11

Computational Quantum Field Theory

11.1 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, biologically motivated problems such as protein folding, aggregation and adhesion as well as related properties of semiflexible polymers, and the intriguing physics of low-dimensional quantum spin systems. 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 a European RTN Network collaboration of 13 teams, and the statistical mechanics of complex networks is studied in collaboration with our partner university in Krakow, Poland.

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 is likely to become the third cornerstone 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 quite powerful compute servers, at the parallel computers of the University computing center, and, upon successful grant application at the national supercomputing centres in Jülich and München on IBM and Hitachi parallel supercomputers. This hierarchy 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 closely integrated into the Graduate School "BuildMoNa": Leipzig School of Natural Sciences – *Building with Molecules and Nano-objects* funded by the German Research Foundation (DFG) within the German Excellence Initiative and the international DFH-UFA Graduate School "Statistical Physics of Complex Systems" with the l'Université Henri Poincaré Nancy, France, supported by the Deutsch-Französische Hochschule. The two Graduate Schools are both "Classes" of the Research Academy Leipzig (RAL), providing the organizational frame for hosting visiting students, offering language courses and for many other practical matters. At the post-graduate level our research projects are embedded into the "Sächsische DFG-Forschergruppe" FOR 877 *From Local Constraints to Macroscopic Transport* and into two of the priority research areas ("Profilbildende Forschungsbereiche (PbF)") and the Centre for Theoretical Sciences (NTZ) of the University. In particular the latter structures are instrumental for our cooperations with research groups in experimental physics and biochemistry.

On an international scale, our research projets are carried out in a wide net of collaborations funded by the German Academic Exchange Service (DAAD), the Alexander-von-Humboldt Foundation though an Institute Partnership with the Jagellonian University in Krakow, Poland, as well as their Fellowship Programme, and the European Commission through the RTN Network "ENRAGE": *Random Geometry and Random Matrices: From Quantum Gravity to Econophysics* and the Incoming Fellowship Programme. In 2008 and a few years to come, our group is hosting Humboldt Research Prize Winner Professor Bernd A. Berg from Florida State University, Tallahassee, USA. Further close contacts and collaborations are also established with research groups in Armenia, Austria, China, France, Great Britain, Israel, Italy, Japan, Poland, Russia, Spain, Sweden, Taiwan, Turkey, Ukraine, and the United States. These contacts are refreshed and furthered through our international Workshop series CompPhys: "New Developments in Computational Physics", taking annually place at the end of November.

Wolfhard Janke

11.2 Free-Energy Barriers of Spin Glasses

A. Nußbaumer, E. Bittner, M. Aust, F. Beyer, W. Janke

In statistical physics there is an on-going debate about the nature of the low-temperature phase of finite-dimensional spin-glass systems. The most prominent theses in the field are the replica symmetry-breaking theory and the phenomenological droplet picture (for some reviews see [1–4]).

Like in the thermodynamic limit of the mean-field spin glass, the frozen phase of a finite system shows an complicated corrugated structure. As a consequence of the disorder and frustration characterising spin glasses in general, there is a rugged free-energy landscape with probable regions and rare event-states. Consequently, conventional Monte Carlo simulations tend to get stuck in local free energy valleys.

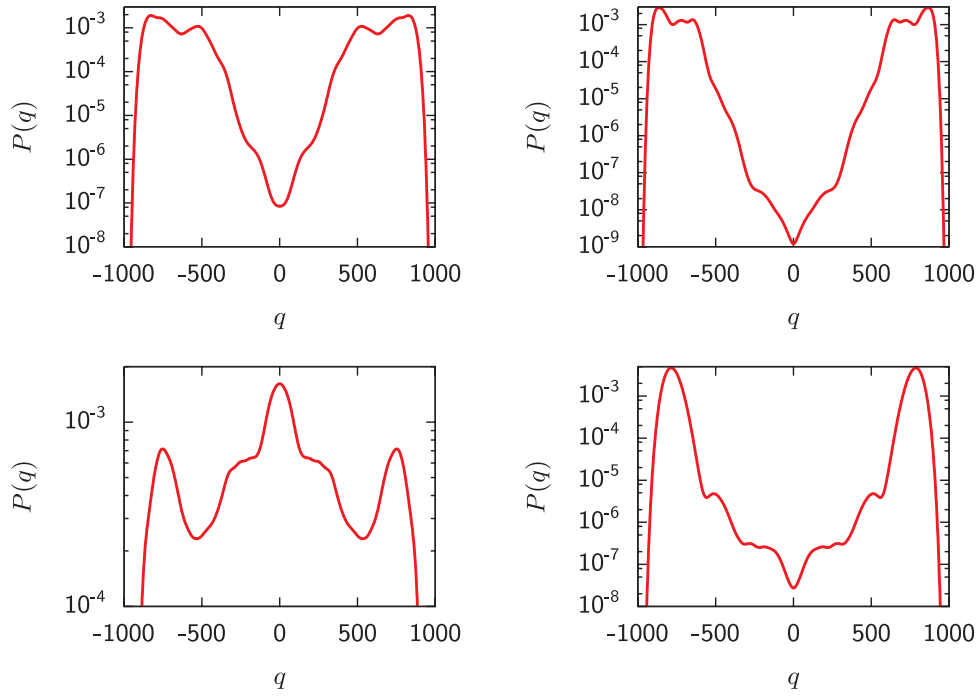

Figure 11.1: Distribution functions $P(q)$ of the Edwards-Anderson Ising model for four different disorder realisations on a $V = 10^3$ lattice in the low-temperature phase. While three realisations have a valley at $q = 0$, one realisation has its maximum at that point.

The project tries to solve this kind of problems using a novel, combined algorithm making use of the parallel tempering method [5] and the multioverlap Monte Carlo algorithm [6]. Large scale simulations on our local computer cluster as well as on the "JUMP" super-computer in Jülich have been performed for the Sherrington–Kirkpatrick mean-field model [7] and the Edwards-Anderson Ising model [8].

The typical outcome for different disorder realisations is shown in Fig. 11.1. To get "physical" results, several thousand different realisations must be averaged, making the vast amount of computer time needed understandable. Parts of our results can be found in [9].

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11.3 Fractals Meet Fractals: Multicritical Behavior of Self-Avoiding Walks on Percolation Clusters

V. Blavatska, W. Janke

It is well established that the scaling properties of long flexible polymer chains are perfectly described within the model of a self-avoiding walk (SAW) on a *regular* lattice [1]. In particular, for the average squared end-to-end distance R^2 and the number of all possible trajectories Z_N of a SAW with N steps on a regular lattice one finds in the asymptotic limit $N \to \infty$:

$$\langle R^2 \rangle \sim N^{2\nu_{\rm SAW}} , \qquad Z_N \sim z^N N^{\gamma_{\rm SAW}-1} , \tag{11.1}$$

where $\nu_{\rm SAW}$ and $\gamma_{\rm SAW}$ are universal exponents that only depend on the space dimensionality d. The properties of a SAW on a regular lattice have been studied in detail, and the values of the universal exponents in (11.1) are known by now with high precision from experiments, computer simulations and theory.

One question of great interest is the influence of structural disorder on the universal properties of a SAW, namely: does the scaling (11.1) hold with modified exponents $\nu^{p_c}_{\rm SAW}$ and $\gamma^{p_c}_{\rm SAW}$ when a SAW resides on a structurally *disordered* (diluted) lattice? The question of how do linear polymers behave in disordered media is not only of academic interest, but is also relevant for understanding transport properties of polymer chains in porous media, such as enhanced oil recovery, gel electrophoresis, gel permeation chromatography, etc. In the present project, we were interested in the special case when the disordered lattice is exactly at the percolation threshold p_c. Here, the SAW is allowed to have its steps only on the percolation clusters.

For simulating SAWs on percolative lattices, we used the pruned-enriched Rosenbluth method (PERM) [2]. Estimates for the critical exponents $\nu^{p_c}_{\rm SAW}$ were obtained by linear least-square fitting. Since we can construct only lattices with a finite linear size L, the scaling laws (11.1) only hold up to some "marginal" number of SAW steps $N_{\rm marg} \sim L^{1/\nu^{p_c}_{\rm SAW}}$. We take this into account when estimating the critical exponents by the linear least-square fitting. The thus obtained values of $\nu^{p_c}_{\rm SAW}$ for $d = 2, 3, 4$ are larger than the corresponding exponents on the pure lattice [3]; presence of disorder leads to stretching of the trajectory of self-avoiding walks. In addition we have also obtained numerical estimates for the exponents $\gamma^{p_c}_{\rm SAW}$ [4, 5].

Both a SAW and a percolation cluster are among the most frequently encountered examples of fractals in condensed matter physics. If two such fractals "meet", multifractal behavior may show up. Following early ideas [6], it was only recently proven in field-theoretical studies [7] that the exponent $\nu^{p_c}_{\rm SAW}$ alone is indeed not sufficient to completely describe the peculiarities of SAWs on percolation clusters. Instead, a whole spectrum $\nu^{(q)}$ of multifractal exponents emerges. Our numerical values for the exponents $\nu^{(q)}$ as a function of q appear to be in an astonishingly perfect agreement with analytical estimates derived from $\varepsilon = 6 - d$ expansions down to $d = 2$ dimensions [8]. The properties of the associated spectral function have been analyzed as well.

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11.4 Critical Properties of High-Temperature XY Graphs

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Based on his space-time approach to quantum mechanics, Feynman [1] developed a profound original picture of Bose–Einstein condensation. In this picture, all the particles in the system execute a random walk in space during the imaginary time interval $\hbar\beta$ ($\hbar$ is Planck's constant and β denotes the inverse temperature). Starting and ending at the same point in space, these particle trajectories form loops. At high temperatures, the individual loops hardly overlap. However, upon lowering the temperature, individual particle trajectories start to overlap and hook up to form longer loops. A particle in such a composite loop moves in imaginary time along a trajectory that does not end at its own starting position, but at that of another particle. Whence, although the initial and final configurations are identical, the participating particles are cyclically permuted. They thereby loose their identity and become indistinguishable. Loops involving, say, w particles wrap the imaginary time axis exactly w times. Upon approaching the condensation temperature from above, loops with arbitrary large winding number appear and signal the formation of a Bose–Einstein condensate.

