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Computational Quantum Field Theory

10.1 Introduction

The Computational Physics Group performs basic research into classical and quantum statistical physics with special emphasis on phase transitions and critical phenomena. In the centre of interest are 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 adsoprtion 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 previous European Research Training Network (RTN) "ENRAGE": *Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*, a collaboration of 13 teams throughout Europe. Moreover, initiated by a bi-national Institute Partnership with the Jagiellonian University in Krakow, Polen, supported by the Alexander von Humboldt (AvH) Foundation the statistical mechanics of complex networks is studied. In April 2012 a new Institute Partnership Grant of the Alexander von Humboldt Foundation with the Institute for Condensed Matter Physics of the National Academy of Sciences in Lviv, Ukraine, commenced with special focus on *Polymers in Porous Environments and on Disordered Substrates*.

The methodology is a combination of analytical and numerical techniques. The numerical tools are currently mainly Monte Carlo computer simulations and exact enumeration techniques. The computational approach to understand physical phenomena 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 as sketched in Fig. 10.1. 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

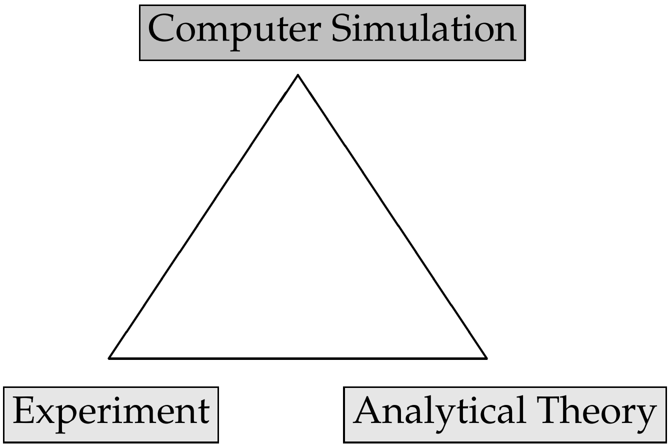

Figure 10.1: Sketch of the relationship between theory, experiment and computer simulation.

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 center, and, upon successful grant application at the national supercomputing centres in Jülich, Stuttgart and München on 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*, the International Max Planck Research School (IMPRS) *Mathematics in the Sciences* and the international DFH-UFA Graduate School *Statistical Physics of Complex Systems* with Université de Lorraine in Nancy, France, supported by the Deutsch-Französische Hochschule. In the second funding period 2011–2013, Coventry University in England has been integrated as an associated partner. The three Graduate Schools are all "Classes" of the Research Academy Leipzig (RALeipzig), providing the organizational frame for hosting visiting students and senior scientists, 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* and the Sonderforschungsbereich/Transregio SFB/TRR 102 *Polymers under Multiple Constraints: Restricted and Controlled Molecular Order and Mobility* together with Halle University. Our group also actively contributes to 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 particularly instrumental for our cooperations with research groups in experimental physics and biochemistry on the one hand and with mathematics and computer science on the other.

On an international scale, our research projects in part initiated by the European RTN "ENRAGE" and the AvH Institute Partnership with the Jagiellonian University in Krakow, Poland, are currently carried out in a wide net of collaborations mainly funded by the German Academic Exchange Service (DAAD) and the Alexander von Humboldt Foundation through the new Institute Partnership with the National Academy of Sciences in Lviv, Ukraine, as well as their Fellowship Programmes. From June 2011 to November 2012 our group has been hosting Professor Handan Arkın-Olgar from Ankara University in Turkey who was awarded an Alexander von Humboldt Fellowship for Experienced Researchers. 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

10.2 Grafted vs Nongrafted Polymers near Attractive Substrates

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The statistical properties of a polymer grafted, i.e. firmly attached at one of its ends, to an attractive substrate [1] are significantly different from those of a polymer that can move freely above that substrate [2]. Especially for the adsorption transition such differences were suggested by a microcanonical analysis of a nongrafted polymer which showed first-order like signals for short extended conformations that get more pronounced with increasing translational entropy of desorbed conformations [3, 4]. To systematically compare the two cases, we employed a combination of canonical and microcanonical analyses over a wide range of surface attraction strengths ϵ_s and temperature T [1]. This way not only the adsorption transition, but also the collapse and freezing transitions of an individual self-interacting polymer in solution were covered.

Our analysis is based on a simple bead-stick model with 12-6 Lennard-Jones (LJ) interaction between nonbonded monomers, a weak bending stiffness and an attraction to a flat substrate that is proportional to a parameter ϵ_s which measures the relative strength compared to the monomer-monomer attraction. This surface attraction is a 9-3 LJ potential obtained by integrating the 12-6 LJ potential over a half space. The polymer is once grafted with one end to the substrate and once considered in a box within which it can move freely. 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 [5].

It turned out that qualitative differences mainly occur at the adsorption transition where four cases need to be differentiated for finite chains: (1) the adsorption of ex-

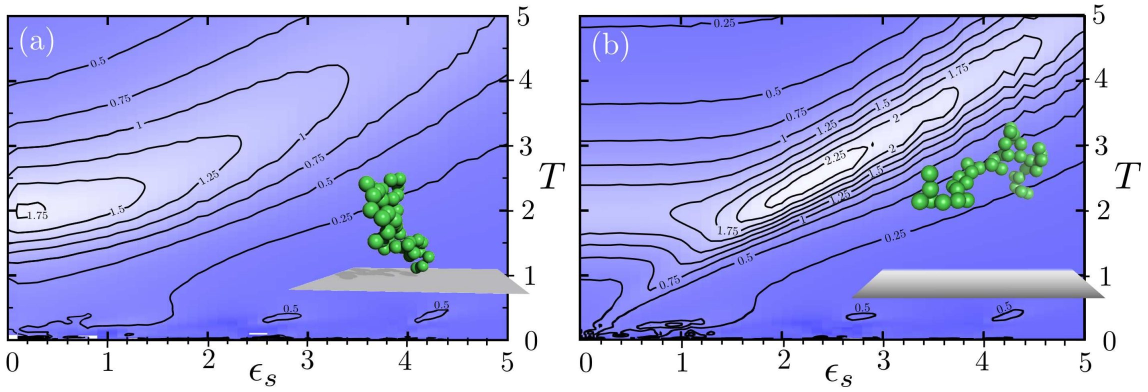

Figure 10.2: Fluctuation of the tensor component of the radius of gyration perpendicular to the substrate $d\left\langle R^2_{\mathrm{gyr},\perp}\right\rangle/dT$ for (a) the grafted and (b) the free polymer as a contour plot versus surface attraction strength ϵ_s and temperature T.

tended nongrafted polymers, (2) the adsorption of extended grafted polymers, (3) the adsorption of globular nongrafted polymers and (4) the adsorption of globular grafted polymers. Only in the first case, the microcanonical entropy, which is proportional to the logarithm of the density of states, gets convex such that the adsorption transition appears first-order-like here. In the cases (2) and (3) a continuous adsorption is observed already for short chains, while in case (4) the adsorption signals get reduced significantly and only a weaker wetting transition is left.

As an example, Fig. 10.2 shows how this is reflected in the temperature derivative of the canonical expectation value of the tensor component of the radius of gyration perpendicular to the substrate. While for the nongrafted polymer a maximum over the whole diagonal $T_{\mathrm{ads}} \propto \epsilon_s$ is visible, this signal is strongly weakened for extended grafted conformations ($\epsilon_s \gtrsim 1.9, T \gtrsim 2$) and even disappears for globular grafted conformations ($\epsilon_s \lesssim 1.9$, $T \lesssim 2$). For grafted chains, in this observable only the collapse transition at $T \approx 2$ is signaled for low ϵ_s values. It is among others this necessary distinction between the adsorption of globular and extended conformations that demonstrates that it is not just the difference in translational, but also in conformational entropy that gives rise to the differences. This has been carefully described and explained in Ref. [1].

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[3] M. Möddel et al.: Phys. Chem. Chem. Phys. **12**, 11548 (2010)
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10.3 Polymer Adsorption onto a Stripe-Patterned Substrate

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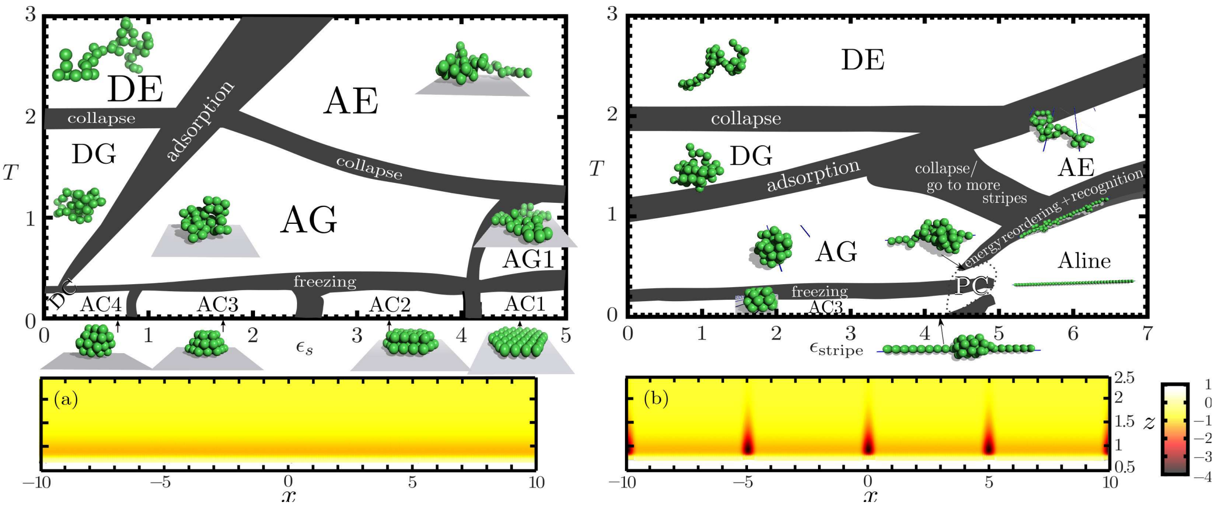

Figure 10.3: (a) On the left the pseudo-phase diagram of the polymer versus temperature and varying ϵ_s for $\epsilon_{\text{stripe}} = 0$ and a heat map of the substrate potential for $\epsilon_s = 1$ is shown – the homogeneous substrate case. (b) On the right the analogous pseudo-phase diagram versus temperature and varying ϵ_{stripe} for $\epsilon_s = 1$ is displayed – the stripe patterned case. Phases with "A/D" are adsorbed/desorbed, while "E", "G", and "C" denote phases with increasing order: expanded, globular, and compact. "PC" is a short form for a region with phase coexistence.

