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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 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 adsorption as well as related properties of homopolymers, and the intriguing physics of low-dimensional quantum spin systems. Our 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, build on the recently concluded European Research Training Network (RTN) "ENRAGE": *Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*, a collaboration of 13 teams throughout Europe. Moreover, within a bi-national Institute Partnership of the Humboldt Foundation 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. Currently we are also exploring the possibilities of the rapidly developing graphics card computing, that is computer simulations on graphics processing units (GPUs) with many cores.

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 centre, 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 Nancy Université, France, supported by the Deutsch-Französische Hochschule. For the latter we submitted in 2010 a successful extension proposal, securing enhanced funding for the period 2011–2014. The two Graduate Schools are both "Classes" of the Research Academy Leipzig (RALeipzig), providing the organizational frame for hosting visiting students, offering language courses, organizing childcare and for many other practical matters. At the post-graduate level our research projects are embedded into the "Sächsische DFG-Forschergruppe" FOR877 *From Local Constraints to Macroscopic Transport*, which also has been successfully extended in 2010 for the period 2011–2014, the International Max Planck Research School (IMPRS) *Mathematics in the Sciences* and into two of the top level research areas ("Profilbildende Forschungsbereiche (PbF)") and the Centre for Theoretical Sciences (NTZ) of the University. Beside "BuildMoNa" 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) and the Alexander von Humboldt Foundation through the Institute Partnership with the Jagiellonian University in Krakow, Poland, as well as their Fellowship Programmes, and in part initiated by the European Research Training Network "ENRAGE". Since 2008 our group is annually hosting the Humboldt Research Prize Winner Professor Bernd A. Berg from Florida State University, Tallahassee, USA, for a few months. Further close contacts and collaborations are 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 topical Workshops and Tutorials and our International Workshop series *CompPhys: New Developments in Computational Physics*, taking annually place at the end of November just before the first advent weekend.

Wolfhard Janke

11.2 Large-Scale Computer Simulations of Spin Glasses

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One of the most challenging problems in the statistical physics of disordered systems is the nature of the low-temperature phase of spin-glass systems such as the short-ranged

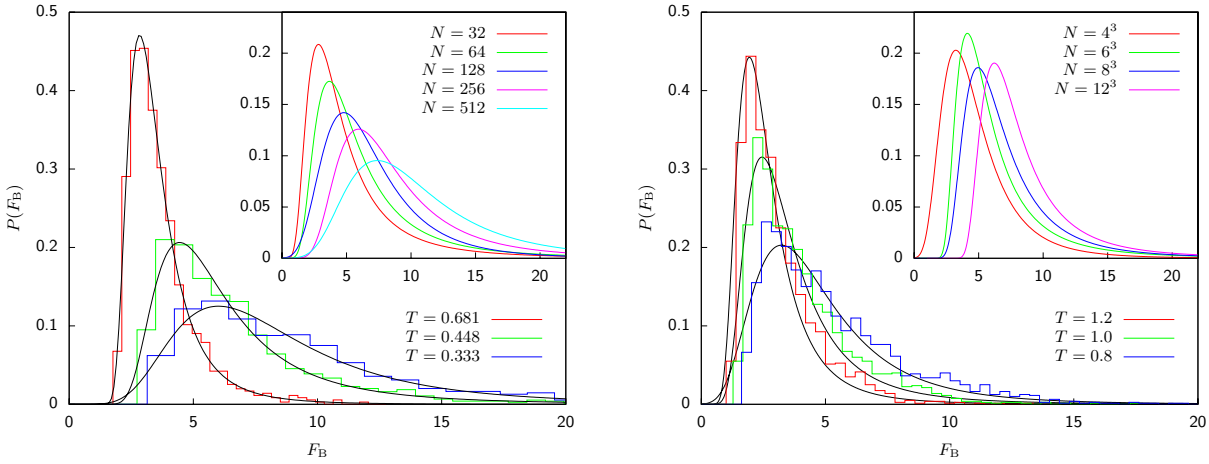

Figure 11.1: Left: Distribution of free-energy barriers F_B for the SK model with $N = 256$ spins at different temperatures. The inset shows the distribution for $T = 1/3$ for different numbers of spins. Right: The same type of graph for the EA model with $N = 4^3$ spins. The inset shows the distribution for $T = 0.8$ for different lattice sizes.

Edwards-Anderson (EA) and mean field Sherrington-Kirkpatrick (SK) models [1–3]. The origin of the numerical problems can be traced back to the combination of disorder and frustration which leads in the spin-glass phase for $T < T_c$ to a rugged free-energy landscape with probable regions separated by rare-event states [4]. Consequently, conventional Monte Carlo simulations tend to get stuck in local free-energy valleys. In this project we try to overcome this kind of problem by using a novel update algorithm which combines the parallel tempering method [5] with the multi-overlap Monte Carlo algorithm [6].

From large-scale computer simulations we obtained the free-energy barriers F_B characterizing these rare-event states. Their distribution becomes broader for lower temperatures and is expected to be represented by a Fréchet extreme-value distribution for fat-tailed distributions [7]. In general, extreme-value statistics can be classified into different universality classes, depending on whether the tails of the original distribution are fat tailed (algebraic), exponential, or thin tailed (decaying faster than exponential). Fitting our data with a generalized extreme-value distribution (GEV),

$$F_{\xi;\mu;\sigma}(x) = \exp\left[-\left(1 + \xi\frac{x-\mu}{\sigma}\right)^{-1/\xi}\right]$$

with $1 + \xi(x - \mu)/\sigma > 0$, we find a shape parameter $\xi > 0$, i.e., a Fréchet distribution. The distributions and fits are shown in Fig. 11.1. The histograms of the SK model for low temperatures show deviations from the Fréchet distribution for small values of F_B, so a much larger number of disorder realizations would be needed to determine both tails of the distribution properly. We determined the parameters σ, μ and ξ for different temperatures and found that σ grows linearly and μ logarithmically with inverse temperature $1/T$, whereas ξ stays more or less constant at $\xi \approx 0.33$. If we keep the temperature fixed and look at the size dependence of the distribution, we find that for a larger number of spins the distribution becomes broader, c.f. the inset of Fig. 11.1 (left). To quantify this behaviour we use the scaling relations $\sigma \propto N^{\alpha(\sigma)}$ and $\mu \propto N^{\alpha(\mu)}$, which lead to $\alpha(\sigma) \approx 0.25$ and $\alpha(\mu) \approx 0.31$ for our lowest temperatures.

We find a temperature dependence of the exponents $\alpha(\sigma)$ and $\alpha(\mu)$ with negative and positive slope for increasing T, respectively. For the EA model we also find fat-tailed distributions, but the broadening of the distribution with increasing number of spins is much weaker than for the SK model, see Fig. 11.1 (right).

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11.3 Shape Anisotropy of Polymers in Disordered Environment

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Topological properties of macromolecules, such as their shape and size, are of interest in various respects. The shape of proteins affects their folding dynamics and motion in a cell and is relevant in comprehending complex cellular phenomena, such as catalytic activity. The hydrodynamics of polymer fluids is essentially affected by the size and shape of individual macromolecules, and polymer shapes also play an important role in determining the molecular weight in gel filtration chromatography.

An obvious shape measure of macromolecules is provided by the normalized average eigenvalues λ_i of the gyration tensor. Their computation is, however, difficult because one must explicitly diagonalize the gyration tensor for each realization in an ensemble of polymers. It was therefore proposed to characterize the asymmetry of polymer conformations by rotationally invariant universal quantities, such as the averaged asphericity $\langle A_d \rangle$ and prolateness $\langle S \rangle$ [1, 2]. $\langle A_d \rangle$ takes on a maximum value of one for a completely stretched, rodlike conformation, and equals zero for spherical form, thus obeying the inequality: $0 \leq \langle A_d \rangle \leq 1$. The quantity $\langle S \rangle$, defined in $d = 3$ dimensions, takes on a positive value for prolate ellipsoidlike conformation, and is negative for oblate shapes, being bounded to the interval $-1/4 \leq \langle S \rangle \leq 2$, cf. Fig. 11.2.

In real physical processes, one is often interested in the behaviour of macromolecules in the presence of structural disorder, e.g., in colloidal solutions or microporous membranes. In particular, a related problem is relevant when studying protein folding dynamics in cellular environments which are highly disordered due to the presence

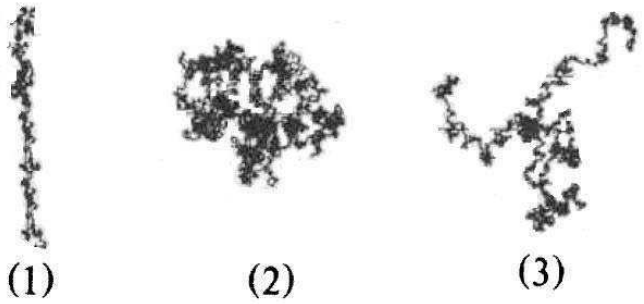

Figure 11.2: Schematic representation of a polymer chain conformation which is (1) rod-like, (2) almost spherical, and (3) oblate.

of a large amount of soluble and insoluble biochemical species occupying up to 40% of the total aquabased volume [3]. It is known that structural obstacles strongly effect protein folding and aggregation as well as their shape characteristics.

In this project we study a minimalistic lattice model [4] in which the allowed sites are restricted to the fractal structure of a percolation cluster and the polymers are modeled by self-avoiding walks [5, 6]. Applying the pruned-enriched Rosenbluth method (PERM) [7], we performed chain-growth computer simulations in $d = 2$ and $d = 3$ and obtained numerical estimates for the averaged asphericity, prolateness, and size ratio [8, 9]. All the shape characteristics increase gradually with increasing polymer chain length – the structure of a fractal percolation cluster drives the longer polymer chain conformations to become more and more prolate. Our results quantitatively indicate that the shape parameters of typical polymer conformations change significantly relative to the obstacle-free case: The shape tends to be more anisotropic and elongated due to the fractal structure of the disordered environment.

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11.4 Scaling Behaviour of Self-Avoiding Walks on Critical Ising Clusters

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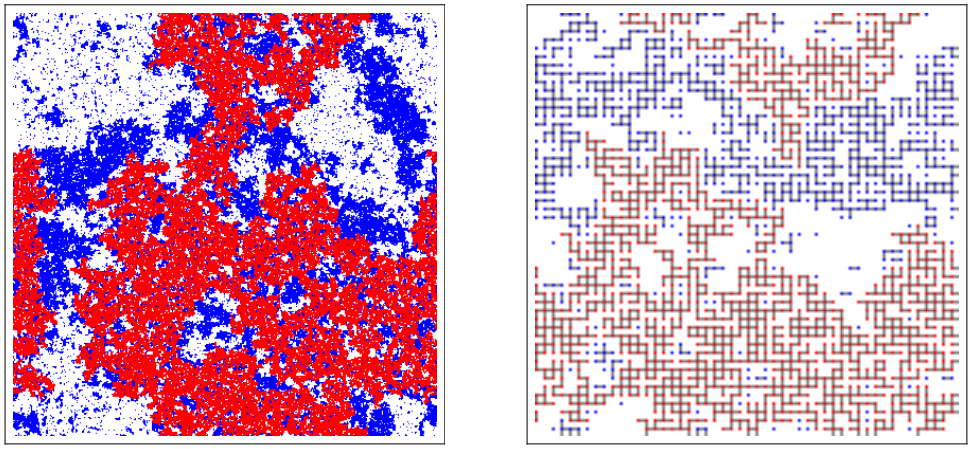
The discrete self-avoiding walk (SAW) is one of the most fundamental systems in the realm of statistical physics: It is the simplest non-trivial model for a polymer, and features universal asymptotic scaling behaviour, which is intimately related to the critical behaviour of spin systems. In particular, the exponent ν describing the scaling of the mean end-to-end distance $\langle R \rangle$ with the number of steps N ($\langle R \rangle \sim N^{\nu}$) is a universal quantity, depending only on fundamental properties of the system such as its dimensionality. Its value is non-integer, in general even non-rational, reflecting the SAW's fractal nature.

The case where the substrate itself has a non-Euclidean, fractal dimension is of particular interest and has attracted a considerable amount of attention in recent decades. Exact mathematical fractals have been investigated [1] as well as percolation clusters [2–4], which are an example of disordered, statistical fractals. However, the understanding of such systems is still far from being exhaustive. We therefore investigated SAWs on clusters occurring for the 2D Ising model at the critical temperature. These represent another type of statistical fractal whose properties have been extensively studied, see [5, 6]. Contrary to the percolation case, the disorder for this system is correlated, which may also effect the scaling behaviour.



(a) (b)

Figure 11.3: Ising model at criticality. In (a), the percolating Fortuin-Kasteleyn cluster is marked in red. Spins on the blue sites have the same alignment, but no connecting bonds to the percolating Fortuin-Kasteleyn cluster. In (b), active bonds between spins are displayed.

Monte Carlo methods were applied to both, creating the Ising clusters and simulating the SAWs. For the creation of the clusters a Swendsen-Wang type algorithm [7] has been used. The SAWs have been sampled using a chain-growth method, the so-called "pruned enriched Rosenbluth method" (PERM) [8]. Three slightly different situations have been studied: In the first cases, the walker was only allowed to move between sites belonging to the lattice-spanning Fortuin-Kasteleyn cluster [9] (red sites in Fig. 11.3(a)), which at criticality is a fractal object. In the second case, the walker

was allowed to visit all connected sites having the same spin direction (blue and red sites in Fig. 11.3(a)). Finally, the walker was only permitted to step between sites which are connected by a bond in the Fortuin-Kasteleyn representation [9] (Fig. 11.3(b)). All three structures have different fractal dimensions, and indeed, three distinct values for the exponent ν have been found. However, a systematic monotonous dependence on the Hausdorff dimension could not be established, indicating that other factors do also play a significant role.

