, *16. Workshop on Lattice Field Theory and Statistical Physics* COVLAT06, Coventry, UK, 29. June – 01. July

E. Bittner: *On the Overlap Probability Distribution in the Sherrington-Kirkpatrick Model*, ENRAGE Network Conf., Edinburgh, 03. – 07. April

E. Bittner: *The Evaporation/Condensation Transition of Ising Droplets*, invited talk, Workshop *Statistical Physics and Low-Dimensional Systems*, Nancy, France, 17. – 19. May

L. Bogacz, Z. Burda, W. Janke, B. Wacław: *A Program Generating Homogeneous Random Graphs with Given Weights*, Spring Meeting of the German Physical Society, Dresden, 27. – 31. March

W. Janke: *Adsorption Phenomena at Hybrid Organic-Inorganic Interfaces*, NIC Workshop CBSB06, Jülich, 06. – 09. June

W. Janke: *Adsorption Phenomena at Hybrid Organic-Inorganic Interfaces*, invited talk, Sitzung des Wissenschaftlichen Rates des NIC, DESY Zeuthen, 21. June

W. Janke: *Adsorption Phenomena at Hybrid Organic-Inorganic Interfaces*, invited talk, 16. Workshop on Lattice Field Theory and Statistical Physics – COVLAT06, Coventry University, UK 29. June – 01. July

W. Janke: *Diluted Magnets – Simulations vs Series Expansions*, invited talk, 3rd Int. Workshop Hangzhou 2006 on *Simulational Physics*, Zhejiang University, Hangzhou, China, 16. – 18. November

W. Janke: *First-Order Phase Transitions*, two invited lectures, Block Course on *Phase Transitions in Statistical Physics and Field Theory* of the Int. Graduate School *Quantum Fields and Strongly Interacting Matter*, Universität Bielefeld, 04. – 09. October

W. Janke: *Fortuin-Kasteleyn Versus Geometrical Clusters*, joint DPG-und ESF-Frühjahrstagung, TU Dresden, 27. – 31. March

W. Janke: *Fortuin-Kasteleyn Versus Geometrical Clusters – Fractal Dimensions and Critical Exponents*, invited talk, Workshop Programme *Stochastic Geometry and Field Theory: From Growth Phenomena to Disordered Systems*, Kavli Institute for Theoretical Physics, University of California Santa Barbara, USA, 06. September

W. Janke: *Geometrical Description of Critical Behaviour*, Seminar zur Theorie der kondensierten Materie, Institut für Theoretische Physik, RWTH Aachen, 31. January

W. Janke: *Geometrical Picture of Phase Transitions*, 31th Conf. Middle European Cooperation in Statistical Physics MECO31, Primošten, Croatia, 23. – 26. April

W. Janke: *Geometrical Picture of Phase Transitions*, invited talk, Atelier Nancy *Statistical Physics and Low Dimensional Systems*, Nancy, France, 17. – 19. May

W. Janke: *Monte Carlo Methods in Classical Statistical Physics*, two invited lectures, Heraeus Summerschool *Computational Many Particle Physics*, Universität Greifswald, 18. – 29. September

W. Janke: *Multi-Scale Modelling and Simulation of Protein Folding*, PAP$_3$A Workshop, Schloß Oppurg, 13. – 14. January

W. Janke: *Picturing Phase Transitions Geometrically*, ENRAGE Network Conf., Edinburgh, UK, 03. – 07. April

W. Janke: *Quenched Connectivity Disorder: Spin Models on Random Lattices and Graphs*, invited talk, Int. Workshop *The World a Jigsaw: Tessellations in the Sciences*, Lorentz Center, Leiden University, The Netherlands, 06. – 10. March

A. Nußbaumer: *Football Fever: goal distributions and non-Gaussian statistics*, CompPhys06 *Workshop on Computational Physics*, Leipzig, 30. November – 02. December

A. Nußbaumer: *Numerical Results for the 3D Edwards-Anderson-Ising Model*, Spring Meeting of the German Physical Society, Dresden, 27. – 31. March

T. Vogel, M. Bachmann, W. Janke: *Polymer Chain Growth on Lattice*, Department of Theoretical Physics, Lund University, Sweden, 06. February

Posters

E. Bittner, W. Janke: *Tails of the Sherrington-Kirkpatrick Model*, 31th Conf. Middle European Cooperation in Statistical Physics MECO31, Primošten, Croatia, 23. – 26. April

K. Goede, M. Bachmann, W. Janke, M. Grundmann: *Specific Adhesion of Peptides on Semiconductor Surfaces in Experiment and Simulation*, 28th Conf. Physics of Semiconductors, Vienna, Austria, 24. – 28. July

G. Gökoğlu, M. Bachmann, C. Çelik, W. Janke: *Conformational Properties of Semiconductor–Binding Synthetic Peptides*, Spring Meeting of the German Physical Society, Dresden, 27. – 31. March

M. Hellmund, W. Janke: *Series Expansions for Percolation and Bond-Diluted Ising Models on Z^D*, Spring Meeting of the German Physical Society, Dresden, 27. – 31. March

C. Junghans, M. Bachmann, W. Janke: *Microcanonical analysis of polymer aggregation*, CompPhys06 *Workshop on Computational Physics*, Leipzig, 30. November – 02. December

