# 10

# Computational Quantum Field Theory

## 10.1 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. These projects are embedded into the joint international DFH-UFA Graduate School "Statistical Physics of Complex Systems" with the l'Université Henri Poincaré Nancy, France, supported by the Deutsch-Französische Hochschule. 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 carried out at the Institute on the Linux cluster GRAWP with 40 Athlon MP1800+ processors, 60 dual-core Opteron 2218 processors, and 18 Opteron 242 processors. Further large-scale computations are performed on 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 "Sächsische Forschergruppe" FOR877 *From Local Constraints to Macroscopic Transport* and the Graduate School "BuildMoNa": Leipzig School of Natural Sciences – *Building with Molecules and Nano-objects* within the Excellence Initiative. These research structures are embedded into the priority research areas ("Profilbildende Forschungsbereiche (PbF)") and the Research Academy Leipzig (RAL), providing in particular the organizational frame for our cooperations with research groups in experimental physics and biochemistry. Also the international DFH-UFA Graduate School with Nancy is integrated into the RAL as a separate "Class". On a wider scale, our research projets 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, Japan, Russia, Spain, Taiwan, Turkey, Ukraine, and the United States.

*Wolfhard Janke*

## 10.2 Free-Energy Barriers of Spin Glasses

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A major open problem in statistical physics is the nature of the "glassy" low-temperature phase of finite-dimensional spin-glass systems. It is still unresolved whether the replica symmetry-breaking theory or the phenomenological droplet picture yields the correct description.

In the thermodynamic limit the frozen phase of the mean-field spin glass shows many stable and metastable states. Such a feature is the consequence of the disorder and the frustration characterising spin glasses in general, leading to a rugged free-energy landscape with probable regions (low free energy) separated by rare-event states (high free energy). But also for finite systems the free-energy landscape shows an intricate, corrugated structure. Therefore, it is hard to measure the free-energy barriers by means of conventional Monte Carlo simulations directly. The aim of this project is

to study the free-energy barriers of the Sherrington-Kirkpatrick (SK) mean field spin-glass model [1] and the three-dimensional Edwards-Anderson (EA) nearest-neighbour model [2] using a combination of the multioverlap Monte Carlo algorithm [3] with parallel tempering methods [4]. By using this combined algorithm we are able to perform simulations at much lower temperatures for the EA model than in previous studies [5]. This is necessary, because for temperatures close to the spin-glass transition significant deviations from the theoretical mean-field prediction were found in both the three- and four-dimensional EA model. Since one possible explanation for these deviations are strong finite-size effects close to the spin-glass transition, by measuring at lower temperatures these effects should become less pronounced.

The fact that there is no explicit order parameter which allows one to exhibit the free-energy barriers led us to use the Parisi overlap parameter [6],

$$q = \frac{1}{N} \sum_{i=1}^{N} s_i^{(1)} s_i^{(2)} \,, \tag{10.1}$$

where the spin superscripts label two independent (real) replicas for the same realization of randomly chosen exchange coupling constants $\mathcal{J} = \{J_{ij}\}$. For given $\mathcal{J}$ the probability density of $q$ is denoted by $P_{\mathcal{J}}(q)$, and the function $P(q)$ is obtained as

$$P(q) = [P_{\mathcal{J}}(q)]_{\text{av}} = \frac{1}{\#J} \sum_{\mathcal{J}} P_{\mathcal{J}}(q) \,, \tag{10.2}$$

where $[\ldots]_{\text{av}}$ symbolises the quenched average and $\#J$ is the number of realizations considered. For a given realization of $\mathcal{J}$ the nontrivial (i.e., away from $q = \pm 1$) minima are related to the free-energy barriers of this disordered system. We are, therefore, interested in the whole range of the probability density $P_{\mathcal{J}}(q)$, for an example see Fig. 10.1.

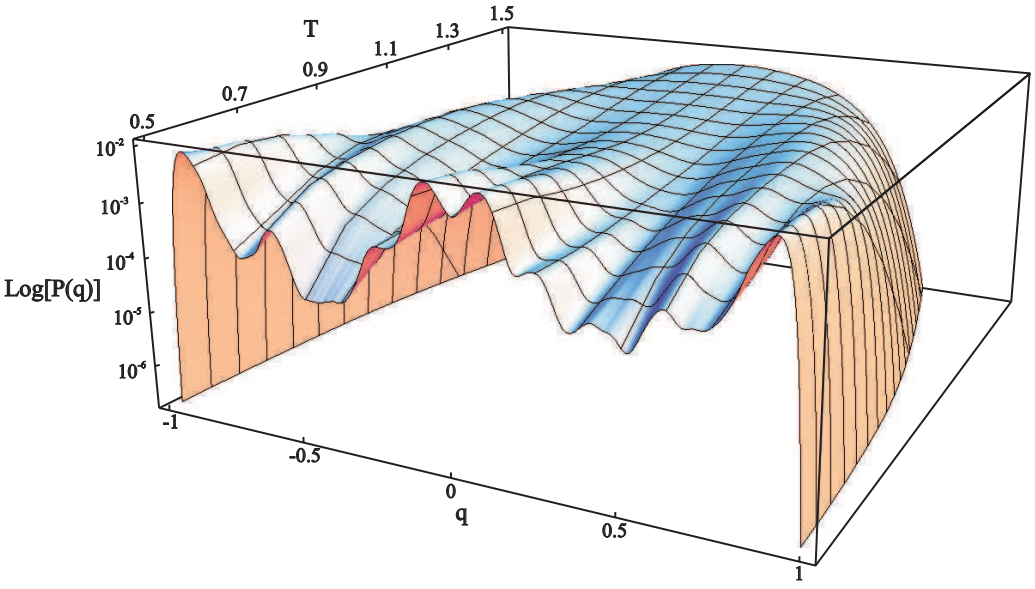


**Figure 10.1:** EA model: The logarithm of the canonical $P(q)$ distribution for a $8^3$ lattice as a function of temperature for a typical disorder realisation.

We found that the free-energy barriers of the SK model are non-self-averaging and distributed according to the Fréchet extreme-value distribution [7]. These particular features were also found for the EA nearest-neighbour model [8] and such similarities support the position that the Parisi replica symmetry breaking solution of the SK model is the limit of the short-range model on a lattice in dimension $d$ when $d \to \infty$, with a proper rescaling of the strength of the Hamiltonian. On the other hand, we also found that the free-energy barriers of the SK model diverge with the theoretically predicted value $\alpha = 1/3$, which is in contrast to our new results for the EA model in three dimensions [8] and previous findings for the three- and four-dimensional EA model [5].

This work is partially supported by the Deutsche Forschungsgemeinschaft (DFG) under grant No. JA483/22-1 and the JUMP supercomputer time grant hlz10 of NIC, Forschungszentrum Jülich.

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## 10.3 Self-Avoiding Walks on Percolation Clusters

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The universal configurational properties of long, flexible polymer chains in a good solvent are perfectly described by the model of self-avoiding walks (SAWs) on a regular lattice [1]. In particular, the average square end-to-end distance $\langle R^2 \rangle$ and the number of configurations $Z_N$ of SAWs with $N$ steps obey the scaling laws:

$$\langle R^2 \rangle \sim N^{2\nu_{\mathrm{SAW}}} , \qquad Z_N \sim z^N N^{\gamma_{\mathrm{SAW}}-1} , \tag{10.3}$$

where $\nu_{\mathrm{SAW}}$ and $\gamma_{\mathrm{SAW}}$ are the universal critical exponents that only depend on the space dimension $d$.

A question of great interest is how SAWs behave on randomly diluted lattices, which may serve as a model of linear polymers in a porous medium. This problem attracts a great attention of researchers [2]. Most interesting is the case when the concentration $p$ of structural defects is exactly at the percolation threshold $p_c$. Studying properties of percolative lattices, one encounters two possible statistical averages. In the first, one considers only incipient percolation clusters whereas the other statistical ensemble includes all the clusters, which can be found in a percolative lattice. For the latter ensemble of all clusters, the SAW can start on any of the clusters, and for an $N$-step SAW, performed on the $i$th cluster, we have $\langle R^2 \rangle \sim l_i^2$, where $l_i$ is the averaged size of the $i$th cluster. We are interested in the former case, when SAWs reside only on the

percolation cluster. In this regime, the scaling laws (10.3) hold with new exponents $\nu_{p_c} \neq \nu_{\mathrm{SAW}}, \gamma_{p_c} \neq \gamma_{\mathrm{SAW}}$ [2, 3]. A hint to the physical understanding of this phenomenon is given by the fact that weak disorder does not change the dimension of a lattice, whereas the percolation cluster itself is a fractal with fractal dimension $d^F_{p_c}$ dependent on $d$. In this way, scaling law-exponents of SAWs change with the dimension $d^F_{p_c}$ of the (fractal) lattice on which the walk resides.

Note that up to date there do also not exist many studies dedicated to Monte Carlo (MC) simulations of our problem and they do still exhibit some controversies. The value for $\nu_{p_c}$ was found in two dimensions to be in a new universality class in a study of Grassberger [4]. In the case of three and four dimensions, there also exist estimates indicating a new universality class, but no satisfactory numerical values have been obtained so far.

In our study, we use the pruned-enriched Rosenbluth method (PERM), proposed in the work of Grassberger [5], taking into account that a SAW can have its steps only on the sites belonging to the backbone of the percolation cluster. In the given problem, we have to perform two types of averaging: the first average is performed over all SAW configurations on a single backbone, the second average is carried out over different realizations of disorder, i.e. over many backbone configurations. We use lattices of size up to $L_{\mathrm{max}} = 300, 200, 50$ in $d = 2, 3, 4$, respectively, and perform averages over 1000 clusters in each case.

Since we can only construct lattices of a finite size $L$, it is not possible to perform very long SAWs on it. For each $L$, the scaling laws (10.3) hold only up to some "marginal" number of SAW steps $N_{\mathrm{marg}}$. We take this into account when analyzing the data obtained; for each lattice size we are interested only in values of $N < N_{\mathrm{marg}}$, which results in effects of finite-size scaling for critical exponents. We find, that for a SAW confined inside a lattice with size $L$ finite-size scaling holds:

$$\langle r \rangle \sim N^{\nu_{p_c}} g\left(\frac{N}{L^{1/\nu_{p_c}}}\right) , \tag{10.4}$$

where $g$ is a scaling function.

Our results bring about numerical values of critical exponents, governing the end-to-end distance of SAWs in a new universality class in two-, three-, and four-dimensional lattices at the percolation thresholds. The effects of finite lattice size are discussed as well.