Bose–Einstein condensation in a dilute uniform Bose gas belongs to the family of critical phenomena described by the XY model which, for computational purposes, can be conveniently formulated on the lattice. The model can then, for example, be represented by graphs on the lattice. In this so-called high-temperature approach, the partition function and correlation functions are calculated by counting graphs on the lattice, with each graph representing a certain contribution. The high-temperature graphs of the XY model physically represent the spatial projections of the particle trajectories of the Bose gas.

By simulating the high-temperature graphs on a cubic lattice (see Fig. 11.2) and using observables originally introduced in the context of percolation theory, we studied the critical properties of the XY model in purely geometrical terms [2]. We determined the fractal dimension of the graphs at the critical point to be $D = 1.7626(66)$, and showed that the diverging length scale characterizing the high-temperature graphs close to the critical point coincides with the thermal correlation length. The value of the fractal dimension of the XY high-temperature graphs is between that of a self-avoiding walk, for which $D = 1.7001(32)$, and that of a Brownian random walk, for which $D = 2$.

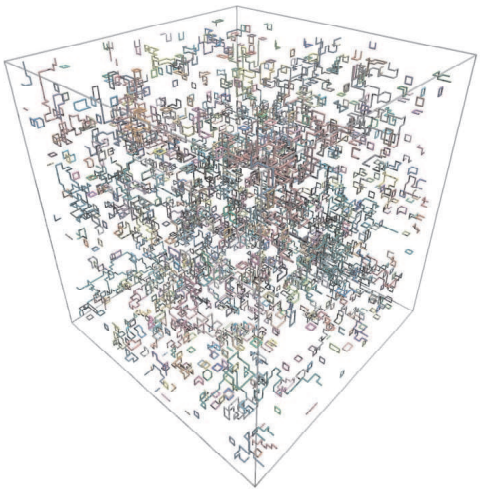

Figure 11.2: Typical high-temperature graphs on a cubic lattice at the temperature where, on average, a single graph spans the lattice.

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11.5 Complex Networks and Non-Equilibrium Systems

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Complex networks [1] are a relatively new branch of physics. An enormous growth of this discipline was triggered by observing in the 90s that many networks like the Internet, the WWW, and social or biological networks display a complex structure which places them between purely random graphs and regular grids. Many models explaining their features have been proposed. However, most of them are solvable only in thermodynamic limit. We study the convergence towards limiting properties for different networks, both analytically and numerically.

We focus mainly on so-called equilibrated networks, that is graphs being maximally random under given constraints, e.g., fixed number of nodes and given degree distribution. Because typical sizes of real-world networks range from $N \sim 10^2$ (small transportation networks) to $N \sim 10^9$ (the WWW), finite-size effects are much stronger than in "classical" systems composed of atoms and particles ($N \sim 10^{23}$). For example, in scale-free networks where the degree distribution $\pi(k) \sim k^{-\gamma}$ has a power-law behavior, due to the finite size N, the distribution $\pi(k)$ decreases rapidly above some k_{cutoff}. The cutoff k_{cutoff} scales as some power α of N. This effect influences many processes like percolation or disease spreading on networks. We discovered that the scaling predicted for very large networks is approached very slowly (sometimes with a logarithmic correction) and is far from being true even for $N = 10^9$ [2]. In contrast, the scaling of the maximal degree $k_{\max} \sim N^{\alpha'}$ is reached much faster and, in general, $\alpha' \neq \alpha$.

Many network models cannot be solved analytically for finite N and one has to turn to Monte Carlo (MC) simulations. We developed a program [3] which generates various kinds of equilibrated networks by MC sampling. Written originally in C, the software has been rewritten in C++ in an object-oriented way and evolved into a library that can be linked to any other program [4].

Our second activity are driven diffusive systems. They are simple models of non-equilibrium systems of particles hopping between sites of a lattice, or more generally, of an arbitrary graph or network. Under certain conditions, such models exhibit condensation of particles – a single site takes an extensive number of particles. Motivated by our previous experience with zero-range processes on networks [5, 6], we study models which have pair-factorized steady states (PFSS). This means that the probability of having a certain configuration of particles factorizes over the pairs of nodes [7]. This is equivalent to an equilibrium model called SOS model [8]. The PFSS allows one to study how node–node interactions influence the condensation. We found that in one dimension the condensate, if it exists, is usually spatially extended to $W \sim N^{\alpha}$ sites, with α depending on the functional form of the hopping rate. We also calculated the envelope of the condensate [9]. We are currently studying the model in higher dimensions, its generalization to random graphs and the factorization over more complicated motifs (triangles, plaquettes, etc.).

This work is partially supported by an Institute Partnership grant "Krakow–Leipzig" (http://www.physik.uni-leipzig.de/~waclaw/AvH) of the Alexander-von-Humboldt Foundation and the EU-Network "ENRAGE".

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11.6 Thickness-Dependent Secondary-Structure Formation of Tubelike Polymers

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By means of computer simulations we studied the thermodynamical behaviour of tube models for simple homopolymers as well as for exemplified hydrophobic-polar heteropolymers [1, 2]. The thickness of the tube in our simulations is controlled by a single parameter, the global radius of curvature, which depends on three-body interactions [3].

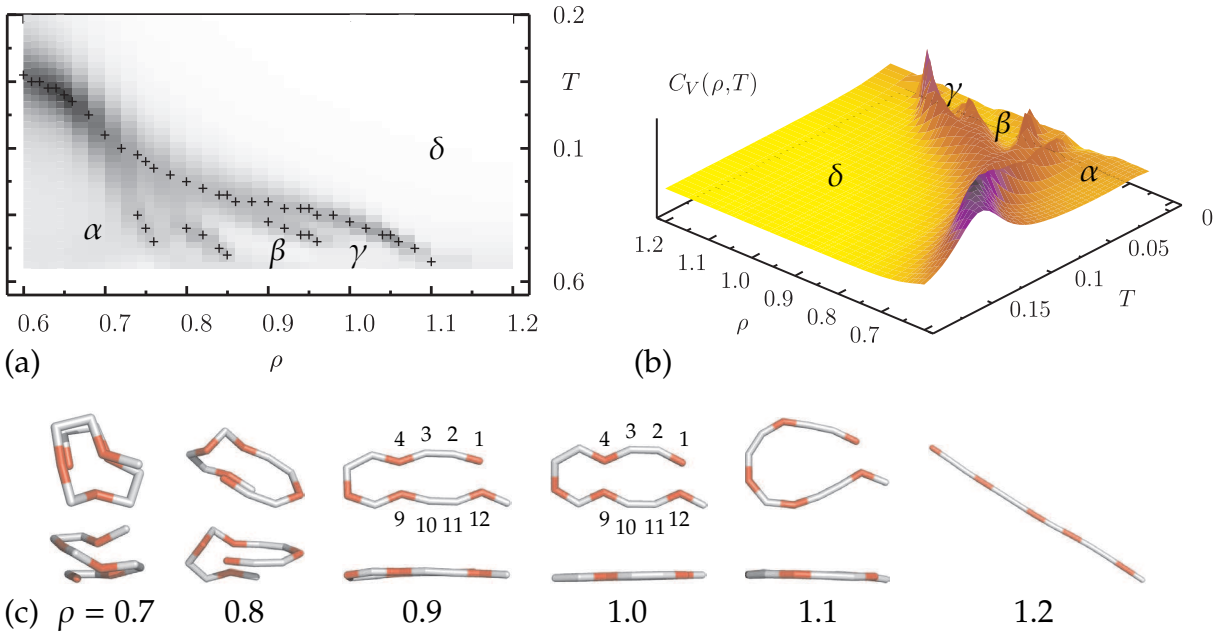

Figure 11.3: Pseudophase diagram and ground-state conformations of the $N = 13$ Fibonacci AB heteropolymer. (**a**) The plot shows the top-view with marked peak positions of the specific heat for various thickness parameters ρ, (**b**) the qualitative view of the specific-heat landscape. The pictures in (**c**) illustrate selected ground-state conformations. Conformations are shown from different viewpoints, "A" monomers are marked by red color (dark gray), "B" monomers are white.

After focusing on ground states of homopolymers and their properties in a preceding step [4], we identified dominant structural pseudophases at finite temperatures, i.e., specific-heat landscapes depending on the thickness parameter ρ and temperature T, representing the conformational phase diagram. Independently of the polymer length, we find four major structural phases. These include helices (α), sheetlike planar structures (β), bended rings (γ) and sprawled random coils (δ). These different secondary structure phases can be assigned to different ranges of the tube thickness. The thickness parameter is therefore suitable for a classification of the structural behaviour of classes of polymers.

Particularly, we introduced the AB tube model for hydrophobic-polar heteropolymers and obtained results for specific sequences of monomers (see Fig. 11.3), which has extensively been studied before without thickness [5]. We showed that a specific monomer sequence can stabilize the general secondary structures. We find, for example, a very pronounced and stable region of β-sheet structures. We further showed that the additional introduction of a bending stiffness plays a subordinate role. This observation is necessary to relate our general results to existing results of special systems. We could in particular reproduce simulational results published within the past years for polymer models without explicit thickness as limiting case of our our study [2].

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11.7 Low-Temperature Behaviour of Elastic Lennard-Jones Polymers

S. Schnabel, M. Bachmann, W. Janke

We developed and applied sophisticated Monte Carlo computer simulation methods to investigate the low-temperature behaviour of an off-lattice model for flexible elastic homopolymers. In this model beads interact via truncated Lennard-Jones potentials and adjacent beads are additionally bonded by a FENE bond potential [1]. Special interest laid on so-called solid-solid transitions, which became accessible by the introduction of a new order parameter that refers to Platonic, Archemedean, and Johnson solids.

Considering the ground-state structures of homopolymers of different sizes, it soon turned out that the obtained structures show wide similarities to low-energy conformations of atomic Lennard-Jones clusters. We mainly found icosahedral structures (see Fig. 11.4) with Mackay or anti-Mackay overlayers [2] and were able to document transitions between both types [3].

As it is well known from former research on Lennard-Jones clusters [4], non-icosahedral structures might play an important role at low temperatures. However, due to the complex shape of the state space it is difficult to identify such structures with standard Monte Carlo methods. Therefore, we divided the conformational space by classifying all structures with respect to the occurrence of icosahedral cells. We then modified the scheme of multicanonical Monte Carlo sampling and applied different weight functions for different classes of conformations. In consequence, we were able to overcome the broken-ergodicity problem and to investigate the solid-solid transitions between structures of icosahedral and non-icosahedral type at extreme low temperatures [5].