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11.5 Mass Transport by Thermal Ratchets

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Non-equilibrium mass transport on nanoscopic scales through ratchet effects or Brownian motors has attracted much attention in the recent literature [1]. The basic ingredients for a ratchet are (i) a periodic but asymmetric potential and (ii) a mechanism to disturb thermal equilibrium, since the second law of thermodynamics forbids a net flux of particles otherwise. The disturbance can be a periodic variation of the potential (pulsating ratchet), a periodic driving force with vanishing average (tilting ratchet) or temperature variations in time (temperature ratchet) or space (Seebeck ratchet). Most ratchets and Brownian motors discussed in the literature consider single (independent) particles, but there are also a few examples using collective effects. Being out-of-equilibrium, Curie's principle predicts a non-zero effect due to the broken symmetry. But in general there is no direct way to predict the strength or even the direction of the effect. On variation of some parameters one even can create a current inversion. So one has to consult computer simulations or do experiments for specific informations.

We proposed a new thermal ratchet setup to model periodic but asymmetric pores filled with a binary liquid mixture with a liquid-liquid phase transition at temperature T_c. The three-dimensional pore geometry sketched in Fig. 11.4 depends on the two dimensionless length ratios $R_{\max}/R_{\min}$ and $L/R_{\max}$. For temperatures periodically switched between two temperatures above and below T_c, one expects asymmetric mass transport, moving the two types of liquids in different directions. The considered system can be classified as a collective temperature ratchet with an entropic potential. The role of the potential is played by the varying diameter of the pores effectively producing entropic barriers. The phase transition is then used to trigger the ratchet effect

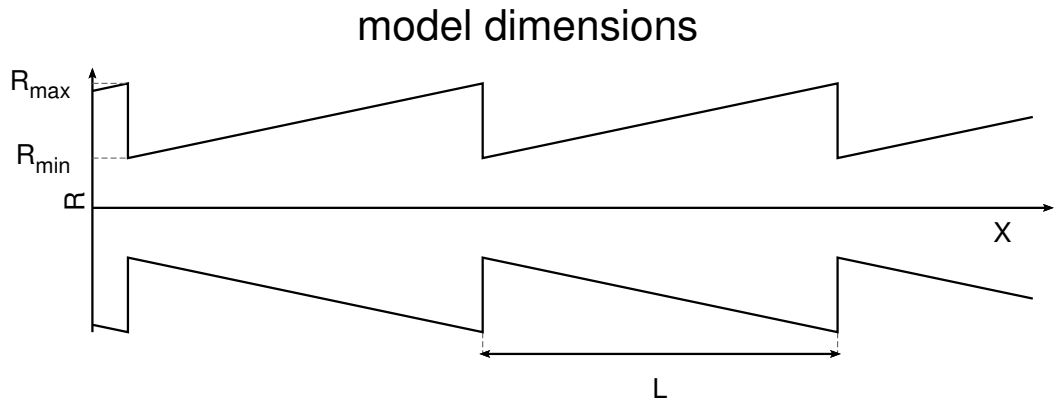

Figure 11.4: Geometry parameters of the proposed ratchet model, characterized by the pore radii $R_{\min}$ and $R_{\max}$ and the segment length L of long three-dimensional channels. In the computer simulations, we set $R_{\max}/R_{\min} = 5$ and $L/R_{\max} = 4$.

by switching between droplet formation and dissolution. This phase transition is the crucial ingredient making the proposed system an example for a generally new class of ratchets.

Computer simulations were performed to provide at least qualitative answers to the problem of how to optimize the profile and the diameter of the pores and the temperature schedule, in order to obtain a maximal ratchet effect. The simulations were kept as simple as possible. This is partly due to the fact that most of the advanced simulation techniques rely on thermal equilibrium to hold [2], whereas for the ratchet effect to occur, this must be broken. In effect, simple random walk simulations (dynamical Monte Carlo) were performed to investigate the driven diffusive behaviour. In a first step, we studied independent "pointlike" random walkers confined to the three-dimensional periodic pores modeled by hard walls forming cells. The geometry parameters were chosen as $R_{\max}/R_{\min} = 5$ and $L/R_{\max} = 4$. Starting all walks from a given fixed position x_0 on the central axis of the pore ($R = 0$), during the first steps a net drift could be observed, before the system reached equilibrium. This simulation would model the part of the ratchet, when one of the two liquids has formed droplets which sit on average at a given position inside each cell, and the temperature is raised above T_c so that now free diffusion is possible. The observed net drift depends in strength and direction on the chosen starting position, also including a neutral position from where no drift would result. In a second step, the average position of the droplets was determined again by independent random walks in the same geometry, but this time the particles had a non-zero extent, making the entropic barriers much more severe. The average position deviated slightly from the neutral position mentioned above, thus leading to a ratchet effect. However, the drift and thus the resulting ratchet effect turned out to be always so small that up to now no reliable predictions for the optimal pore geometry of this model system could be obtained.

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11.6 Stochastic Transport Models

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Stochastic transport processes out-of-equilibrium are of importance in many different fields of physics. Examples are traffic flow, ranging from macroscopic applications to pedestrian or car traffic down to the intracellular level, force propagation in granular media, aggregation and fragmentation of clusters, and many others [1]. The transport is classically modeled by probabilities for hopping events from one site to another. Since such processes are in general out-of-equilibrium and specified in terms of dynamical rules without any energy concept, it is difficult to predict and classify the possible stationary states and to identify transitions between phases like a liquid phase or a phase with a condensate ("traffic jam") that are associated with the different stationary states. In particular one observes the phenomenon of spontaneous symmetry breaking already in one-dimensional systems, in which the symmetry breaking manifests itself in the spontaneous formation of a condensate: A finite fraction M' of constituent particles condenses onto a finite extension W in space (sometimes even on a single site) in the thermodynamic limit, in which the number of particles M along with the volume N is sent to infinity, with the density $\rho = M/N$ fixed.

In this joint DFG project with the Jacobs University Bremen and in collaboration with the University of Edinburgh we concentrate on a class of models which lead to steady states that factorize over the links of arbitrary connected graphs, so-called pair-factorized steady states (PFSS) [2–4]. This enables at least partially an analytic treatment of the transport properties. For systems in one and two dimensions we derive the phase structure from these states, in particular the transition from a liquid phase to a phase with a condensate. In one dimension we predict the critical mass density at the transition, the shape of the condensate, and its scaling with the system size. The shape of the condensate is not universal, but can be tuned from an extended to a localized one via the competition of local (K) and ultralocal (p) interactions that are implemented in the hopping rates. In the equivalent language of solid-on-solid (SOS) models in the context of surface roughening [5] this corresponds to the energy $E = -\ln K(|m-n|) - (1/2)\left[\ln p(m) + \ln p(n)\right]$ of an interface within a 1+1-dimensional space (where the interface refers to the envelope of occupation numbers m and n at neighboring sites) [6]. The resulting phase diagram for the choice $K(x) \propto \exp(-x^\beta)$ and $p(m) \propto \exp(-m^\gamma)$ and the exponent α in the predicted scaling behaviour of the condensate extension, $W \sim M'^\alpha$, are shown in Fig. 11.5.

Many of these usually approximate analytic predictions for pair-factorized steady states have been confirmed by computer simulations of the hopping events. This also allowed us to study dynamic properties of the condensation process which is governed by a time scale $\tau \propto M^\delta$, where the dynamical exponent δ depends on symmetry properties of the hopping dynamics: For a spatially *asymmetric* hopping rule we find $\delta \approx 2$, whereas for *symmetric* hopping $\delta \approx 3$, similar to the previously observed behaviour of simpler, ultralocal zero-range processes (ZRPs).

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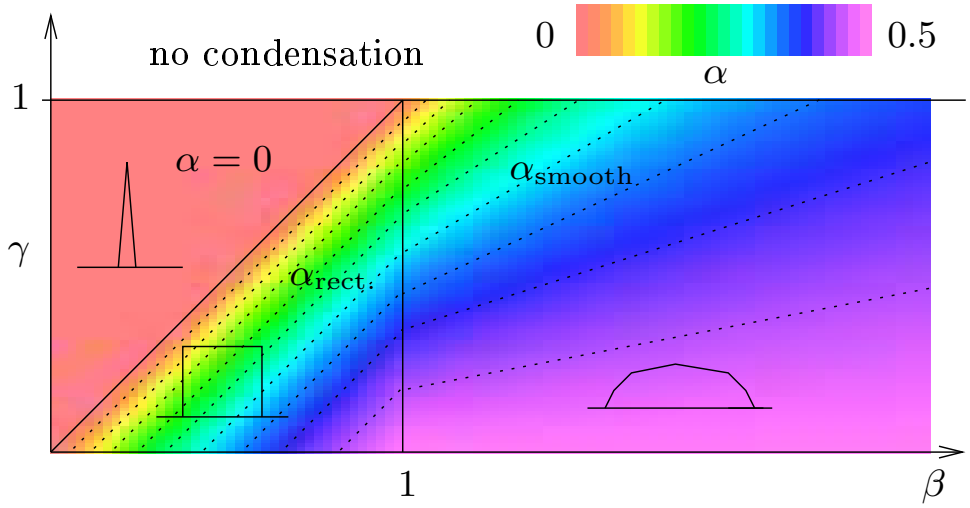

Figure 11.5: Phase diagram for $K(x) \sim e^{-x^\beta}$ and $p(m) \sim e^{-m^\gamma}$. Values of the exponent α in the scaling law for the extension W of the condensate with the number M' of condensed particles, $W \simeq M'^\alpha$, $\alpha_{\rm rect} = (\beta-\gamma)/(\beta-\gamma+1)$ for a rectangular and $\alpha_{\rm smooth} = (\beta-\gamma)/(2\beta-\gamma)$ for a smooth condensate, are represented by the color (gray) code. The dotted lines show $\alpha = 0.05, 0.1, \ldots, 0.45$ (from left to right).

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11.7 Birth of the First Large Condensation Droplet

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The "birth" of the first large droplet in condensation phenomena is an important problem in many physical systems, ranging from atoms to colloids to macromolecules. With early theoretical work dating back to the 1960s, this problem has been taken up many times and further advanced both analytically and numerically. Yet, there are still many open questions we try to answer in this project. One goal is to evaluate by how much asymptotic theoretical predictions are affected by finite-size effects. A second goal is to test the degree of universality suggested by the analytical treatment. Finally, we also study the free-energy barrier associated with the "birth" of the first large droplet.

The results of our extensive Monte Carlo simulations of the two-dimensional Ising lattice-gas model [1–3] clearly confirm the asymptotic predictions of Biskup et al. [4, 5] and extend them to practically accessible system sizes. The observed finite-size scaling behaviour matches perfectly with the predicted infinite-volume limit. By comparing

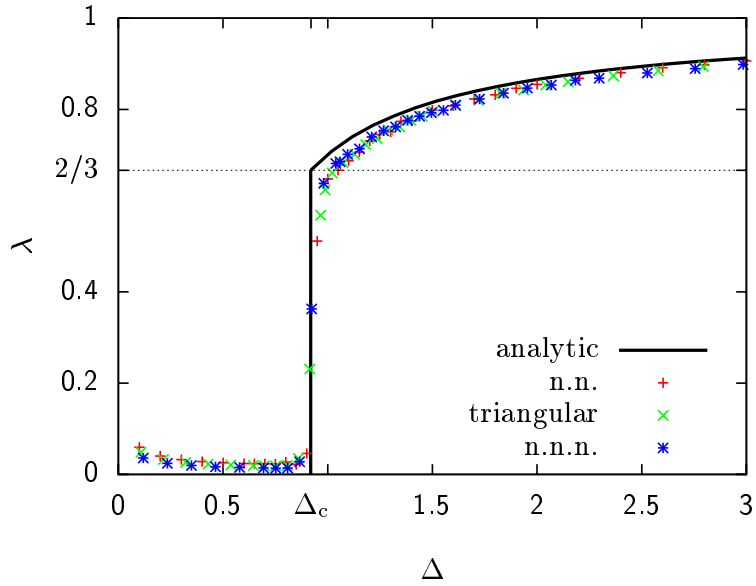

Figure 11.6: Comparison of the fraction λ of particles in the largest droplet for the three considered Ising models: NN square, NN triangular, and NNN square lattice. In all three cases the lattice size is $L = 640$ and the simulation temperature was chosen as $T \approx 0.66\, T_c$.

square and triangular lattices with next-neighbour (NN) interactions and a square lattice with next-nearest-neighbour (NNN) interactions, we obtained recently compelling evidence for the insensitivity of the droplet condensation mechanism to microscopic details provided the reduced temperature T/T_c is kept fixed [6], see Fig. 11.6. For technical reasons, the mathematical work of Biskup et al. only applies to *square* lattices with *NN* couplings. Our results thus show that the theoretical arguments can indeed be carried over to other lattice types and interactions as well, as expected on physical grounds. All simulations were performed in thermal equilibrium and the suppression of droplets of intermediate size could be unambiguously verified.

We also measured the distribution of the fraction λ of particles in the largest droplet [6]. The observed double-peak structure at the evaporation/condensation transition point implies a free-energy barrier, similar to a first-order phase transition. By analyzing the ratio of peak maximum to minimum in simulations with fixed magnetisation (adjusted such that the two maxima agree) for different lattice sizes L, we clearly observe an exponential scaling $\simeq \exp(c\, L^{2/3})$ compatible with the theoretical expectation. Alternatively, by measuring (integrated) autocorrelation times τ_{int} in simulations with the magnetisation fixed directly at the evaporation/condensation point, we also find a compatible asymptotic scaling behaviour $\tau_{\text{int}} \simeq \exp(c\, L^{2/3})$. In both cases, however, the parameter c is difficult to determine reliably with the present data sets. Presumably much larger lattices are needed to arrive at a firm estimate.

Currently we are performing simulations and analyses for the three-dimensional case, where a similar behaviour is expected in the thermodynamic limit. In three dimensions it appears, however, numerically much harder to reach the scaling region. Once the relevant length scales are fully understood, off-lattice simulation studies with Lennard-Jones particles in a similar vein would be a very interesting future project with many applications of practical relevance.