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Naturally occuring substrates almost exclusively exist with heterogeneities not just on the macroscopic, but also on the micro- or nanoscopic level. Consequently, after we developed an in-depth understanding of the statistical equilibrium behaviour of a generic self-attracting polymer model close to an attractive homogeneous substrate in recent years [1–5], the question arose how this behaviour gets modified if hetereogenities are introduced on the substrate.

The goal was to see the influence on the level of the whole pseudo-phase diagram, where "pseudo" refers to the finiteness of the simulated chain length. Since already the phase diagram of the polymer near the homogeneous substrate is very rich in transitions (cf. Fig. 10.3(a)), to extract any meaningful results the chosen surface heterogeneity needs to be easily controllable and preferably simple.

Our choice was to add to the previously investigated [1–5] bulk energy term and 9-3 Lennard-Jones (LJ) attraction between each monomer and the substrate an attractive cosine-square potential of distance $D = 5$ such that the energy of the system in total is

$$E_{\text{bulk}} = 4 \sum_{i=1}^{N-2} \sum_{j=i+2}^{N} \left(r_{ij}^{-12} - r_{ij}^{-6} \right) + \frac{1}{4} \sum_{i=1}^{N-2} \left(1 - \cos \vartheta_i \right) , \tag{10.1}$$

that is strongly dominated by a 12-6 Lennard-Jones (LJ) attraction between non-neighboring monomers, and

$$E_{\text{sur, stripe}}(x, z) = \begin{cases} \left(\frac{2}{15} z^{-9} - z^{-3} \right) \left[\epsilon_s + \epsilon_{\text{stripe}} \cos^2 \left(\pi \left(\operatorname{mod} \left(x + \frac{D}{2}, D \right) - \frac{D}{2} \right) \right) \right], & \text{if} \left| \operatorname{mod} \left(x + \frac{D}{2}, D \right) - \frac{D}{2} \right| \le \frac{1}{2} \\ \left(\frac{2}{15} z^{-9} - z^{-3} \right) \epsilon_s, & \text{else.} \end{cases}$$

(10.2)

The impact of those stripes was described in detail with an emphasis on the onset of the "recognition" transition below which the polymer perfectly adapts the shape of the stripe. Despite some striking differences, many conclusions drawn for the adsorption of a single polymer on a homogeneous substrate remain valid in the more general hetereogeneous case [6].

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[5] M. Möddel et al.: in Proceedings of the *NIC Symposium 2012*, eds. K. Binder, G. Münster, M. Kremer, John von Neumann Institute for Computing, Jülich, NIC Series, Vol. **45**, p. 277 (2012)
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10.4 Exact Enumeration of Polymer Adsorption onto a Stripe-Patterned Surface

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In recent years, polymers have received a great deal of attention from both experimental and theoretical researchers. However, a complete description of the properties of these materials does not currently exist. Therefore, further research is needed. This particular study is part of an ongoing effort to try to understand these systems and is focused on the adsorption of single polymer chains. Previous theoretical studies have provided phase diagrams that lay the foundations for understanding polymer adsorption. This particular study focuses on a single polymer chain in a confined volume and its adsorption onto a stripe-patterned surface.

A minimalistic simple-cubic lattice model was used where the chain is represented by an interacting self-avoiding walk (ISAW) and was confined between an attractive patterned wall and a steric wall with no interaction whatsoever. The pattern consisted of parallel stripes of defined width and separation. The complete system as well as the patterned surface are illustrated in Fig. 10.4. Besides the pattern parameters, entropy and three energy scales define the phase diagram of the system: chain-surface attraction ϵ_s, chain-pattern attraction ϵ_str and chain self-attraction ϵ_m. The energy of the polymer was defined as a function of the different types of contacts $E(n_\mathrm{s}, n_\mathrm{str}, n_\mathrm{m}) = -\epsilon_\mathrm{s} n_\mathrm{s} - \epsilon_\mathrm{str} n_\mathrm{str} - \epsilon_\mathrm{m} n_\mathrm{m}$. One of the coupling constants (ϵ_s) was used to set the scale of the temperature of the system, whereas the other two were expressed as fractions of it. This allowed for the systematic study of a total of four parameters on the properties of the system.

Chains of lengths up to $N = 19$ monomers were studied using the method of exact enumeration. The influence of the energy scales and pattern parameters on the system was analysed with the help of temperature vs. chain-pattern attraction phase diagrams. These diagrams were constructed by means of both canonical and microcanonical

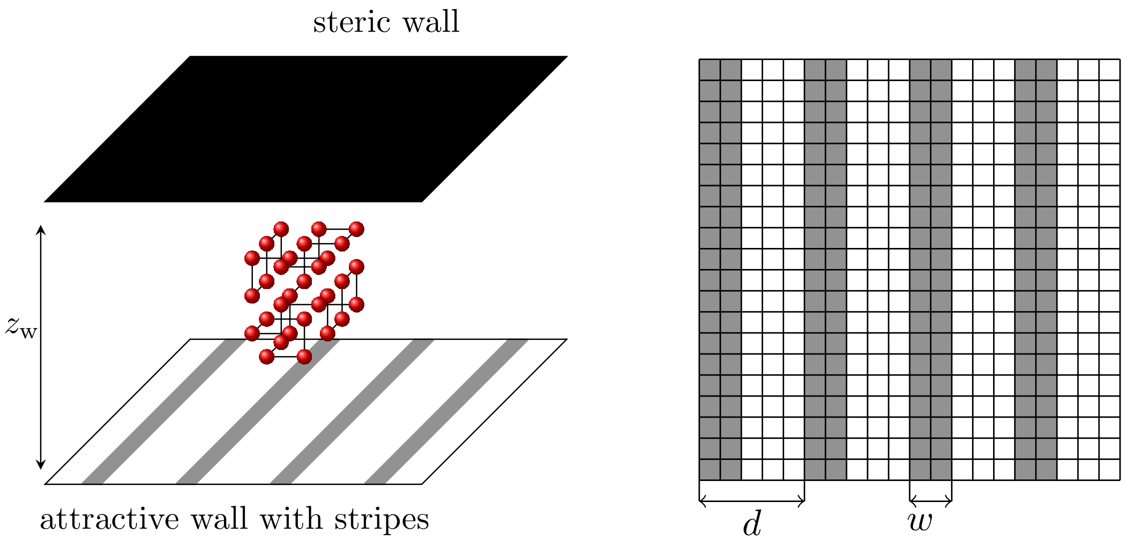

Figure 10.4: Sketch of an ISAW in a cavity of height z_{w}. The width of the attractive stripes (in grey) is controlled by the parameter w and the stripe distance by the parameter d.

analysis of the simulation data. The results are comparable to those from another study of a similar system using an off-lattice polymer model [1]. Although the two models yield quantitatively different results, both show comparable qualitative behaviour.

The effects of the confinement volume on the phase diagram were found to be considerable when the separation between both walls is $O(N)$. For distances between $O(10 \times N)$ and $O(100 \times N)$, minor differences of the transition temperatures were found. The results from the non-grafted chain were also compared with the results for a chain grafted to a stripe. However, the grafted chain was considered to be too short and was not analysed in detail.

These findings are important since substantial progress has very recently been made in experimental techniques. More importantly, it is now possible to visualise single chains, enabling the verification of theoretical models against experimental data as part of a future collaborative research.

[1] M. Möddel: *Statistical Equilibrium Behaviour of Finite Polymers Near Attractive Substrates*, PhD thesis, Universität Leipzig (2012)

10.5 Polymers Adsorbing onto a Fractal Surface

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The study of polymers near disordered surfaces is of great importance since most naturally occurring substrates are rough and energetically (or structurally) inhomogeneous and surface heterogeneity is known to have a crucial effect on polymer adsorption phenomena [1]. As most chemical substrates are proved to be of fractal nature, studying the

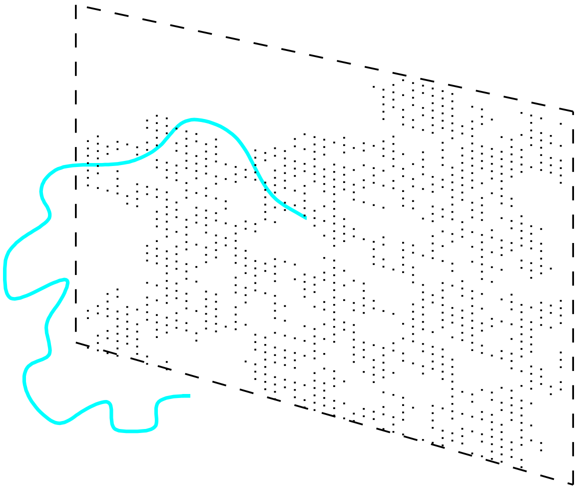

Figure 10.5: Sketch of a polymer grafted to a site of an attractive percolation cluster.

influence of such a non-trivial surface geometry is of particular interest. It is established that the adsorption process is enhanced (diminished) when the fractal dimension of the substrate is larger (smaller) than that of a plain Euclidean surface [2].

As order parameter one considers the fraction of the average number of monomers N_s adsorbed to the surface and the total length N of the polymer chain, obeying for long chains the scaling law $\langle N_s \rangle / N \sim N^{\phi_s - 1}$ where ϕ_s is the surface crossover exponent [3]. In the language of lattice models, where polymers can be represented by self-avoiding random walks (SAWs) [4], disordered surfaces can be modeled as a two-dimensional regular lattice with randomly distributed attractive sites. Fractal properties emerge at the percolation threshold where a spanning percolation cluster of attractive sites with fractal dimension $d_s^{p_c} = 91/49 \approx 1.89 < 2$ appears [5], cf. Fig. 10.5.