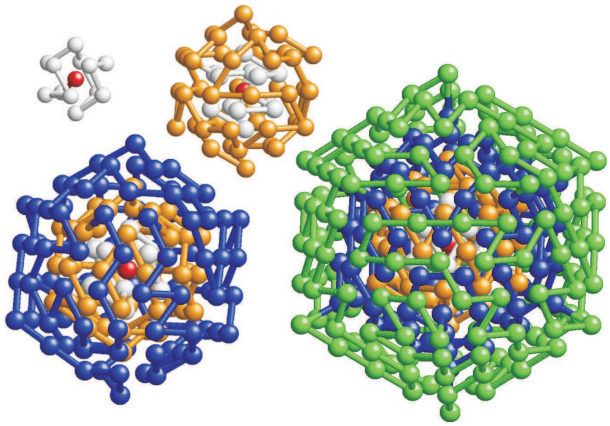

Figure 11.4: Ground-state conformations for homopolymers of "magic" sizes (N = 13, 55, 147, 309) that form complete icosahedra. Due to the high symmetry and the almost spherical shape, these structures are of high stability and dominate the low-temperature behaviour of these polymers.

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11.8 Statistical Mechanics of Aggregation and Crystallization for Semiflexible Polymers

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Cluster formation and crystallization of polymers are processes which are interesting for technological applications, e.g., as new materials with certain mechanical properties or nanoelectronic organic devices and polymeric solar cells. From a biophysical point of view, the understanding of (de)fragmentation in semiflexible biopolymer systems like actin networks and also peptide oligomerization is of substantial relevance. This requires a systematic analysis of polymeric cluster formation processes, in particular, for small polymer complexes on the nanoscale, where surface effects are competing noticeably with structure-formation processes in the interior of the aggregate.

By means of multicanonical computer simulations, we have investigated thermodynamic properties of the aggregation of interacting semiflexible polymers. We analyzed a mesoscopic bead–stick model, where nonbonded monomers interact via van der Waals forces. The aggregation of semiflexible polymers turns out to be a process, in which the constituents experience strong structural fluctuations [1], similar to peptides in coupled folding-binding cluster formation processes. In contrast to a recently studied related proteinlike hydrophobic-polar heteropolymer model [2, 3], aggregation and crystallization are separate processes here. However, in analogy to the heteropolymer study, we find that the first-order-like aggregation transition of the complexes is accompanied by strong system-size dependent hierarchical surface effects. These are called backbending effects, because the caloric (or microcanonical) temperature decreases with increasing energy. This is a direct consequence of the fact that the aggregation of polymers is a phase-separation process with entropy reduction [4].

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11.9 Conformational Mechanics of Polymer Adsorption Transitions at Attractive Substrates

M. Möddel, M. Bachmann, W. Janke

We used thermal fluctuations of energetic and structural quantities obtained by multicanonical computer simulations to identify a variety of pseudophases of a semiflexible

off-lattice homopolymer near an attractive substrate. Introducing a solvent parameter ϵ_s, that is related to the strength of the surface attraction, the solubility-temperature phase diagram is constructed and discussed (Fig. 11.5) [1].

Although the computational expense for an accurate exploration of such a broad parameter range restricted us to investigate rather short chains, we identified the following conformational pseudophases and pseudophase transitions:

- Crystalline structures in the regimes of compact phases: We identified maximally compact desorbed conformations in bulk (DC) or adsorbed at the substrate (AC), semi-spherical compact conformations (AC2a) that are distorted by the surface but not layered, double-layer conformations (AC2b), and single-layer conformations (AC1).

- Adsorbed conformations in the globular and expanded (random-coil) phases: Here, three conformational pseudophases were distinguished: unstructured 3D surface-attached globular conformations (AG), expanded dissolved but planar adsorbed conformations (AE1), and 3D expanded random-coil-like adsorbed conformations (AE2).

- Desorbed conformations: Compact conformations (DC) are separated by the freezing transition from globular conformations (DG). At even higher temperatures above the well known θ-transition, random-coil conformations are found (DE).

These results are in nice quantitative coincidence with recent lattice results [2] which demonstrates the ability of such coarse-grained models to capture the general adsorption behavior of polymers near attractive surfaces.

With the density of states, estimated in the multicanonical recursion, we then performed a microcanonical analyses that focused on the adsorption transition, where a convex intruder of the microcanonical entropy can be observed for short chains. A typical signal for a phase separation process. This, however, vanishes for increasing chain lengths and decreasing surface attraction.

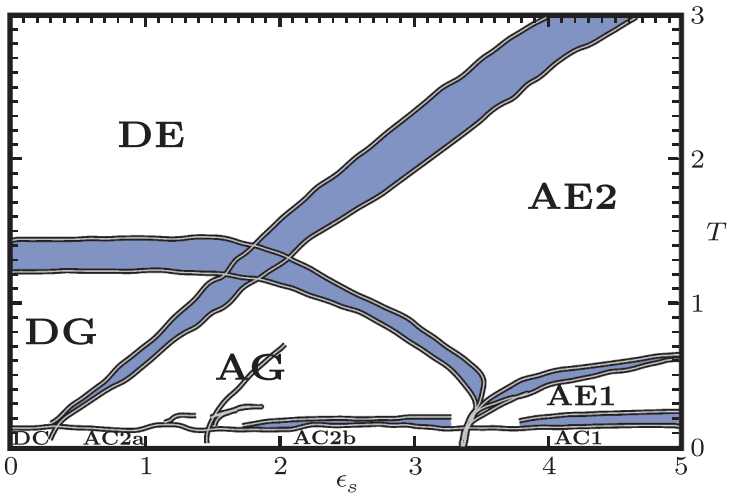

Figure 11.5: Phase diagram of the 20mer. The colored stripes separate the individual conformational phases described in the text.

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11.10 Microscopic Mechanism of Specific Peptide Adhesion to Semiconductor Substrates

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In the past few years, the interest in hybrid interfaces formed by "soft" molecular matter and "hard" solid substrates has rapidly grown as such systems promise to be relatively easily accessible candidates for novel biosensors or electronic devices. The enormous progress in high-resolution microscopy and in biochemical engineering of macromolecules is the major prerequisite for studies of hybrid systems and potential applications [1]. One particularly important problem is the self-assembly and adhesion of polymers, proteins, or protein-like synthetic peptides to solid materials such as, e.g., metals [2] and semiconductors [3–5]. Peptide and substrate-specific binding affinity is particularly relevant in pattern recognition processes [6]. Basic theoretical considerations of simplified polymer–substrate and protein–substrate models have predicted complex pseudophase diagrams [7, 8].

In bacteriophage display experiments, only a few peptides out of a library of 10^9 investigated sequences with 12 amino acid residues were found to possess a particularly strong propensity to adhere to (100) gallium-arsenide (GaAs) surfaces [3]. The sequence-specificity of adsorption strength is a remarkable property, but the question remains how it is related to the individual molecular structure of the peptides. We expect that *relevant* mutations of sites in the amino-acid sequence can cause a change of the binding affinity. Indeed, one key aspect of our study is to provide evidence that proline is a potential candidate for switching the adsorption propensities to cleaned (100) silicon (Si) substrates.

In this project, we show by means of experimental and computational analyses that the adsorption properties of mutated synthetic peptides at semiconductors exhibit a clear sequence-dependent adhesion specificity. Our simulations of a novel hybrid peptide-substrate model reveal the correspondence between proline mutation and binding affinity to a clean silicon substrate. After synthesizing the theoretically suggested amino-acid sequences with different binding behaviour, we could confirm the relevance of the selective mutations upon adhesion in our subsequent atomic force microscopy experiments [9].

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11.11 Quantum Critical Phenomena in Uniform and Mixed Heisenberg Spin Chains

R. Bischof, W. Janke

By means of quantum Monte Carlo (QMC) simulations (continuous imaginary time loop algorithm) [1] and quantum reweighting methods [2] we investigate quantum critical phenomena and low-temperature properties of various versions of the 1D quantum Heisenberg model, which is one of the most fundamental models of quantum magnetism and is related to high-temperature superconductors [3]. Furthermore it exhibits various zero-temperature quantum critical phenomena, depending on the specific choice of spins and different types of coupling mechanisms. Specifically, we have investigated the uniform $S = 1/2$ Heisenberg spin chain with bond alternation and alternating quantum chains of mixed spins, consisting of two different kinds of spin, S_a and S_b, that appear alternatingly in pairs [4].

The low-temperature properties of quantum spin chains depend significantly on the size of spins involved. Uniform chains of half-odd integer spins have no energy gap between the ground state and first excited states (i.e., they are quantum critical), whereas chains with integer spins do show an excitation gap [5]. Above that, spin chains can be driven to and away from criticality by tuning appropriate parameters (such as bond alternation, exchange anisotropy, next-nearest-neighbour interaction, spin–phonon coupling, etc.). While there exists wide literature about quantum critical phenomena in uniform chains, mixed spin chains have yet rarely been considered.

The twist order parameter, as introduced in [6], is well suited to signal quantum phase transitions between different valence bond configurations in various 1D quantum spin systems. At non-zero temperature we have found the formation of a plateau in the twist order parameter around the (zero temperature) quantum critical point. We have investigated the possibility that this plateau is related to the quantum critical region that fans out from the quantum critical point. However, up to the present accuracy of our simulations the data does not support this conjecture [7].

Supplemented by exact Lanczos diagonalisation and extrapolation algorithms we could extract estimates of the critical exponents of the mixed spin models under investigation. We are currently examining the presence of multiplicative logarithmic corrections in mixed spin chains. These corrections have been found in the uniform $S = 1/2$ Heisenberg model [8].