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11.8 Hierarchies in Peptide Nucleation Transitions

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Understanding cooperative effects leading to structure formation of polymers is a challenging problem of statistical mechanics and thermodynamics. An important example is the aggregation of macromolecules which can be considered as a special case of nucleation processes. In biosystems, the aggregation of peptides can lead to plaque formation, often with disastrous consequences. A prominent example is the aggregation of Aβ peptides in the human brain which is associated to the neurodegenerative Alzheimer's disease.

Structural properties of interacting polymers can be well described by means of simple, coarse-grained "bead-stick" models with typically Lennard-Jones interactions among the monomers [1–3]. In this work [4] we considered the aggregation of up to four peptide chains with 13 monomers each, modeled by the minimalistic hydrophobic-polar AB model [5, 6] where only two types of residues, hydrophobic (A) and hydrophilic (B) ones, line up in a linear heteropolymer sequence. All four chains have the same Fibonacci sequence $AB_2AB_2ABAB_2AB$ [4]. Employing multicanonical computer simulations we determined the density of states $g(E)$, giving immediately the microcanonical entropy $S(E) = k_B \ln g(E)$ and temperature $T(E) = [\partial S(E)/\partial E]^{-1}$ [1–3]. The entropy turned out to be a convex curve in the aggregation transition region as is characteristic for a first-order-like nucleation transition of a finite system [7, 8]. The details of the transition regime are high-lighted in Fig. 11.7 where the (microcanonical) temperature $T(E)$ is shown. In this plot the various stages or subphases of the nucleation prosess are clearly reflected by the oscillations in the transition region. Representative conformations in the different structural phases are depicted in the right panel.

For high energies $e > e_{\text{frag}} \approx 0.05$ all chains can form individual conformations, almost independently of each other, and are hence fragmented. If two chains aggregate (subphase 1 in Fig. 11.7), the translational entropy of the individual chains is reduced by $k_B \ln V$, where V is the volume (corresponding to the simulation box size), but this is overcompensated by the more favorable (= lower) energy of the aggregate compared to the fragmented chains. Here, the energy associated with the interaction between different chains, i.e., the cooperative formation of *inter*-chain contacts between residues of different peptides, is highly relevant. In a subsequent step an additional peptide joins the two-peptide cluster and the system enters subphase 2. This procedure continues

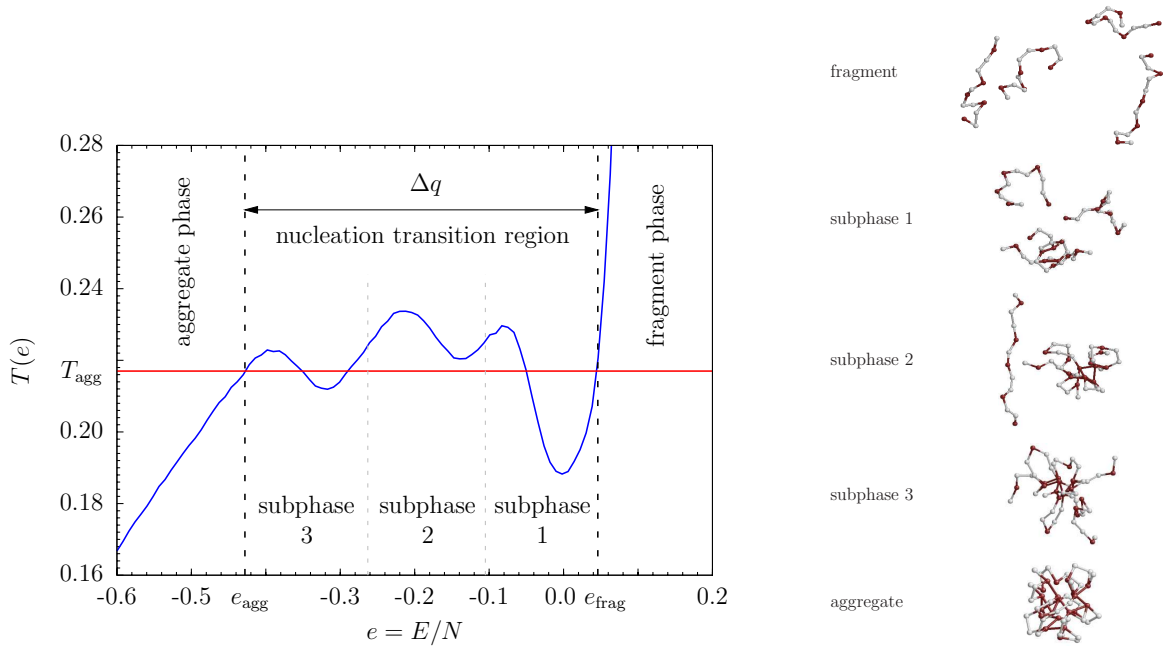

Figure 11.7: Left: Microcanonical temperature in the nucleation transition regime. The horizontal so-called Maxwell line marks the aggregation temperature T_{agg} , obtained by a Gibbs construction [7]. Right: Representative conformations in the different structural subphases of the peptide aggregation process.

until for $e < e_{agg} \approx -0.43$, conformations of a single, entangled aggregate, composed of all four peptide chains forming a hydrophobic core, dominate.

Our data thus show that heteropolymer aggregation can be understood as a composite nucleation processes consisting of hierarchical subphase transitions, each of which exhibits features of first-order-like transitions. A closer look into the data reveals that with an increasing number of chains the strength of the subphase transitions becomes weaker and weaker. This suggests that in the thermodynamic limit of infinitely many chains the first-order nucleation process is composed of an infinite number of infinitesimally "weak" first-order-like subphase transitions.

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11.9 Polymer Crystallization with Advanced Multicanonical Monte Carlo Methods

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This project is devoted to numerical investigations of the freezing or crystallization transition of a single elastic polymer [1, 2]. In the model that we employ the bond length is adaptive in a way that highly symmetric conformations can form in the crystalline phase. By means of multicanonical Monte Carlo computer simulations we identified a nontrivial systematic chain-length dependence that is associated with the type of growth of the nucleus. However, a conventional scaling behaviour has not been found – it simply does not exist. This is also known from atomic clusters [3]. A particularly sharp transition signal from fluctuating quantities, such as the specific heat, is obtained for "magic" chain lengths $N = 13, 55, 147, 309, \ldots$. In these cases almost perfect icosahedra can form which are particularly stable and typically represent the core cells in the structure formation of longer chains [1, 2].

To arrive at these results a couple of algorithmic improvements were necessary which we developed along the way [4]. First, we introduced energy-dependent step lengths of the proposed Monte Carlo moves that enable a novel general optimization scheme for systems with continuous degrees of freedom. Key to this idea is a bias correction in the acceptance criterium. Applying this procedure to multicanonical sampling with a flat energy distribution one obtains constantly high acceptance rates everywhere in energy space and hence reliable estimates of the density of states over several *thousands* of orders of magnitudes.

The second methodological improvement concerns the types of proposed update moves. We proposed two bond-exchange moves which allow the reordering of polymer bonds without alteration of monomer positions, cf. Fig. 11.8(a) and (b). Moreover, with the monomer cut-and-paste update sketched in Fig. 11.8(c) we introduced a novel Monte Carlo move which increased the efficiency of the simulation further in two ways. First, the update allows the tunneling of energy barriers in the solid phase and second, it performs larger changes in the unstructured globular and random-coil phases.

The third class of improvements deals directly with the multicanonical method. By enabling variations in system size at runtime we extended the multicanonical ensemble to treat also the monomer number in a "dynamical" way. This led to an additional gain in efficiency since the thus modified algorithm was able to circumvent certain energy barriers or to penetrate them where they are low, i.e., at their "weak" points. As a result we obtained information about the entire state space over a large polymer-size interval from a single simulation. Finally, confronted with the problem of broken ergodicity and low-temperature solid-solid transitions, we developed a second extension to the standard multicanonical technique. Due to the application of additional weight functions it is possible to retain ergodicity and to reach "hidden" ground states by circumventing the "blocking" states at intermediate temperatures. Although we yet have demonstrated the potential of this method for homopolymers only, it is a general approach and, in combination with suitable order parameters, it might lead to substantial

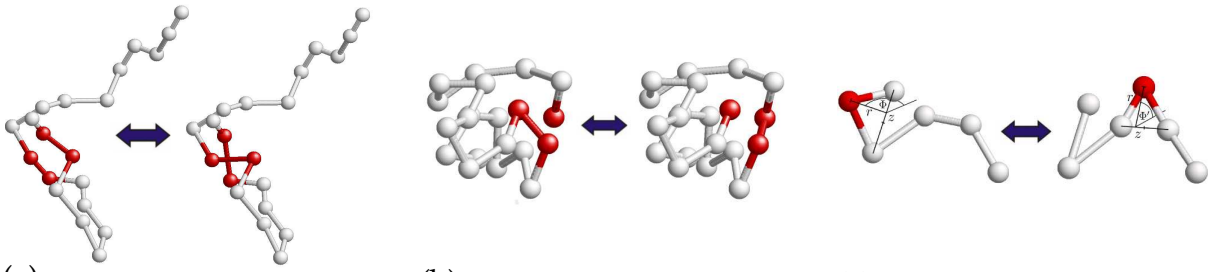

Figure 11.8: (a) Bond-exchange, (b) end-bond-exchange, and (c) monomer cut-and-paste update moves.

progress in the investigation of many other systems as well.

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11.10 The Influence of Grafting onto Freezing, Collapse and Adsorption of a Single Polymer in Solution

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In our previous studies of macromolecular adsorption transitions [1, 2] it turned out that a combined canonical and microcanonical analysis is able to reveal some properties that are hidden in a purely canonical approach [3]. We therefore extended this method to all other transitions a polymer of finite length close to an attractive substrate undergoes [4]. We studied a simple bead-stick model with 12–6 Lennard-Jones (LJ) interaction between nonbonded monomers, a weak bending stiffness and an attractive interaction with a flat substrate at $z = 0$ that is proportional to a parameter ϵ_s. This surface attraction is a 9–3 LJ potential obtained by integrating the 12–6 LJ potential over a half space and, e.g., $\epsilon_s = 5$ roughly gives a surface attraction that exceeds the monomer-monomer attraction by a factor of five. To evaluate the influence of the translational entropy and the restrictions of the commonly studied grafted case, the polymer is once considered in a box within which it can move freely and once with one end grafted to the substrate.

The goal was to rediscover all transitions in the microcanonical entropy, which is proportional to the logarithm of the density of states. To this end we analyzed its slope and curvature as well as other observables as a function of energy. For an example, see Fig. 11.9. This provides additional information, e.g., about the nature of the transition. Due to the finite size of the polymer the two ensembles are not equivalent and also the nature of the transition can still differ from the limiting infinite-size behaviour as was

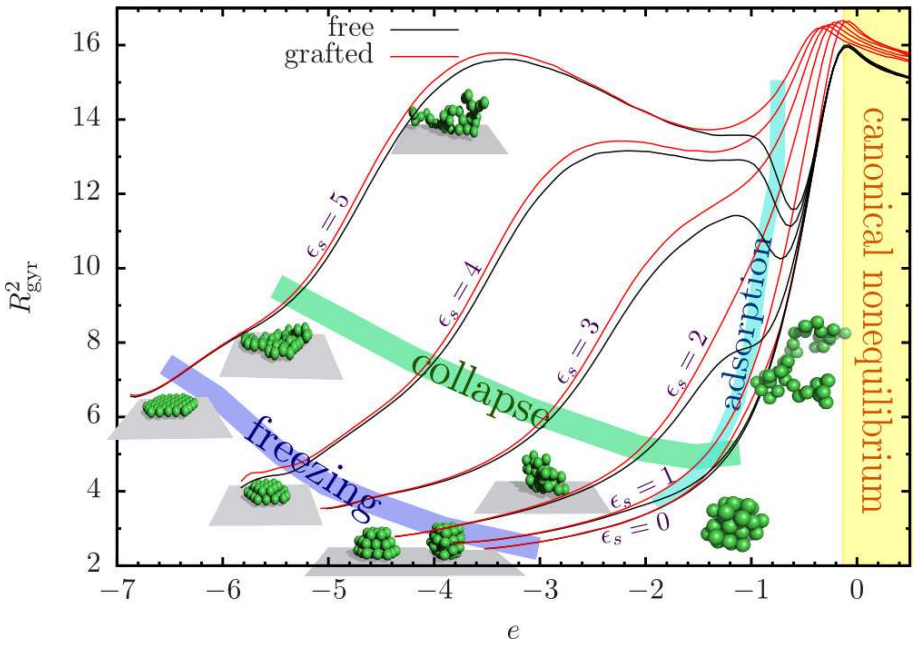

Figure 11.9: The radius of gyration squared R^2_{gyr} versus energy per monomer e for several surface attraction strengths ϵ_s. The energy regimes of the main transitions are indicated and the pseudophases are illustrated by exemplified conformations. Depending on ϵ_s the collapse occurs at higher or lower e than the adsorption.

indeed found for the freezing and adsorption transitions. The former is not strongly affected by the grafting, since the fraction of forbidden conformations due to the constraint is comparable above and below the freezing. But the first-order-like nature of this transition only arises if the chain exceeds a certain length, whereas short chains exhibit a continuous freezing transition. The adsorption transition, however, is strongly affected by the grafting. Here, both, the translational and conformational entropy of desorbed polymers are much stronger restricted by the grafting than of adsorbed polymers. One consequence is a first-order-like adsorption for short free chains and strong surface attraction, while grafted polymers always adsorb continuously.

All simulations were performed with the parallel tempering Monte Carlo method that allowed to highly parallelize the simulation and obtain good statistics over the whole energy range [4].

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11.11 Thermodynamics of Polymer Adsorption to a Flexible Membrane

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The interaction of macromolecules with cell membranes is essential for almost all biological processes. Membrane proteins like glycoproteins and transmembrane proteins govern the exchange of signals, small molecules, and ions between the intra- and extracellular solvent. Membrane embedded receptors are specific for the binding of ligands. The conformational changes caused by the binding process can, e.g., trigger cellular motion, drug delivery, or enzymatic catalysis.