We have studied this problem with the help of the pruned-enriched Rosenbluth method (PERM) [6] for simulating the polymer chains. We examined the behaviour of the components of the radius of gyration $\overline{\langle R^2_{g\|} \rangle}$, $\overline{\langle R^2_{g\perp} \rangle}$ in directions parallel and perpendicular to the surface and obtained $\nu_2^{p_c} = 0.772 \pm 0.006$ [7, 8] for the critical exponent that governs the scaling of the size of a polymer adsorbed onto a fractal substrate. This value is compatible with $\nu_2^{p_c} = 0.782 \pm 0.003$ for a polymer strictly confined onto a two-dimensional percolating cluster [9], but significantly larger than $\nu_2 = 0.742 \pm 0.006 \approx 3/4$ for a plain homogeneous surface [7]. Examining the peak structure of the heat capacity, we estimated for the surface crossover exponent $\phi_s^{p_c} = 0.425 \pm 0.009$, compared to $\phi_s = 0.509 \pm 0.009$ for the plain surface [7]. As expected, the adsorption is diminished, when the fractal dimension of the surface is smaller than that of the plain Euclidean surface due to the smaller number of contacts of monomers with attractive sites.

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10.6 Ground-State Properties of a Polymer Chain Inside an Attractive Sphere Potential

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Investigating basic structure formation mechanisms of biomolecules at different interfaces is one of the major challenges of a large variety of modern interdisciplinary research and possible applications in nanotechnology. Knowledge of the origin of structure formation is an important prerequisite for the understanding of polymer adhesion to metals and semiconductors [1], biomedical implants [2], and biosensors [3]. The adsorption behaviour can also influence cellular motion, drug delivery, and other biological processes. The advances in designing and manipulating biomolecules at solid substrates on the nanoscale open new challenges for potential nanotechnological applications of hybrid organic-inorganic interfaces.

Recently, some progress has been achieved in the understanding of general properties of the conformational behaviour of homopolymers and heteropolymers near substrates. In most cases, the substrates are considered to be planar [4]. In this work, we considered a simple off-lattice coarse-grained polymer model inside of an attractive sphere, for which we have recently constructed the finite-temperature phase diagram [5]. Here, we focused on the ground-state properties caused by different attraction strengths ϵ of the sphere within the frame of generalized-ensemble simulations [6]. In a comparative analysis based among others on various (invariant) shape parameters related to the eigenvalues of the gyration tensor, a classification of the structures formed in the accompanying adsorption process has been achieved.

The distributions of all successive pairs of virtual bond angles $\Theta_i = \pi - \vartheta_i$ and torsion angles Φ_i in the low-temperature regime ($T < 0.2$) for different values of the surface attraction strength ϵ are shown in Fig. 10.6. It is one of the most remarkable results of our study that for different parameter values of the polymer-attractive sphere system, we get conformations that fit perfectly to the inner wall of the sphere. A careful comparison with results for flat substrates has recently been presented in Ref. [7].

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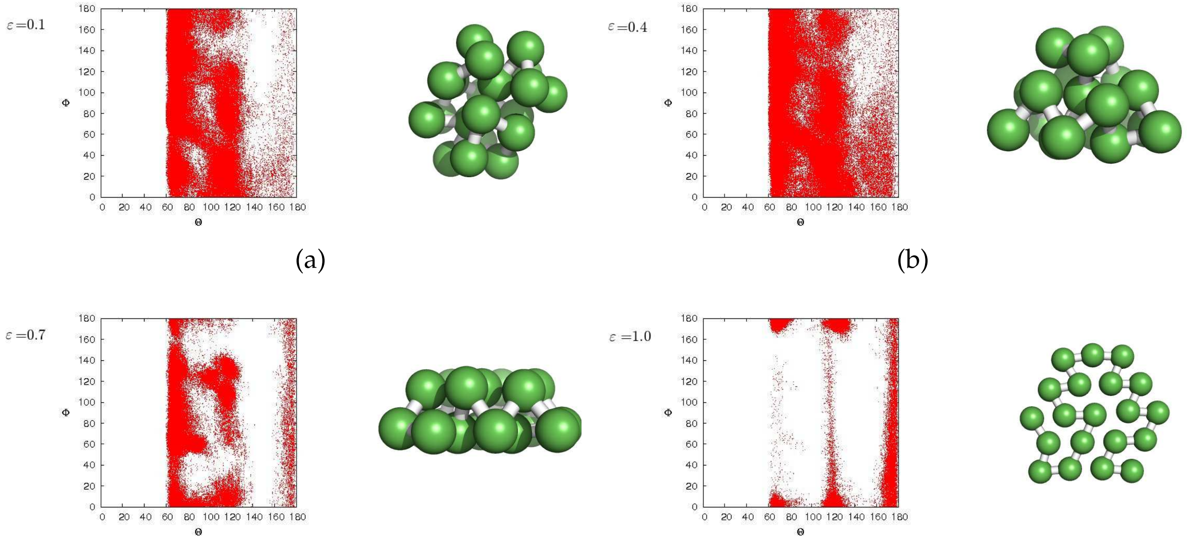

(a) (b)

(c) (d)

Figure 10.6: Bond and torsion angle distributions for (a) $\epsilon = 0.1$, (b) $\epsilon = 0.4$, (c) $\epsilon = 0.7$, (d) $\epsilon = 1.0$ and the associated conformations of the global energy minimum. The distribution of the torsion angles has reflection symmetry and therefore only the positive interval is shown.

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10.7 Thermodynamics of a Model Protein in Spherical Confinement

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We have performed Monte Carlo computer simulations in generalized ensembles of a model protein confined in a spherical cage to investigate the dynamics of the folding mechanism [1]. The problem of whether proteins are misfolded or aggregated or, on the contrary, fold properly more promptly in spatial confinement has recently attracted much interest [2, 3]. A detailed understanding of this subject would play a key role for finding treatments to diseases caused by misfolding of proteins. Our goal is thus to analyze the thermodynamics of the folding mechanism and to investigate whether the folding mechanism is controlled or not in a confining environment. To do so we have employed exhaustive multicanonical Monte Carlo simulations by using a minimalistic AB model where hydrophobic residues are labeled by A and the polar or hydrophilic

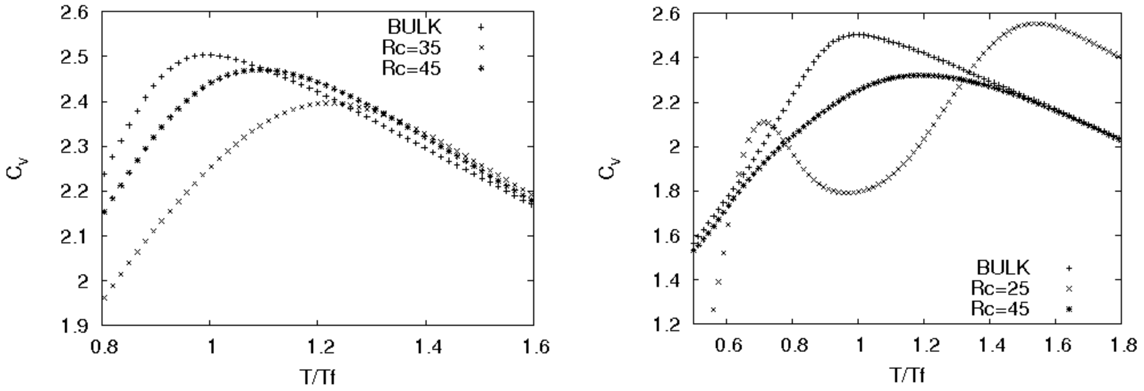

Figure 10.7: Specific heat as a function of temperature for the AB model protein $BA_6BA_4BA_2BA_2B_2$ in a spherical confinement with sphere radius R_c. The temperature T is given in units of the folding temperature T_f in the bulk. *Left:* Purely repulsive potential. *Right:* Attractive potential.

ones by B [4, 5]. Adjacent residues or monomers are connected by rigid covalent bonds. Thus, their distance is kept fixed and set to unity. The contact interaction is replaced by a distance- and residue-dependent $12-6$ Lennard-Jones potential accounting for short-range excluded volume repulsion and long-range interaction. An additional interaction accounts for the bending energy of any pair of successive bonds. In this study, we focused on the folding of a model protein with 20 residues arranged in the sequence $BA_6BA_4BA_2BA_2B_2$.

The model protein is enclosed by a sphere of radius R_c. Apart from the steric hindrance effect, we assumed two different types of wall interactions, one with a purely repulsive wall potential and another that exhibits an attractive part close to the inner sphere wall. By monitoring the specific heat as a function of temperature, we observe in the first, purely repulsive case merely a monotonic finite-size scaling shift of the folding temperature, cf. Fig. 10.7 (left). The second case with attractive wall interaction is much more interesting since here, for small enough sphere radius R_c, the protein is first adsorbed to the (inner) surface of the sphere and in a second step the folding takes place. This is indicated by the two peaks of the specific heat for $R_c = 25$ in Fig. 10.7 (right) [6].

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10.8 Effects of Spherical Confinement on Phase Transitions of a Simple Model for Flexible Polymers

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We used our recently developed "Polymer Framework" for Monte Carlo simulations to investigate a simple bead-stick model for a flexible homopolymer. This model features two different pseudo-phase transitions, the collapse transition which distinguishes the random coil and the globular phase and the freezing transition which distinguishes the globular and a crystal like phase. Our model is so simple, that we cannot claim to observe quantities for any specific polymer or biopolymer, but it is also so generic, that it should reflect the qualitative behaviour of any flexible chain-like object. Especially, we are interested in the case where we confine this polymer to a spherical cage as illustrated in Fig. 10.8 and how this confinement influences the two pseudo-phase transitions of our model. On the one hand, confinements are very important for all kind of biopolymers such as proteins, DNA or RNA, because their natural habitat are crowded environments like micelles or chaperon-like cages, where a spherical cage could be considered as a first-order approximation for these environments. For synthetic polymers the behaviour inside a confinement could be also very important for different kinds of technical applications which try to combine polymers with novel materials.

To investigate the thermodynamic behaviour of our model, we need to calculate different thermodynamic observables, such as the energy, the end-to-end distance or the radius of gyration and their thermodynamic derivatives, over a broad temperature range. For this propose we use the parallel tempering Monte Carlo technique [1, 2], which enables us not only to calculate all desired observables over a temperature range, it also helps us to overcome technical problems arising from the complex energy landscape which even such a simple model features [3].