C. Junghans, U.H.E. Hansmann: *Cross-Check Methods in Protein Simulations*, From Computational Biophysics to Systems Biology 2006, FZ Jülich, 06. – 09. June

C. Junghans, U.H.E. Hansmann: *Modern Methods in Protein Simulations*, Spring Meeting of the German Physical Society, Dresden, 27. – 31. March

A. Kallias, W. Janke, M. Bachmann: *Thermodynamics and Folding Kinetics of Coarse-Grained Protein Models*, Spring Meeting of the German Physical Society, Dresden, 27. – 31. March

E. Lorenz, W. Janke: *Phase-Ordering and Ageing Phenomena in q-State Potts Models with $q = 3$ and 8*, Spring Meeting of the German Physical Society, Dresden, 27. – 31. March

S. Mitternacht, S. Schnabel, A. Irbäck, M. Bachmann, W. Janke: *Solution Behavior of Semiconductor-Binding Peptides*, CompPhys06 *Workshop on Computational Physics*, Leipzig, 30. November – 02. December

J. Schluttig, M. Bachmann, W. Janke: *Comparing Thermodynamics of the AB Protein Model in Monte Carlo and Molecular Dynamics Simulations*, Spring Meeting of the German Physical Society, Dresden, 27. – 31. March

S. Schnabel, M. Bachmann, W. Janke: *Folding Channels for Coarse-Grained Heteropolymer Models*, Spring Meeting of the German Physical Society, Dresden, 27. – 31. March

T. Vogel, M. Bachmann, W. Janke: *Application of New Chain Growth Algorithms for Lattice Polymers*, Spring Meeting of the German Physical Society, Dresden, 27. – 31. March

T. Vogel, M. Bachmann, W. Janke: *Collapse and Freezing Transitions of Polymers on Regular Lattices*, CompPhys06 *Workshop on Computational Physics*, Leipzig, 30. November – 02. December

S. Wenzel, L. Bogacz, W. Janke: *Quantum Monte Carlo Simulations of Dimerized Heisenberg Models*, Spring Meeting of the German Physical Society, Dresden, 27. – 31. March

S. Wenzel, L. Bogacz, W. Janke: *Quantum Monte Carlo Simulations of Dimerized Heisenberg Models*, 31th Conf. Middle European Cooperation in Statisitical Physics MECO31, Primošten, Croatia, 23. – 26. April

S. Wenzel, A.M.J. Schakel, W. Janke: *Percolation of Vortex Networks in the U(1) Lattice Higgs Model*, 3rd Int. Workshop on Simulational Physics, Hangzhou, China, 16. – 18. November

S. Wenzel, A.M.J. Schakel, W. Janke: *Percolation of Vortex Networks in the U(1) Lattice Higgs Model*, CompPhys06 *Workshop on Computational Physics*, Leipzig, 30. November – 02. December

9.20 Graduations

Diploma

- Thomas Haase
  2D/3D Crossover beim Isingmodell – Optimierung des Spin-1 Modells
  October 2006
- Christoph Junghans
  Aggregation of Mesoscopic Protein-Like Heteropolymers
  October 2006

9.21 Guests

- PD Dr. Thomas Neuhaus
  NIC Jülich
  NTZ-Kolloquium/TKM-Seminar, 11. April 2006: *Global Radius of Curvature and its Applications in Polymer Physics*, 11. – 12. April 2006
- Dr. Thorsten Pöschel
  Charité Berlin
  NTZ-Kolloquium, 11. May 2006: *Instabilities in Driven Granular Gases*, 11. – 12. May 2006
- Dr. Tommaso Roscilde
  MPI für Quantenoptik, Garching
  NTZ-Kolloquium, 22. May 2006: *Exploring New Quantum Phases of Correlated Matter via Lattice Disorder: The Route of Quantum Spin Systems*, 22. – 23. May 2006
- Dr. Alain Billoire
  DSM/SphT CE Saclay, Gif-sur-Yvette, France
  NTZ-Kolloqium, 22. June 2006: *Finite-Size Effects in the Sherrington-Kirkpatrick Model*, 22. – 23. June 2006
- Prof. Dr. Lawrence S. Schulman
  Clarkson University, Potsdam, USA
  NTZ/Department-Kolloquium, 27. June 2006: *Imaging Dynamics: Phase transitions, Clusters, and Geometry*, 27. – 28. June 2006
- Prof. Dr. Karl Heinz Hoffmann
  TU Chemnitz
  NTZ-Kolloquium, 06. July 2006: *Dynamics on Energy Landscapes*, 06. – 07. July 2006
- Prof. Dr. Friederike Schmid
  Universität Bielefeld
  NTZ/Department-Kolloquium, 18. July 2006: *Statistical Physics of Molecular Recognition: Some Insights from Simple Model Systems*, 18. – 19. July 2006
- Prof. Dr. Frank Steiner
  Universität Ulm
  NTZ-Kolloquium, 09. November 2006: *Die kosmische Mikrowellenhintergrundstrahlung als Fenster zum frühen Universum*, 09. – 10. November 2006
- Prof. Dr. Volker Dohm
  RWTH Aachen
  NTZ/Department-Kolloquium, 30. November 2006: *Universality and Diversity of Critical Phenomena*, 29. November – 01. December 2006