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11.12 Unconventional Quantum Criticality in 2D Dimerized Heisenberg Models

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Low-dimensional quantum spin systems are a central research topic in condensed matter physics as they effectively explain many of ordering phenomena in real life materials (e.g. magnetism in the clean cuprates). In the particular the antiferromagnetic Heisenberg model defined by the Hamiltonian

$$\mathcal{H} = \sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \mathbf{S}_j = \sum_{\langle i,j \rangle} J_{ij} \left(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \right) \tag{11.2}$$

is at the forefront of such research. Repeated interest in this model stems from the possibility to study the effect of competing interactions or quantum fluctuations on the ground-state properties of an interacting many-body quantum system. Motivated by the pressure induced disorder-order quantum phase transition in Mott insulators like $TlCuCl_3$ [1], we address in this project so-called dimerized Heisenberg models, in which the lattice spins $\mathbf{S}_i$ interact via two different non-equivalent couplings J and J',

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j + J' \sum_{\langle i,j \rangle'} \mathbf{S}_i \mathbf{S}_j \,, \qquad \alpha = J'/J \,, \tag{11.3}$$

in a regular manner as depicted in Fig 11.6. Access to quantum critical physics can be gained by varying the parameter $\alpha = J'/J$. In this project, we have carried out extensive quantum Monte Carlo simulations based on the stochastic series expansion (SSE) approach [2] of the quantum phase transition in dimerized Heisenberg models in order to verify the applicability of the nonlinear sigma model (NLSM) to characterize quantum critical phenomena. This theory predicts a standard 3D $O(3)$ description for Heisenberg models.

Our most surprising result is that of a novel universality class triggered by special geometric arrangements of the strong couplings J' in Fig. 11.6c. While we find total agreement with $O(3)$ criticality for the ladder and plaquette models of Fig. 11.6(a,b), our Monte Carlo data for the staggered model indicates different critical exponents β/ν

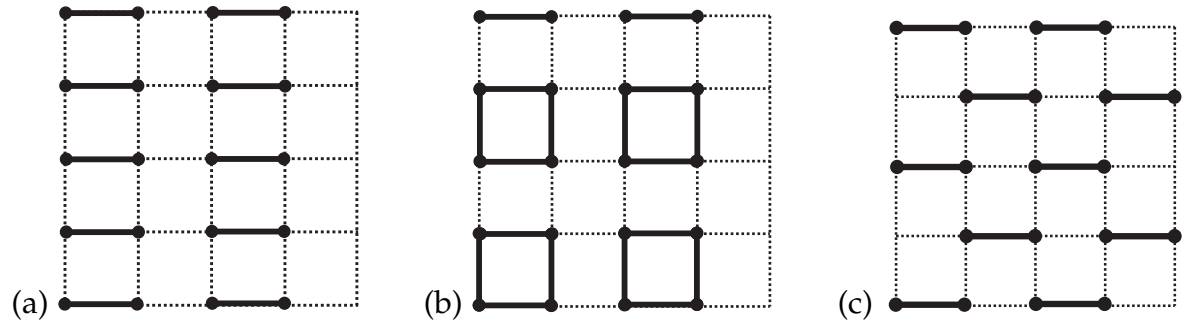

Figure 11.6: Examples of dimerized Heisenberg models on the square lattice in form of (**a**) the ladder model, (**b**) the plaquette model, (**c**) the staggered model. Dashed bonds indicate couplings J whereas thick bonds indicate J' interactions.

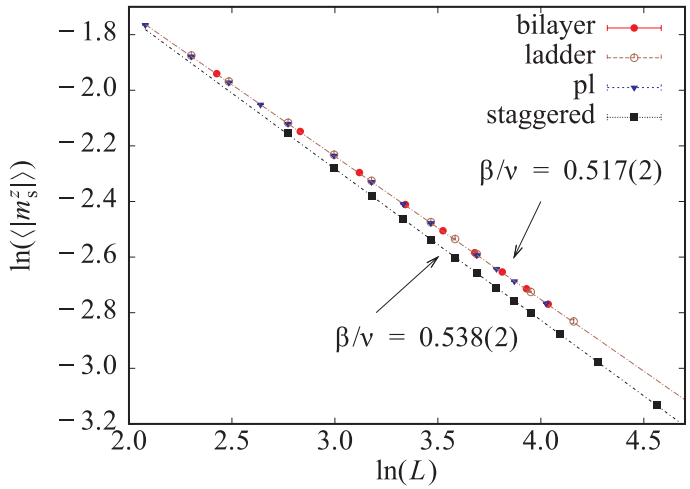

Figure 11.7: Finite-size scaling analysis of the sublattice magnetization in different dimerized Heisenberg models at the quantum critical point. The data for the staggered model indicates a deviation from the anticipated value $\beta/\nu = 0.5188(3)$ [3].

characterizing the sublattice magnetization order parameter m_s^z. This effect is illustrated in Fig. 11.7, where a finite-size analysis of the magnetization at the quantum critical point is performed [4, 5].

In case of the staggered model, further simulations show deviations from the standard theory in experimentally accessible quantities like the critical uniform magnetic susceptibility at finite temperatures. Initial analytical derivations and simulations of other dimerized Heisenberg models suggest that the novel unconventional behaviour could be related to topological terms that appear in the effective action in certain cases. In result, the Heisenberg model continues to be an even richer playground of quantum phenomena than anticipated until today.

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11.13 Thermodynamics of Heisenberg Ferromagnets in a Magnetic Field

I. Juhász Junger*, D. Ihle*, L. Bogacz†, W. Janke

*Theory of Condensed Matter Workgroup
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The thermodynamic properties magnetization, magnetic susceptibility, transverse and longitudinal correlation lengths, and specific heat of 1D ferromagnetic chains and of 2D ferromagnet layers with arbitrary spin S in a magnetic field are investigated by a second-order Green-function theory. In addition, quantum Monte Carlo simulations for $S = 1/2$ and $S = 1$ are performed by using the stochastic series expansion (SSE) method [1]. Good agreement between the results of both approaches is found [2]. The field dependence of the position of the maximum in the temperature dependence of the susceptibility fits well to a power law at low fields and to a linear increase at high fields. The maximum height decreases according to a power law in the whole field region. The longitudinal correlation length may show an anomalous temperature dependence: a minimum followed by a maximum with increasing temperature.

Considering the specific heat in one dimension and at low magnetic fields, two maxima in its temperature dependence for both the $S = 1/2$ and $S = 1$ ferromagnets are found. For $S > 1$, only one maximum occurs, as in the 2D ferromagnets. Relating the theory to experiments on the $S = 1/2$ quasi-one-dimensional copper salt TMCuC $[(CH_3)_4NCuCl_3]$, a fit to the magnetization as a function of the magnetic field yields the value of the exchange energy, which is used to make predictions for the occurrence of two maxima in the temperature dependence of the specific heat.

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11.14 Universal Aspects of the Evaporation/Condensation of Ising Droplets

A. Nußbaumer, E. Bittner, W. Janke

In a seminal work [1] we showed in 2006 that the behaviour of droplets that live on a 2D Ising lattice, with a Hamiltonian defined as

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \,, \qquad \sigma_i = \pm 1 \,, \tag{11.4}$$

is compatible with the prediction made by Biskup et al. [2, 3] already for relatively small system sizes L. There, an analytical curve is derived that, adapted to the case of the Ising model, yields the amount of magnetisation that is consumed in the largest droplet of the

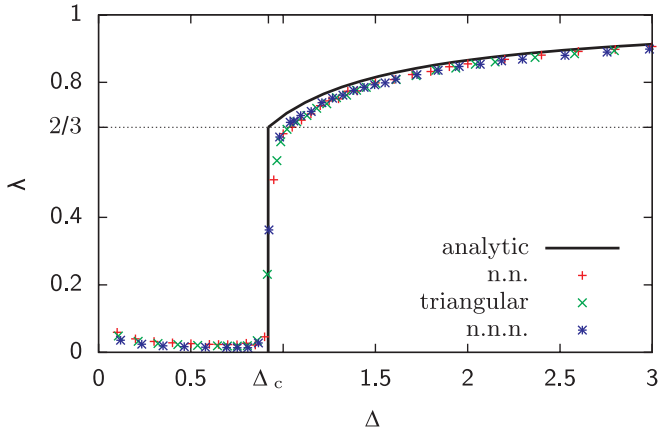

Figure 11.8: The fraction λ of the excess magnetisation that builds up the largest droplet in dependence of the parameter Δ that in turn is a function of the magnetisation and some system specific constants, like the spontaneous magnetisation and others. Independent of the three different lattice types (square lattice nearest-neighbour (n.n.): +, triangular: $\times$, and square lattice next-nearest-neighbour (n.n.n.): $*$) the theoretical curve (solid line) is nicely approached. The small differences to the theoretical prediction can be attributed to the finite size ($L = 640$) of the simulated systems.

system. With the help of computer simulations, using the so-called "multicanonical" algorithm [4], we were able to obtain precise results for systems up to size $L = 640$ – even in the two-phase region, where the metastable behaviour of a solid or liquid and a gaseous phase with an greatly increased autocorrelation time makes the relative errors larger. The details of our investigations can be found in [5].

By extending our work of 2006, we redid our simulation using different lattice types. Using our numerical data we now have strong arguments that the rigorous results of Biskup et al. for the 2D square lattice Ising model with nearest neighbour (n.n.) interactions are indeed independent of the underlying geometry of the lattice and the range of interactions (see Fig. 11.8), providing thus a universal description of the evaporation/condensation process.

As a future prospect, we intend to look at the 3D case and possibly also add some off-lattice simulations using a Lennard–Jones potential.

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11.15 Anisotropy of the Interface Tension of the 3D Ising Model

E. Bittner, A. Nußbaumer, W. Janke

In many physical systems with discrete symmetry the anisotropy of the interface tension can play an important role for various phenomena, including equilibrium

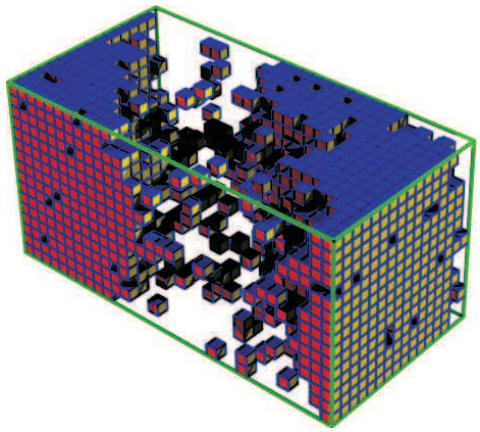

Figure 11.9: Plot of a typical configuration with two 110 interfaces.

droplet shapes [1] and the interfacial roughening transition [2]. For sufficiently strong anisotropy, facets, edges, or even corners can be identified in the equilibrium droplet shape. Due to the anisotropy of the interface tension in the 3D Ising model, the shape of the equilibrium droplet at some finite temperature is not spherical and has, in principle, to be determined by the Wulff construction [3]. Since the 3D Ising model with nearest-neighbour interaction is not exactly solvable, no analytical results are available for the interfacial free energy and the Wulff construction can only be done using an effective model of the angle-depending interface tension. Only for temperatures not too far below the critical temperature one can use the spherical approximation and, therefore, it is important to know how large the anisotropy is for a given temperature.