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## 10.4 Percolation of Vortices and Monopoles in the 3D Abelian Lattice Higgs Model

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The Abelian Higgs model with a compact gauge field formulated on a three-dimensional (3D) lattice possesses an intriguing phase structure. In addition to the Higgs state where the photon acquires a mass, it exhibits a state in which electric charges are confined. The richness of the model, which serves as a toy model for quark confinement, stems from the presence of two types of topological excitations: vortex lines and magnetic monopoles. The former are similar to the defect lines found in superfluid liquids. The latter are point defects in three dimensions which arise because of the compactness of the $U(1)$ gauge group. In the pure 3D compact Abelian gauge theory, these monopoles lead to confinement of electric charges for all values of the gauge coupling. The coupling to the scalar theory preserves this confinement state and gives in addition rise to a Higgs state. For sufficiently small values of the Higgs self-coupling parameter $\lambda$, the two ground states are separated by a first-order transition as sketched in Fig. 10.2. For $\lambda$ larger than a critical value $\lambda_c$, which depends on the value of the gauge coupling, the two states are no longer separated by a transition where thermodynamic observables become singular, i.e., it is always possible to cross over from one ground state to the other without encountering a thermodynamic singularity. Because of this, the Higgs and confinement states were thought to constitute a single phase, despite profound differences in physical properties.

In [1], we argued that the phase diagram is more refined than implied by this picture. We conjectured that although analytically connected, the two ground states can be considered as two distinct phases. In the confinement phase the monopoles must form

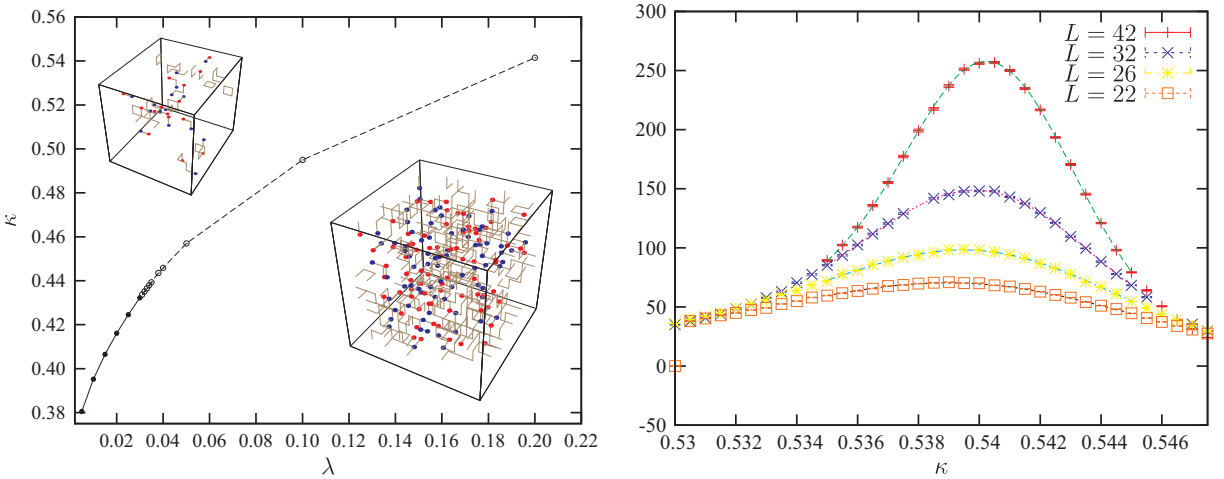


**Figure 10.2:** *Left:* Phase diagram of the $U(1)$ Lattice Higgs in dependence on two coupling constants. While for small $\lambda$ the type of the transition line is of first order (*black dots*), the line continues as a Kertész line (*open dots*) with no thermal phase transition. The insets show typical configurations of the vortex network in the two phases. *Right:* Diverging susceptibility of the maximal cluster size at the Kertész line.

a plasma which means that they are no longer tightly bound in pairs as in the Higgs phase, cf. the typical configuration plots in Fig. 10.2. Since the tension of the vortex lines connecting the monopoles and antimonopoles is finite in the Higgs phase and zero in the confinement phase, we argued that the phase boundary is uniquely defined by the vanishing of the vortex line tension, irrespective of the order of the phase transition.

In addition to open vortex lines the system also possesses closed vortex lines which are expected to be characterized by the same line tension. Because of the finite line tension, large vortex loops are exponentially suppressed in the Higgs phase. Upon approaching the phase boundary, the line tension becomes smaller so that the vortex network can grow larger and the overall line density increases. Finally, at the phase boundary where the line tension vanishes, vortices can grow arbitrarily large at no energy cost. The phase boundary between the Higgs and confinement phase is therefore expected to be marked by a proliferation of (open and closed) vortex lines. The vortices proliferate both in the region where the transition is first-order and in the region where it is not. A line along which geometrical objects proliferate, yet thermodynamic quantities and other local gauge-invariant observables remain nonsingular has become known as a Kertész line [2]. Such a line was first discussed in the context of spin clusters in the 2D Ising model in an applied magnetic field.

In our Monte Carlo study [3] we investigated this vortex proliferation scenario by studying the behavior of the vortex network directly. Because vortices are geometrical objects, their analysis is amenable to the methods developed in percolation theory [4]. As one of our main results we find that along the Kertész line, percolation observables have the usual percolation exponents. In addition, we verified that the vortex network displays discontinuous behavior in the region where the phase boundary consists of a first-order transition.

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## 10.5 Geometric Properties of the Three-Dimensional Ising and XY Models

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The relation between thermal phase transitions of lattice spin systems and the percolation problem has been in the focus of intense research for at least three decades. Clusters of 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*). While the geometric clusters are not yet the proper objects in general, it turned out that, in fact, a close relation between thermal phase transitions and percolation can be established by considering *stochastically* defined clusters (or droplets) as they occur in the Fortuin–Kasteleyn (FK) or Coniglio–Klein (CK) representation of the Potts model. Using this type of clusters, the Potts model can be shown to be equivalent to a site-bond correlated percolation problem [2] such that the corresponding critical exponents agree exactly.

In this sprit we have recently developed a new approach in which the high-temperature (HT) series expansion of lattice spin models is used to study their critical properties in a geometric percolation picture. In this approach, the partition function and correlation functions are calculated by counting graphs on the lattice, with each graph representing a certain contribution. Traditionally, such an expansion is carried out exactly to a given order by enumerating all possible ways a graph of given size and topology can be drawn on the lattice. This exact approach, involving combinatorial and graph-theoretical algorithms, is notoriously challenging and laborious, with each additional order requiring typically about the same amount of effort needed for all previous orders combined.

To circumvent this problem, we apply here Monte Carlo simulations to sample the graph configurations stochastically, cf. Fig. 10.3. At high temperatures, only a few small graphs generated this way can be found scattered throughout the lattice. As the temperature is lowered, graphs start to fill the lattice by growing larger and becoming more abundant. At temperatures below the critical temperature, the lattice becomes filled with graphs. A typical graph configuration now consists of one big graph spanning the entire lattice and a collection of much smaller graphs (see Fig. 10.4). The steady increase in the number of occupied links and the appearance of graphs spanning the lattice as the temperature is lowered are reminiscent of a percolation process. The use of percolation observables therefore suggests itself to analyze the graph configurations. For these observables to have bearing on the critical properties of the model under investigation, it is necessary that the HT graphs percolate right at the thermal critical point. The fractal structure of closed and open graphs then encodes the standard critical exponents [3].

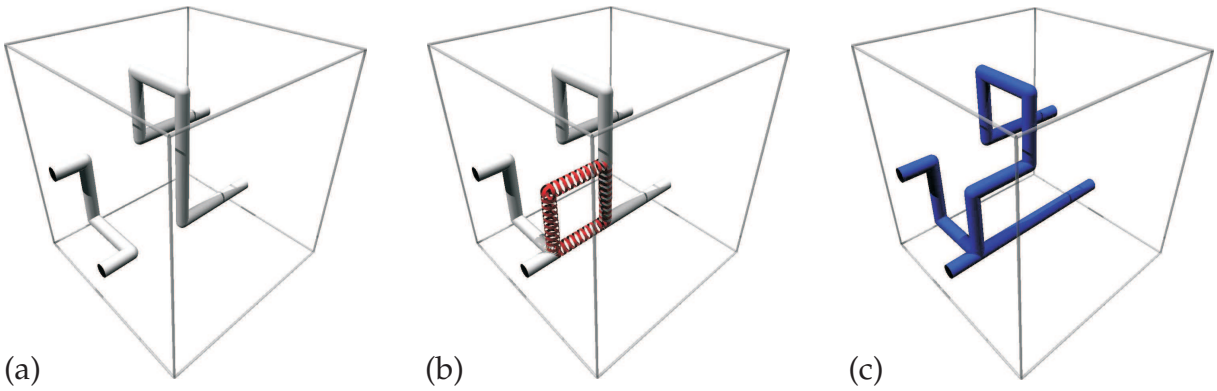


**Figure 10.3:** An existing Ising HT graph on a cubic lattice (**a**) is updated with the help of a chosen plaquette (**b**) into a new graph (**c**).

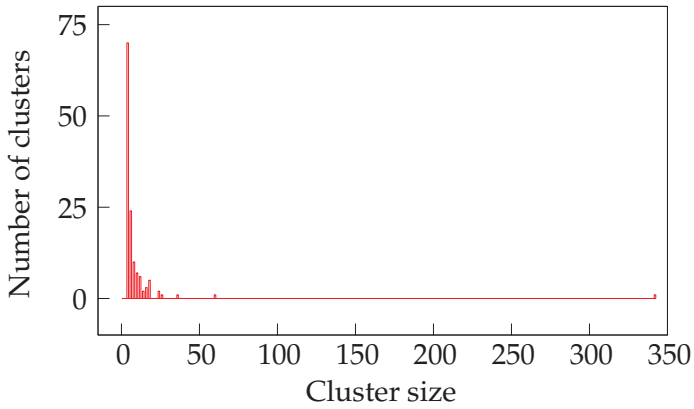


**Figure 10.4:** Distribution of Ising HT graphs on a cubic lattice of linear size $L = 24$ at the percolation threshold. Note the presence of a single big graph and many much smaller graphs.

We have verified this scenario for the HT graphs of the three-dimensional Ising and XY models on a simple cubic lattice with periodic boundary conditions [4]. The graphs are shown to indeed percolate right at the (thermal) Curie critical point. The diverging length scale relevant to the graphs in the vicinity of the percolation threshold is shown to be provided by the spin correlation length. By applying finite-size scaling techniques, the fractal dimension of the HT graphs at criticality is estimated to be $D = 1.7349(65)$ for the Ising and $D = 1.7626(66)$ for the XY model, which both are, via general scaling relations, in good agreement with the standard thermal critical exponents.

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## 10.6 Statistical Mechanics of Complex Networks

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Recent progress in understanding the structure and function of complex networks [1] has been largely influenced by the application of methods of statistical physics. We use these tools to investigate the properties of different models of networks as well as dynamical processes taking place on them. We also study matter-network interactions, that is situations when not only the network governs the behavior of some matter field placed on it, but also the matter field can have an influence on the network. For all problems, we apply both analytical and Monte Carlo methods.