It is therefore an important problem to investigate the conformational behaviour of a polymer interacting with a *flexible*, *fluctuating* substrate such as a membrane under thermal conditions. So far much work has been dedicated to the identification of structural transitions polymers and peptides experience when adsorbing to *solid* substrates [1–3]. In this project we extend these studies by considering a simple coarse-grained off-lattice model system consisting of a polymer grafted to a fluctuating substrate and performing extensive generalized-ensemble Monte Carlo computer simulations [4]. Adjacent monomers of the polymer are tied together by a finitely extensible nonlinear elastic (FENE) potential and all monomers interact pairwise via a standard 12–6 Lennard-Jones (LJ) potential. The fluctuating substrate is modeled by a tethered membrane with the individual building segments (nodes) again tied together by a FENE potential according to a square lattice structure with $L_x \times L_y$ nodes in total. Finally, the interaction between the polymer, which is anchored at the membrane center, and the membrane is modeled by another LJ potential between all pairs of monomers and membrane nodes.

By means of extensive parallel tempering Monte Carlo simulations we have shown that the system exhibits a rich phase behaviour ranging from highly ordered, compact to extended random coil structures and from desorbed to completely adsorbed or even partially incorporated conformations, cf. Fig. 11.10. These findings are summarized in a pseudophase diagram indicating the predominant class of conformations as a function of the external parameters temperature and polymer-membrane interaction strength. By comparison with adsorption to a stiff membrane surface it is shown that the flexibility of the membrane gives rise to qualitatively new behaviour. At low temperatures, we found the membrane adapting its structure such that it partially incorporates the polymer. This leads to the "embedded compact" (MC), oblate shaped and the "embedded expanded" (ME), almost linearly stretched conformations shown in Fig. 11.10, which both most clearly reflect the influence of the back-reaction between polymer and membrane fluctuations.

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[2] M. Möddel et al.: J. Phys. Chem. B **113**, 3314 (2009)

[3] M. Möddel et al.: Phys. Chem. Chem. Phys. **12**, 11548 (2010); and *Adsorption of finite polymers in different thermodynamic ensembles*, to appear in Comp. Phys. Commun., in print (2011)

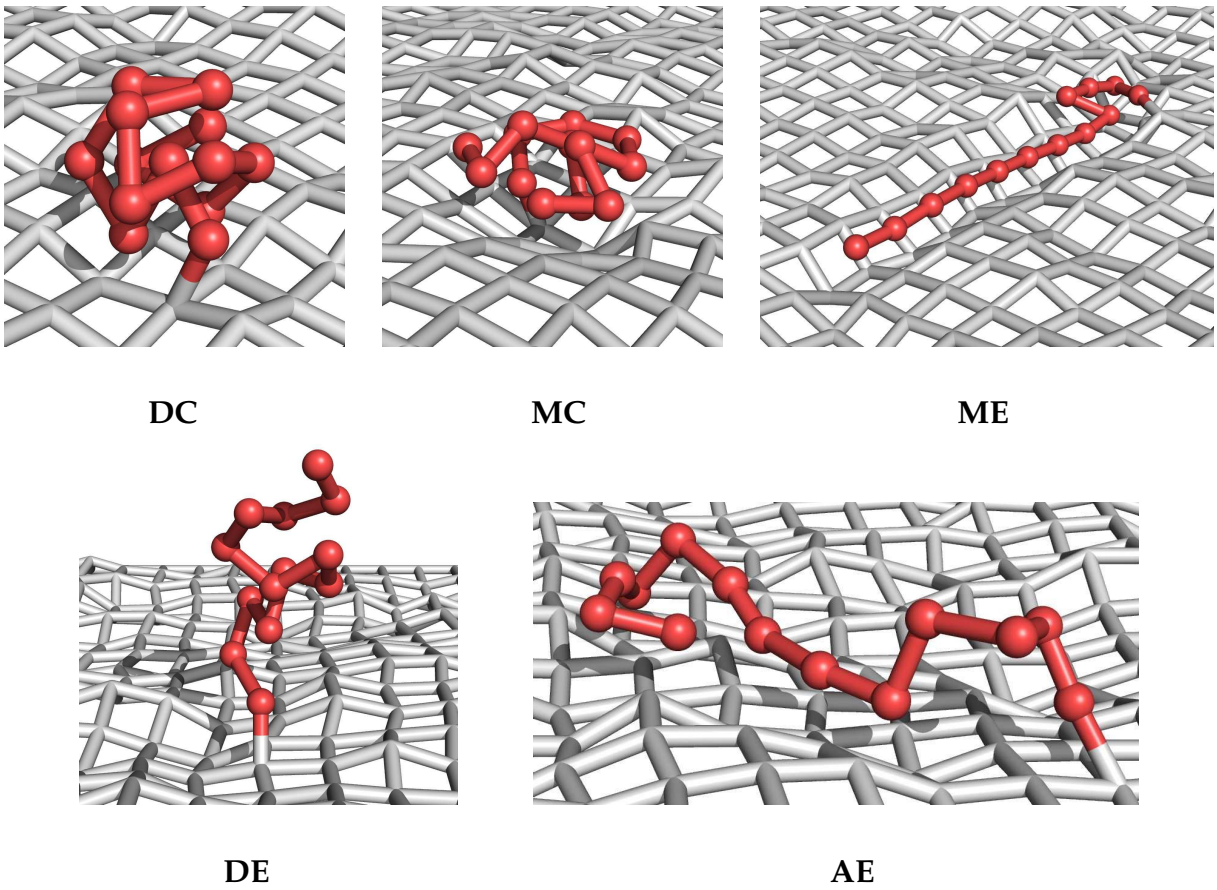

Figure 11.10: Typical conformations of a polymer grafted to a flexible membrane. The letter code classifies the polymer shapes (DC: desorbed compact; MC and ME: embedded compact and expanded; DE and AE: desorbed and adsorbed expanded).

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11.12 Microscopic Mechanism of Peptide Adhesion to Semiconductor Substrates: Simulations and Experiments

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[‡]Institut für Biochemie
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In the past few years, the interest in hybrid systems consisting of "soft" molecular matter and "hard" material substrates has rapidly grown as these are relatively easily accessible candidates for novel biosensors or electronic devices [1]. One important

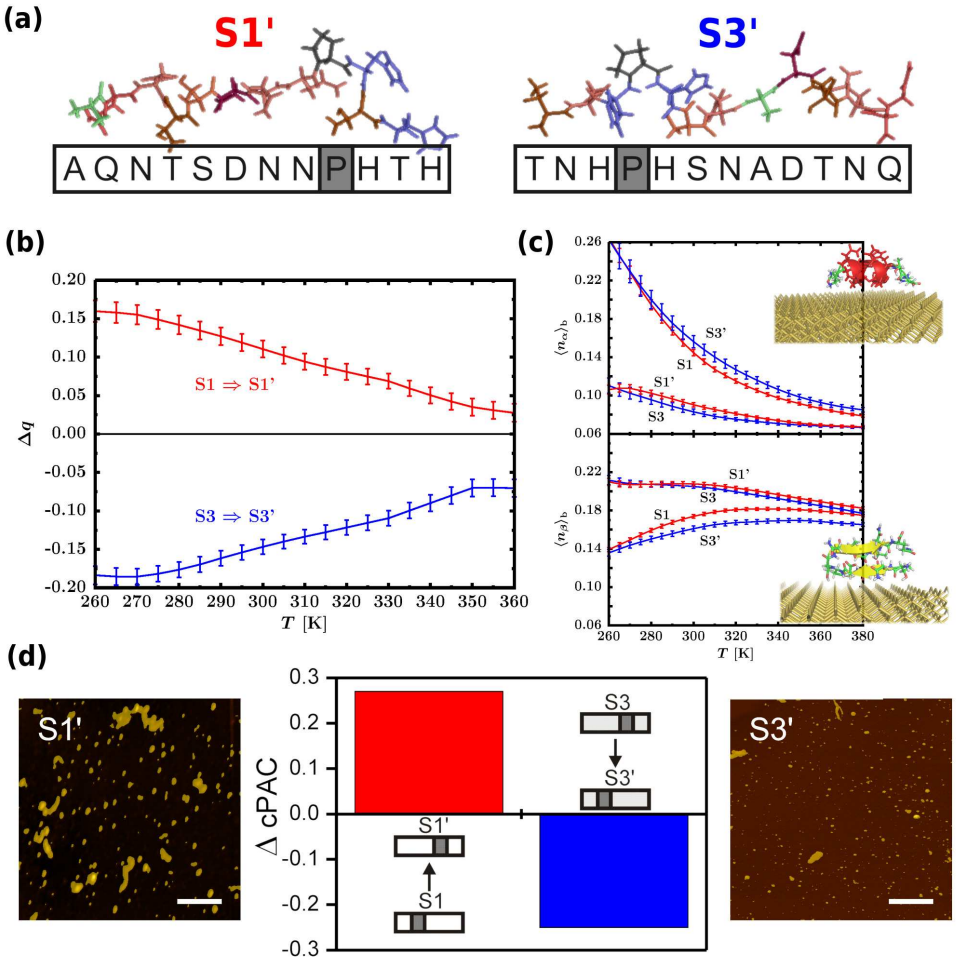

Figure 11.11: Reversed adsorption propensity of (a) the proline-mutated peptides S1′ and S3′. (b) Adsorption parameter Δq and (c) α-helix content $\langle n_\alpha \rangle_b$ and β-strand content $\langle n_\beta \rangle_b$ of bound peptides versus temperature as obtained in our computer simulations. The peptide conformations depicted in the insets are the identified (but at room temperature rather weakly occupied) lowest-energy structures representing the preferred trends in secondary-structure formation. (d) Confirmation by AFM experiments (scale bar = 1 mm) at room temperature.

property is the adhesion propensity of polymers, proteins, or protein-like synthetic peptides to solid materials such as, e.g., metals [2] and semiconductors [3–5]. Basic theoretical considerations of simplified polymer-substrate [6, 7] and protein-substrate [8] models have predicted complex pseudophase diagrams.

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 it is not yet understood how this is related to the individual molecular structure of the peptides. In this joint project with experimentalists and biochemists within the BuildMoNa collaborative project we show by means of computer simulations and experiments that the adsorption properties of synthetic peptides at semiconductor surfaces exhibit a clear sequence-dependent adhesion specificity [9]. Our Monte Carlo simulations of a novel hybrid peptide-substrate model reveal “in silico” in particular the strong correlation between

proline mutation and binding affinity to a clean (100) silicon substrate. Subsequently, in atomic force microscopy (AFM) experiments with the mutated amino-acid sequences synthesized according to our theoretical predictions, we could confirm "in vitro" the relevance of the selective mutations upon adhesion, cf. Fig. 11.11.

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[6] M. Bachmann, W. Janke: Phys. Rev. Lett. **95**, 058102 (2005); Phys. Rev. E **73**, 041802 (2006)
[7] M. Möddel et al.: J. Phys. Chem. B **113**, 3314 (2009); Phys. Chem. Chem. Phys. **12**, 11548 (2010)
[8] M. Bachmann, W. Janke: Phys. Rev. E **73**, 020901(R) (2006)
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11.13 Replica-Exchange Simulations of Polymers on GPUs

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Computer simulations have become a fundamental pillar in physics. This is particularly apparent in structural biophysics and polymer physics, where many-body interactions and disorder effects cannot be tackled by means of analytical approaches alone. However, despite large advances in the design of central processing unit (CPU) architectures, the computation time for simulations on single CPU systems can become interminable. One way around this problem is parallel computing using a message passing interface (MPI) on clusters or multithreaded programming on multicore CPUs. A currently rapidly emerging third approach are computations on graphics processing units (GPUs) with their massively parallel architecture (see Fig. 11.12), whose power has been driven originally mainly by the professional computer gaming industry. With the latest release of NVIDIA's convenient programming language CUDA, GPUs have also become quite popular in scientific applications [1, 2].

The purpose of this project was to evaluate whether GPU simulations can also quite efficiently be performed for off-lattice polymer models without the need of highly sophisticated tricks of implementation. By employing straightforward parallel tempering (replica-exchange) Monte Carlo simulations, we investigated the possible speed-up provided by the massive parallelization on GPUs. We tested the two GT200-based GPUs Tesla C1060 and GTX285 with 240 cores and NVIDIA's new generation Fermi-based GTX480 card with 480 cores. As reference CPU system one core of a quadcore Xeon E5620 processor was considered [3, 4].

With the most naive implementation of distributing the replica of the parallel tempering algorithm over the cores, only moderate speed-up factors of about 6 to 9 could

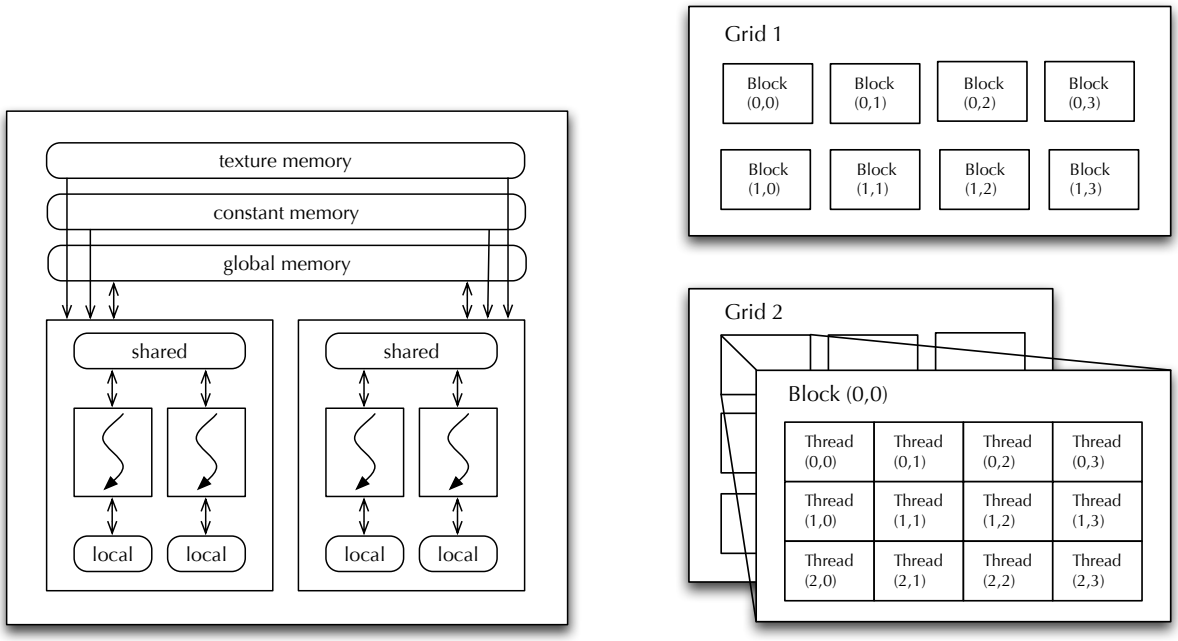

Figure 11.12: Memory layout on a GPU device (left) and grids with thread blocks (right).

be achieved. Having observed that, an improved version was implemented with a parallel calculation of the energy function. This implementation is much faster than the CPU version, when more than 2 replica are simulated. The maximum speed-up factor for the Tesla C1060 card is 68, for the GTX285 card it is 78 and for the Fermi-based GTX480 card even 130. Furthermore it is possible to access multiple graphics cards in a single workstation from one and the same program with no extra effort. Also nodes of established cluster computers can be equipped with GPUs, a combination of the traditional message passing interface (MPI) and CUDA is used in such a scenario. Thus GPUs promise great gains in productivity as well as energy efficiency and are already now on their way to enter the architecture of the next-generation supercomputers [5, 6].