The Hamiltonian of our system is given by a Lennard-Jones potential which corresponds to the excluded-volume and attractive parts of the monomer-monomer interaction, a cosine potential which introduces a bending stiffness to our model and a spherical cage which restricts the phase space of the polymer to a sphere with radius R_S:

$$
\begin{aligned}
H = {} & 4\sum_{i=1}^{N-2}\sum_{j=i+2}^{N}\left(\frac{1}{r_{ij}^{12}}-\frac{1}{r_{ij}^{6}}\right)+\kappa\sum_{i=1}^{N-2}(1-\cos\theta_i) \\
& \times\begin{cases} 1 & \text{if all } |r_i| < R_S \\ \infty & \text{if any } |r_i| \geq R_S \end{cases} .
\end{aligned}
\tag{10.3}
$$

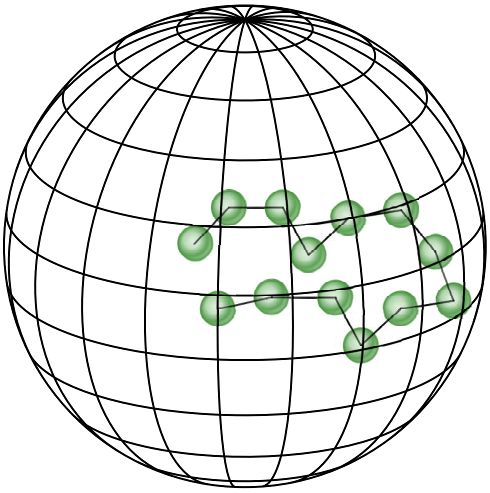

Figure 10.8: Sketch of a polymer fluctuating inside a spherical cage.

Our main goal was to determine the transition temperatures $T_{\rm max}$ of the pseudo-phase transitions and the dependency of $T_{\rm max}$ on the radius of the spherical cage. Good indicators for the transition temperature are the maxima of the temperature derivative of several thermodynamic observables, for example of the radius of gyration, $\frac{d}{dT}\langle R^2_{\rm gyr}\rangle$, see Fig. 10.9. For the freezing transition we observe hardly any change in the position of the phase transition, except for very small radii where the polymer is pressed into very artificial high-energy states due to the repulsive part of the Lennard-Jones potential. In contrast to the freezing transition, the transition temperature of the collapse transition shows a clear dependence on the radius of the sphere. We found the following power law for this dependency, where $T^{\Theta,N}_{\rm max}$ is the transition temperature in the confined case of the collapse transition for a fixed length N of the polymer and $T^{\Theta,N}_c$ is the transition temperature for the free case:

$$|T^{\Theta,N}_{\rm max} - T^{\Theta,N}_c| = A\left(\frac{N^{\frac{1}{2}}}{R_S}\right)^{3.63(15)} . \tag{10.4}$$

The amplitude A is the same for all N. Another notable effect is that the direction of the shift of the transition temperature is opposite to what has been observed in simulations of different realistic models for specific proteins [4–6]. This may depend on the flexibility of the polymer: Our polymer is a very flexible one and most proteins are relatively stiff. The clarification of this question is the objective of further investigations.

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[6] M. Bilsel et al.: in Proceedings of the NIC Workshop *From Computational Biophysics to Systems Biology (CBSB11) – Celebrating Harold Scheraga's 90th*

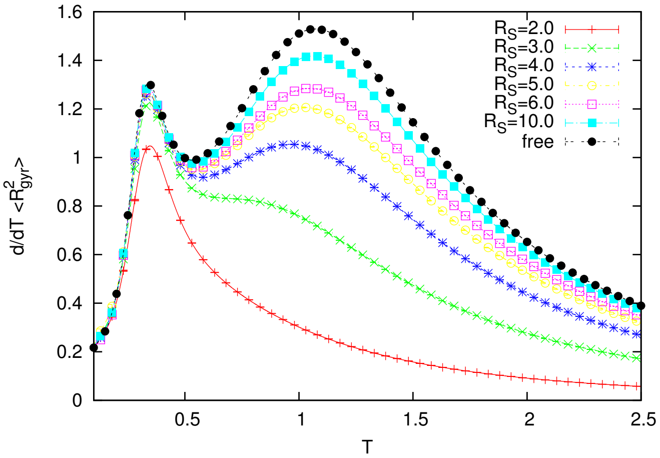

Figure 10.9: The derivative of the radius of gyration, $\frac{d}{dT}\langle R^2_{\mathrm{gyr}}\rangle$, of a 14mer inside spherical cages with different radii.

Birthday, eds. P. Carloni, U.H.E. Hansmann, T. Lippert, J.H. Meinke, S. Mohanty, W. Nadler, O. Zimmermann, John von Neumann Institute for Computing, Forschungszentrum Jülich, IAS Series Vol. **8**, p. 21 (2012)

10.9 Polymer Aggregation Modeled by Interacting Self-Avoiding Walks

J. Zierenberg, A. Tretbar, W. Janke

In order to investigate aggregation of flexible polymers in large systems, we decided to consider interacting self-avoiding walks as a simplified model. This model has been applied to a variety of problems such as protein folding or surface adsorption and yielded good qualitative results. The Hamiltonian of the system is given by

$$\mathcal{H} = -\left(\epsilon_{\mathrm{intra}} n_{\mathrm{intra}} + \epsilon_{\mathrm{inter}} n_{\mathrm{inter}}\right), \tag{10.5}$$

where $n_{\mathrm{intra}}, n_{\mathrm{inter}}$ are the number of contacts of the polymers with themselves and with each other, respectively. This simple but straightforward model allowed to capture the qualitative results for few-polymer aggregation of a coarse-grained model investigated by our group [1].

We applied Metropolis and Parallel Multicanonical [2] simulations to systems with different number of polymers of fixed length and density. It was possible to observe an aggregation process with decreasing temperature, see Fig. 10.10. At the transition temperature, we observed a double peak in the energy distribution with decreasing probability for the intermediate regime, indicating a first-order phase transition. For increasing system sizes, the Metropolis algorithm showed difficulties in the low-temperature regime such that the application of the more sophisticated multicanonical method became more and more necessary. To this end, we successfully applied the "Polymer Framework", developed recently in our group.

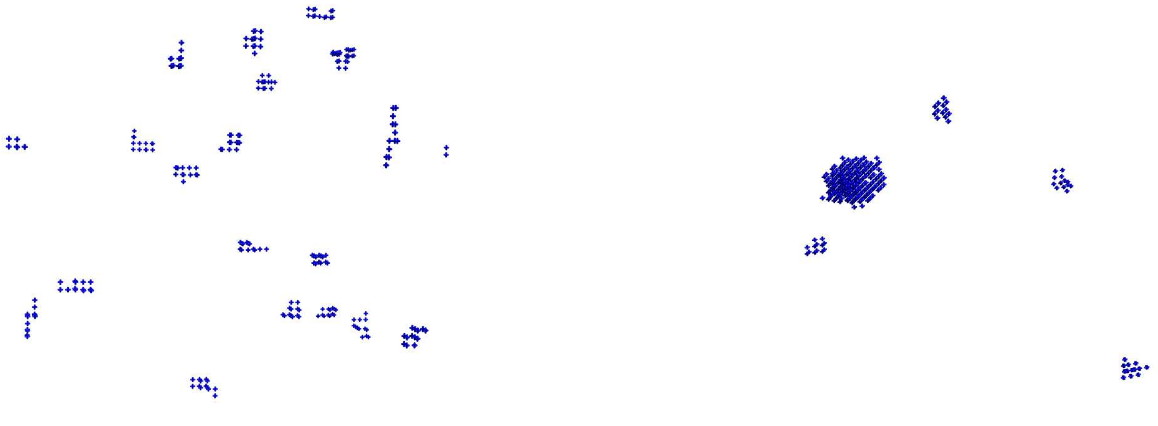
(a) (b)

Figure 10.10: Example of the aggregation process for 20 interacting self-avoiding walks of length 13: (a) High-temperature fluctuations and (b) low-temperature aggregation.

The transition temperature of the aggregation was observed to depend on the number of polymers, the length of the polymers and the density. The explicit dependencies are currently under investigations. Still, the rich parameter space combined with the accessible numeric effort promise interesting insight into the aggregation phenomenon of flexible polymers.

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[2] J. Zierenberg et al.: Comput. Phys. Comm. **184**, 1155 (2013)

10.10 Random Heteropolymer Models

V. Blavatska*, W. Janke

*Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, Lviv, Ukraine

A subject of great interest in both chemical and biological physics are the conformational properties of long heteropolymer chains. Typical examples are proteins, consisting of sequences of amino acid residues, connected by peptide bonds. The conformations of individual macromolecules are controlled by the type of monomer-monomer interactions. In general, the constituents (monomers) of macromolecules in an aqueous environment can be characterized as hydrophilic or hydrophobic, depending on their chemical structure. Hydrophilic residues tend to form hydrogen bonds with surrounding water molecules, whereas the hydrophobic monomers effectively attract each other and tend to form a dense hydrophobic core.