An example of a problem we study in connection with structural properties of networks are finite-size effects in equilibrated graphs [2]. These are graphs which are maximally random under given constraints. The possible constraints are, for instance, fixing the total number of nodes and links, excluding multiple- and self-connections, or imposing a tree structure. Finite-size effects in graphs are very strong, much stronger than in more "typical" physical systems, where the number of degrees of freedom is of order $10^{23}$. In networks, however, the typical number of nodes $N$ is between $10^3$ (transportation networks) to $10^9$ (the World Wide Web). Moreover, since complex networks have in general infinite fractal dimension, their "surface" is very large in comparison to the volume. This, together with power-law degree distributions of many networks is the reason why very large corrections to solutions in the thermodynamic limit appear. We study these corrections by means of analytical methods and also with the help of advanced Monte Carlo procedures like, e.g., multicanonical simulations.

Apart from the structural properties we also study their influence on the dynamics on networks. A very simple model we consider is the zero-range process (ZRP) [3], where some particles hop between nodes along existing connections between them. Particles jump according to a very local rule: the probability that a particle will move to another site depends only on the occupation of the departure node. Because of its simplicity, this model can be treated analytically in many aspects. It has, however, a very rich behavior. For instance, in networks with inhomogeneous degrees of nodes, that is when nodes have various numbers of nearest neighbors, a phenomenon called condensation occurs. This means that a finite fraction of particles resides on a single node. This can be viewed as a prototype of traffic jamming. We study conditions under which the condensate is formed, a typical time it takes to build the condensate from a uniform background, and its mean life time [4].

We also investigate the interplay between the network and the matter. The prototype of such a system is a modified ZRP, where we allow the network to rearrange itself in parallel to the particle dynamics. Different rules for rewiring connections lead to different effects. But even if we rewire links at random, there is an interesting transition from the condensed to a liquid phase provided that the rewiring rate is large enough. It turns out that if the node with maximal number of neighbors migrates fast through the network, the condensate has no time to grow up [5].

On the other hand, if the network dynamics is very slow, it can be considered as quenched disorder from the particles point of view. The averaging over the disorder can lead to a very interesting effect: for networks with properly tuned degree distribution, the distribution of particles shows a power law, exactly as it has been observed in the ZRP on homogeneous networks [6].

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## 10.7 Studies of Structure Formation Processes Employing Mesoscopic Models for Polymers and Proteins

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With several thermodynamic and kinetic questions regarding polymer and protein folding, aggregation and adsorption at solid substrates in mind, we have investigated by means of sophisticated Monte Carlo [1–6] and thermostated Molecular Dynamics simulations [7] mesoscopic models for homo- and heteropolymers. Usually, polymer structure formation processes require semilocal or even nonlocal cooperativity of the monomers involved. In good solvents, secondary structures such as helices and sheets, for example, are formed on relatively small scales, whereas the hydrophobic collapse requires an optimal formation of all monomers in a highly compact shape. If it comes to crystallization, the monomers can even arrange in symmetric structures. Because of the mesoscopic nature of tertiary structure formations processes, simplified models can be employed to analyze characteristic features of such conformational transitions.

Therefore, we have likewise analyzed hydrophobic collapse, crystallization, as well as compact hydrophobic-core formation with mesoscopic models for the folding of flexible homopolymers and hydrophobic-polar heteropolymers, the aggregation of polymers, and the adsorption of polymers at attractive solid substrates. The main advantage of these models is the possibility to perform systematic, comparative studies regarding different aspects. In a detailed analysis of a simple heteropolymer model based on the effective attraction of nonbonded hydrophobic monomers (mimicking the "hydrophobic effect" in good solvents) [8], we could show that typical folding characteristics known from natural proteins are also observed on mesoscopic scales, i.e., without explicitly taking into account interactions on nanoscales [1, 2]. One such typical folding behavior is two-state folding, where only ensembles of folded and denatured protein structures occur. In this case, folding and unfolding times depend exponentially on the temperature near the transition state [3].

By investigating the nucleation transition of small peptides and polymers with mesoscopic models, we have also found that the aggregation of polymers and peptides is a phase separation process, in which the loss of entropy due to surface effects entails an decrease of temperature with increasing energy ("backbending effect") [4–6].

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## 10.8 Conformational Transitions of Flexible Polymers

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The nature of conformational freezing transitions of single flexible polymers and their relations to colloidal systems is little understood. Systems of finite length that can computationally be studied do not reveal a clear picture at all. This is actually not surprising as the large conformational entropy of frozen polymer conformations leads to the assumption that the solid phase is largely amorphous and frustrated. In contrast, very large systems are known to form crystalline structures with long-range order in order to optimize energetically favored short-range monomer-monomer contacts. The reason for the complexity of the structural behavior of small polymers is the competition between surface effects in order to reduce interfacial free energy and the tendency to form lattice structures in the interior.

Even in lattice models, the diversity of lowest-energy conformations can be observed [1]. For polymers of different lengths on the simple-cubic lattice, we have found a remarkably systematic pattern of the freezing transition which can be explained by lattice effects of the finite-length systems. In fact, the high precision of our data allows us to reveal a noticeable difference in the behavior of "magic" chain lengths that allow for cubic or cuboid conformations. In these cases, an energy gap exists between the ground-state conformations and the first excitations. This peculiarity causes a first-order-like pseudotransition which is typically more pronounced than the separate freezing transition. Surprisingly, this effect vanishes widely for polymers with slightly longer chain lengths. The freezing temperature decreases with increasing chain length until the next "magic" length is reached. Polymers on the face-centered cubic lattice behave similarly, but the relevant geometries are more complex.

Employing a flexible polymer model with highly elastic covalent bonds, polymer freezing behaves similar like atomic cluster formation at low temperatures (Lennard–Jones cluster) [2]. There are also "magic numbers" of atoms or monomers, for which almost perfect geometric structures form (see Fig. 10.5 for an icosahedral structure of a 147mer). A particularly important shape is the regular icosahedron with 20 equilateral triangular faces and it is known to be the basic capsid structure of spherical viruses, on which the capsomer proteins assemble. For chain lengths different from "magic" numbers, overlayers form on the outer faces. Depending on the kind of monomer arrangement on the surface, so-called Mackay or anti-Mackay layers are distinguished. Actually, the different strategies how clusters grow with increasing chain lengths make a uniform description of the freezing transition for flexible polymers quite intricate. The situation seems to be even more difficult for polymers with nonflexible bonds (such as proteins), as regular tertiary structures can hardly be identified.

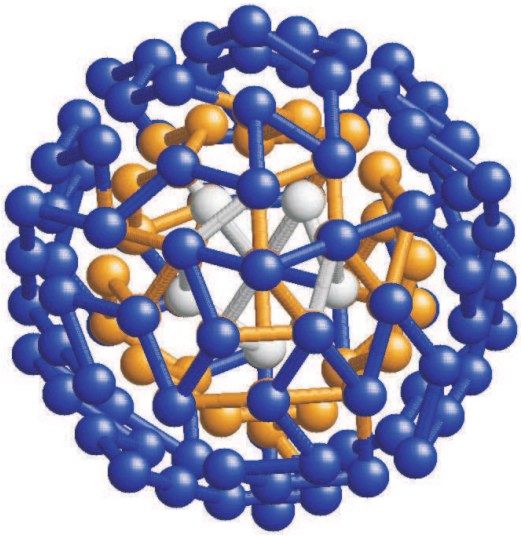

**Figure 10.5:** Optimal volume-filling icosahedral shape of a flexible polymer with elastic bonds. The linear polymer consists of 147 monomers and as such it is of "magic" length.

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[2] S. Schnabel et al.: *Liquid-Solid Transitions of Flexible Polymers*, Leipzig preprint (2008)

## 10.9 Thickness-Dependent Secondary–Structure Formation of Tubelike Polymers

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By means of Monte Carlo methods, we have investigated conformational ground-state and thermodynamic properties of a simple model for flexible polymer classes with explicit thickness [1]. The thickness constraint, which is introduced via the global radius of curvature [2] of a polymer conformation, accounts for the excluded volume induced by the polymer side chains. In our detailed analysis of ground states and conformational phases of short tubelike polymers, we find that, depending on the thickness, known secondary structures like helices and turns, but also ringlike conformations and stiff rods are intrinsic topologies of such tubelike objects. Explicit dipole-dipole interactions resulting in the formation of hydrogen bonds, which in natural polymers stabilize secondary structures are, thus, not a necessary prerequisite for forming secondary structures. Furthermore, we clearly find that the thickness of polymers noticeably influences the ability to form structural segments which naturally occur in conformations of linear polymers, such as proteins.

For the identification of underlying *secondary* structure segments like helices and strands, the generic modeling of volume exclusion by means of pair potentials is not

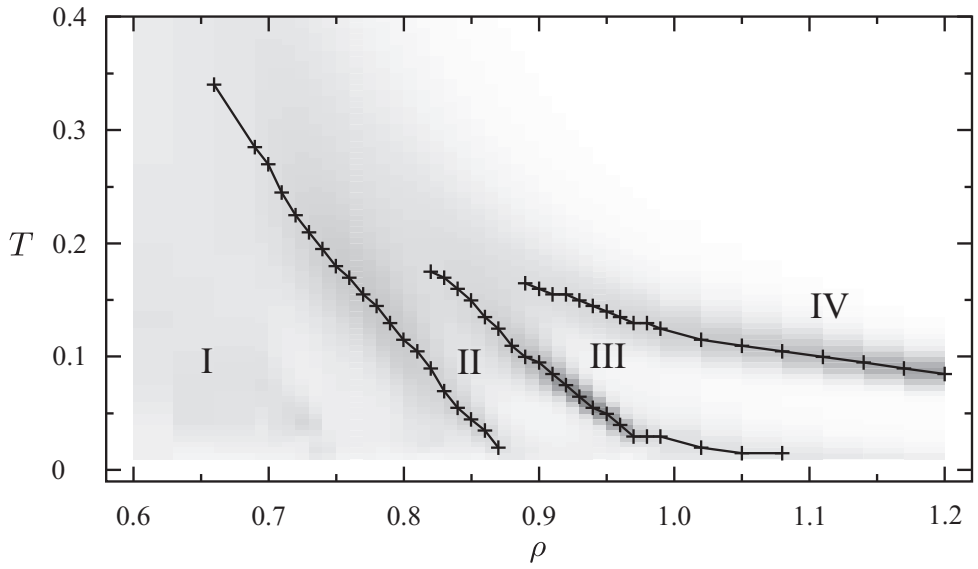


**Figure 10.6:** Hundreds of simulations revealed a clear structure of the temperature–thickness pseudophase diagram of secondary structures for classes of short tubelike polymers. Dominant structures in the principal phases are found to be helical (I), sheetlike (II), ringlike (III), or random coils/rods (IV).

sufficient. Rather, the formation of such segments requires the cooperative behavior of adjacent monomers, i.e., in addition to pairwise repulsion, information about the relative position of the monomers to each other in the chain is necessary to effectively model the competition between noncovalent monomeric attraction and short-range repulsion due to volume exclusion effects [3]. The simplest way to achieve this in a general, unspecific mesoscopic model is to introduce a hard single-parameter thickness constraint and, thus, to consider a polymer chain rather as a three-dimensional tube than as a one-dimensional, linelike object [4, 5].