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[6] The Green500 List: Environmentally responsible supercomputing, http://www.green500.org

11.14 Ground-State Analysis of Tip4p Water Parameterizations in the Ice I_h Phase

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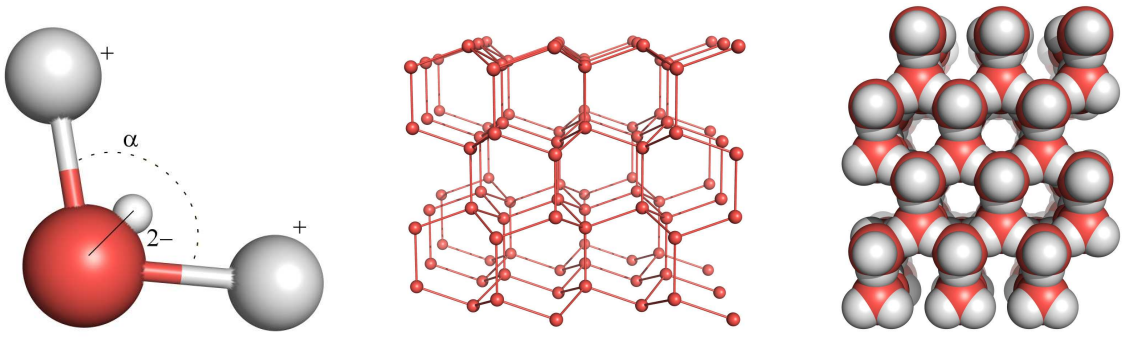
Today, many computer simulations are performed in order to investigate processes on a biological or chemical scale, often involving water molecules. Simulating over large temperature ranges, it has to be ensured that the water model behaves correctly over the whole range. Because of its frequent use, we investigated the Tip4p (*4-point-transferable-intermolecular-potential*) water model [1], with four points of interaction (see Fig. 11.13). It describes rigid molecules with 12–6 Lennard-Jones (LJ) interaction between oxygen atoms (r_{OO}) and Coulomb interaction between charges q_i , q_j from different molecules. The interaction Hamiltonian between two molecules (a, b) is given by

$$\mathcal{H}^{ab} = k_C \sum_{i}^{\text{in a}} \sum_{j}^{\text{in b}} \left(\frac{q_i q_j}{r_{ij}} \right) + \frac{TipA}{r_{OO}^{12}} - \frac{TipC}{r_{OO}^{6}}, \tag{11.1}$$

where k_C is the Coulomb constant and $TipA$, $TipC$ are specified by the parameterization [1–3].

In our study, we analyzed the ground states of water molecules in the ordinary ice phase (ice I_h) known from day-to-day life. In this phase, the oxygen atoms are arranged in a hexagonal lattice (see Fig. 11.13), forming tetrahedra with their four nearest neighbors. A valid ground-state configuration requires that exactly one hydrogen atom lies between two neighboring oxygen atoms. Thus, there exist multiple (in principle degenerate) ground states [4, 5].



(a) (b) (c)

Figure 11.13: (a) Tip4p water model with a rigid angle α and 4 points of interaction, namely the two hydrogen atoms (white), the oxygen atom (red) and the oxygen charge (small white) shifted along the dipole out of the oxygen, (b) hexagonal lattice formed by the oxygen positions in the ordinary ice phase, and (c) spherical occupation of the water molecules in the hexagonal layer, showing vacant shafts.

It was possible to show that the Tip4p water model provides stable hexagonal ice I_h ground states, with the lattice constant depending on the parameterization and the ground-state energy degeneration being slightly lifted [6].

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11.15 Quantum Critical Phenomena in Uniform and Mixed Heisenberg Spin Chains

R. Bischof, W. Janke

The quantum Heisenberg model (which, here, stands synonymously for all its generalizations) is one of the most fundamental models of quantum magnetism. High-temperature superconducting cuprates can be successfully described as 1D and 2D quantum antiferromagnets at low doping. Above that, it exhibits a rich variety of zero-temperature quantum critical phenomena, depending on the specific choice of spins and different types of coupling mechanisms. 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 [1]. 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.

In order to investigate quantum critical phenomena of mixed anisotropic Heisenberg (XXZ) spin chains with bond alternation we use self-implemented versions of the continuous time loop algorithm [2] and Lanczos exact diagonalization. Specifically, we consider two different mixed 1D quantum XXZ models consisting of two different kinds of spins, $S_a = 1/2$ and $S_b = 1$ or $3/2$, that appear alternatingly in pairs [3]. By successful generalization of recently proposed quantum reweighting methods [4] to improved estimators of the loop algorithm, we have been able to determine the phase diagram in the XY-like region to high precision. In the following analysis we could establish a line of continuously varying critical exponents which strongly suggests that mixed spin chains are in the Gaussian universality class characterized by a central charge of $c = 1$. Furthermore, we could show the presence of logarithmic corrections in our mixed spin models at the SU(2) symmetric isotropic point. These logarithmic corrections influence the scaling and finite-size scaling behaviour on all length scales, which makes the extraction of critical exponents particularly difficult. It is well known that the homogeneous spin chains of $S = 1$ do exhibit such types of corrections [5].

We have identified several scaling dimensions that can all be parametrized in terms of one fundamental parameter, a typical sign of the Gaussian universality class. To this end we proposed novel string-like order parameters as a generalization of the

disorder parameters of the quantum Ashkin–Teller model. For the $S = 1$ chain our generalization corresponds to the order parameter of the dimerized phase in contrast to the usual string order parameter of the Haldane phase. These new order parameters offer access to scaling dimensions that differ from those of spin operators, and thus the validity of scaling relations can be tested with higher accuracy.

Another exotic order parameter is called twist order parameter, as introduced in [6]. It is particularly well suited to signal quantum phase transitions between different valence bond configurations in various 1D quantum spin systems. Despite its potential to accurately give pseudo-critical points in quantum Monte Carlo simulations, the scaling behaviour of the twist order parameter has not yet been studied. Our attempts to identify scaling behaviour seem to fail due to the inherently non-local nature of the twist order parameter, even though according to [6] a scaling dimension can be assigned.

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11.16 Re-Examining the Quantum Compass Model with Screw-Periodic Boundary Conditions

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Due to its connection to interesting quantum phenomena ranging from orbital order in transition metal compounds to topologically protected qbits [1–3] the so-called compass model has recently attracted much interest in the literature. In two dimensions the model is defined by the Hamiltonian

$$\mathcal{H} = (1/4) \sum_i \left(J_x \sigma_i^x \sigma_{i+e_x}^x + J_z \sigma_i^z \sigma_{i+e_z}^z \right) , \tag{11.2}$$

where σ are the usual Pauli operators, J_x, J_y coupling constants and e_x, e_z unit vectors in x and z direction. Although simple looking at first sight, this Hamiltonian is rather hard to study. It was shown to possess rich physics ranging from highly degenerate ground states to quantum phase transitions to an exciting thermal phase transition. In a recent Letter [4] it was proposed that directional order in the quantum compass model is rather stable against dilution, which is not the case for the classical model.

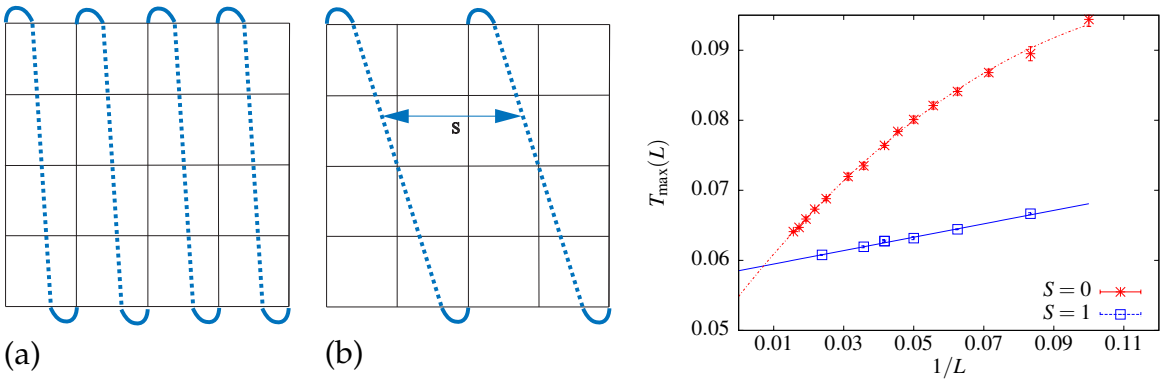

Figure 11.14: Left: Illustration of screw-periodic boundary conditions along the y-axis with pitch parameter (a) $S = 1$ and (b) $S = 2$. Right: Finite-size scaling plot of the pseudocritical temperatures for the quantum compass model from the susceptibility maxima comparing periodic ($S = 0$) and screw-periodic boundary conditions ($S = 1$). The latter clearly lead to a considerable improvement of the finite-size scaling behaviour.

To investigate these questions in more detail, we have performed a comprehensive study of the two-dimensional (2D) compass model on square lattices for classical and quantum spin degrees of freedom using Monte Carlo computer simulations [5]. We employed state-of-the-art implementations using Metropolis, stochastic series expansion (SSE) and parallel tempering (PT) techniques to obtain the critical ordering temperatures and critical exponents. In the classical case we compared the finite-size scaling (FSS) behaviour of ordinary periodic boundary conditions with so-called annealed boundary conditions. We found that periodic boundary conditions suffer from extreme finite-size effects, which might be caused by closed loop excitations on the torus, so that one needs to go to very large lattice sizes to see the true asymptotic scaling behaviour. Our numerical results are at odds with recent literature on the subject which we can trace back to neglecting these strong finite-size effects on periodic lattices. Our analysis showed, however, that one arrives at quite different conclusions when these effects are properly taken into account [5]. This observation may also have an impact on previous conclusions for the quantum model concerning dilution effects because a precise estimate of the critical temperature T_c enters crucially into this analysis [4].

The precision of our results for the quantum model, however, was still rather low compared to the classical case. It was therefore a challenging goal to devise and analyze special boundary conditions for the quantum model with improved FSS behaviour compared to periodic boundary conditions. To this end, we recently re-examined the model and, in fact, obtained several significant improvements [6]. First, for the classical case, we proposed an improved update scheme which builds on the Wolff cluster algorithm in one-dimensional subspaces of the configuration space. This allowed us to study much larger classical systems up to $L = 512$ and to provide compelling evidence for the presence of strongly anomalous scaling for periodic boundary conditions which is much worse than anticipated before. Second, for both the classical and the quantum case, we proposed to work with screw-periodic boundary conditions [7] sketched in Fig. 11.14, which do not make use of extended configuration spaces of the annealed boundary schemes and demonstrated that they completely remove the problem with

finite-size scaling. In particular for the quantum problem the use of screw-periodic boundary conditions gives a considerably improved estimate for the critical temperature (cf. Fig. 11.14) which should be of interest for future studies on the compass model. The origin of the anomalous scaling for periodic boundary conditions is also discussed.

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11.17 Monte Carlo Simulations with the Worm Algorithm

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About a decade ago, Prokof'ev and Svistunov [1] have introduced a novel Monte Carlo update scheme for spin models and lattice field theories that, although based on local updates, does away with critical slowing down almost completely. Their algorithm is based on the high-temperature series expansion of the partition function Z, leading to closed lines or loops of non-zero bond variables, and of the spin-spin correlation function $\langle s_{i_0} s_{j_0} \rangle$, containing an open line or chain of non-zero bonds connecting the lattice sites i_0 and j_0 [2]. This so-called *worm algorithm* generates loop configurations through the motion of the end points of the *open* line – the "head" and "tail" of a "worm". A loop is generated in this scheme when the head bites the tail, or through a "back bite" where the head erases a piece (bond) of its own body and thereby leaves behind a detached loop and a (possibly drastically) shortened open chain. Typical conformations of the chain immersed into the background of loops are depicted in Fig. 11.15.

Recently we have evaluated the performance of the worm algorithm for the two-dimensional Ising model where two equivalent high-temperature representations are possible: one with unrestricted bond occupation numbers $N_b = 0, 1, 2, \ldots$ and another with restricted bond occupation numbers $N_b = 0, 1$. There is, however, no reason to believe that also the quantitative dynamical behaviour of the worm update algorithm is the same for the two formulations. Our numerical tests on square lattices show that the restricted representation with $N_b = 0, 1$ is slightly favorable.