We determine the interface tension for the 100, 110 and 111 interface of the simple-cubic Ising model with nearest-neighbour interaction (see Fig. 11.9) using novel simulation methods [4]. To overcome the droplet/strip transition and the droplet nucleation barrier we use a newly developed combination of the multimagnetic algorithm with the parallel tempering method. We investigate a large range of inverse temperatures to study the anisotropy of the interface tension in detail and show that at given T/T_c the anisotropy of the interface in three dimensions is larger than in two dimensions. However, down to 0.7 T_c it never exceeds 3 %, so that in most cases the isotropic approximation for droplet condensation phenomena should be sufficiently accurate.

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11.16 Autocorrelation Times and the Parallel Tempering Algorithm

E. Bittner, A. Nußbaumer, W. Janke

We introduce a new update scheme to systematically improve the efficiency of parallel tempering Monte Carlo simulations (PT) [1] by taking into account the temperature

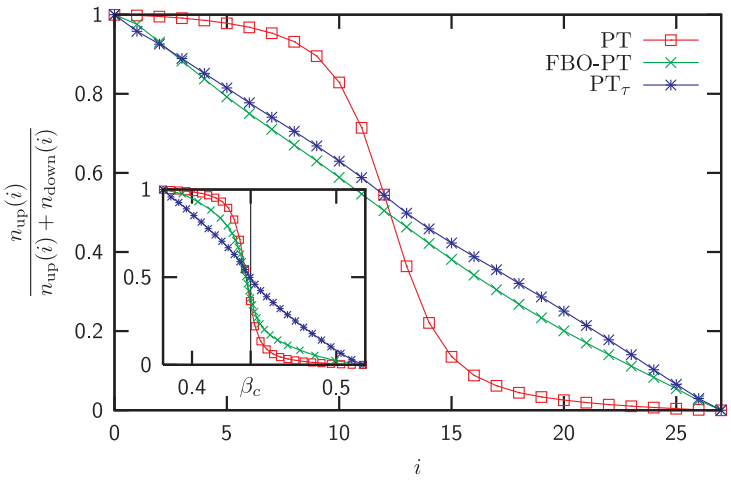

Figure 11.10: Fraction of replica which wander from the smallest inverse temperature β to the largest as a function of the replica index i for the 2D Ising model (with linear lattice size $L = 80$). The simulations without optimization exhibit a sharp decline close to the critical inverse temperature β_c, as one can see in the inset. Taking the canonical correlation times $\tau_{\rm can}$ into account (PT$_\tau$), the fraction decreases, for the same set of temperatures, almost linearly.

dependence of autocorrelation times. In contrast to previous attempts (FBO-PT) [2] the temperatures are not dynamically adjusted but chosen in such a way that the acceptance rate for proposed exchanges of all adjacent replica is about 50%. We show that by adapting the number of sweeps between the parallel tempering moves to the canonical autocorrelation time, the average round-trip time of a replica between the lowest and the highest temperatures is significantly decreased and, therefore, the efficiency of the parallel tempering algorithm is considerably improved, cf. Fig. 11.10. We illustrate the new algorithm (PT$_\tau$) [3] with results for the 2D Ising model and the 3D Edwards–Anderson Ising spin glass.

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11.17 Football Fever

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Analyzing football score data with statistical techniques, we investigate how the not purely random, but highly co-operative nature of the game is reflected in averaged properties such as the probability distributions of scored goals for the home and away teams. As it turns out, especially the tails of the distributions are *not* well described

by the Poissonian or binomial model resulting from the assumption of uncorrelated random events. Instead, a good effective description of the data is provided by less basic distributions such as the negative binomial one or the probability densities of extreme-value statistics. To understand this behaviour from a microscopical point of view, however, no waiting time problem or extremal process need be invoked. Instead, modifying the Bernoulli random process underlying the Poissonian model to include a simple component of *self-affirmation* seems to describe the data surprisingly well and allows to understand the observed deviation from Gaussian statistics. The phenomenological distributions used before can be understood as special cases within this framework. We analyzed historical football score data from many leagues in Europe as well as from international tournaments, including data from all past tournaments of the "FIFA World Cup" series, and found the proposed models to be applicable rather universally. In particular, we analysed the results of the German women's premier football league and considered the two separate German men's premier leagues in the East and West during the cold war times and the unified league after 1990 to see how scoring in football and the component of self-affirmation depend on cultural and political circumstances [1].

The main task of the "Wissenschaftssommer" exhibition within the frame of the "Jahr der Mathematik" in July 2008 on the Augustusplatz in Leipzig was to motivate visitors to participate and to deal with the mathematical topics of the individual booths. To illustrate the meaning of statistical properties we chose the football score data described above and to incorporate the visitors we rented two football tables, see Fig. 11.11. With the help of over 2500 visitors we were able to collect more then 1000 table football results, which we analysed on-site and found a good agreement with our model. A detailed report on the results can be found in [2].

Figure 11.11: Football fever infected visitors of the "Wissenschaftssommer", from left to right former Foreign Minister K. Kinkel, Vice-Rector Research of the University of Leipzig Prof. Dr. M. Schlegel, Lord Mayor of Leipzig B. Jung, and Parliamentary State Secretary to the Federal Minister of Education and Research T. Rachel.

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11.18 Funding

Excellence Initiative, Graduate School "BuildMoNa": Leipzig School of Natural Sciences – Building with Molecules and Nano-objects
W. Janke (Principal Investigator)
DFG

Forschergruppe 877: From Local Constraints to Macroscopic Transport
W. Janke (Principal Investigator)
DFG

RTN-Network "ENRAGE": Random Geometry and Random Matrices: From Quantum Gravity to Econophysics
W. Janke (Principal Investigator)
EU MRTN-CT-2004-005616

Host of EU Marie Curie Incoming Fellowship: SAWs on Fractals, Dr. Viktoria Blavatska (Lviv, Ukraine)
W. Janke
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Dynamik und Statik von Spingläsern
W. Janke
DFG Ja 483/22-1

Phasenübergänge in Systemen mit einschränkender Geometrie
W. Janke
DFG Ja 483/23-1 and 2

Investigation of Thermodynamic Properties of Lattice and Off-Lattice Models for Proteins and Polymers
M. Bachmann and W. Janke
DFG Ja 483/24-1 and 2

Molecular Conformation Mechanics of Proteins and Polymers
W. Janke
DFG Ja 483/24-3

"Deutsch-Französisches Doktorandenkollegium (DFDK)" with "Co-tutelle des Thèse": Statistical Physics of Complex Systems, jointly with l'Université Henri Poincaré, Nancy I, France
W. Janke (with B. Berche)
Deutsch-Französische Hochschule, CDFA-02-07

Statistical Mechanics of Complex Networks
W. Janke (with Z. Burda)

Alexander von Humboldt Foundation "Institutspartnerschaft" with the Jagellonian University, Krakow, Poland, 3.4-Fokoop-DEU/1117877

Numerical Approaches to Protein Folding
W. Janke (with A. Irbäck)
DAAD-STINT Collaborative Research Grant with the University of Lund, Sweden, D/05/26016

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W. Janke
Alexander von Humboldt Foundation

Grant for full support of 75 participants of the *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, Dresden

Monte Carlo Simulationen der Statik und Dynamik von Spingläsern
E. Bittner, W. Janke
NIC Jülich (computer time grant for "JUMP"), hlz10

Protein and Polymer Models
M. Bachmann, W. Janke
NIC Jülich (computer time grant for "JUMP"), hlz11

Quantum Monte Carlo Simulations of Quantum Spin Models
W. Janke
NIC Jülich (computer time grant for "JUMP"), hlz12

Dimerized Heisenberg Models
S. Wenzel
Studienstiftung des deutschen Volkes

11.19 Organizational Duties

M. Bachmann

- Scientific Secretary of the Workshop *LEILAT08 – 18. Workshop on Lattice Field Theory and Statistical Physics* ITP, Universität Leipzig, 26. – 28. June 2008
- Scientific Secretary of the Workshop *CompPhys08 – 9. International NTZ-Workshop on New Developments in Computational Physics*, ITP, Universität Leipzig, 27. – 29. November 2008
- Referee: Phys. Rev. Lett., J. Am. Chem. Soc., IEEE/ACM Transact. Comput. Biol. Bioinf., Phys. Rev. A, Phys. Rev. E, J. Phys. A, Eur. J. Phys. D, Biophys. Rev. Lett., Comput. Phys. Commun., J. Comput. Chem., Macromolecules, Phys. Chem. Chem. Phys.
- Reviewer: Engineering and Physical Sciences Research Council (EPSRC) UK, National Science Foundation (NSF) USA

E. Bittner

- 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 – 18. 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. June – 04. July 2008
- Scientific Secretary of the Workshop *CompPhys08 – 9. International NTZ-Workshop on New Developments in Computational Physics*, ITP, Universität Leipzig, 27. – 29. November 2008
- Scientific Secretary of the Workshop *CompPhys09 – 10. International NTZ-Workshop on New Developments in Computational Physics*, ITP, Universität Leipzig, 26. – 29. November 2009
- Referee: Phys. Rev. Lett., Phys. Rev. E, J. Phys. A, Eur. J. Phys. B, Comput. Phys. Commun.