We studied the conformational transitions in heteropolymers within the frames of a lattice model containing two types of monomers A and B, N_A monomers of type A and $N_B = N - N_A$ monomers of type B. Such a model can describe in particular the sequences of hydrophobic and hydrophilic residues in proteins [1] and polyampholytes with oppositely charged groups [2]. Restricting ourselves only to short-range

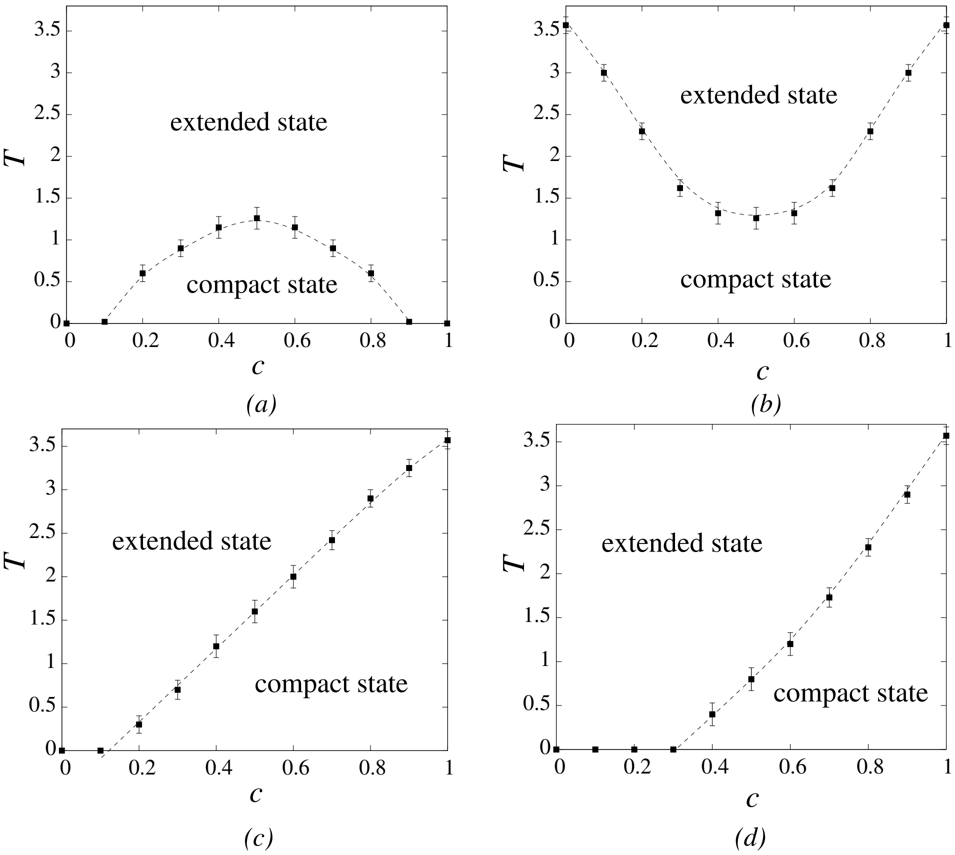

Figure 10.11: Phase diagrams of heterogeneous polymer chains in T-c space. (a) model 1, (b) model 2, (c) model 4, (d) model 5.

interactions between any pair of monomers residing on neighboring lattice sites that are not connected by a covalent bond, we considered 5 different parametrizations of this model. In particular, model 1 ($\varepsilon_{AA} = \varepsilon_{BB} = 1, \varepsilon_{AB} = -1$) where like monomers repel and opposite ones attract each other, refers to strongly screened Coulomb interactions [2]. The model 3 ($\varepsilon_{AA} = 1, \varepsilon_{BB} = \varepsilon_{AB} = 0$) is a particular case of model 1 and corresponds to a polymer chain containing charged (A) and neutral (B) monomers. Model 4 ($\varepsilon_{AA} = -1, \varepsilon_{BB} = \varepsilon_{AB} = 0$) refers to the (minimal) HP model [5] with hydrophobic (A) and hydrophilic (B) monomers. Models 2 ($\varepsilon_{AA} = \varepsilon_{BB} = -1, \varepsilon_{AB} = 1$) and 5 ($\varepsilon_{AA} = -1, \varepsilon_{BB} = 1, \varepsilon_{AB} = 0$) can be considered as generalizations of the two above mentioned cases.

Applying the pruned-enriched Rosenbluth chain-growth algorithm (PERM) [3] we analyzed numerically the transitions from an extended into a compact state as function of the inhomogeneity ratio $c = N_A/N$ for all five heteropolymer chain models [4]. In model 3, unlike the other models, the polymer chain expands its size with lowering the temperature due to the repulsion between monomers, and the polymer chain remains in an extended state at any temperature. As it shown in Figure 10.11, in model 2, the so-called θ-transition between an extended and compact state is always present at any value of inhomogeneity ratio c, whereas models 1, 4 and 5 remain in an extended state when the concentration of attracting monomers is too small to cause a transition into the compact state. Note also that at small concentration of attractive monomers, the chains can attain the compact state only when they are long enough and have enough attractive nearest-neighbour contacts to overcome the conformational entropy. In the limiting case $c = 1$, models 2, 4 and 5 describe homogeneous polymer chains with nearest-neighbour attractions (for model 2 also $c = 0$) with known value of the transition temperature $T_\theta = 3.717(3)$ [3].

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10.11 Exact Enumeration of Self-Avoiding Walks on Multidimensional Critical Percolation Clusters

N. Fricke, T. Peschel, W. Janke

The self-avoiding walk (SAW) is one of the most fundamental models in statistical physics. Its asymptotic scaling behaviour is characterized by universal exponents, which are assumed to be valid for a range of systems, from SAWs on a square lattice to flexible polymers in good solvents. The exponents are independent of details such as the lattice type, but they do depend on the dimensionality of the system.

While SAWs on regular lattices are relatively well understood, their behaviour in crowded disordered environments still holds many questions. A paradigmatic case are SAWs on critical percolation clusters, see [1, 2]. At the percolation threshold, the lattice is disordered on all length scales and the clusters have non-integer fractal dimensions. It is natural to assume that the clusters' Hausdorff dimension will take role of the Euclidean dimension for SAWs on regular lattices. However, there are a number of other fractal dimensions that might also be relevant. It has even been argued that only the cluster backbone (Fig. 10.12), the part of the cluster that remains when all singly connected "dangling ends" are removed, should determine the SAW's scaling behaviour. While this is probably not the case, it is clear that the backbone plays a crucial role. Treatment of the problem with standard numerical tools has proved difficult, and the few existing analytical results are controversial.

We recently developed a new method to efficiently enumerate all SAW conformations on a critical cluster or its backbone [3, 4]. Exploiting the clusters' low connectivity and self-similarity, it outperforms the best Monte Carlo methods [5]. We have now generalized the method to systems of arbitrary dimensionality, and recent optimizations have made it possible to handle 10^4 SAW steps with 10^{1000} conformations. Preliminary measurements of SAWs of 10^3 steps already yielded good estimates for the scaling exponents on critical clusters in up to seven dimensions. More extensive simulations, which will shed some light on the role of the fractal dimensions, are ongoing.

[1] B. Barat, B.K. Chakrabarti: Phys. Rep. **258**, 377 (1995)

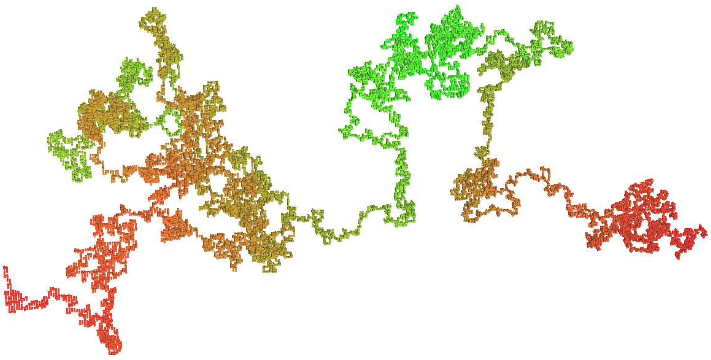

Figure 10.12: Backbone of a three-dimensional critical percolation cluster. Coloring indicates chemical distance to the origin.

[2] V. Blavatska, W. Janke: Europhys. Lett. **82**, 66006 (2008); Phys. Rev. Lett. **101**, 125701 (2008)
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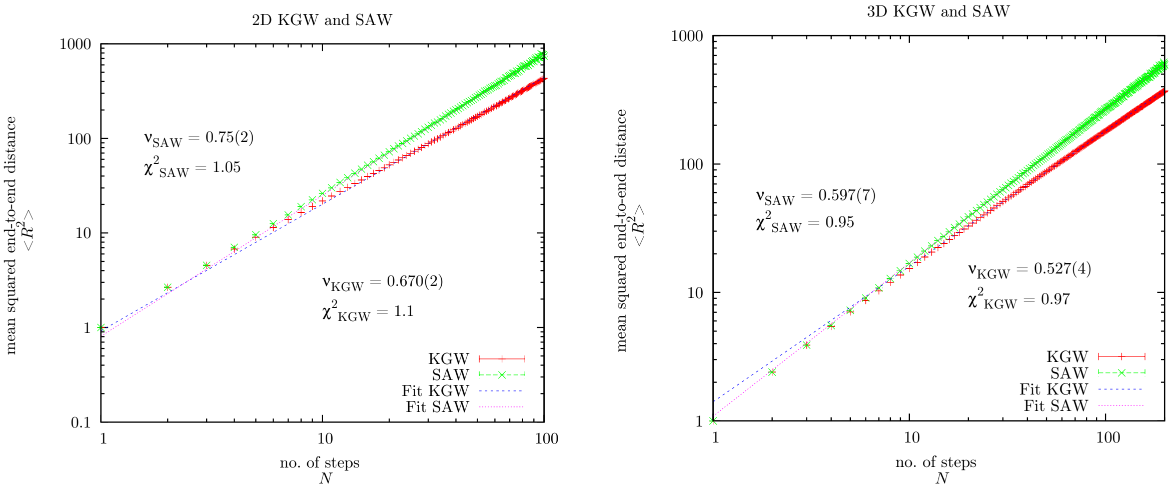
10.12 Kinetic Growth Random Walks

J. Bock, N. Fricke, W. Janke

Random walks are a field of interest in statistical physics since the 1950s. They are a basic model of polymers and are investigated in various forms, e.g., the simple random walk, the self-avoiding walk (SAW) or the kinetic growth walk (KGW). A special interest lies in their universal scaling behaviour with respect to their end-to-end distance R and chain length N, $\sqrt{\langle R^2 \rangle} \sim N^\nu$, where ν denotes the universal exponent. Measurements were done by our group for self-avoiding walks in two and three dimensions on regular lattices and diluted lattices [1, 2].

We revisited kinetic growth random walks for two reasons in particular: First they have not been under investigation since the early 1990s and the results from that time were to be evaluated by nowadays computational possibilities. Second to compare these results to those of the self-avoiding walks. To this end, two algorithms were used, the Rosenbluth-Rosenbluth and pruned-enriched Rosenbluth chain-growth algorithm (PERM). The results of our work [3] for regular lattices are shown in Fig. 10.13. The difference between KGW and SAW is obvious and quite similar results were obtained on diluted lattices. The comparison with previous results is shown in Table 10.1. For the 2D case, our results are similar to the work done bei Kremer and Lyklema [4] and in 3D we are between Kremer and Lyklema and Majid [5]. Also in the case of diluted lattices we obtained different results for SAW and KGW, hence we can conclude both walks behave differently and are not the same.