The worm algorithm is perfectly suited for pursuing the loop-gas approach to lattice spin systems providing an alternative description in terms of fluctuating geometrical

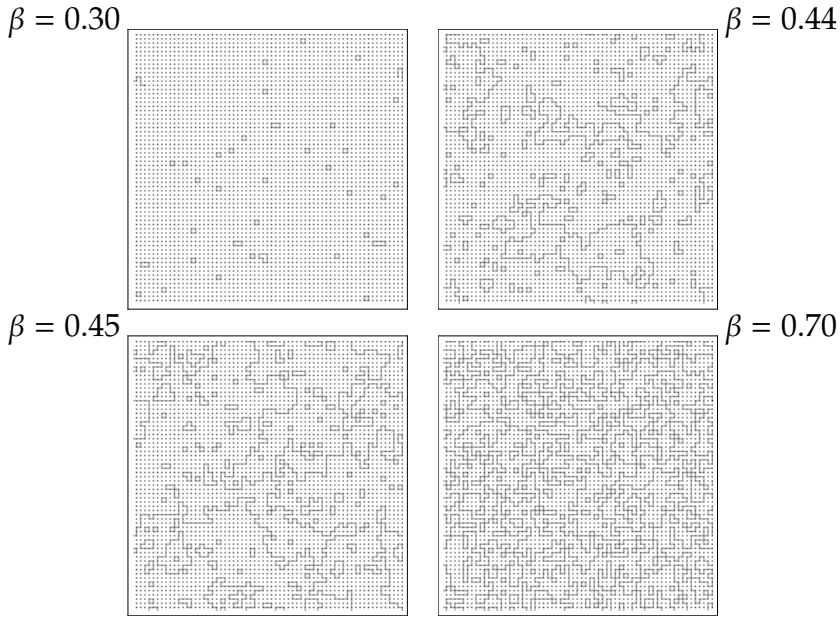

Figure 11.15: Typical high-temperature graph configurations on a 64×64 square lattice (where $\beta_c = 1/k_B T_c = 0.440\,686\ldots$) with periodic boundary conditions.

objects, the loops. Physical observables are no longer estimated by sampling an ensemble of spin configurations, but by sampling a grand canonical ensemble of (mostly closed) lines, known as a *loop gas*, instead. The weight of a given high-temperature graph is typically determined by its total size, the number of intersections, and the number of loops contained in the tangle. In relativistic quantum field theories formulated on a space-time lattice, the high-temperature expansion is replaced by the strong-coupling expansion, representing the hopping of particles from one lattice site to the next, which is closely connected to Feynman's space-time approach to quantum theory [3].

As a first application we performed Monte Carlo "worm" simulations for the two-dimensional Ising or O(1) loop model on a honeycomb lattice [4] and used concepts from percolation theory – the paradigm of a geometrical phase transition – and the theory of self-avoiding random walks to analyze the critical behaviour of the model in terms of observables that naturally arise in a loop-gas approach, e.g., the radius of gyration of loops and chains or the end-to-end distance of chains [5, 6]. The honeycomb lattice serves as a prototype because here ambiguities in the loop interpretation can be avoided due to its coordination number $z = 3$ (on a square lattice with $z = 4$, for example, "knots" are possible). Furthermore, for the Ising model on this lattice various exact results are known, which provide a yardstick for our numerical results and also for the feasibility of our approach in general.

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11.18 Self-Adaptive Simulations of Critical Phenomena

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In the past few years much attention has been paid to improved simulations of first-order phase transitions and systems with rugged free-energy landscapes where generalized ensembles techniques (umbrella, multicanonical, Wang-Landau, parallel/simulated tempering sampling) [1] proved to be very successful. For critical phenomena, on the other hand, the merits of this non-Boltzmann sampling approach have been fully appreciated only quite recently [2]. Here one often needs an extended temperature range around the critical point when analyzing second-order phase transitions by means of finite-size scaling analyses. To cover the complete "desired" temperature range in a single simulation for each lattice size, we combined in Ref. [2] multibondic sampling [3] with the Wang-Landau recursion [4], where the precise meaning of "desired" follows from a careful finite-size scaling (FSS) analysis of all relevant observables [5].

In this project we developed an alternative method based on the parallel-tempering algorithm [6] combined with cluster updates [7] and an improved adaptive routine [8] to determine the "desired" temperature range. The performance of our method is assessed by monitoring the integrated autocorrelation time $\tau_{\mathrm{int}}(T_i, L)$ for each replica at temperature T_i and system size L. If the requested overlap of the energy histograms for the different replica is chosen appropriately, the needed number of replica N_{rep} of the parallel tempering algorithm stays constant as a function of L. In this case the maximum of $\tau_{\mathrm{int}}(T_i, L)$ over all replica, that is the relevant time scale of the full self-adaptive algorithm, scales only weakly $\propto L^z$. For the energy we obtain $z = 0.27$ in 2D and $z = 0.62$ in 3D, cf. Fig. 11.16, which is asymptotically a great improvement over the multibondic Wang-Landau method with $z \approx 1.05$ in both dimensions [9]. But also for moderate system sizes we gain one to two further orders of magnitude in the performance compared to our earlier method in Ref. [2], which is, however, already a great improvement over the standard multicanonical variant.

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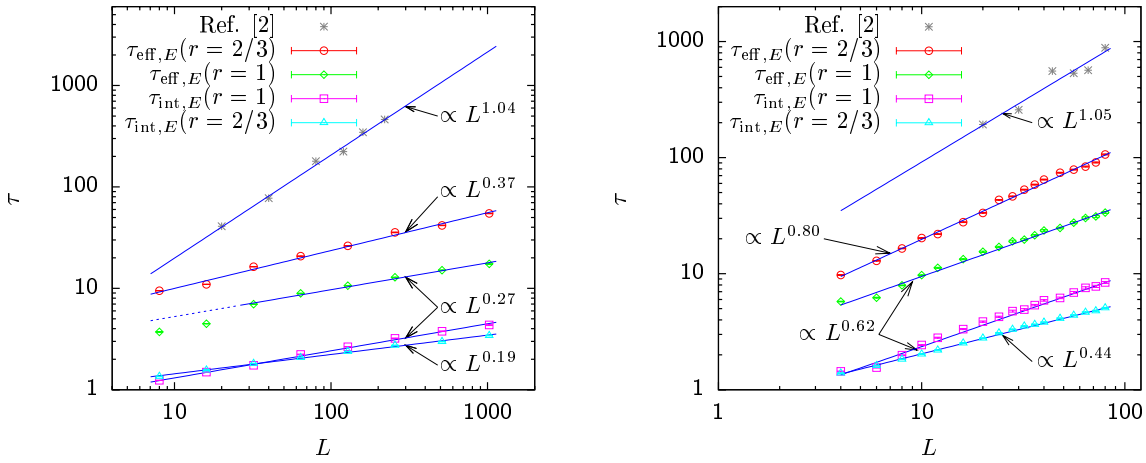

Figure 11.16: Autocorrelation times τ_{int} and τ_{eff} for the energy of the Ising model in 2D (left) and 3D (right). Here $\tau_{\mathrm{eff}} = N_{\mathrm{rep}}\,\tau_{\mathrm{int}}$ with N_{rep} being the number of replica of the parallel tempering algorithm. The parameter r determines the size of the "desired" temperature range [2, 9].

11.19 Critical Amplitude Ratios of the Baxter-Wu Model

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One of the central results of the theory of phase transitions and critical phenomena is the formulation of the universality hypothesis [1, 2]. According to the theory, all systems with the same dimensionality, the same symmetry of the ordered phase and the same number of order parameters are described by the same set of critical exponents at the critical point [2]. Additionally, thermodynamic functions vary with temperature in such a way that some combinations of their critical amplitudes take the same values for all systems within a universality class [3]. A typical example is provided by the scaling relation for the magnetic susceptibility χ which in the vicinity of the critical temperature T_c behaves according to $\chi \sim \Gamma_{\pm}|T/T_c - 1|^{-\gamma}$, where γ is the critical exponent and Γ_+ and Γ_- denote the critical amplitudes in the high- and low-temperature phase, respectively. The ratio $R_\chi = \Gamma_+/\Gamma_-$ is then such a universal amplitude ratio.

Special interest in the properties of universality classes derives from cases in which for some representative models the singular behaviour is complicated by logarithmic corrections [4]. This is for instance the case for the two-dimensional 4-state Potts model which gives the name to this specific universality class. Another two-dimensional model which belongs to the same universality class, but *without* logarithmic corrections to its singular behaviour, is the Baxter-Wu model on a triangular lattice [5].

The objective of this project was to investigate the influence of the logarithmic corrections by estimating the critical amplitudes of the Baxter-Wu model numerically and comparing them with the universal amplitude ratios available for the 4-state Potts model (e.g., $R_\chi = 6.5 \pm 0.4$ [6]). To this end we simulated the model with the traditional Metropolis Monte Carlo algorithm and analyzed the magnetization and polarization in the ordered phase, and the energy, specific heat and magnetic susceptibility in both phases. One of our central findings for the Baxter-Wu model is the result $R_\chi = 3.9 \pm 0.1$ [7], which is in very good agreement with approximate analytical estimates [8, 9] for this

ratio predicting $R_\chi = 4.013$ and $R_\chi = 4.02$, but clearly deviates from the estimate [6] for the 4-state Potts model. This clearly indicates that the numerical estimate for the 4-state Potts model is strongly affected by logarithmic corrections, despite all the care exercised in the analysis [6]. Also for other universal combinations involving the specific-heat and magnetization amplitudes we obtained for the Baxter-Wu model perfect agreement with analytical approximations [7].

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11.20 Geometrothermodynamics Applied to Black Holes

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†Applied Mathematics Research Centre, Coventry University, United Kingdom

The application of information geometric ideas to statistical mechanics using a metric on the space of states, as pioneered by Ruppeiner [1] and Weinhold [2], has proved to be a useful alternative approach to characterizing phase transitions [3, 4]. The results obtained by using either the Ruppeiner or Weinhold metric (which are conformally related to each other) were found to be consistent in these applications. Some puzzling anomalies become apparent, however, when these methods are applied to the study of black hole thermodynamics. A possible resolution was suggested by Quevedo et al. [5] who emphasized the importance of Legendre invariance in thermodynamic metrics. They found physically consistent results for various black holes when using a Legendre invariant metric, which agreed with a direct determination of the properties of phase transitions from the specific heat. Recently, information geometric methods have been employed by Wei et al. [6] to study the Kehagias-Sfetsos (KS) black hole in Hořava-Lifshitz gravity [7, 8]. The formalism suggests that a coupling parameter in this theory plays a role analogous to the charge in Reissner-Nordström black holes or angular momentum in the Kerr black hole and the calculation of the specific heat shows a singularity which may be interpreted as a phase transition. When the curvature of the Ruppeiner metric is calculated for such a theory, it does not, however, show a singularity at the phase transition point. We show in this project that the curvature of a particular Legendre invariant ("Quevedo") metric for the KS black hole is singular at

the phase transition point [9]. We contrast the results for the Ruppeiner, Weinhold and Quevedo metrics and in the latter case investigate the consistency of taking either the entropy or mass as the thermodynamic potential [9].

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11.21 Cross Correlations in Statistical Error Estimation

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The success of Monte Carlo computer simulations, in particular Markov chain based methods, is largely due to the development and refinement of a number of advanced simulation techniques such as cluster algorithms and generalized-ensemble methods. Equally important to the efficient generation of simulation data, however, is their correct and optimal analysis. This includes finite-size scaling (FSS) approaches [1], turning the limitation to finite system sizes into a systematic tool for accessing the thermodynamic limit, reweighting techniques [2], yielding continuous functions of estimates from a single simulation, and statistical tools for error estimation such as the jackknife and other resampling schemes [3].

Of these techniques, the statistical error analysis appears to have received the least attention. In particular the effects of cross correlations have been mostly neglected to date (see, however, Refs. [4–6]), but are only systematically being discussed following our recent suggestion [7, 8]. In this project, we investigate how such cross correlations lead to systematically wrong estimates of statistical errors of averaged or otherwise combined quantities when a naive analysis is employed, and how a statistically correct analysis can be easily achieved within the framework of the jackknife resampling method. Furthermore, one can even take benefit from the presence of such correlation effects for significantly reducing the variance of estimates without substantial additional effort. We demonstrate the practical relevance of these considerations for a finite-size scaling study of the Ising model in two and three dimensions and report in some cases improvement factors of up to 10 in simulation time [9]. A typical example for averaging correlated data is shown in Fig. 11.17.

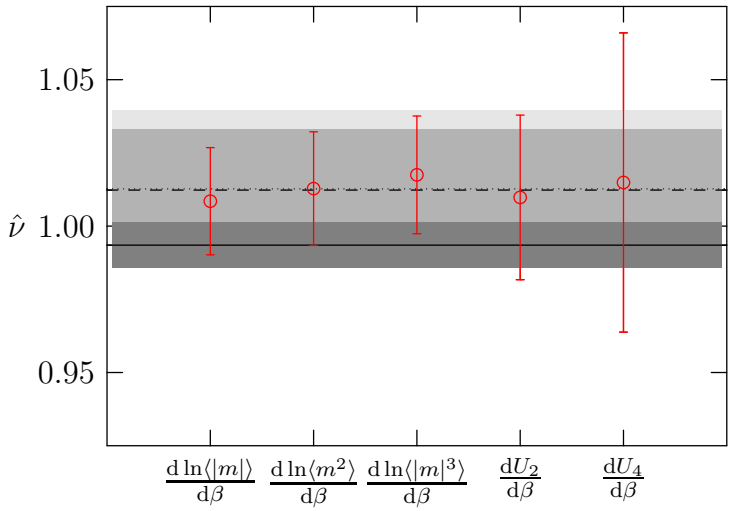

Figure 11.17: Mutually correlated estimates of the critical exponent ν of the 2D Ising model from finite-size scaling fits of the indicated observables (circles). The (almost identical) dotted and dashed lines indicate the plain average and the error-weighted mean, respectively. The covariance-weighted mean corresponds to the solid line. While counterintuitive at first sight, this is the statistically correct averaging procedure for correlated data.The shaded areas indicate the corresponding one-sigma error intervals of the mean values.