We have also analyzed in detail the phase diagram of flexible polymers that does not only allow for the classification of possible thermodynamic conformational phases of a single polymer with fixed thickness (see Fig. 10.6). Performing various simulations for different thicknesses enabled us also to resolve the phase behavior with respect to the thickness constraint. This means that the we have identified the structure of the conformational space of *classes* of polymers, parametrized by their thickness. Although we employ a generic model for flexible polymers, we find that the thickness constraint is an intrinsic source of an effective stiffness. The main result of our analysis is that the tube thickness is also responsible for the capability of a polymer to form secondary structures. Indeed, we clearly find helical and sheet-like structures which are dominant in different pseudophases.

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## 10.10 Computer Simulation and Experimental Analysis of Peptide Adhesion at Semiconductor Substrates

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In this project, we have investigated solvent properties and adsorption behavior of short synthetic proteins. From experiments [1–3], it is known that some of these peptides possess a specific adsorption characteristics at semiconductor surfaces like, for example, silicon (Si) and gallium-arsenide (GaAs) with certain crystal orientations at the surface. It could be shown in these experiments that permutations and pointwise mutations of the amino acid sequences can cause noticeably changes in the adsorption behavior of the peptides. In our simulation study, our main interest was devoted to an amino-acid sequence that exhibits good binding propensity to the (100) surface of GaAs and poor binding strength to Si(100) and to a peptide with the same amino acid contents but with randomly permuted sequence. In the latter case, the adsorption strength to Si(100) improved noticeably. It is one of the main objectives of our project to get deeper insights into specific properties of peptide binding to semiconductor substrates by means of single-molecule Monte Carlo computer simulations of a hybrid model that enables a detailed analysis of the thermodynamics of folding and adsorption properties on atomic scales. On the other hand, it is required that the model is sufficiently simple allowing for an efficient simulation. The particular complexity of the problem lies in the competition of the folding and the adsorption transitions, both affecting the conformational changes of the peptides under the influence of thermal fluctuations.

In a first step, we have analyzed solvent properties of these peptides [4]. For that purpose, we performed simulated tempering computer simulations employing a simplified implicit-water all-atom protein model that had recently been developed in the Lund group [5, 6]. Although unstructured conformations dominate at room temperature, we found surprisingly clear evidence that the peptide with good Si(100) binding strength and the peptides with small Si(100) binding propensities exhibit different tendencies in forming secondary-structure (i.e., $\alpha$-helical and $\beta$-stranded) segments. We could also identify the amino acid proline and its different position in the sequences we compared with each other as being relevant for the different trends in structure formation. By a pairwise mutation regarding the proline positions, we could also show that then the trends of secondary-structure formation reverse.

In order to check our experimentally not yet verified prediction that this trend reversal also changes the binding propensity to Si(100) substrates, we have developed and analyzed in the second part of the project an extension of the peptide model, where the interaction with a Si(100) substrate has been incorporated [7]. In our model, the Si substrate is considered as bare and flat. This approach is justified, as our experiments revealed that the Si(100) substrate is not yet noticeably oxidized while the peptide adsorption process proceeds. The multicanonical computer

simulations we performed with this model not only confirmed qualitatively the experimentally observed Si(100) binding specificity of the different peptides; we also found that the position changes of proline in the sequences actually reverse also the binding propensity of the peptides as predicted from our studies of the peptides' solvent behavior.

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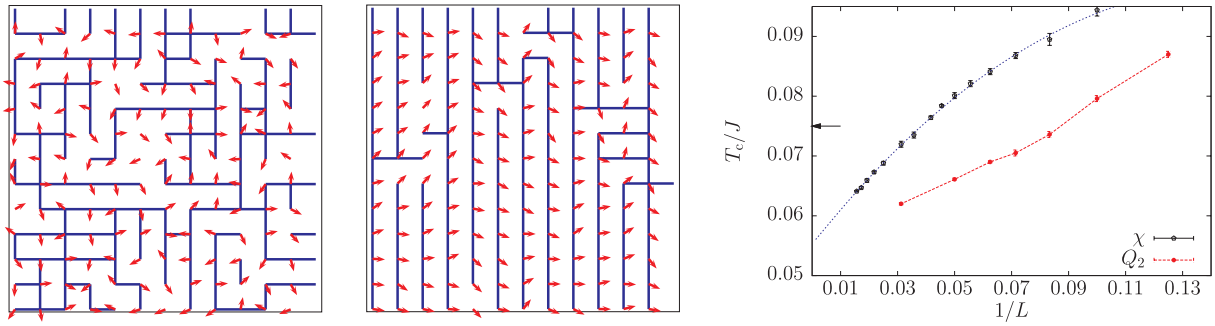
## 10.11 Directional-Ordering in the Two-Dimensional Compass Model

S. Wenzel, W. Janke

The so-called compass model with quantum spin-degrees of freedom is a possible realization of a system that topologically protects Qbits from decoherence [1] and has, as such, prompted recent theoretical investigations. The model is a spin model on a simple square lattice (in two-dimensions), defined by the Hamiltonian

$$\mathcal{H} = \sum_i \left( J_x S_i^x S_{i+e_x}^x + J_y S_i^y S_{i+e_y}^y \right) , \tag{10.5}$$

where $S = (S^x, S^y)$ is a two-component spin on sites $i$ and $J_x$, $J_y$ are the coupling constants. This Hamiltonian looks very similar to an ordinary XY model but differs




(a) (b) (c)

**Figure 10.7:** (**a**) Sketch of spin configurations in the disordered state and (**b**) in the ordered state where thick lines indicate bonds carrying the important energy contributions. The pictures are obtained from simulations of the classical model. (**c**) The critical temperature $T_c$ obtained from finite-size scaling of the susceptibility at different lattice sizes $L$. Our result is at variance with a recent estimate (indicated by the arrow) in the literature.

from it crucially in that the interactions in the system are strangely non-isotropic. The $x$-component of the spin interacts only with nearest neighbor spins in $x$-direction and the $y$-component in $y$-direction, respectively.

We study this model for the case $J_x = J_z$ employing state-of-the-art quantum Monte Carlo methods based on the so-called stochastic series expansion (SSE) [2]. By investigating the quantity $D = |E_x - E_y|$ (the difference between mean energy in $x$ and $y$ direction), we show that there is a finite-temperature phase transition between a disordered state ($T > T_c$) and an ordered state. This ordered state is not magnetic but rather like a nematic phase oriented with equal probability in $x$ or $y-$direction (see Fig. 10.7a,b). By performing comprehensive simulations of the model we were able to determine the critical temperature $T_c$ and the critical exponents of this transition. Our results reported in [3] improve previous values in the literature considerably and provide a first real benchmark for future studies (see Fig. 10.7c).

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## 10.12 Quantum Critical Phenomena and Quantum Spin Systems

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In this project we study the quantum Heisenberg model, which is one of the most fundamental models of quantum magnetism. Several aspects of this model are studied in relation to a theoretical understanding of quantum phase transition.

Firstly, so called mixed spin chains in one dimension (1D) are considered. The low temperature properties of those chains 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 [1]. However, even integer spin chains can be driven to quantum criticality by tuning the bond alternation of the coupling strength.

We have investigated quantum chains of mixed spins [2, 3]. By means of quantum Monte Carlo (QMC) simulations (continuous imaginary time loop 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 $S_a = 1/2$ and $S_b = 1$, $S_a = 1/2$ and $S_b = 3/2$ as well as $S_a = 1$ and $S_b = 3/2$. The analysis of the QMC results is supplemented by exact Lanczos diagonalisation. Under the aspect of conformal invariance theory [4], extrapolation methods have been applied to determine central charge and critical exponents of the models under investigation.

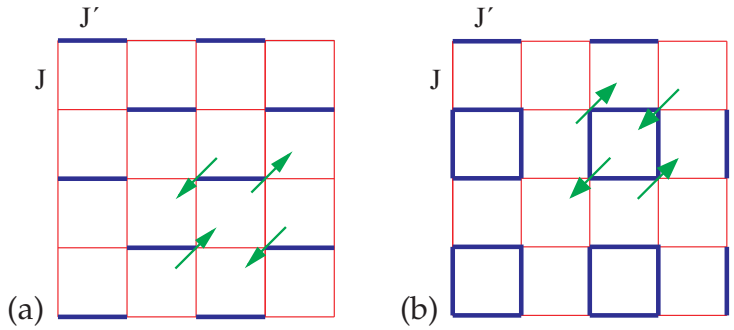


**Figure 10.8:** Two-dimensional Heisenberg models on the square lattice with antiferrogmagnetic couplings $J$ and $J'$. Varying the ratio $J/J'$ drives the system through a quantum phase transition, which is the main object of this project.

Secondly, we study the quantum phase transition from a Néel ordered to a disordered (dimer) state in two-dimensional antiferrogments possessing two different kinds of nearest neighbor interactions $J$ and $J'$ (see Fig. 10.8). To this end, we employ the stochastic series expansion (SSE) [5] algorithm. Our main interest is to study the critical exponents of the phase transitions. We compare the effect of several geometric arrangements of the bonds and our current high-precission data suggests that $O(3)$ Heisenberg universality class might be broken in case of Fig. 10.8a.

Thirdly, we have investigated quantum ferromagnets in an external magnetic field. Here we performed for one-dimensional chains and two-dimensional layers a careful comparison of analytical approaches with numerical quantum Monte Carlo simulations using the SSE method, paying special attention to a peculiar double-peak structure of the specific heat and the behaviour of correlation lengths as a function of temperature in dependence on the spin quantum number $S$ [6].

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## 10.13 Evaporation/Condensation of Ising Droplets

E. Bittner, A. Nußbaumer, W. Janke

In our present research project we continued an ongoing approach to theoretically investigate the evaporation/condensation transition in liquid/gas or solid/gas mixtures by means of computer simulations. More precisely, we use the two and three-dimensional spin-1/2 Ising model, having a Hamiltonian

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \,, \qquad \sigma_i = \pm 1 \,, \tag{10.6}$$

where $J = 1$ is an interaction constant and $\sigma_i = \pm 1$ is a spin located at the lattice site $i$. The symbol $\langle ij \rangle$ denotes the pairs of interacting spins defined by the underlying lattice. In two dimensions we select the square lattice, triangular lattice and the next-nearest-neighbour lattice all of size $L \times L$ while in three dimensions only the cubic lattice of size $L \times L \times L$ was taken into account. Certainly, the idea is, that (e.g.) positive spins correspond to particles while negative spins correspond to vacancies. Then, an interpretation as lattice gas is possible.