(a) 2D walks of length 250 and fit range (10:250). (b) 3D walks of length 200 and fit range (13:148).

Figure 10.13: Comparison of (a) two-dimensional (2D) and (b) three-dimensional (3D) kinetic growth walks (KGWs) and self-avoiding walks (SAWs).

Table 10.1: Comparison of the exponent ν for KGWs with previous results.

Authors	ν
Majid [5]	$\nu_{2D} = 2/3; \nu_{3D} = 1/2$
Lam, Zhang [6]	$\nu_{2D} = 0.646$
Kremer, Lyklema [4]	$\nu_{2D} = 0.68; \nu_{3D} = 0.525$
Pietronero [7]	$\nu_{2D} = 3/4; \nu_{3D} = 3/5$
our work	$\nu_{2D} = 0.682(2); \nu_{3D} = 0.520(1)$

[1] V. Blavatska, W. Janke: Europhys. Lett. **82**, 66006 (2008); Phys. Rev. Lett. **101**, 125701 (2008)
[2] N. Fricke, W. Janke: Europhys. Lett. **99**, 56005 (2012)
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[5] I. Majid et al.: Phys. Rev. Lett. **55**, 1257 (1984)
[6] P.M. Lam, Z.Q. Zhang: Z. Phys. B **69**, 65 (1984)
[7] L. Pietronero: Phys. Rev. Lett. **55**, 2025 (1985)

10.13 Semiflexible Polymers in Hard-Disk Disorder

S. Schöbl, J. Zierenberg, W. Janke

The conformational properties of polymers exposed to disordered media are strongly affected by the surrounding disorder potential. For the case of flexible polymers, the impact of disorder on polymers has already been discussed since long [1–3]. The special case of geometrical constraining environments has been investigated recently in, e.g., Ref. [4]. It is expected that geometrical restrictions to chain conformations also play a crucial role for biological systems. In these systems, however, polymers may no

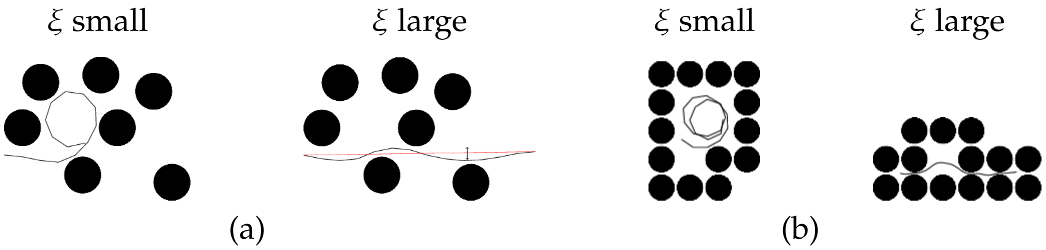

Figure 10.14: Sketch to elucidate the idea of softening and stiffening for polymers with small and large persistence length ξ at (a) low and (b) high occupation probabilities, respectively. The double-headed arrow indicates the width of the thermal fluctuations of the polymer.

longer be assumed flexible and models of moderately stiff polymers, called semiflexible polymers, are introduced. The stiffness is characterized by the persistence length ξ. On length scales shorter than the persistence length, the polymers behave like stiff rods; on longer scales, they exhibit entropic flexibility and random coiling occurs. The geometrical restrictions of the environment along with the intrinsic stiffness of the polymers lead to an interesting phenomenology, which, in contrast to the case of flexible polymers, is to date only partially understood [5, 6].

In this work we used an off-lattice growth algorithm [7] and multicanonical simulations to examine the equilibrium properties of a pinned semiflexible polymer exposed to a quenched random potential consisting of hard disks [8]. The disks are arranged on the sites of a square lattice. We build up on Ref. [4], where flexible polymers exposed to hard-disk disorder assembled on the sites of a square lattice were investigated. We extend the polymer model to comprise bending stiffness. In computer simulations, the appropriate polymer model is the Heisenberg chain model which in the continuum limit becomes the worm-like chain, also called the Kratky-Porod model [9].

We found that the polymer, depending on the ratio of persistence length and void space extension, either crumples up (small ξ) or straightens (large ξ) for increasing density of the potential (see Fig. 10.14). Besides, the periodic structure of the lattice is reflected in the distribution functions of the polymer. Furthermore, we found that the distributions – in the case of pinning the polymer at one end – strongly reflect the local cluster structure of the disorder. Leaving the constraint of pinning lets the polymer escape local cavities and gain entropy in larger void-space clusters. The corresponding distributions for pinned and non-pinned polymers differ considerably. Equipped with this finding, a challenging next step is to investigate the behaviour of semiflexible polymers in hard-disk fluid disorder.

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10.14 Polymer Framework: A Tool Box for fast Programming of Monte Carlo Simulations

M. Marenz, J. Zierenberg, W. Janke

We have started to create an environment for writing fast and efficient Monte Carlo (MC) simulations for arbitrary polymer models. Simulations of such systems yield a better understanding of the behaviour of polymers in specific circumstances [1], or may provide a good initial guess for creating new ones with specific properties [2]. There are a lot of different Molecular Dynamics (MD) programs available, which are capable of simulating biological or synthetic polymers. However, their abilities to perform MC simulations are rather limited because sophisticated update algorithms are, if at all, implemented only rudimentary. Although MC techniques, in contrast to MD, cannot investigate dynamical properties, they are very convenient for investigating phase transitions and the general character of phase space of arbitrary models in a very efficient manner. The efficiency comes from the broad range of improved MC techniques and the possibility to design a suitable propagation of the system as a Markov process freely.

Unfortunately there exists no widely-used program for MC simulations of polymers. To write a single program which implements all these techniques and possibilities at the same time and still remains efficient is nearly impossible. The alternative, writing a new program from scratch for every demand could be very annoying. That is one reason, why we developed a framework for MC simulations of polymers. The aim of this framework is to provide an environment in the C++ programming language, allowing to perform MC simulations for specific problems in a short time. Another goal of the framework is the expandability. Thus, one can add new methods, potentials, systems and update methods, without adjusting all other parts of the framework. To achieve this goal we divided the problem into single parts, which fit into each other. One can imagine every part as a brick, which can be combined in order to construct a simulation.

There are five basic building blocks: The smallest building blocks are the atoms. The next block is the system, which combines all needed atoms and defines the Hamiltonian of the physical system. On top of the system are the last two main building blocks, the update move and the MC technique. Moves define single updates of the system, propagating from the current state to the next one. Additionally a constraint can be added to every move, in order to simulate a polymer in confinement. An organogram of the simulation framework is sketched in Fig. 10.15.

Until now, we have implemented several MC techniques such as parallel tempering [3], multicanonical [4] and Wang-Landau [5]; for recent reviews, see [6, 7]. As system there are all kinds of linear polymers available, such as simple bead-spring or bead-stick models, with Lennard-Jones, spring, FENE and bending potentials. Adding further pair or bending potentials is extremely simple. We have also implemented confinement constraints such as steric walls, a sphere or a barbell.

As first examples, we are looking at the behaviour of a homopolymer in two different confinements, a polymer inside a sphere and inside a barbell. One important question here is to what extent the confinement modifies the phase transition properties compared to those of a free polymer.

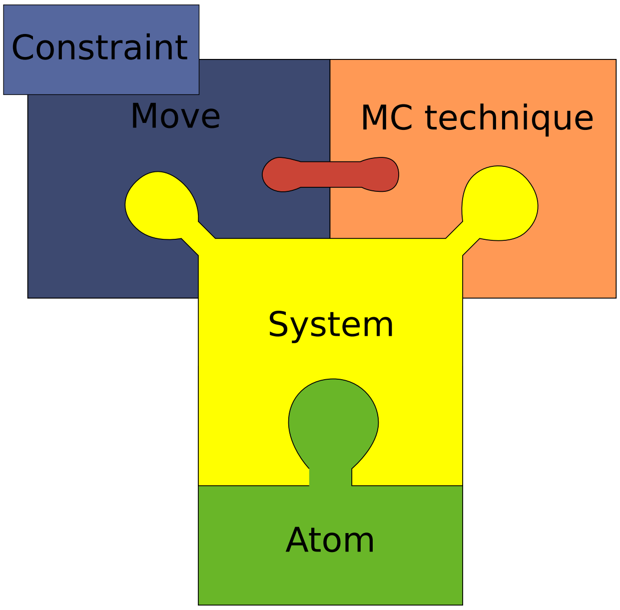

Figure 10.15: The five basic building blocks of the MC simulations framework.

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[2] M. Bachmann et al.: Angew. Chem. Int. Ed. **49**, 9530 (2010) [Angew. Chem. **122**, 9721 (2010) (in German)]
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10.15 The Effect of Multiple Inherent Time Scales on the Dynamics of the Binary Frustrated Unit

D. Labavić[*], H. Nagel, W. Janke, H. Meyer-Ortmanns[*]

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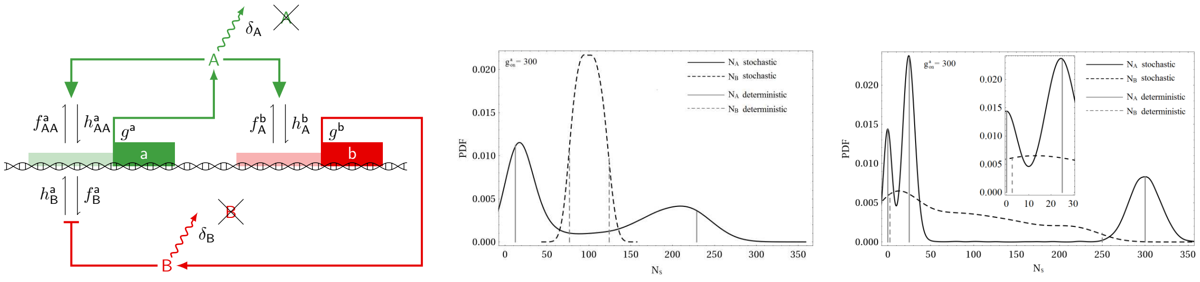
The motif of a self-activating species A that also activates another species B, which in turn represses its activator A, is often found in biological systems, particularly in those featuring inherent oscillatory behaviour. In such biological systems a source of delay in the interaction is essential for the observed dynamics. Thus different time scales are present in the interaction of the species. In this research, we investigated how such different inherent time scales lead to distinct dynamics in a stochastic description of such a system.