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W. Janke (Principal Investigator)
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Dynamik und Statik von Spingläsern
W. Janke
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W. Janke
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M. Bachmann and W. Janke
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Molecular Conformation Mechanics of Proteins and Polymers
W. Janke
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Mass Transport Models on Networks
W. Janke (twin project with H. Meyer-Ortmanns, Jacobs University Bremen)
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E. Bittner and W. Janke
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M. Bachmann and W. Janke
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Quantum Monte Carlo Simulations of Quantum Spin Models
W. Janke
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Quanten Monte Carlo Simulationen von (ungeordneten) Quantenspinsystemen
R. Bischof
Landesgraduiertenstipendium

11.23 Organizational Duties

Elmar Bittner

- Co-organizer of the contribution *Fußball-Fieber statistisch betrachtet*, 11. Leipziger Buchmesse-Akademie, Book Fair Leipzig (with W. Janke, A. Nußbaumer), Neue Messe, Leipzig, 20. March 2010
- Co-organizer of the contribution *Fußball-Fieber wissenschaftlich betrachtet*, Studieninformationstag der Universität Leipzig, Campus Augustusplatz (with W. Janke, A. Nußbaumer), Leipzig, 8. May 2010
- Referee for Physical Review Letters, Physical Review E, Journal of Physics A, European Journal of Physics B, Computer Physics Communications

Wolfhard Janke

- Director, Naturwissenschaftlich-Theoretisches Zentrum (NTZ), Universität Leipzig
- Member of the Board of the Faculty of Physics and Earth Sciences, 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
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- Specialist Editor, Computer Physics Communications (CPC), Elsevier, Amsterdam, The Netherlands
- Editor "Computational Sciences", Lecture Notes of Physics, Springer, Berlin, Heidelberg, Germany
- Editor "Computational Physics", Central European Journal of Physics, Krakow, Poland
- Member of Editorial Board, Condens. Matter Phys., Lviv, Ukraine
- Permanent Member of the "International Advisory Board", *Conference of the Middle European Cooperation in Statistical Physics (MECO)*
- Member of International Organization Committee of the 10th International Conference *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)), Washington DC, USA, 11.–16. July 2010
- Member of the Programme Committee for the *European Conference on Complex Systems 2011 (ECCS'11)*, Vienna, Austria, 12.–16. September 2011
- Co-organizer of the contribution *Fußball-Fieber statistisch betrachtet*, 11. Leipziger Buchmesse-Akademie, Book Fair Leipzig (with E. Bittner, A. Nußbaumer), Neue Messe, Leipzig, 20. March 2010

- Co-organizer of the contribution *Fußball-Fieber wissenschaftlich betrachtet*, Studieninformationstag der Universität Leipzig, Campus Augustusplatz (with E. Bittner, A. Nußbaumer), Leipzig, 8. May 2010
- Co-organizer of the contribution *Fußballfieber wissenschaftlich betrachtet*, *Lange Nacht der Wissenschaft* (with A. Nußbaumer), Universität Leipzig, 24. September 2010
- Organizer of the "BuildMoNa" Theory Module *Probability in Physics* (with K. Kroy), Universität Leipzig, 10.–11. November 2010
- Organizer of the Workshop *CompPhys10* – 11th International NTZ Workshop on *New Developments in Computational Physics*, ITP, Universität Leipzig, 25.–27. November 2010
- Organizer of the Workshop *CompPhys11* – 12th International NTZ Workshop on *New Developments in Computational Physics*, ITP, Universität Leipzig, 24.–26. November 2011
- External Reviewer for Humboldt-Stiftung (AvH); Deutsche Forschungsgemeinschaft (DFG); Studienstiftung des deutschen Volkes; the Jeffress Memorial Trust, Bank of America, Virginia, USA; "Fond zur Förderung der wissenschaftlichen Forschung (FWF)", Österreich; "The Royal Society", Great Britain; The "Engineering and Physical Sciences Research Council (EPSRC)", Great Britain; The University of Warwick, England, Great Britain; Coventry University, England, Great Britain; CECAM, Lausanne, Switzerland; National Science Foundation (NSF), USA; Natural Sciences and Engineering Research Council of Canada (NSERC), Canada; Israel Science Foundation, Israel
- Referee for Physical Review Letters, Physical Review B, Physical Review E, Journal of Chemical Physics, Europhysics Letters, Physics Letters A, Physics Letters B, The European Physical Journal B, Physica A, Proceedings of the Royal Physical Society, Journal of Physics A, Computer Physics Communications, JSTAT, Journal of Statistical Physics, New Journal of Physics, International Journal of Modern Physics C

Andreas Nußbaumer

- Co-organizer of the contribution *Fußball-Fieber statistisch betrachtet*, 11. Leipziger Buchmesse-Akademie, Book Fair Leipzig (with E. Bittner, W. Janke), Neue Messe, Leipzig, 20. March 2010
- Co-organizer of the contribution *Fußball-Fieber wissenschaftlich betrachtet*, Studieninformationstag der Universität Leipzig, Campus Augustusplatz (with E. Bittner, W. Janke), Leipzig, 8. May 2010
- Co-organizer of the contribution *Fußballfieber wissenschaftlich betrachtet*, *Lange Nacht der Wissenschaft* (with W. Janke), Universität Leipzig, 24. September 2010

11.24 External Cooperations

Academic

- Institut für Festkörperforschung (IFF-2) and Institute for Advanced Simulation (IAS-2), Forschungszentrum Jülich
  PD Dr. Michael Bachmann, Dr. Thomas Vogel

- Institute of Physics, Jagiellonian University, Kraków, Poland
  Prof. Dr. Piotr Białas, Dr. Leszek Bogacz, Prof. Dr. Zdzisław Burda
- CEA/Saclay, Service de Physique Théorique, France
  Dr. Alain Billoire
- Institut für Physik, Universität Mainz
  Prof. Dr. Kurt Binder, Dr. Hsiao-Ping Hsu, Prof. Dr. Friderike Schmid, Dr. Martin Weigel
- Laboratoire de Physique des Matériaux (UMR CNRS No 7556), Nancy Université, France
  Prof. Dr. Bertrand Berche, Dr. Christophe Chatelain, Dr. Olivier Collet, Prof. Dr. Malte Henkel, Dr. Dragi Karevski
- Groupe de Physique des Matériaux (UMR CNRS No 6634), Université de Rouen, France
  Dr. Pierre-Emmanuel Berche
- SUPA, School of Physics and Astronomy, University of Edinburgh, Scotland, UK
  Dr. Richard A. Blythe, Prof. Dr. Martin Evans, Dr. Bartłomiej Wacław
- Istituto Nazionale di Fisica Nucleare, Sezione di Milano-Bicocca, Milano, Italy
  Prof. Dr. Pablo Butera
- Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich
  Prof. Dr. Peter Grassberger, PD Dr. Thomas Neuhaus
- IAC-1, Universität Stuttgart
  Prof. Dr. Rudolf Hilfer, Anjan Prasad Gantapara
- Complex Systems Division, Department of Theoretical Physics, Lunds Universitet, Lund, Sweden
  Prof. Dr. Anders Irbäck, Simon Mitternacht
- Department of Mathematics and the Maxwell Institute for Mathematical Sciences, Heriot-Watt University, Edinburgh, Scotland, UK
  Prof. Dr. Desmond A. Johnston
- Applied Mathematics Research Centre, Coventry University, England, UK
  Dr. Ralph Kenna, PD Dr. Christian von Ferber
- Inst. für Theoretische Physik, FU Berlin
  Prof. Dr. Hagen Kleinert
- Max-Planck Institut für Physik komplexer Systeme, Dresden
  Dr. Andreas Läuchli
- Atominstitut, TU Wien, Austria
  Prof. Dr. Harald Markum, Dr. Rainer Pullirsch
- Jacobs Universität Bremen
  Prof. Dr. Hildegard Meyer-Ortmanns
- Applied Mathematics, Universitat Pompeu Fabra, Barcelona, Spain
  Dr. Ramon Villanova
- EPF Lausanne, Switzerland
  Dr. Sandro Wenzel

- Engineering of Physics, Ankara University, Turkey
  Prof. Dr. Handan Arkın (Olgar)
- Dept. of Physics, Hacettepe University, Ankara, Turkey
  Prof. Dr. Tarik Çelik, Gökhan Gökoğlu
- Institute for Condensed Matter Physics, National Academy of Sciences, Lviv, Ukraine
  Dr. Viktoria Blavatska, Prof. Dr. Yurij Holovatch
- Yerevan Physics Institute, Yerevan, Armenia
  Prof. Dr. David B. Saakian
- Landau Institute for Theoretical Physics, Chernogolovka, Russia
  Prof. Dr. Lev N. Shchur
- Banaras Hindu University, Varanasi, India
  Prof. Dr. Sanjay Kumar
- Dept. of Physics, Florida State University, Tallahassee, USA
  Prof. Dr. Bernd A. Berg
- Dept. of Physics, Michigan Technological University, Houghton, USA
  Prof. Dr. Ulrich H.E. Hansmann
- Center for Simulational Physics, The University of Georgia, Athens, USA
  Prof. Dr. David P. Landau, Dr. Stefan Schnabel
- The University of Tokyo, Japan
  Prof. Dr. Nobuyasu Ito
- Nagoya University, Japan
  Prof. Dr. Yuko Okamoto
- Laboratory of Statistical and Computational Physics, Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan
  Prof. Dr. Chin-Kun Hu
- Zhejiang Institute of Modern Physics, Zhejiang University, Hangzhou, P.R. China
  Prof. Dr. He-Ping Ying, Prof. Dr. Bo Zheng

11.25 Publications

Journals

M. Bachmann, K. Goede, A. Beck-Sickinger, M. Grundmann, A. Irbäck, W. Janke: *Microscopic Mechanism of Specific Peptide Adhesion to Semiconductor Substrates*, Angew. Chem. Int. Ed. **49**, 9530–9533 (2010)

M. Bachmann, K. Goede, A. Beck-Sickinger, M. Grundmann, A. Irbäck, W. Janke: *Mikroskopischer Mechanismus der spezifischen Adhäsion von Peptiden an Halbleitersubstraten*, Angew. Chem. **122**, 9721–9724 (2010)

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, Physics Procedia **7**, 19–28 (2010)

V. Blavatska, W. Janke: *Fractals Meet Fractals: Self-Avoiding Random Walks on Percolation Clusters*, in *Computer Simulations in Condensed Matter Physics XXII*, ed. by D.P. Landau, S.P. Lewis, H.-B. Schüttler, Physics Procedia **3**, 1431–1435 (2010)

V. Blavatska, W. Janke: *Shape Anisotropy of Polymers in Disordered Environment*, J. Chem. Phys. **133**, 184903-1–7 (2010)

W. Janke, D.A. Johnston, R. Kenna: *Geometrothermodynamics of the Kehagias-Sfetsos Black Hole*, J. Phys. A: Math. Theor. **43**, 425206-1–11 (2010)

W. Janke, T. Neuhaus, A.M.J. Schakel: *Critical Loop Gases and the Worm Algorithm*, Nucl. Phys. B **829**, 573–599 (2010)

M. Möddel, W. Janke, M. Bachmann: *Systematic Microcanonical Analyses of Polymer Adsorption Transitions*, Phys. Chem. Chem. Phys. **12**, 11548–11554 (2010)

A. Nußbaumer, E. Bittner, W. Janke: *Free-Energy Barrier at Droplet Condensation*, Prog. Theor. Phys. Suppl. **184**, 400–414 (2010)

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, Physics Procedia **7**, 52–62 (2010)

L.N. Shchur, W. Janke: *Critical Amplitude Ratios of the Baxter-Wu Model*, Nucl. Phys. B **840**, 491–512 (2010)

B. Wacław, J. Sopik, W. Janke, H. Meyer-Ortmanns: *Mass Condensation on Networks*, J. Phys.: Conf. Ser. **246**, 012011-1–11 (2010)

M. Weigel, W. Janke: *Error Estimation and Reduction with Cross Correlations*, Phys. Rev. E **81**, 066701-1–15 (2010)

S. Wenzel, W. Janke, A. Läuchli: *Re-examining the Directional-Ordering Transition in the Compass Model with Screw-Periodic Boundary Conditions*, Phys. Rev. E **81**, 066702-1–9 (2010)

in press

V. Blavatska, W. Janke: *Θ-Polymers in Crowded Media under Stretching Force*, to appear in Comput. Phys. Commun., in print (2011)

J. Gross, W. Janke, M. Bachmann: *Massively Parallelized Replica-Exchange Simulations of Polymers on GPUs*, to appear in Comput. Phys. Commun., in print (2011)

J. Gross, W. Janke, M. Bachmann: *A GPU Approach to Parallel Replica-Exchange Polymer Simulations*, to appear in *Computer Simulations in Condensed Matter Physics XXIV*, ed. by D.P. Landau, S.P. Lewis, H.-B. Schüttler, Physics Procedia, in print (2011)

W. Janke, T. Neuhaus, A.M.J. Schakel: *Worms Exploring Geometrical Features of Phase Transitions*, to appear in *Computer Simulations in Condensed Matter Physics XXIV*, ed. by D.P. Landau, S.P. Lewis, H.-B. Schüttler, Physics Procedia, in print (2011)

C. Junghans, W. Janke, M. Bachmann: *Hierarchies in Nucleation Transitions*, to appear in Comput. Phys. Commun., in print (2011)

M. Möddel, W. Janke, M. Bachmann: *Adsorption of Finite Polymers in Different Thermodynamical Ensembles*, to appear in Comput. Phys. Commun., in print (2011)

S. Schnabel, W. Janke, M. Bachmann: *Advanced Multicanonical Monte Carlo Methods for Efficient Simulations of Nucleation Processes of Polymers*, to appear in J. Comput. Phys., in print (2011)

Talks

E. Bittner: *Free-Energy Barrier of the Evaporation/Condensation Transition*, Spring Meeting of the German Physical Society, Universität Regensburg, 21.–26. March 2010