W. Janke

- Director, Naturwissenschaftlich-Theoretisches Zentrum (NTZ) of 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 of 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 Spring School on *Monte Carlo Simulations of Disordered Systems*, ITP, Universität Leipzig, 30. March – 04. April 2008
- Organizer of the Workshop *LEILAT08 – 18. 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. June – 04. July 2008
- Organizer of the Workshop *CompPhys08 – 9. International NTZ-Workshop on New Developments in Computational Physics*, ITP, Universität Leipzig, 27. – 29. November 2008
- Organizer of the 34. 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

- Organizer of the Workshop *CompPhys09 – 10. International NTZ-Workshop on New Developments in Computational Physics*, ITP, Universität Leipzig, 26. – 29. November 2009
- Member of International Organization Committee of the 10. Int. Conf. *Path Integrals* (with L.S. Schulman (USA), M. Gutzwiller (USA), A. Inomata (USA), J.R. Klauder (USA), D. Fujikawa (Japan) und Chookyu Lee (South Korea)), planned for Seoul, South Korea, Summer 2010
- 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 (DFG); Studienstiftung des deutschen Volkes; The Jeffress Memorial Trust, Bank of America, USA; Fond zur Förderung der wissenschaftlichen Forschung (FWF), Austria; The Royal Society, UK; 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. Che. Phys., Europhys. Lett., Phys. Lett. A, Phys. Lett. B, Eur. Phys. J. B, Physica A, Proc. Roy. Phys. Soc., J. Phys. A, Comput. Phys. Commun., J. Stat. Mech. Theor. Exp., New J. Phys., Int. J. Mod. Phys. C

A. Nußbaumer

- Co-organizer of the contribution *Football Feaver* to the "Wissenschaftssommer" exhibition within the frame of the "Jahr der Mathematik", Universität Leipzig, 28. June – 04. July 2008

T. Vogel

- Scientific Secretary, Naturwissenschaftlich-Theoretisches Zentrum (NTZ) of the Zentrum für Höhere Studien (ZHS), Universität Leipzig

11.20 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, Université de Rouen, France
  Dr. Pierre-Emmanuel Berche
- School of Mathematical and Computer Sciences, Heriot-Watt University, Edinburgh, UK
  Prof. Dr. Desmond A. Johnston
- School of Physics and Astronomy, University of Edinburgh, UK
  Richard A. Blythe
- School of Mathematical and Information Sciences, Coventry University, UK
  Dr. Ralph Kenna, PD Dr. Christian von Ferber
- Department of Physics, Hacettepe University, Ankara, Turkey
  Dr. Handan Arkin, Prof. Dr. Tarik Çelik, 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. Peter Grassberger, Prof. Dr. U. Hansmann, 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
- Istituto Nazionale di Fisica Nucleare, Sezione di Milano-Bicocca, Milano, Italy
  Prof. Dr. Pablo Butera
- Banaras Hindu University, Varanasi, India
  Prof. Dr. Sanjay Kumar
- Brunel University of West London, UK
  Dr. Gernot Akemann
- Institut für Theoretische Physik, Freie Universität Berlin, Germany
  Prof. Dr. Hagen Kleinert, Dr. Adriaan M.J. Schakel
- IAC-1, Universität Stuttgart
  Prof. Dr. Rudolf Hilfer
- Institut für Theoretische Physik, Universität Duisburg-Essen, Germany
  PD Dr. Axel Pelster
- Institut für Theoretische Physik, Universität Bielefeld, Germany
  Prof. Dr. Friderike Schmid
- School of Engineering and Science, 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
- Zhejiang Institute of Modern Physics, Zhejiang University, Hangzhou, P.R. China
  Prof. Dr. He-Ping Ying, Prof. Dr. Bo Zheng

11.21 Publications

Journals

M. Bachmann, W. Janke: *Minimalistic Hybrid Models for the Adsorption of Polymers and Peptides to Solid Substrates*, Phys. Part. Nucl. Lett. **5**, 243 (2008)

B.A. Berg, W. Janke: *Multibondic Cluster Algorithm for Finite-Size Scaling Studies of Critical Phenomena*, Comput. Phys. Commun. **179**, 21 (2008)

E. Bittner, W. Janke: *A Boundary Field Induced First-Order Transition in the 2D Ising Model: Numerical Study*, J. Phys. A **41**, 395 001 (2008)

E. Bittner, A. Nußbaumer, W. Janke: *Make Life Simple: Unleash the Full Power of the Parallel Tempering Algorithm*, Phys. Rev. Lett. **101**, 130 603 (2008)

E. Bittner, A. Nußbaumer, W. Janke, M. Weigel: *Fußballfieber beim Wissenschaftssommer: Eine mathematisch-empirische Nachlese*, Universität Leipzig Journal **6**/2008, 22 (2008)

V. Blavatska, C. von Ferber, Y. Holovatch: *Scaling of Complex Polymers: New Universality Classes and Beyond*, Philos. Mag. **88**, 4085 (2008)

V. Blavatska, W. Janke: *Scaling Behavior of Self-Avoiding Walks on Percolation Clusters*, Europhys. Lett. **82**, 66 006 (2008)

V. Blavatska, W. Janke: *Multifractality of Self-Avoiding Walks on Percolation Clusters*, Phys. Rev. Lett. **101**, 125 701 (2008)

M. Hasenbusch: *The Binder Cumulant at the Kosterlitz-Thouless Transition*, J. Stat. Mech. P08 003 (2008)

M. Hasenbusch: *Monte Carlo Study of the Three-Dimensional XY Universality Class: Universal Amplitude Ratios*, J. Stat. Mech. P12 006 (2008)

M. Hasenbusch, F. Parisen Toldin, A. Pelissetto, E. Vicari: *Multicritical Nishimori Point in the Phase Diagram of the ±J Ising Model on a Square Lattice*, Phys. Rev. E **77**, 051 115 (2008)

M. Hasenbusch, F. Parisen Toldin, A. Pelissetto, E. Vicari: *Universal Dependence on Disorder of Two-Dimensional Randomly Diluted and Random-Bond ±J Ising Models*, Phys. Rev. E **78**, 011 110 (2008)

M. Hasenbusch, A. Pelissetto, E. Vicari: *The Critical Behavior of 3D Ising Spin Glass Models: Universality and Scaling Corrections*, J. Stat. Mech. L02 001 (2008)

M. Hasenbusch, A. Pelissetto, E. Vicari: *Critical Behavior of Three-Dimensional Ising Spin Glass Models*, Phys. Rev. B **78**, 214 205 (2008)

I. Juhász Junger, D. Ihle, L. Bogacz, W. Janke: *Thermodynamics of Heisenberg Ferromagnets with Arbitrary Spin in a Magnetic Field*, Phys. Rev. B **77**, 174 411 (2008)

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)

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)

J. Schluttig, M. Bachmann, W. Janke: *Comparative Molecular Dynamics and Monte Carlo Study of Statistical Properties for Coarse-Grained Heteropolymers*, J. Comput. Chem. **29**, 2603 (2008)

B. Wacław, L. Bogacz, W. Janke: *Approaching the Thermodynamic Limit in Equilibrated Scale-Free Networks*, Phys. Rev. E **78**, 061 125 (2008)

B. Wacław, Z. Burda: *Counting Metastable States of Ising Spin Glasses on Arbitrary Graphs*, Phys. Rev. E **77**, 041 114 (2008)

B. Wacław, Z. Burda, W. Janke: *Power Laws in Zero-Range Processes on Random Networks*, Eur. Phys. J. B **65**, 565 (2008)

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)

S. Wenzel, L. Bogacz, W. Janke: *Evidence for an Unconventional Universality Class from a Two-Dimensional Dimerized Quantum Heisenberg Model*, Phys. Rev. Lett. **101**, 127 202 (2008)

S. Wenzel, W. Janke: *Monte Carlo Simulations of the Directional-Ordering Transition in the Two-Dimensional Classical and Quantum Compass Model*, Phys. Rev. B **78**, 064 402 (2008); publisher's Note: Phys. Rev. B **78**, 099 902(E) (2008)

F.T. Winter, W. Janke, A.M.J. Schakel: *Geometric Properties of the Three-Dimensional Ising and XY Models*, Phys. Rev. E **77**, 061 108 (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, Lecture Notes in Physics **736** (Springer, Berlin 2008) p 203

M. Bachmann, W. Janke: *Conformational Transitions in Molecular Systems*, in: *Path Integrals – New Trends and Perspectives*, ed. by W. Janke, A. Pelster (World Scientific, Singapore 2008) p 531

M. Bachmann, W. Janke: *Mesoscopic Properties of Molecular Folding and Aggregation Processes*, Proc. BIFI 2008 Int. Conf. *Large Scale Simulations of Complex Systems, Condensed Matter and Fusion Plasma*, Zaragoza, Spain, 6.–8. February 2008, ed. by P. Bruscolini, J. Clemente-Gallardo, P. Echenique, J.F. Sáenz-Lorenzo, F. Castejón, AIP Conf. Proc. Volume **1071**, 1 (2008)

R. Bischof, W. Janke: *Critical Exponents of Mixed Quantum Spin Chain*, in: *Path Integrals – New Trends and Perspectives*, ed. by W. Janke, A. Pelster (World Scientific, Singapore 2008) p 514

E. Bittner, W. Janke: *Vortex-Line Percolation in a Three-Dimensional Complex $|\psi|^4$ Theory*, in: *Path Integrals – New Trends and Perspectives*, ed. by W. Janke, A. Pelster (World Scientific, Singapore 2008) p 493

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

V. Blavatska, W. Janke: *Self-Avoiding Walks on Fractals: Scaling Laws*, in: *Path Integrals – New Trends and Perspectives*, ed. by W. Janke, A. Pelster (World Scientific, Singapore 2008) p 585

V. Blavatska, C. von Ferber, Y. Holovatch: *Star Polymers in Correlated Disorder*, in: *Path Integrals – New Trends and Perspectives*, ed. by W. Janke, A. Pelster (World Scientific, Singapore 2008), p 549

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

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, Lecture Notes in Physics **736** (Springer, Berlin 2008) p 1

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

W. Janke, A. Pelster (Eds.): *Path Integrals – New Trends and Perspectives* (World Scientific, Singapore 2008)

A. Nußbaumer, E. Bittner, W. Janke: *Evaporation/Condensation of Ising Droplets*, in: *Path Integrals – New Trends and Perspectives*, ed. by W. Janke, A. Pelster (World Scientific, Singapore 2008) p 525

S. Schnabel, M. Bachmann, W. Janke: *Different Kinds of Protein Folding Identified with a Coarse-Grained Heteropolymer Model*, in: *From Computational Biophysics to Systems Biology (CBSB08)*, ed. by U.H.E. Hansmann, J.H. Meinke, S. Mohanty, W. Nadler, O. Zimmermann, NIC Series Vol. **40** (John von Neumann Institute for Computing, Jülich 2008) p 369