For these systems it is known, that for temperatures $T$ below the critical temperature $T_c$ the magnetisation $m = M/V = \sum_i \sigma_i / V$ has in the infinite-volume limit ($V = L^2 \to \infty$) a value of $m_0(T) \neq 0$. Assuming that the majority of spins has a positive sign, i.e. $\sigma_i = +1$, then, on a microscopic level, at every given time there is a fixed amount of spins $V(1 - m_0)/2$ in the system that are overturned and therefore have a negative sign. If we artificially increase the number of overturned spins by a macroscopic amount, then the magnetisation decreases and we can pose the question what happens to the extra $-1$-spins. One possible answer is that the system forms a droplet of the "wrong phase" that has the same magnitude of the spontaneous magnetisation but the opposite sign, i.e., this phase consists of negative majority spins with some overturned spins within. If all additional $-1$-spins are "absorbed" into this phase, and if this phase is compact, then there is only one (large) droplet with negative magnetisation. The total magnetisation is then given by a contribution $m_0(V - v)$ from the positive phase (background) of volume $V - v$ and a contribution $-m_0 v$ from the negative phase of volume $v$ giving

$$M = m_0(V - v) - m_0 v = m_0 V - 2m_0 v \; . \tag{10.7}$$

We can measure the volume of this droplet and it must hold

$$\frac{v}{V} = \frac{m_0 - m}{2m_0} \; . \tag{10.8}$$

In order to do so we performed simulations in the low-temperature phase at $T = 1.5$ at constant magnetisation (Kawasaki dynamics). The choice of the temperature is a trade-off between a fast spin-flip (pseudo-)dynamics and an increase of the correlation length in the vicinity of the critical temperature of the model. At a certain temperature, the infinite-system correlation length exceeds the system size $L$. Then, a percolating cluster builds up which effectively would prevent us from measuring a droplet in the system – which is our main interest.

Figure 10.9(a) shows the droplet size for various values of the magnetisation $m$ (every point is a single simulation). Clearly, only for large system sizes and small values of the magnetisation $m$ the theoretical value (10.8) of the droplet is approached. For $L \geq 160$ and large values of $m$, a kink in the droplet size becomes visible and the droplet size rapidly reaches zero. The position of this drop-off is moving for larger system sizes towards $m_0$ while the height of the drop-off is decreasing. Apparently, the assumption that *all* extra spins form a droplet is not correct but only a part of them form the droplet while the rest stays in the background. For values of the magnetisation larger than the drop-off value, there is no droplet at all, i.e., in this case all extra spins contribute to the fluctuations in the background and the maximal droplet volume is of the order one.

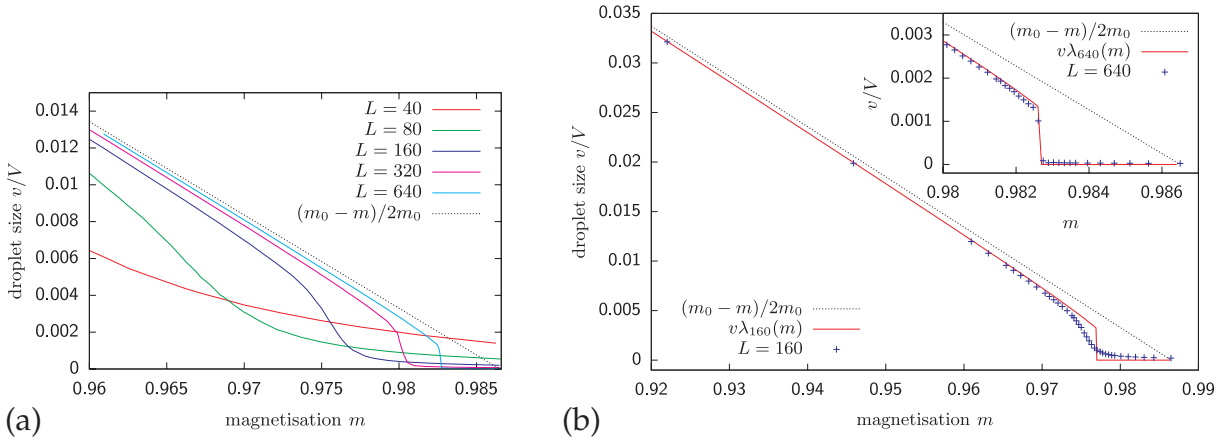


**Figure 10.9:** (**a**) Relative droplet volume $v/V$ for the 2D Ising model at the temperature $T = 1.5$ and for different system sizes from $L = 40$ to $L = 640$. The abscissa ranges from $m_{\min} = 0.96$ to the value of the spontaneous magnetisation $m_{\max} = m_0(1.5) = 0.9865$. The *dashed line* shows (10.8); for the measured values a combination of Hoshen–Kopelman and flood-fill algorithm was used. Similar plots can be found in [1, 2]. (**b**) Relative droplet volume $v/V$ for the 2D Ising model at the temperature $T = 1.5$ and system sizes $L = 160$ and $L = 640$ (*inset*). The *dashed line* shows (10.8) and the *blue '+' symbols* indicate the measured values. The *solid red line* represents the theoretical curve modified by the factor $\lambda_L(m)$.

In recent work Biskup et al. [3, 4] were able to proof this behaviour in the case of the two-dimensional Ising model rigorously. They give an analytic expression for $\lambda_L(m)$, the fraction of the additionally overturned spins that help to form the droplet. Then, the actual droplet volume is not $v(m)$ but $\lambda_L(m)v(m)$. Furthermore, for values $m > m_c$ there is no large minority droplet at all and consequently $\lambda_L(m) = 0$. At $m = m_c$ the value of $\lambda_L$ jumps to 2/3, marking the position where the system makes a transition from a one-phase state (evaporated) to a two-phase state (evaporated/condensed), thereby absorbing 2/3 of the extra −1-spins into the droplet. For lower values of the magnetisation the fraction $\lambda_L(m)$ gradually increases to 1 and the actual droplet size approaches that of (10.8). In Fig. 10.9b we show the data for $L = 160$ and $L = 640$ (inset) from Fig. 10.9 again but additionally the (red) solid curve shows the finite size corrected theoretical value of the droplet size $\lambda_L(m)v(m)$.

More details can be found in [5] and the recent detailed work in [6].

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## 10.14 Boundary Field Induced First-Order Transition in the 2D Ising Model

E. Bittner, W. Janke

Wetting transitions are phase transitions in the surface layer of bulk systems which are induced by symmetry-breaking surface fields. The Ising model with a boundary magnetic field is a simple model for such a wetting problem, because the Ising ferromagnets have the same critical behaviour as the analogous case of gas-fluid transitions, as has been pointed out by Nakanishi and Fisher [1]. The use of the Ising model with short range interactions for wetting studies has not only the advantage that one can use all the advanced simulation techniques, which have been developed for the Ising model. Especially in two dimensions (2D), there are also a lot of theoretical results available for comparison.

The Ising model with a uniform boundary magnetic field on one side of a square lattice has been completely solved by McCoy and Wu [2], whereas the Ising model with a uniform bulk field can only be solved at the critical temperature. For configurations with other fixed boundary spins or equivalently infinite boundary magnetic fields or finite boundary magnetic fields some exact results have also been found. In a recent paper, Clusel and Fortin [4] presented an alternative method to that developed by McCoy and Wu to obtain some exact results for the 2D Ising model with a general boundary magnetic field and for finite-size systems. Their method is based on the fermion representation of the Ising model using a Grassmann algebra. They applied this method to study the first-order transition induced by an inhomogeneous boundary magnetic field in the 2D Ising model [5]. By taking the thermodynamic limit exactly for a given geometry of the lattice, they obtained a simple equation for the transition line and also a threshold for the aspect ratio $\zeta_s = L_x/L_y \simeq 1/4$, where this line moves into the complex plane. This vanishing of the transition line indicates the crossover from 1D behaviour for $L_x \ll L_y$ to 2D behaviour at large $\zeta$, which can be seen in the boundary spin-spin correlation function.

The aim of this work is to check some of the predictions by carrying out Monte Carlo simulations of this model and to extend the results to parameter ranges and for observables where analytic solutions cannot be found. Data were first obtained for $\zeta = 0.2 < \zeta_s$. For this value of the aspect ratio we find the phase diagram as predicted by Clusel and Fortin [5], cf. Fig. 10.10a. Here the thick line indicates the transition from the fully magnetized state to a state with an interface extended across the bulk. To check the nature of this transition we measured the probability density for the magnetization as a function of the boundary magnetic field $H$ at constant temperature $T$ and estimated the interface tension, cf. Fig. 10.10b. We find a good agreement with the infinite-volume transition boundary magnetic field given by Clusel and Fortin [5] and for all cuts of constant temperature $T$ a clearly nonzero interface tension. We also performed simulations at various constant values of the boundary magnetic field $H > 0$ and chose the temperature such that the peaks of the probability density for the magnetization are of equal height. The infinite-volume extrapolation tends to increase with system size and yields a clearly nonzero interface tension and the transition point converges to the analytical value. Furthermore, we checked the critical behaviour along the line of second-order transitions at $T = T_c$. To this end we performed a finite-

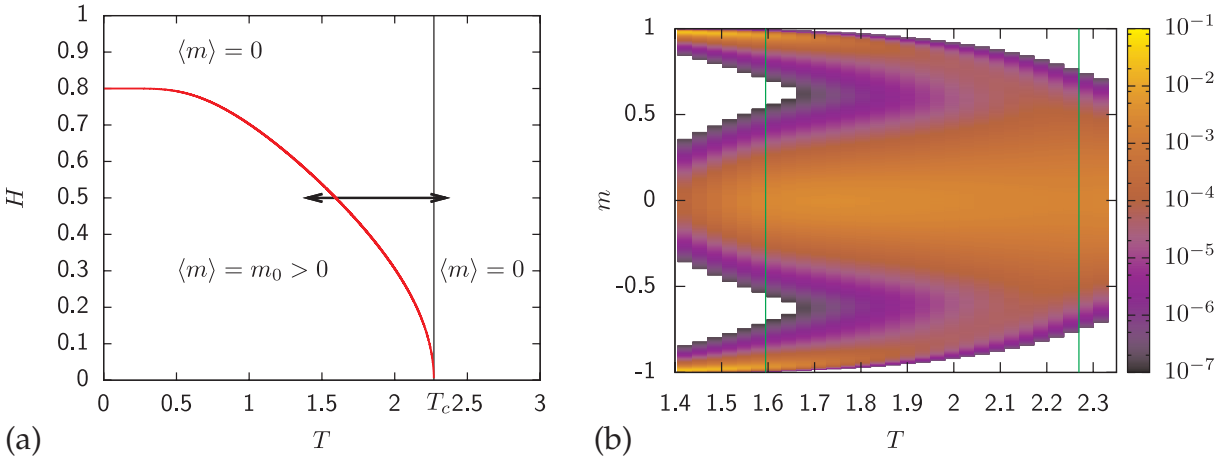


**Figure 10.10:** (**a**): The phase diagram for a system with $\zeta = 0.2$. The *thick line* shows the first-order transition given by Clusel and Fortin [5] and the *thin line* indicates the second-order bulk phase transition. The *double headed arrows* show the parameters of the Monte Carlo simulation. (**b**): The probability density for the magnetization as a function of temperature at the constant boundary magnetic field $H = 0.5$ for $L_x = 20$ and $L_y = 100$. The *vertical lines* indicate the value of the temperature $T$ at which the peaks are of equal height and the critical temperature $T_c \approx 2.269$ of the bulk phase transition.

size scaling (FSS) analysis at $H = 0.5$ and determined the transition point and some critical exponents. Moreover, we studied the spin-spin correlation function for which no analytical results are available.