E. Bittner: *Free-Energy Barriers of the 3D Edwards-Anderson-Ising Spin Glass Model*, Spring Meeting of the German Physical Society, Universität Regensburg, 21.–26. March 2010

E. Bittner: *Parallel Tempering Cluster Algorithm for Computer Simulations of Critical Phenomena*, StatPhys24 Conference, Cairns, Australia, 18.–23. July 2010

E. Bittner: *Replica-Exchange Cluster Algorithm*, MASCOS Workshop on Monte Carlo Algorithms in Statistical Physics, University of Melbourne, Australia, 27.–29. July 2010

W. Janke: *Formation/Dissolution of Equilibrium Droplets*, PbF2 Workshop, Universität Leipzig, 13. January 2010

W. Janke: *Computer Simulation Studies of Macromolecules*, Global Challenges for Sustainable Development: GSSD'2010 – Sustainable Chemistry & Related Areas, Université européenne de Bretagne (UEB), Rennes, France, 25.–26. February 2010

W. Janke: *Generalized Ensemble Simulations of Molecular Systems*, invited talk, 239th American Chemical Society National Meeting, San Francisco, USA, 21.–25. March 2010

W. Janke: *Computer Simulations of Macromolecular Systems in Generalized Ensembles*, SFG FOR877 Meeting, MPI-CBG, Dresden, 28. April 2010

W. Janke: *Exploring Critical Loop Gases with Worms*, Lattice Seminar, Humboldt Universität zu Berlin, 21. June 2010

W. Janke: *Polymers in Crowded Environment under Stretching Force: Globule-Coil Transitions*, Conference on Computational Physics (CCP 2010), NTNU Trondheim, Norway, 23.–26. June 2010

W. Janke: *Unconventional Quantum Phase Transition of Coupled Spin Dimers*, StatPhys24 Conference, Cairns, Australia, 18.–23. July 2010

W. Janke: *Error Estimation and Reduction with Cross Correlations*, invited talk, MASCOS Workshop on Monte Carlo Algorithms in Statistical Physics, University of Melbourne, Australia, 27.–29. July 2010

W. Janke: *Exploring Random-Graph Ensembles with Worms*, invited talk, NORDITA Workshop *Random Graphs and Networks*, Stockholm, Sweden, 01.–03. November 2010

W. Janke: *Monte Carlo Simulations and Critical Phenomena*, Physikalisches Kolloquium, Bergische Universität Wuppertal, 29. November 2010

W. Janke: *Computer Simulations of Macromolecular Systems*, invited talk, NORDITA Workshop *Random Geometry and Applications*, Stockholm, Sweden, 03. December 2010

W. Janke: *The Ising Model in Statistical Physics I*, IMPRS Ringvorlesung *Discrete Structures in Physics*, International Max Planck Research School, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, 14. December 2010

M. Möddel: *Systematic Microcanonical Analyses of Polymer Adsorption Transitions*, Global Challenges for Sustainable Development: GSSD'2010 – Sustainable Chemistry & Related Areas, Université européenne de Bretagne (UEB), Rennes, France, 25.–26. February 2010

M. Möddel: *First-Order-Like Behavior at the Adsorption Transition of Short Polymers in the Microcanonical Ensemble*, Spring Meeting of the German Physical Society, Regensburg, 21.–26. March 2010

M. Möddel: *Thermodynamics of a Finite Homopolymer Near an Attractive Substrate*, Computational Biology Cluster Seminar, Forschungszentrum Jülich, Germany, 16. June 2010

M. Möddel: *Systematic Microcanonical Analyses of Polymer Adsorption Transitions*, Conference on Computational Physics (CCP 2010), NTNU Trondheim, Norway, 23.–26. June 2010

M. Möddel: *Grafted and Non-Grafted Polymer Adsorption in Different Thermodynamical Ensembles*, Seminar of the CDFA-DFDK, Nancy, France, 6. July 2010

Posters

M. Aust, M. Dvoyashkin, J. Kärger, R. Valiullin, W. Janke: *Particle Dynamics in Nano-Structured Channels*, SFG-FOR877–Defense Symposium, Universität Leipzig, 1.–2. July 2010

R. Bischof, W. Janke: *Critical Exponents and Phase Diagram of Mixed Spin Chains with Bond Alternation and Exchange Anisotropy*, 35th Conference of the Middle European Cooperation in Statistical Physics *MECO35*, Pont-à-Mousson, France, 15.–19. March 2010

R. Bischof, W. Janke: *Universality Class of Mixed Quantum Spin Chains*, Conference on Computational Physics (CCP 2010), NTNU Trondheim, Norway, 23.–26. June 2010

E. Bittner, W. Janke: *Replica-Exchange Cluster Algorithm*, NIC Symposium 2010, Forschungszentrum Jülich, 24.–25. February 2010

E. Bittner, W. Janke: *Free-Energy Barrier of the Evaporation/Condensation of Ising Droplets*, 35th Conference of the Middle European Cooperation in Statistical Physics *MECO35*, Abbaye des Prémontrés, Pont-à-Mousson, 15.–19. March 2010

M.H. Gerlach, W. Janke: *Monte Carlo Study of the Droplet-Strip Transition in the Two-Dimensional Ising Model*, 11th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys10*, Universität Leipzig, 25.–27. November 2010

A.P. Gantapara, W. Janke, R. Hilfer: *Flat Histogram Monte Carlo Study of the Order Parameter Distribution*, Spring Meeting of the German Physical Society, Regensburg, 21.–26. March 2010

J. Gross, W. Janke, M. Bachmann: *Multithreading Monte Carlo Simulations of Polymer Models*, Spring Meeting of the German Physical Society, Regensburg, 21.–26. March 2010

J. Gross, W. Janke, M. Bachmann: *Massively Parallelized Replica-Exchange Simulations of Polymers on GPUs*, Workshop *BioScience 2010*, Forschungszentrum Jülich, 15.–19. November 2010

W. Janke, V. Blavatska: *Polymers in Crowded Environment Under Stretching Force: Globule-Coil Transitions*, Spring Meeting of the German Physical Society, Regensburg, 21.–26. March 2010

W. Janke, K. Kroy: *Polymer Conformations and Diffusive Transport in Disordered Environments*, SFG-FOR877–Defense Symposium, Universität Leipzig, 1.–2. July 2010

S. Karalus, W. Janke, M. Bachmann: *Cutting the Energy Range in Multicanonical Monte Carlo Simulations*, Spring Meeting of the German Physical Society, Regensburg, 21.–26. March 2010

M. Marenz, A. Nußbaumer, W. Janke: *Worm Algorithm in Ordered and Disordered Media*, 11th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys10*, Universität Leipzig, 25.–27. November 2010

M. Möddel, W. Janke, M. Bachmann: *Microcanonical Analyses of Polymer Adsorption*, 35th Conference of the Middle European Cooperation in Statistical Physics *MECO35*, Pont-à-Mousson, France, 15.–19. March 2010

M. Möddel, W. Janke, M. Bachmann: *Systematic Microcanonical Analyses of Polymer Adsorption*, Spring Meeting of the German Physical Society, Regensburg, 21.–26. March 2010

M. Möddel, W. Janke, M. Bachmann: *Systematic Microcanonical Analyses of Polymer Adsorption*, 3rd Scientific Symposium of the Graduate School *BuildMoNa*, Universität Leipzig, 29.–30. March 2010

M. Möddel, W. Janke, M. Bachmann: *Microcanonical Analyses of Polymer Adsorption*, Workshop *BioScience 2010*, Forschungszentrum Jülich, 15.–19. November 2010

M. Müller, M. Bachmann, T. Neuhaus: *Towards Optimized Parallel Tempering*, 11th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys10*, Universität Leipzig, 24.–27. November 2010

H. Nagel, B. Wacław, W. Janke: *Time Scale of Mass Condensation in Stochastic Transport with Pair Factorized Steady States*, 11th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys10*, Universität Leipzig, 24.–27. November 2010

A. Nußbaumer, E. Bittner, W. Janke: *Gibbs-Thomson Effect in the Ising Model*, 11th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys10*, Universität Leipzig, 24.–27. November 2010

S. Schöbl, K. Kroy, W. Janke: *Effect of Disorder on Equilibrium Conformations of Semiflexible Polymers*, 35th Conference of the Middle European Cooperation in Statistical Physics *MECO35*, Pont-à-Mousson, France, 15.–19. March 2010

S. Schöbl, K. Kroy, W. Janke: *Effect of Disorder on Equilibrium Conformations of Semiflexible Polymers*, 3rd Scientific Symposium of the Graduate School *BuildMoNa*, Universität Leipzig, 29.–30. March 2010

M. Wiedenmann, A. Nußbaumer, E. Bittner, W. Janke: *Evaporation/Condensation Transition of 3D Ising Droplets*, 35th Conference of the Middle European Cooperation in Statistical Physics *MECO35*, Pont-à-Mousson, France, 15.–19. March 2010

M. Wiedenmann, A. Nußbaumer, E. Bittner, W. Janke: *Monte Carlo Study of the Evaporation/Condensation Transition of Ising Droplets*, 3rd Scientific Symposium of the Graduate School *BuildMoNa*, Universität Leipzig, 29.–30. March 2010

J. Zierenberg, B.A. Berg, W. Janke: *Structure of the Tip4p Water Model in the Ice I_h Phase*, 11th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys10*, Universität Leipzig, 25.–27. November 2010

11.26 Graduations

Diploma

- Hannes Nagel
  Mass Condensation in Stochastic Transport Processes and Complex Networks
  19. February 2010
- Jonathan Groß
  Multithreading Monte Carlo Simulationen eines minimalistischen Polymermodells
  26. February 2010
- Niklas Fricke
  Self-Avoiding Walks on Disordered Lattices
  01. July 2010
- Steffen Karalus
  Thermodynamics of Polymer Adsorption to a Flexible Membrane
  20. September 2010
- Martin Marenz
  Worm Algorithm in Ordered and Disordered Media
  25. November 2010

Master

- Johannes Zierenberg
  Tip4p Water Model in the Ice I_h Configuration
  21. December 2010

Bachelor

- Benjamin Winkler
  Nichtgleichgewichtsrelationen vom Jarzynski-Typ zur Bestimmung von Grenzflächenspannungen
  23. August 2010
- Kieran Austin
  Exakte Enumeration von Polymeren an Oberflächen
  29. October 2010

11.27 Guests

- Mario Collura
  Nancy Université, France
  01. January – 30. June 2010
- Prof. Dr. Nihat Berker
  Sabanci University, Istanbul, Turkey, and MIT, Boston, USA
  Anisotropy Effects and Impurity Induced Antiferromagnetism: Renormalization-Group Theory of d=3 Electronic Models
  29.–30. January 2010

- Dr. Thomas Vogel
  IFF-2 and IAS-2, Forschungszentrum Jülich, Germany
  08.-12. March 2010
- Prof. Dr. Bernd A. Berg
  Florida State University, Tallahassee, USA
  Research Prize Winner of the Alexander von Humboldt Foundation
  Search for Non-Perturbative Mechanisms to Generate a W Boson Mass
  11. May – 31. July 2010
- Dr. Viktoria Blavatska
  Institute for Condensed Matter Physics, Lviv, Ukraine
  Humboldt Fellow/FOR877 guest
  Shape Anisotropy of Polymers in Disordered Environment
  07. April – 18. June 2010
- Jeremi Ochab
  Jagiellonian University, Krakow, Poland
  Epidemics on Networks
  01. October – 31. December 2010
- Marcin Zagorski
  Jagiellonian University, Krakow, Poland
  02.–06. October 2010
- Prof. Dr. Herbert Wagner
  LMU Munich, Germany
  BuildMoNa Tutorial *Probability in Physics*
  09.–12. November 2010
- Dr. Richard Blythe
  University of Edinburgh, UK
  BuildMoNa Tutorial *Probability in Physics*
  09.–12. November 2010
- Dr. Martin Weigel
  Universität Mainz, Germany
  Performance Potential for Simulating Spin Models on GPU
  23.–28. November 2010
- Dr. Ralph Kenna
  Coventry Univ., UK
  Size Matters, Except Perhaps for Pure Mathematicians
  24.–27. November 2010
- Dr. Sandro Wenzel
  EPF Lausanne, Switzerland
  Critical Properties of the 120 Degree Model for Orbital Ordering
  24.–27. November 2010
- Prof. Dr. Antun Balaz
  Scientific Computing Laboratory, Institute of Physics, University of Belgrade, Serbia
  Fast Converging Path Integrals for Time-Dependent Potentials
  24.–28. November 2010

- Prof. Dr. Ferenc Iglói
  Institute of Theoretical Physics, Research Institute for Solid State Physics and Optics, Budapest, Hungary
  Infinite Disorder Scaling of Random Quantum Magnets in Three and Higher Dimensions
  24.–28. November 2010
- PD Dr. Thomas Neuhaus
  Jülich Supercomputing Centre, Forschungszentrum Jülich, Germany
  More on Quantum Adiabatic Computations
  24.–28. November 2010
- Prof. Dr. J.J. Ruiz-Lorenzo
  Univ. Extremadura, Badajoz, Spain
  Ising Spin-Glass Transition in Magnetic Field out of Mean-Field: Numerical Simulations and Experiments
  24.–28. November 2010
- Marcin Zagorski
  Jagiellonian University, Krakow, Poland
  Model Gene Regulatory Networks under Mutation-Selection Balance
  24.–28. November
- Dr. Stefan Schnabel
  University of Georgia, Athens, USA
  On the Low-Temperature Behavior of a Geometrically Frustrated Heisenberg Antiferromagnet
  24. November – 31. December 2010
- Prof. Dr. Harald Markum
  TU Wien, Austria
  Formulation of Time from Aristotle to Monte Carlo Simulations and to Noncommutative Geometry
  25.–26. November 2010
- Prof. Dr. A. Hartmann
  Universität Oldenburg, Germany
  Large-Deviation Properties of Largest Component for Random Graphs
  26.–27. November 2010
- Prof. Dr. Bernd A. Berg
  Florida State University, Tallahassee, USA
  From Data to Probability Densities without Histograms
  16.–17. December 2010