T. Vogel, M. Bachmann, W. Janke: *Freezing and Collapse of Flexible Polymers*, in: *From Computational Biophysics to Systems Biology (CBSB08)*, ed. by U.H.E. Hansmann, J.H. Meinke, S. Mohanty, W. Nadler, O. Zimmermann, NIC Series Vol. **40** (John von Neumann Institute for Computing, Jülich 2008) p 405

B. Wacław, L. Bogacz, Z. Burda, W. Janke: *Monte Carlo Methods for Generation of Random Graphs*, in: *Path Integrals – New Trends and Perspectives*, ed. by W. Janke, A. Pelster (World Scientific, Singapore 2008) p 342

Talks

M. Aust: *Outlook on a New Thermal Ratchet Theme Based on a Binary Liquid Mixture*, SFG-Meeting and Guest Kolloquia, Leipzig, Germany 25. September 2008

M. Bachmann: *Thermodynamics and Kinetics of a Proteinlike Heteropolymer Model*, 72. DPG Spring Meeting, Berlin, Germany 25. – 29. February 2008

M. Bachmann: *Conformation Mechanics of Molecular Structure Formation Processes*, Seminar talk, Max-Planck-Institut für Polymerforschung, Mainz, Germany, 04. March 2008

M. Bachmann: *Nanopatterns of Macromolecules*, Project meeting, Martin-Luther-Universität Halle-Wittenberg, Germany, 09. May 2008

M. Bachmann: *Conformational Mechanics of Molecular Structure Formation Processes*, Habilitation talk, Universität Leipzig, Germany, 17. July 2008

M. Bachmann: *Mesoscopic Modeling of Protein Assemblies*, Presentation at the Evaluation Panel Meeting "Computational Biology", Forschungszentrum Jülich, Germany, 07. – 08. October 2008

R. Bischof: *Quantum Phase Transitions in Mixed Quantum Spin Chains*, Seminar talk, Deutsch-Französische Hochschule (Collège Doctoral), Université Henri Poincaré, Nancy, France, 04. February 2008

R. Bischof: *Quantum Monte Carlo Investigation of Mixed Quantum Spin Chains*, Seminar talk, Universität des Saarlandes, Saarbrücken, Germany, 05. February 2008

E. Bittner: *Autocorrelation Times and the Parallel Tempering Algorithm*, 72. DPG Spring Meeting, Berlin, Germany 25. – 29. February 2008

E. Bittner: *Free-Energy Barriers in Spin Glasses: Mean-Field vs Short-Range Models*, invited talk, "ENRAGE" Network School on Monte Carlo Simulations of Disordered Systems, Leipzig, Germany, 30. March – 04. April 2008

E. Bittner: *Autocorrelation Times and the Parallel Tempering Algorithm*, 33. Conf. Middle European Cooperation Stat. Phys. (MECO33), Puchberg/Wels, Austria, 14. – 16. April 2008

V. Blavatska: *Multifractality of Self-Avoiding Random Walks on Percolation Clusters*, 72. DPG Spring Meeting, Berlin, Germany 25. – 29. February 2008

V. Blavatska: *Copolymer Stars in Porous Media*, XI. International Workshop on Complex Systems, Andalo, Italy, 17. – 20. March 2008

V. Blavatska: *Self-Avoiding Walks on Disordered Lattices: Scaling Laws*, "ENRAGE" Network School on Monte Carlo Simulations of Disordered Systems, Leipzig, Germany, 30. March – 04. April 2008

V. Blavatska: *Multifractality of Self-Avoiding Walks on Percolation Clusters*, ENRAGE Network Meeting, University of Oxford, UK, 15. – 19. September 2008

V. Blavatska: *Random Walks on Percolation Clusters: Multifractal Effects*, 9. Int. NTZ-Workshop "New Developments in Computational Physics" (CompPhys08), Leipzig, Germany, 27. – 29. November 2008

M. Hasenbusch: *The Spin-Glass Transition in the Three-Dimensional EAI Model*, invited talk, "ENRAGE" Network School on Monte Carlo Simulations of Disordered Systems, Leipzig, Germany, 30. March – 04. April 2008

M. Hasenbusch: *Strings, Interfaces and the Ising Model*, 18. Int. Workshop "Lattice Field Theory and Statistical Physics" (Leilat08), Universität Leipzig, Germany, 26. – 28. June 2008

M. Hasenbusch: *Kosterlitz-Thouless transition of thin films in the 3D XY universality class*, 9. Int. NTZ-Workshop "New Developments in Computational Physics" (CompPhys08), Leipzig, Germany, 27. – 29. November 2008

W. Janke: *Modeling and Simulation of Biological Macromolecules*, invited talk, Int. Conf. *Large-Scale Simulations of Complex Systems, Condensed Matter and Fusion Plasma* (BiFi2008), Universidad de Zaragoza, Spain, 06. – 08. February 2008

W. Janke: *Numerical Estimation of Baxter-Wu Critical Amplitudes*, 72. DPG Spring Meeting, Berlin, Germany 25. – 29. February 2008

W. Janke: *Universal Aspects of Ising Droplets*, 33. Conf. Middle European Cooperation Stat. Phys. (MECO33), Puchberg/Wels, Austria, 14. – 16. April 2008

W. Janke: *Universal Aspects of Ising Droplets*, invited talk, Atelier Nancy *Statistical Physics and Low Dimensional Systems 2008*, Université Nancy, France, 21.–23. May 2008

W. Janke: *Condensation in Zero-Range Processes on Inhomogeneous Networks*, invited talk, Workshop *Transport Processes in Physics and Biology*, Jacobs University, Bremen, Germany, 26.–28. May 2008

W. Janke: *Percolating Excitations – A Geometrical View of Phase Transitions*, invited talk, 13. Claude Itzykson Meeting, Saclay, France, 09.–11. June 2008

W. Janke: *Random Walks on Percolation Clusters I and II*, two invited talks, ENRAGE Network Meeting, University of Oxford, Oxford, UK, 15.–19. September 2008

W. Janke: *Quantum Phase Transitions in Dimerized Heisenberg Models*, invited talk, 24. Max Born Symposium, University of Wroclaw, Poland, 25.–27. September 2008

W. Janke: *Droplet Condensation and Evaporation*, ICP Seminar, Universität Stuttgart, Germany, 11. November 2008

W. Janke: *Quantum Phase Transitions of Coupled Spin Dimers*, Physik-Kolloquium der Freien Universität Berlin, Germany, 12. December 2008

M. Möddel: *Conformational Mechanics of Polymer Adsorption Transitions at Attractive Substrates*, Seminar talk, Deutsch-Französische Hochschule (Collège Doctoral), Université Henri Poincaré, Nancy, France, 13. October 2008

A. Nußbaumer: *Free-Energy Barriers of Spin Glasses*, 72. DPG Spring Meeting, Berlin, Germany 25.–29. February 2008

A. Nußbaumer: *Free-Energy Barriers of Spin Glasses*, 18. Int. Workshop "Lattice Field Theory and Statistical Physics" (Leilat08), Universität Leipzig, Germany, 26.–28. June 2008

A. Nußbaumer: *Free-Energy Barriers of Spin Glasses*, Seminar "Theory of Condensed Matter Physics", RWTH Aachen, Germany, 01. July 2008

A. Nußbaumer: *Free-Energy Barriers of Spin Glasses*, 9. Int. NTZ-Workshop "New Developments in Computational Physics" (CompPhys08), Leipzig, Germany, 27.–29. November 2008

S. Schnabel: *Conformational Transitions of Flexible Polymers*, 72. DPG Spring Meeting, Berlin, Germany 25.–29. February 2008

S. Schnabel: *Solution Behavior of Semiconductor-Binding Peptides*, 1. BuildMoNa Workshop, Leipzig, Germany, 16./17. October 2008

S. Schnabel: *Low Temperature Behavior of the Lennard-Jones Polymer*, 9. Int. NTZ-Workshop "New Developments in Computational Physics" (CompPhys08), Leipzig, Germany, 27.–29. November 2008

T. Vogel: *Ground-state Properties of Thick Flexible Polymers*, 72. DPG Spring Meeting, Berlin, Germany 25. – 29. February 2008

T. Vogel: *Freezing and Collapse of Flexible Lattice Polymers*, 18. Int. Workshop "Lattice Field Theory and Statistical Physics" (Leilat08), Universität Leipzig, Germany, 26. – 28. June 2008

B. Wacław: *A Monte Carlo Method for Generation of Random Graphs*, 72. DPG Spring Meeting, Berlin, Germany 25. – 29. February 2008

B. Wacław: *Introduction to Complex Networks*, "ENRAGE" Network School on Monte Carlo Simulations of Disordered Systems, Leipzig, Germany, 30. March – 04. April 2008

B. Wacław: *Finite-Size Effects in Growing Networks*, Seminar of Statistical Physics Division, LPTMS, CNRS Orsay, France, 24. April 2008

B. Wacław: *On the Number of Metastable States in Ising Spin Glasses*, Seminar of Statistical Physics Division, LPTMS, CNRS Orsay, France, 24. April 2008

B. Wacław: *Statistical Physics of Mass Transport Models*, invited talk, Workshop "Transport Processes in Physics and Biology", Jacobs University, Bremen, Germany, 26. – 28. May 2008

B. Wacław: *Approaching the Thermodynamic Limit: Cutoffs in Scale-Free Networks*, invited talk, CREEN Workshop, Norwich Research Park, Norwich, UK, 24. June 2008

B. Wacław: *Cutoffs and Maximal Degrees in Scale-Free Networks*, "ENRAGE" Network Meeting on Random Geometry and Random Matrices, University of Oxford, UK, 15. – 19. September 2008

B. Wacław: *Localization of Maximal Entropy Random Walk*, 9. Int. NTZ-Workshop "New Developments in Computational Physics" (CompPhys08), Leipzig, Germany, 27. – 29. November 2008

S. Wenzel: *Evidence of Unconventional Universality Class in a Two-Dimensional Dimerized Quantum Heisenberg Model*, Atelier Nancy *Statistical Physics and Low Dimensional Systems 2008*, Nancy, France, 21. – 23. May 2008