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## 10.15 Multibondic Cluster Algorithm with Wang–Landau Sampling for Finite-Size Scaling Studies of Critical Phenomena

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When studying equilibrium properties of statistical physics systems by means of Markov chain Monte Carlo (MCMC) simulations, it has turned out that it is often advantageous to work with so-called "generalized" ensembles [1]; for reviews see, e.g., [2, 3]. While the power of this approach is well documented for first-order phase transitions and complex systems such as spin glasses or peptides (small proteins) [4],

this is surprisingly not the case for second-order phase transitions and associated critical phenomena. In this 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. The desired extended energy range can, in principle, be covered by performing a Wang-Landau recursion for the spectral density followed by a multicanonical simulation with fixed weights. However, in the conventional approach one loses the advantage of cluster algorithms, which can reduce critical slowing down at second-order phase transitions dramatically.

We have therefore developed a combination of multibondic cluster simulations with the Wang-Landau recursion [5]. We furthermore show that by careful finite-size scaling considerations the relevant energy range to be covered by the simulations can be estimated a priori [6, 7]. This turned out to be an important aspect of our method. We have performed thorough tests of these ideas for 2D and 3D Ising models and obtained improvements over the conventional Wang-Landau/multicanonical approach by power laws in the lattice size [5–7].

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## 10.16 Funding

*Numerical Studies of Protein Folding*
M. Bachmann
Deutsche Forschungsgemeinschaft (DFG) Fellowship for extended research visit of the Computational Biology & Biological Physics Group at Lunds Universitet (Lund, Sweden)

*Mesoscopic Models for Protein Folding*
M. Bachmann
Wenner-Gren Research Fellowship in the group of Prof. Dr. A. Irbäck in the Computational Biology & Biological Physics Group at Lunds Universitet (Lund, Sweden)

*Excellence Initiative, Graduate School "BuildMoNa": Leipzig School of Natural Sciences – Building with Molecules and Nano-objects*

W. Janke (Principal Investigator)
Deutsche Forschungsgemeinschaft (DFG)

*From Local Constraints to Macroscopic Transport*
W. Janke (Principal Investigator)
Deutsche Forschungsgemeinschaft (DFG) "Forschergruppe 877"

*International Conference ENRAGE – Random Geometry and Random Matrices: From Quantum Gravity to Econophysics, 17. – 22. May 2009*
W. Janke (Organizer)
Max-Planck-Institut für Physik komplexer Systeme in Dresden

*Host of the Alexander von Humboldt Research Prize Winner Bernd A. Berg (Florida State University, Tallahassee, USA)*
W. Janke
Alexander von Humboldt Foundation

*Host of EU Marie Curie Incoming Fellowship: SAWs on Fractals, Dr. Viktoria Blavatska (Lviv, Ukraine)*
W. Janke
EU Grant No. MIF1-CT-2006-021867

*"Deutsch-Französisches Doktorandenkollegium (DFDK)" with "Co-tutelle des Thèse", jointly with l'Université Henri Poincaré, Nancy I (with B. Berche): Statistical Physics of Complex Systems*
W. Janke
Deutsch-Französische Hochschule

*Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*
W. Janke
EU RTN-Network "ENRAGE", Grant No. MRTN-CT-2004-005616

*Dynamik und Statik von Spingläsern*
W. Janke
Deutsche Forschungsgemeinschaft (DFG), Grant No. JA483/22-1

*Investigation of Thermodynamic Properties of Lattice and Off-Lattice Models for Proteins and Polymers*
M. Bachmann and W. Janke
Deutsche Forschungsgemeinschaft (DFG), Grant Nos. JA483/24-1 and 2

*Phasenübergänge in Systemen mit einschränkender Geometrie*
W. Janke
Deutsche Forschungsgemeinschaft (DFG), Grant Nos. JA483/23-1 and 2

*Two-Dimensional Magnetic Systems with Anisotropy*
W. Janke
EU Marie Curie Development Host Fellowship, Grant No. IHP-HPMD-CT-2001-00108

*Numerical Approaches to Protein Folding*
W. Janke (with A. Irbäck)
DAAD-STINT Collaborative Research Grant with the University of Lund, Sweden, Grant No. D/05/26016

*Quantum Monte Carlo Studies of Valence Bond Solid Transitions*
W. Janke (with B. Zheng)
DAAD Collaborative Research Grant with the Zhejiang University, Hangzhou, P.R. China, Grant No. D/05/06935

*Statistical Mechanics of Complex Networks*
W. Janke (with Z. Burda)
Alexander von Humboldt Foundation "Institutspartnerschaft" with the Jagellonian University, Krakow, Poland

*Monte Carlo Simulations of Self-Avoiding Walks on the Percolation Cluster*
V. Blavatska (Lviv, Ukraine)
Host of Alexander von Humboldt Foundation Fellowship

*Statistical Mechanics of Networks Interacting with Matter*
B. Wacław (Jagellonian University, Krakow, Poland)
Host of DAAD Fellowship

*Monte Carlo Simulationen der Statik und Dynamik von Spingläsern*
E. Bittner and W. Janke
NIC Jülich (computer time grant for "JUMP"), Grant No. hlz10

*Protein and Polymer Models*
M. Bachmann and W. Janke
NIC Jülich (computer time grant for "JUMP"), Grant No. hlz11

*Quantum Monte Carlo Simulations*
W. Janke
NIC Jülich (computer time grant for "JUMP"), Grant No. hlz12

*Quantum Monte Carlo Simulations*
S. Wenzel
Studienstiftung des deutschen Volkes

## 10.17 Organizational Duties

M. Bachmann

- Scientific Secretary of the Workshop *CompPhys07 – 8th NTZ-Workshop on Computational Physics*, ITP, Universität Leipzig, 29. November – 01. December 2007
- Scientific Secretary of the Workshop *LEILAT08 – 18th Workshop on Lattice Field Theory and Statistical Physics* ITP, Universität Leipzig, 26. – 28. June 2008
- Scientific Secretary of the Workshop *CompPhys08 – 9th NTZ-Workshop on Computational Physics*, ITP, Universität Leipzig, 27. – 29. November 2008

- Referee: Phys. Rev. Lett., J. Am. Chem. Soc., IEEE/ACM Transact. Comp. Biol. Bioinf., Phys. Rev. A, Phys. Rev. E, J. Phys. A, Eur. J. Phys. D, Biophys. Rev. Lett., Comput. Phys. Commun., J. Comput. Chem.
- Reviewer: Engineering and Physical Sciences Research Council (EPSRC), UK; National Science Foundation (NSF), USA

E. Bittner

- Scientific Secretary of the Workshop *CompPhys07 – 8th NTZ-Workshop on Computational Physics*, ITP, Universität Leipzig, 29. November – 01. December 2007
- Scientific Coordinator of the Spring School on *Monte Carlo Simulations of Disordered Systems*, ITP, Universität Leipzig, 30. March – 04. April 2008
- Scientific Secretary of the Workshop *LEILAT08 – 18th Workshop on Lattice Field Theory and Statistical Physics* ITP, Universität Leipzig, 26. – 28. June 2008
- Co-organizer of the contribution *Football Feaver* to the "Wissenschaftssommer" exhibition within the frame of the "Jahr der Mathematik", Universität Leipzig, 28. Juni – 04. July 2008
- Scientific Secretary of the Workshop *CompPhys08 – 9th NTZ-Workshop on Computational Physics*, ITP, Universität Leipzig, 27. – 29. November 2008
- Referee: Phys. Rev. Lett., Phys. Rev. E, J. Phys. A, Eur. J. Phys. B, Comput. Phys. Commun.

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 Sciences", Lecture Notes in Physics, Springer, Berlin, Heidelberg
- Editor "Computational Physics", Central European Journal of Physics
- Member of Editorial Board, Condens. Matter Phys.
- Permanent Member of "International Advisory Board", *Conference of the Middle European Cooperation in Statistical Physics (MECO)*
- Organizer of the Symposium *Finite-Size Effects at Phase Transitions* within the 71st German Physics Spring Meeting ("Physiker-Tagung") 2007 (with W. Selke, RWTH Aachen), Universität Regensburg, 27. – 28. March 2007
- Organizer of the 9th Int. Conf. *Path Integrals – New Trends and Perspectives* (with A. Pelster, Universität Duisburg-Essen) Max-Planck-Institut für Physik komplexer Systeme (MPI-PKS), Dresden, 23. – 28. September 2007
- Organizer of the Workshop *Statistical Mechanics of Complex Networks* (with P. Bialas, Z. Burda, J. Jurkiewicz, and G. Rodgers), Jagellonian University, Krakow, Poland, 02. – 04. November 2007
- Organizer of the Workshop *CompPhys07 – 8th NTZ-Workshop on Computational Physics*, ITP, Universität Leipzig, 29. November – 01. December 2007
- Organizer of the Spring School on *Monte Carlo Simulations of Disordered Systems*, ITP, Universität Leipzig, 30. March – 04. April 2008
- Organizer of the Workshop *LEILAT08 – 18th Workshop on Lattice Field Theory and*

*Statistical Physics* (with A. Schiller, ITP, TET) ITP, Universität Leipzig, 26. – 28. June 2008
- Co-organizer of the contribution *Football Feaver* to the "Wissenschaftssommer" exhibition within the frame of the "Jahr der Mathematik", Universität Leipzig, 28. Juni – 04. July 2008
- Organizer of the Workshop *CompPhys08 – 9th NTZ-Workshop on Computational Physics*, ITP, Universität Leipzig, 27. – 29. November 2008
- Organizer of the The 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34* (with S. Trimper, Martin-Luther-Universität Halle-Wittenberg), ITP, Universität Leipzig, 29. March – 01. April 2009
- Organizer of the International Conference *ENRAGE – Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*, Max-Planck-Institut für Physik komplexer Systeme in Dresden, 17. – 22. May 2009
- Member of International Organization Committee of the 10th International Conference *Path Integrals*, planned for Seoul, South Korea, August 2009
- Chair of the Review Panel: Mid-Term Evaluation of the Research Programme "Scientific Computing" of the Helmholtz-Gemeinschaft, Forschungszentrum Jülich, June 2007
- Member of the Review Panel: Mid-Term Evaluation of the Research Programme "Condensed Matter Physics, PNI and Nanoelectronics" of the Helmholtz-Gemeinschaft, Forschungszentrum Jülich, October 2007
- Member of the Review Panel of the AQAS "Akkreditierungsverfahren" of the Master Studies Curriculum "Computer Simulation in Science", Bergische Universität Wuppertal, January 2008
- Reviewer: Humboldt-Stiftung; Deutsche Forschungsgemeinschaft; Studienstiftung des deutschen Volkes; Jeffress Memorial Trust, Bank of America, Virginia, USA; "Fond zur Förderung der wissenschaftlichen Forschung (FWF)", Österreich; "The Royal Society", UK; The "Engineering and Physical Sciences Research Council (EPSRC)", UK; The University of Warwick, UK; Coventry University, UK; CECAM, Lyon, France; National Science Foundation (NSF), USA; Israel Science Foundation, Israel
- 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. R. Phys. Soc., J. Physics A, Comput. Phys. Commun., J. Stat. Mech., New J. Phys., Int. J. Mod. Phys. C