(a) (b) (c)

Figure 10.16: (a) Implementation of the basic motif as a genetic circuit. (b), (c) Probability density functions for populations N_A, N_B of species A, B respectively for a fast (b) and slow (c) time scale of gene activation. For slow genes (c) the bifurcation picture changes and attractors split up.

We considered a realization as a genetic circuit where two kinds of a proteins act as species A and B. The mechanism of activation and repression is modeled after genetic promoter sequences encoded before their respective regulated genes: The binding of a specific protein to an activating or inhibiting promoter region respectively increases or decreases the expression rate of the protein associated to that gene, cf. Fig. 10.16.

In previous work [1] we found that one source of delay can be introduced by making the species B-protein expression and decay slower than that of the A-protein and could observe oscillations. Depending on the amount of delay, these oscillations are the consequence of a limit cycle and large excursions from a fixed point in a Hopf–type bifurcation.

Here we identified and investigated the effect of a second source of delay in the activation/repression mechanism itself [2]. The corresponding time scale is defined by the binding rates of the proteins to the genes promoter regions. Employing Monte Carlo simulations as well as coarse-graining methods in the time domain we were able to identify distinct dynamic behaviours when the time scale of activation is much faster than that of species A, as fast as A and as slow as B. The bifurcational patterns change with the inherent time scales, too.

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10.16 Condensation Shapes in a Stochastic Mass Transport Model

E. Ehrenpreis, H. Nagel, W. Janke

Generic examples for stochastic mass transport processes are traffic flow, 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 usually out-of-equilibrium, it is in general

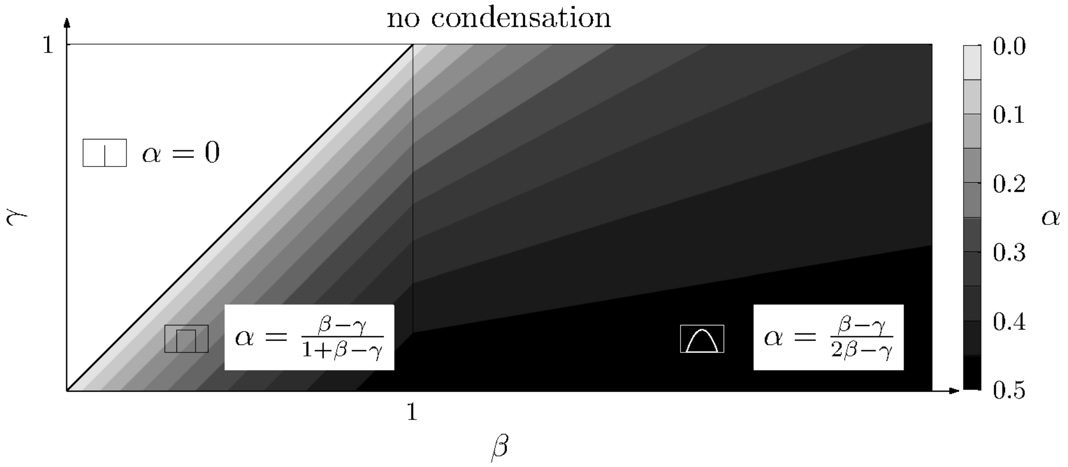

Figure 10.17: Theoretically predicted phase diagram for $K(x) \sim e^{-x^\beta}$ and $p(m) \sim e^{-m^\gamma}$, exhibiting condensed phases with point-like, rectangular and parabolic shapes (from left to right). The predicted value of the exponent α in the scaling law for the condensate extension W with the number M' of condensed particles, $W \simeq M'^\alpha$, is indicated by the gray code.

difficult to predict possible stationary states. Still, under certain circumstances it is possible to identify a transition between a liquid-like phase and a phase with a condensate (e.g., a "traffic jam") that are associated with different stationary states. In the condensate a finite fraction M' of constituent particles condenses onto a finite extension W in space, sometimes even onto a single site. This is an example of spontaneous symmetry breaking which, in contrast to equilibrium systems, can happen here even in a one-dimensional system.

In previous analytical work [2–4] we concentrated on a class of models with steady states that factorize over the links of arbitrary connected graphs, so-called pair-factorized steady states (PFSS). This property enables at least partially an analytic treatment of the transport properties. In one dimension we could predict the critical mass density at the condensation transition and in particular the condensate shape which turned out to be non-universal. Rather, by the competition of local (K) and ultralocal (p) interactions governing the hopping rates, it can be tuned from "extended" to "point-like" [5]. The resulting phase diagram for the choice $K(x) \propto \exp(-x^\beta)$ and $p(m) \propto \exp(-m^\gamma)$ and the analytically predicted exponent α in the scaling law for the condensate extension, $W \sim M'^\alpha$, are shown in Fig. 10.17.

The analytical treatment is based on several approximations. To assess their accuracy, we have performed extensive computer simulations of the hopping events and determined the phase diagram numerically [6]. As a result we find very nice agreement with the theoretical prediction. This is demonstrated in Fig. 10.18 where the measured condensate shapes are displayed in the β-γ plane. By performing power-law fits of the condensate widths W against the number of constituent particles M', we obtain in most parts of the β-γ plane very good agreement with the predicted values of the exponent α at a 1% accuracy level.

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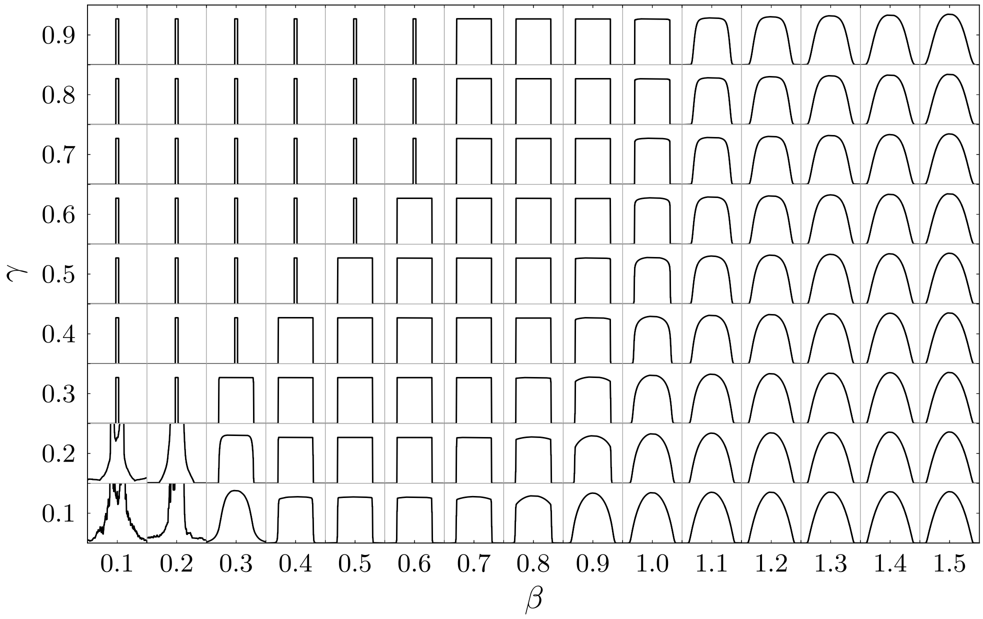

Figure 10.18: Numerically determined characteristic condensate shapes for systems of various β and γ at a condensate volume of about 10^5 masses. The shapes are derived from averages over many measured condensate states. The point-like shapes in the upper left region of the parameter space have not been identified with the present techniques.

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10.17 Mixed Heisenberg Spin Chains: Theory and Quantum Monte Carlo Simulations

R. Bischof, W. Janke

The original Heisenberg model (developed by Heisenberg during his time in Leipzig) and its variants are the basis for understanding quantum magnetism. For instance high-temperature superconducting cuprates can be successfully described as 1D and 2D quantum antiferromagnets at low doping. Depending on the size of the spins and types of coupling mechanisms, the model exhibits a rich variety of zero-temperature quantum critical phenomena. It is well known that 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]. Moreover by tuning appropriate parameters (such as bond alternation, exchange anisotropy, next-nearest-neighbour interaction, spin-phonon coupling, etc.), spin chains can be driven to or away from criticality.

In this project we consider mixed anisotropic Heisenberg (XXZ) spin chains with bond alternation for which much less is known than for uniform chains. Specifically, our focus is on two different mixed quantum XXZ chains consisting of two different kinds of spins, $S_a = 1/2$ and $S_b = 1$ or $3/2$, that appear alternatingly in pairs [2]. In order to investigate their quantum critical properties we employ self-implemented versions of the continuous time loop algorithm [3] and Lanczos exact diagonalization. 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 and could establish a line of continuously varying critical exponents. This 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 the 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].

By invoking conformal field theory, 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. As a consequence, the validity of scaling relations can be tested with higher accuracy [6].

Another exotic order parameter is the twist order parameter [7] that is particularly well suited to signal quantum phase transitions between different valence-bond configurations in 1D chains. Despite its potential to accurately locate pseudo-critical points in quantum Monte Carlo simulations, its scaling behaviour 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 [6], even though according to [7] a scaling dimension can be assigned.

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10.18 Multicanonical Analysis of the Gonihedric Ising Model and its Dual

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Models of fluctuating random surfaces are of great interest in various disciplines of physics or biology. Amongst others, they appear in the treatment of complex networks of membranes [1]. The gonihedric Ising model originates from high-energy physics as a possible discretisation of the area swept out by a string worldsheet moving through spacetime [2]. The name comprises the greek words gonia (angle) and hedra (face) as a reminder of the origin.

A two-dimensional surface is considered to be the assembly of plaquettes in the dual lattice of a three-dimensional lattice of spins. Whenever contiguous spins have opposite signs, such a plaquette is introduced separating the two spins. By changing the spin configuration one effectively alters the surface configuration. Modifying the tendency of spins to align by fine-tuning of the Hamiltonian of the spin system therefore induces different properties to the surface [3, 4].

A strong first-order phase transition can be seen in the special case of surfaces that do not suffer an energy penalty upon self-intersection, as well as glassy dynamics upon cooling in simulations. This phase transition has been analysed using canonical Monte Carlo simulations on dual representations of the model [5], leading to inconsistent results introduced by hysteresis effects.