S. Wenzel: *Quantum Criticality in Dimerized Heisenberg Models*, 18. Int. Workshop "Lattice Field Theory and Statistical Physics" (Leilat08), Universität Leipzig, Germany, 26. – 28. June 2008

S. Wenzel: *The Quantum Compass Model and Extensions*, Seminar talk, Institut für Theoretische Physik III, Universität Stuttgart, 16. June 2008

S. Wenzel: *On Quantum Phase Transitions and Unconventional Behavior in a 2D Quantum Heisenberg Model*, Seminar talk, SFB/TRR 21 (Stuttgart, Ulm, Tübingen), Universität Stuttgart, 14. July 2008

S. Wenzel: *Unconventional Quantum Phase Transitions in Two-Dimensional Quantum Magnets*, 1. BuildMoNa Workshop, Leipzig, Germany, 16./17. October 2008

S. Wenzel: *Quantum Phase Transitions in Dimerized Heisenberg Models*, Condensed Matter Seminar, EPFL Lausanne, Switzerland, 19. November 2008

S. Wenzel: *Dimerized Heisenberg Models*, 9. Int. NTZ-Workshop "New Developments in Computational Physics" (CompPhys08), Leipzig, Germany, 27. – 29. November 2008

Posters

M. Aust, E. Bittner, W. Janke: *Equilibrium Properties of the Wang-Landau Algorithm*, 72. DPG Spring Meeting, Berlin, Germany 25. – 29. February 2008

M. Aust, E. Bittner, W. Janke: *Balance During Wang-Landau Recursion Simulations*, 9. Int. NTZ-Workshop "New Developments in Computational Physics" (CompPhys08), Leipzig, Germany, 27. – 29. November 2008

F. Beyer, E. Bittner, W. Janke: *Techniques Accelerating the Dynamics of Simulations of Complex Systems*, 72. DPG Spring Meeting, Berlin, Germany 25. – 29. February 2008

R. Bischof, W. Janke: *Formation of a Plateau in the Twist Order Parameter of the Bond Alternating Antiferromagnetic $S = 1/2$ Heisenberg Spin Chain*, 9. Int. NTZ-Workshop "New Developments in Computational Physics" (CompPhys08), Leipzig, Germany, 27. – 29. November 2008

E. Bittner, A. Nußbaumer, W. Janke, M. Weigel: *Football Fever: Goal Distributions and Non-Gaussian Statistics*, Economics and Psychology of Football 2008, Innsbruck, Austria, 29. – 30. May 2008

E. Bittner, A. Nußbaumer, W. Janke, M. Weigel: *Football Fever*, "Wissenschaftssommer" exhibition within the frame of the "Jahr der Mathematik", Leipzig, Germany, 28. June – 04. July 2008

E. Bittner, W. Janke: *Replica-Exchange Cluster Algorithm*, 9. Int. NTZ-Workshop "New Developments in Computational Physics" (CompPhys08), Leipzig, Germany, 27. – 29. November 2008

V. Blavatska, W. Janke: *Multifractal Properties of Self-Avoiding Walks on Percolation Clusters*, 33. Conf. Middle European Cooperation Stat. Phys. (MECO33), Puchberg/Wels, Austria, 14. – 16. April 2008

M. Möddel, M. Bachmann, W. Janke: *Conformational Mechanics of Polymer Adsorption Transitions at Attractive Substrates*, 72. DPG Spring Meeting, Berlin, Germany 25. – 29. February 2008

M. Möddel, M. Bachmann, W. Janke: *Conformational Mechanics of Polymer Adsorption Transitions at Attractive Substrates*, Jülich Soft Matter Days 2008, Bonn, Germany, 11. – 14. November 2008

A. Nußbaumer, E. Bittner, W. Janke: *Free-Energy Barriers of Spin Glasses*, "ENRAGE" Network School on Monte Carlo Simulations of Disordered Systems, Leipzig, Germany, 30. March – 04. April 2008

A. Nußbaumer, E. Bittner, W. Janke: *Free-Energy Barriers of Spin Glasses*, 33. Conf. Middle European Cooperation Stat. Phys. (MECO33), Puchberg/Wels, Austria, 14. – 16. April 2008

S. Schnabel, S. Mitternacht, M. Bachmann, W. Janke, A. Irbäck: *Solution Behavior of Semiconductor-Binding Peptides*, 1. Scientific Symposium of BuildMoNa, Leipzig, Germany, 07./08. February 2008

S. Schnabel, M. Bachmann, W. Janke: *Conformational Transitions of Flexible Polymers*, 33. Conf. Middle European Cooperation Stat. Phys. (MECO33), Puchberg/Wels, Austria, 14. – 16. April 2008

S. Schnabel, M. Bachmann, W. Janke: *Folding Channels for Coarse-Grained Polymer Models*, Workshop "From Computational Biophysics to Systems Biology" (CBSB08), Forschungszentrum Jülich, Germany, 19. – 21. May 2008

T. Vogel, T. Neuhaus, M. Bachmann, W. Janke: *Ground-State Properties of Thick Flexible Polymers*, "ENRAGE" Network School on Monte Carlo Simulations of Disordered Systems, Leipzig, Germany, 30. March – 04. April 2008

T. Vogel, T. Neuhaus, M. Bachmann, W. Janke: *Ground-State Properties of Thick Flexible Polymers*, 33. Conf. Middle European Cooperation Stat. Phys. (MECO33), Puchberg/Wels, Austria, 14. – 16. April 2008

T. Vogel, M. Bachmann, W. Janke: *Freezing and Collapse of Flexible Polymers*, Workshop "From Computational Biophysics to Systems Biology" (CBSB08), Forschungszentrum Jülich, Germany, 19. – 21. May 2008

T. Vogel, T. Neuhaus, M. Bachmann, W. Janke: *Ground-State Properties of Thick Flexible Polymers*, 9. Int. NTZ-Workshop "New Developments in Computational Physics" (CompPhys08), Leipzig, Germany, 27. – 29. November 2008

S. Wenzel, W. Janke: *Quantum Monte Carlo Study of the 2D Quantum Compass Model*, 1. Scientific Symposium of BuildMoNa, Leipzig, Germany, 07./08. February 2008

S. Wenzel, W. Janke: *Quantum Monte Carlo Study of the 2D Quantum Compass Model*, 72. DPG Spring Meeting, Berlin, Germany 25. – 29. February 2008

S. Wenzel, W. Janke: *Directional Ordering in the 2D Classical and Quantum Compass Model*, 33. Conf. Middle European Cooperation Stat. Phys. (MECO33), Puchberg/Wels, Austria, 14. – 16. April 2008

S. Wenzel, W. Janke: *Directional Ordering in the 2D Classical and Quantum Compass Model*, International Workshop on "Unconventional Phases and Phase Transitions in Strongly Correlated Electron Systems", Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany, 04. – 07. June 2008

S. Wenzel, L. Bogacz, W. Janke: *Criticality in Dimerized Heisenberg Models*, International Workshop on "Unconventional Phases and Phase Transitions in Strongly Correlated Electron Systems", Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany, 04. – 07. June 2008

S. Wenzel, W. Janke: *The 2D Compass Model*, 9. Int. NTZ-Workshop "New Developments in Computational Physics" (CompPhys08), Leipzig, Germany, 27. – 29. November 2008

M. Wiedenmann, A. Nußbaumer, E. Bittner, W. Janke: *Monte Carlo Study of the Evaporation/Condensation Transition of Ising Droplets*, 1. Scientific Symposium of BuildMoNa, Leipzig, Germany, 07./08. February 2008

M. Wiedenmann, A. Nußbaumer, E. Bittner, W. Janke: *Monte Carlo Study of the Evaporation/Condensation Transition of Ising Droplets*, 72. DPG Spring Meeting, Berlin, Germany 25. – 29. February 2008

11.22 Graduations

Habilitation

- Dr. Michael Bachmann
  Conformational Mechanics of Molecular Structure Formation Processes
  July 2008

Diploma

- Mathias Aust
  Generalized Ensemble Simulations of Disordered Systems
  May 2008
- Frank Beyer
  Monte Carlo Simulation Techniques and Minimal Energy States in the Edwards-Anderson Spin-Glass Model
  February 2008
- Monika Möddel
  Thermodynamics of Molecular Adsorption Processes on Mesocopic Scales
  May 2008
- Micha Wiedenmann
  Monte Carlo Study of the Evaporation/Condensation Transition of 3D Ising Droplets
  February 2008

11.23 Guests

- Prof. Dr. David P. Landau
  Unversity of Georgia, Athens, USA
  30. March – 02. April 2008
- Prof. Dr. Andrea Pelissetto
  University of Rome, Italy
  30. March – 02. April 2008

- Prof. Dr. Bertrand Berche, Dr. Christophe Chatelain, Jean-Charles Walter
  Université Henri Poincaré, Nancy, France
  31. March – 04. April 2008
- Andrzej Görlich
  Jagellonian University, Krakow, Poland
  31. March – 04. April 2008
- Marcin Zagorski
  Jagellonian University, Krakow, Poland
  30. March – 05. April 2008
- Prof. Dr. Bernd A. Berg
  Florida State University, Tallahassee, USA
  01. May – 30. June 2008
- PD Dr. Stefan Wessel
  Universität Stuttgart
  07. – 08. May 2008
- Christoph Junghans
  Max-Planck-Institut für Polymerforschung, Mainz
  15. – 16. May 2008
- Dr. Shura Hayryan
  Academia Sinica, Taipei, Taiwan
  16. May 2008
- Prof. Dr. Sanjay Kumar
  Banaras Hindu University, Varanasi, India
  19. May 2008
- Prof. Dr. Anders Sandvik
  Boston University, USA
  17. June 2008
- Prof. Dr. Sanjay Kumar
  Banaras Hindu University, Varanasi, India
  03. July 2008
- Prof. Dr. Robert H. Swendsen
  Carnegie Mellon University, Pittsburgh, USA
  30./31. July 2008
- Jean-Charles Walter
  Université Henri Poincaré, Nancy, France
  07. – 29. November 2008
- Prof. Dr. Peter Young
  University of California at Santa Cruz, USA
  26. – 30. November 2008
- Xavier Durang
  Université Henri Poincaré, Nancy, France
  26. – 30. November 2008

- Prof. Dr. Herbert Wagner
  Ludwig-Maximilians-Universität München
  04. – 05. December 2008