## 10.18 External Cooperations

**Academic**

- EU RTN-Network "ENRAGE" – *Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*
  research collaboration with 13 teams throughout Europe
- Deptartment 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, Prof. Dr. Malte Henkel, Dr. Dragi Karevski
- 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, England, UK
  Dr. Ralph Kenna, PD Dr. Christian von Ferber
- 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, Lund, Sweden
  Prof. Dr. Anders Irbäck, Simon Mitternacht
- John von Neumann-Institut für Computing (NIC), Forschungszentrum Jülich, Germany
  Prof. Dr. U. Hansmann, Prof. Dr. Peter Grassberger, PD Dr. Thomas Neuhaus
- Institut für Physik, Universität Mainz
  Prof. Dr. Kurt Binder, Dr. Hsiao-Ping Hsu, Dr. Martin Weigel
- 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, Germany
  Prof. Dr. Hagen Kleinert, Dr. Adriaan M.J. Schakel
- IAC-1, Universität Stuttgart, Germany
  PD Dr. Rudolf Hilfer
- Universität Duisburg-Essen, Germany
  PD Dr. Axel Pelster
- Institut für Theoretische Physik, Universität Bielefeld, Germany
  PD Dr. Thomas Neuhaus, Prof. Dr. Friderike Schmid
- Jacobs Universität Bremen, Germany
  Prof. Dr. Hildegard Meyer-Ortmanns
- Institute of Physics, Jagellonian University, Kraków, Poland
  Prof. Dr. Zdzisław Burda, Prof. Dr. Piotr Bialas, Dr. Leszek Bogacz
- 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, P.R. China
  Prof. Dr. He-Ping Ying, Prof. Dr. Bo Zheng

## 10.19 Publications

**Journals**

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

E. Bittner, A. Nußbaumer, W. Janke, M. Weigel: *Self-Affirmation Model for Football Goal Distributions*, Europhys. Lett. **78**, 58 002 (2007)

L. Bogacz, Z. Burda, W. Janke, B. Wacław: *Balls-in-Boxes Condensation on Networks*, Chaos **17**, 026 112 (2007)

L. Bogacz, Z. Burda, W. Janke, B. Wacław: *Free Zero-Range Processes on Networks*, Proc. SPIE **6601**, 66010V (2007)

K. Goede, M. Bachmann, W. Janke, M. Grundmann: *Specific Adhesion of Peptides on Semiconductor Surfaces in Experiment and Simulation*, AIP Conf. Proc. **893**, 611 (2007)

C. Junghans, M. Bachmann, W. Janke: *Thermodynamics of Peptide Aggregation Processes: An Analysis from Perspectives of Three Statistical Ensembles*, J. Chem. Phys. **128**, 085 103 (2008)

A. Kallias, M. Bachmann, W. Janke: *Thermodynamics and Kinetics of a Gō Proteinlike Heteropolymer Model with Two-State Folding Characteristics*, J. Chem. Phys. **128**, 055 102 (2008)

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, W. Janke: *Monte Carlo Study of the Droplet Formation-Dissolution Transition on Different Two-Dimensional Lattices*, Phys. Rev. E **77**, 041 109 (2008)

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)

T. Vogel, M. Bachmann, W. Janke: *Freezing and Collapse of Flexible Polymers on Regular Lattices in Three Dimensions*, Phys. Rev. E **76**, 061 803 (2007)

B. Wacław, L. Bogacz, Z. Burda, W. Janke: *Condensation in Zero-Range Processes on Inhomogeneous Networks*, Phys. Rev. E **76**, 046 114 (2007)

S. Wenzel, E. Bittner, W. Janke, A.M.J. Schakel: *Percolation of Vortices in the Abelian Lattice Higgs Model*, Nucl. Phys. B **793**, 344 (2008)

**Books**

M. Bachmann, W. Janke: *Thermodynamics of Protein Folding from Coarse-Grained Models' Perspectives*, in: *Rugged Free Energy Landscapes: Common Computational Approaches to Spin Glasses, Structural Glasses and Biological Macromolecules*, ed. by W. Janke, Lect. Notes Phys. **736** (Springer, Berlin 2008), p 203

E. Bittner, A. Nußbaumer, W. Janke: *Free-Energy Barriers of Spin Glasses*, in: *NIC Symposium 2008* , NIC Series, Vol. **39**, ed. by G. Münster, D. Wolf, M. Kremer (John von Neumann Institute for Computing, Jülich 2008), p 229

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

W. Janke: *Monte Carlo Methods in Classical Statistical Physics*, in: *Computational Many-Particle Physics*, ed. by H. Fehske, R. Schneider, A. Weiße, Lect. Notes Phys. **739** (Springer, Berlin 2008) p 79

W. Janke: *Rugged Free-Energy Landscapes – An Introduction*, in: *Rugged Free Energy Landscapes: Common Computational Approaches to Spin Glasses, Structural Glasses and Biological Macromolecules*, ed. by W. Janke, Lect. Notes Phys. **736** (Springer, Berlin 2008) p 1

W. Janke (Ed.): *Rugged Free Energy Landscapes: Common Computational Approaches to Spin Glasses, Structural Glasses and Biological Macromolecules*, Lect. Notes Phys. **736** (Springer, Berlin 2008)

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) p 123

C. Junghans, M. Bachmann, W. Janke: *Phase Separation in Peptide Aggregation Processes – Multicanonical Study of a Mesoscopic Model*, in: *From Computational Biophysics to Systems Biology (CBSB07)*, NIC Series, Vol. **36**, ed. by U.H.E. Hansmann, J. Meinke, S. Mohanty, O. Zimmermann (John von Neumann Institute for Computing, Jülich 2007) p 169

**in press**

M. Bachmann, W. Janke: *Conformational Transitions in Molecular Systems*, in: Proc. Int. Conf. *Path Integrals – New Trends and Perspectives*, ed. by W. Janke, A. Pelster (World Scientific, Singapore 2008)

M. Bachmann, W. Janke: *Minimalistic Hybrid Models for the Adsorption of Polymers and Peptides to Substrates*, Phys. Part. Nuclei (2008)

B.A. Berg, W. Janke: *Multibondic Cluster Algorithm for Finite-Size Scaling Studies of Critical Phenomena*, Comp. Phys. Commun. (2008)

B.A. Berg, W. Janke: *Wang-Landau Multibondic Cluster Approach to Simulations of Second-Order Transitions*, in: *Computer Simulations in Condensed Matter Physics XX*, ed. by D.P. Landau, S.P. Lewis, H.-B. Schüttler (Springer, Heidelberg 2008)

R. Bischof, W. Janke: *Critical Exponents of Mixed Quantum Spin Chain*, in: Proc. Int. Conf. *Path Integrals – New Trends and Perspectives*, ed. by W. Janke, A. Pelster (World Scientific, Singapore 2008)

E. Bittner, W. Janke: *Vortex-Line Percolation in a Three-Dimensional Complex $|\psi|^4$ Theory*, in: Proc. Int. Conf. *Path Integrals – New Trends and Perspectives*, ed. by W. Janke, A. Pelster (World Scientific, Singapore 2008)

V. Blavatska, W. Janke: *Scaling Behavior of Self-Avoiding Walks on Percolation Clusters*, Europhys. Lett. (2008), arXiv:0804.2988 (cond-mat.dis-nn)

V. Blavatska, W. Janke: *Self-Avoiding Walks on Fractals: Scaling Laws*, in: Proc. Int. Conf. *Path Integrals – New Trends and Perspectives*, ed. by W. Janke, A. Pelster (World Scientific, Singapore 2008)

W. Janke, A. Pelster (Eds.): *Path Integrals – New Trends and Perspectives*, Proceedings of the International Conference, MPI PKS Dresden, 23.–28. September 2007 (World Scientific, Singapore 2008)

I. Juhász Junger, D. Ihle, L. Bogacz, W. Janke: *Thermodynamics of Heisenberg Ferromagnets with Arbitrary Spin in a Magnetic Field*, Phys. Rev. **B** (2008), arXiv:0802.3395

A. Nußbaumer, E. Bittner, W. Janke: *Evaporation/Condensation of Ising Droplets*, in: Proc. Int. Conf. *Path Integrals – New Trends and Perspectives*, ed. by W. Janke, A. Pelster (World Scientific, Singapore 2008)

A. Nußbaumer, E. Bittner, T. Neuhaus, W. Janke: *Universality of the Evaporation/ Condensation Transition*, in: *Computer Simulations in Condensed Matter Physics XX*, ed. by D.P. Landau, S.P. Lewis, H.-B. Schüttler (Springer, Heidelberg 2008)

J. Schluttig, M. Bachmann, W. Janke: *Comparative Molecular Dynamics and Monte Carlo Study of Statistical Properties for Coarse-Grained Heteropolymers*, J. Comp. Chem. (2008)

B. Wacław, L. Bogacz, Z. Burda, W. Janke: *Monte Carlo Methods for Generation of Random Graphs*, in: Proc. Int. Conf. *Path Integrals – New Trends and Perspectives*, ed. by W. Janke, A. Pelster (World Scientific, Singapore 2008)

B. Wacław, Z. Burda: *Counting Metastable States of Ising Spin Glasses on Arbitrary Graphs*, Phys. Rev. E (2008)

F.T. Winter, W. Janke, A.M.J. Schakel: *Geometric Properties of the Three-Dimensional Ising and XY Models*, Phys. Rev. E (2008)

**Talks**

M. Bachmann: *Intrinsic Structural Properties of Mesoscopic Models for Protein Folding and Aggregation*, 71st DPG Spring Meeting, Regensburg, 26. – 30. March 2007

M. Bachmann: *Specific Polymer and Peptide Adsorption to Attractive Solid Substrates*, CECAM Workshop "Modelling the Interaction of Biomolecules with Inorganic Surfaces", Lyon, France, 25. – 27. July 2007

M. Bachmann: *Specific Polymer and Peptide Adsorption to Attractive Solid Substrates*, Mini-Symposium "Adsorption Properties of Polymers and Proteins", Lund, Sweden, 07. March 2007

M. Bachmann: *Specific Polymer and Peptide Adsorption to Attractive Solid Substrates*, Seminar talk, Institut für Theoretische Physik, Martin-Luther-Universität Halle-Wittenberg, 24. January 2007

M. Bachmann: *Statistical Conformation Mechanics of Protein Folding, Aggregation, and Adsorption Transitions*, 9th Int. Conf. "Path Integrals – New Trends and Perspectives PI07", Dresden, 23. – 28. September 2007

E. Bittner: *Complex Eigenvalues of the Dirac Operator in Two-Color QCD with Chemical Potential*, "ENRAGE" Network School on Random Matrices and Random Geometry, Barcelona, Spain, 16. – 20. April 2007

E. Bittner: *Evaporation/Condensation Transition of Ising Droplets*, Seminar talk, Institut für Theoretische Physik (B), RWTH Aachen, 06. November 2007

E. Bittner: *Vortex-Line Percolation in a Three-Dimensional Complex $|\psi|^4$ Theory*, 9th Int. Conf. "Path Integrals – New Trends and Perspectives PI07", Dresden, 23. – 28. September 2007

M. Hasenbusch: *The Critical Behavior of 3D Ising Glass Models: Universality and Scaling Corrections*, 8th Int. NTZ-Workshop "New Developments in Computational Physics – CompPhys07", Universität Leipzig, 29. November – 01. December 2007

W. Janke: *Adsorption Phenomena at Hybrid Organic–Inorganic Interfaces*, invited talk, SFB 418 International Workshop *Soft meets Hard*, Lutherstadt Wittenberg, 13. – 15. September 2007

W. Janke: *Droplet Evaporation/Condensation Transition*, FOR 877 Workshop, Universität Leipzig, 27. November 2007

W. Janke: *Exploring Free-Energy Landscapes of Peptide Folding and Aggregation*, invited talk, Atelier Nancy *Statistical Physics and Low Dimensional Systems 2007*, Université Nancy, France, 23. – 25. May 2007

W. Janke: *Exploring Free-Energy Landscapes of Peptide Folding and Aggregation*, invited talk, EMBIO Workshop 2007, Interdisziplinäres Zentrum für Bioinformatik (IZBI), Universität Leipzig, 17. – 19. May 2007

W. Janke: *Finite-Size Adapted Wang-Landau/Multibondic Cluster Simulations for Second-Order Phase Transitions*, Symposium *Finite-Size Effects*, 71st DPG Spring Meeting, Regensburg, 26. – 30. March 2007

W. Janke: *Geometrical Picture of Criticality*, Physics Seminar, Complex Systems Division, Lund University, Sweden, 02. February 2007

W. Janke: *Geometrical Picture of Phase Transitions*, Physics Seminar, School of Engineering and Science, Jacobs University Bremen, 07. May 2007

W. Janke: *Microcanonical Analyses of Peptide Aggregation Processes*, CBSB Workshop 2007, NIC, Forschungszentrum Jülich, 02. – 04. May 2007

W. Janke: *Microcanonical Analyses of Peptide Aggregation Processes*, invited talk, CECAM Workshop *Modelling the Interaction of Biomolecules with Inorganic Surfaces*, ENS Lyon, France, 25. – 27. July 2007

W. Janke: *Modeling and Simulation of Biological Macromolecules*, Physikalisches Kolloquium, Technische Universität Chemnitz, 13. June 2007

W. Janke: *Modeling and Simulation of Biological Macromolecules*, Theorie-Kolloquium, Martin-Luther-Universität Halle-Wittenberg, 27. June 2007

W. Janke: *Multibondic Cluster Algorithm for Finite-Size Scaling Studies of Second-Order Phase Transitions*, CCP2007 – Conference on Computational Physics, Brussels, Belgium, 05. – 08. September 2007

W. Janke: *Nano-Structured Channels: Computer Simulations and Finite-Size Scaling*, Workshop, Universität Leipzig, 05. April 2007

W. Janke: *Spin Clusters and Loop Gases on Random Graphs*, ANet07 Conference, Jagellonian University, Krakow, Poland, 02. – 04. November 2007

W. Janke: *The LEIPZIG Team*, EU Network ENRAGE Midterm Review Meeting, Utrecht, The Netherlands, 06. September 2007

W. Janke: *Universal Aspects of Evaporation/Condensation Transition*, Physik-Kolloquium, Technische Universität Ilmenau, 03. July 2007

W. Janke: *Universality of Evaporation/Condensation Transition*, invited talk, 20th Ann. Workshop, University of Georgia, Athens, USA, 19. – 23. February 2007

A. Nußbaumer: *Football Fever: Goal Distributions in Football*, 71st DPG Spring Meeting, Regensburg, 26. – 30. March 2007

S. Schnabel: *Impact of Peptide Structure on Semiconductor Binding*, 71st DPG Spring Meeting, Regensburg, 26. – 30. March 2007

S. Schnabel: *Multicanonical Simulation of a Coarse Grained Heteropolymer Model*, Seminar talk, Deutsch-Französische Hochschule (Collège Doctoral), Université Henri Poincaré Nancy, France, 22. October 2007

S. Schnabel: *Multicanonical Simulation of a Coarse Grained Heteropolymer Model*, Seminar talk, Institut für Theoretische Physik, Universität Kassel, 11. July 2007

T. Vogel: *Freezing and Collapse of Flexible Polymers*, 8th Int. NTZ-Workshop "New Developments in Computational Physics – CompPhys07", Universität Leipzig, 29. November – 01. December 2007

B. Wacław: *Balls-in-Boxes Models on Networks*, ANet07 Conference, Jagellonian University, Krakow, Poland, 02. – 04. November

B. Wacław: *Multicanonical Simulations of Complex Networks*, 8th Int. NTZ-Workshop "New Developments in Computational Physics – CompPhys07", Universität Leipzig, 29. November – 01. December 2007

S. Wenzel: *Finite-Size Scaling of Quantum Phase Transitions in 2d Heisenberg Models*, Seminar talk, Deutsch-Französische Hochschule (Collège Doctoral), Université Henri Poincaré Nancy, France, 17. September 2007

S. Wenzel: *On the Phase Structure of 3D Abelian One-Higgs Model on the Lattice*, 8th Int. NTZ-Workshop "New Developments in Computational Physics – CompPhys07", Universität Leipzig, 29. November – 01. December 2007

**Posters**

M. Bachmann, C. Junghans, W. Janke: *Microcanonical Analysis of Polymer Aggregation*, Workshop on "Computer Simulations of Soft Matter and Biosystems", Heidelberg, 14. – 16. March 2007

E. Bittner, W. Janke: *Boundary Field Induced First-Order Transition in the 2D Ising Model: Numerical Study*, 71st DPG Spring Meeting, Regensburg, 26. – 30. March 2007

E. Bittner, A. Nußbaumer, W. Janke: *Replica-Exchange Cluster Algorithm*, 8th Int. NTZ-Workshop "New Developments in Computational Physics – CompPhys07", Universität Leipzig, 29. November – 01. December 2007

E. Bittner, A. Nußbaumer, W. Janke: *Replica-Exchange Cluster Algorithm*, CCP2007 – Conference on Computational Physics, Brussels, Belgium, 05. – 08. September 2007

E. Bittner, A. Nußbaumer, W. Janke: *The Evaporation/Condensation Transition of Ising Droplets*, XXIII Int. Conf. Statistical Physics of the Int. Union for Pure and Applied Physics (IUPAP) – Statphys 23, Genova, Italy, 09. – 13. July 2007

V. Blavatska, W. Janke: *Multifractal Properties of Self-Avoiding Walks Percolation Clusters*, 8th Int. NTZ-Workshop "New Developments in Computational Physics – CompPhys07", Universität Leipzig, 29. November – 01. December 2007

V. Blavatska, W. Janke: *Self-Avoiding Walks on Fractals: Scaling Laws*, 9th Int. Conf. "Path Integrals – New Trends and Perspectives PI07", Dresden, 23. – 28. September 2007

A. Nußbaumer, E. Bittner, W. Janke: *Evaporation/Condensation of Ising Droplets*, 8th Int. NTZ-Workshop "New Developments in Computational Physics – CompPhys07", Universität Leipzig, 29. November – 01. December 2007

A. Nußbaumer, E. Bittner, W. Janke: *Evaporation/Condensation of Ising Droplets*, 9th Int. Conf. "Path Integrals – New Trends and Perspectives PI07", Dresden, 23. – 28. September 2007

A. Nußbaumer, E. Bittner, W. Janke: *Evaporation/Condensation Transition on Different Ising Lattices*, CCP2007 – Conference on Computational Physics, Brussels, Belgium, 05. – 08. September 2007

S. Schnabel, S. Mitternacht, A. Irbäck, M. Bachmann, W. Janke: *Solution Behavior of Semiconductor-Binding Peptides*, 71st DPG Spring Meeting, Regensburg, 26. – 30. March 2007

T. Vogel, M. Bachmann, W. Janke: *Collapse and Freezing Transitions of Polymers on Regular Lattices*, 71st DPG Spring Meeting, Regensburg, 26. – 30. March 2007

T. Vogel, M. Bachmann, W. Janke: *Collapse and Freezing Transitions of Polymers on Regular Lattices*, CECAM Tutorial *Programming Parallel Computers*, Forschungszentrum Jülich, 22. – 26. January 2007

S. Wenzel, E. Bittner, A.M.J. Schakel, W. Janke: *Percolation of Vortex Networks in the $U(1)$ Lattice Higgs Model*, 71st DPG Spring Meeting, Regensburg, 26. – 30. March 2007

## 10.20 Guests

- Dr. Meik Hellmund
  Mathematisches Institut, Universität Leipzig, Germany
  26. April 2007

- Prof. Dr. Bernd Berg
  Florida State University, Tallahassee, USA
  14. – 16. June 2007
- Prof. Dr. Ramon Villanova
  Universitat Pompeu Fabra, Barcelona, Spain
  21. – 26. June 2007
- Prof. Dr. Rainer Klages
  School of Mathematical Sciences, Queen Mary, University of London, UK
  26. – 27. June 2007
- Prof. Dr. Bernhard Mehlig
  Göteborg University, Sweden
  28. – 29. June 2007
- Jean-Charles Walter
  Université Nancy, France
  October – December 2007
- Prof. Dr. Wolfgang Paul
  Institut für Physik, Universität Mainz, Germany
  07. – 09. November 2007
- Oleksandr Kapikranian
  Université Nancy, France
  October – November 2007
- Thierry Platini
  Université Nancy, France
  October – December 2007
- Prof. Dr. Joan Adler
  Technion, Haifa, Israel
  27. November – 02. December 2007
- Prof. Dr. Piotr Bialas
  Jagellonian University, Krakow, Poland
  09. – 15. December 2007