We investigated the discontinuous phase transition in the original model and its dual representation with multicanonical simulations that are tailored to overcome slow dynamics in first-order transitions caused by phase coexistence [6]. In finite systems and a temperature-driven transition, this is reflected by double-peak distributions of the energy as shown in Fig. 10.19. The finite-size scaling needed to extract properties of the infinite system shows a very interesting behaviour. For Potts-like models, there exists a rigorous theory for peak locations of response functions such as the specific heat or Binder's energy cumulant [7, 8]. The leading contribution of the finite-size correction is expected to be of the order of the inverse volume. For the gonihedric Ising model and its dual, our data suggests a finite-size scaling ansatz, where the leading correction is increased by one power of the system size compared to the theory for Potts-like models. Only then we obtain good agreement between the transition temperatures of the original model and its dual representation. We found that the unusual scaling ansatz still coincides with the theory when taking the exponential ground-state degeneracy of the models into account [9].

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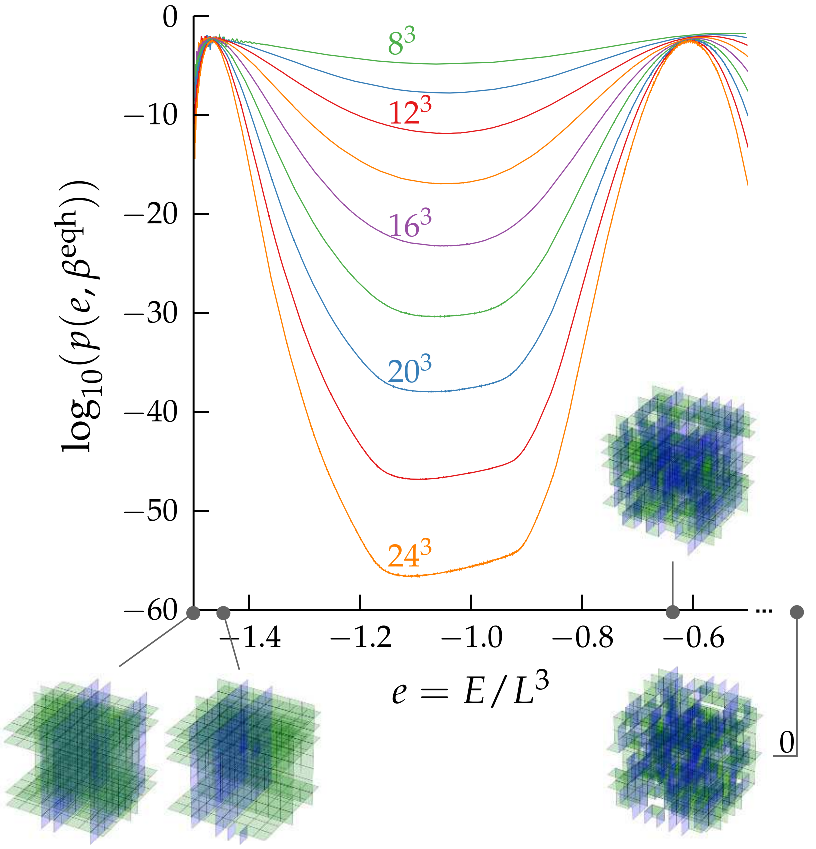

Figure 10.19: Energy probability density of the gonihedric Ising model near the phase transition temperature for various lattice sizes. The rare states between the peaks are strongly suppressed but sufficiently sampled by the multicanonical algorithm. Exemplary configurations for some energies of a cubic lattice with linear size $L = 8$ are depicted as well.

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10.19 Microcanonical Flat-Histogram Sampling

S. Schnabel, W. Janke

Starting from the Metropolis method in 1953 a number of algorithms have been developed to handle complex problems in statistical physics. In many of them estimators of quantities like the density of states or the partition function are in some way derived from histograms, i.e., from measured distributions over a suitable parameter, which is usually the energy of the system. This process can involve the reweighting of a histogram, the determination of the eigenvector of the transition matrix, or – in case of the Wang-Landau method – the adjustment of the algorithm's dynamic at run time while aiming at a flat histogram. Once the density of states is available it can be used

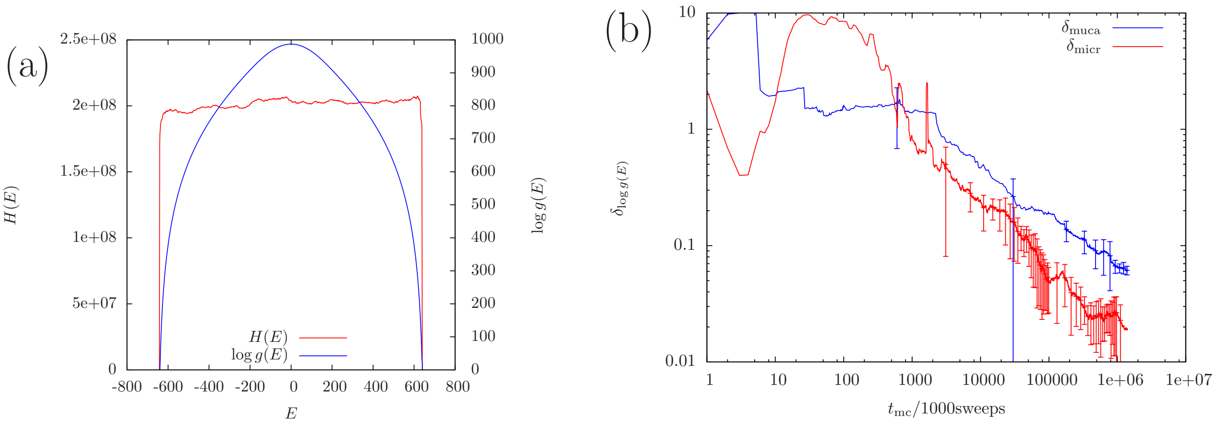

Figure 10.20: (a) The algorithm is able to determine the density of states $g(E)$ over a few hundred orders of magnitude with a high enough precision to produce a flat histogram $H(E)$. (b) Estimating the density of states from microcanonical averages leads to smaller errors (red) compared to a conventional multicanonical simulation (blue).

to obtain thermodynamic quantities like the specific heat or the mean energy. As mentioned, this approach is based on one or more histograms and derived results inherit the comparatively large statistical errors associated with them.

Alternatively, the phase space of a system can as well be analyzed by means of a microcanonical temperature [1] which can be calculated based on gradient and Hessian of the Hamiltonian [2]. It is in principle possible to go one step further and integrate this microcanonical temperature, thus constructing the density of states and use it in turn to drive the Monte Carlo process. This way, shortcomings of the histogram approach would be avoided. However, the calculation of the Hessian is computational expensive and such a method would, therefore, in most cases not be practical.

Using the concept of statistical processes we were able to obtain a slightly different formula where the Hessian is replaced by the Laplacian which can be calculated much faster. The expression becomes particularly simple for spin models with continuous degrees of freedom and we applied the algorithm to the well-known classical Heisenberg model.

We found that the algorithm converges and that the produced histogram is constant over the entire energy range indicating that the estimate of the density of states is accurate [Fig. 10.20(a)]. We consider this an achievement since the main objective of this method is not to balance the histogram but to calculate microcanonical averages. In comparison to established flat-histogram methods our algorithm is faster, i.e. produces results with higher precision in less time. Moreover, even a multicanonical simulation starting with already well-tuned weights (which could be considered a close-to-optimum histogram-based technique) soon has a larger error than the microcanonical sampling [Fig. 10.20(b)].

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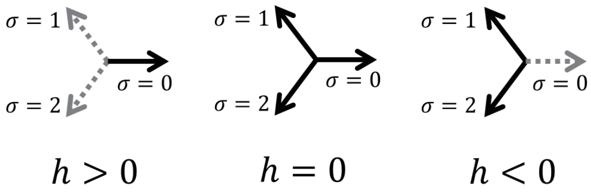

Figure 10.21: Schematic sketch illustrating the behaviour of the spins of the three-state Potts model in an external magnetic field h.

10.20 Simulated Tempering and Magnetizing Simulations of the Three-State Potts Model

T. Nagai*, Y. Okamoto*, W. Janke

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The three-state Potts model in an external magnetic field has several interesting applications in condensed matter physics and serves as an effective model for quantum chromodynamics [1]. When one of the three states per spin is disfavoured in an external (negative) magnetic field (see Fig. 10.21), the other two states exhibit Z_2 symmetry and one expects a crossover from Potts to Ising critical behaviour.

To study such a crossover in a two-dimensional parameter space, generalized-ensemble Monte Carlo simulations are a useful tool [2]. Inspired by recent multi-dimensional generalizations of generalized-ensemble algorithms [3], the "Simulated Tempering and Magnetizing" (STM) method has been proposed by two of us and first tested for the classical Ising model in an external magnetic field [4]. In the conventional simulated tempering (ST) scheme [5] the temperature is considered as an additional dynamical variable besides the spin degrees of freedom. The STM method is a generalization to a two-dimensional parameter space where both the temperature *and* the magnetic field are treated as additional dynamical variables. Recently we have extended this new simulation method to the two-dimensional three-state Potts model and by this means generated accurate numerical data in the temperature-field plane [6].

Our STM simulations were performed for lattice sizes $L = 5, 10, 20, 40, 80$, and 160 with the total number of sweeps varying between about 160×10^6 and 500×10^6, where a sweep consisted of N single-spin updates with the heat-bath algorithm followed by an update of either the temperature T or the field h. By this means one can easily sample a wide range of the two-dimensional parameter space and it is straightforward to compute a two-dimensional map of any thermodynamic quantity that can be expressed in terms of the energy and magnetization. As an example, Fig. 10.22 shows (a) the specific heat and (b) the susceptibility for $L = 80$. We see a line of phase transitions starting at the Potts critical point at $h = 0$, $T_c^{\mathrm{Potts}} = 1/\ln(1+\sqrt{3}) = 0.9950$ which approaches for strong negative magnetic fields the Ising model limit with a critical point at $h \to -\infty$, $T_c^{\mathrm{Ising}} = 1/\ln(1+\sqrt{2}) = 1.1346$. By means of finite-size scaling analyses we confirmed that along this transition line the critical exponents indeed fall

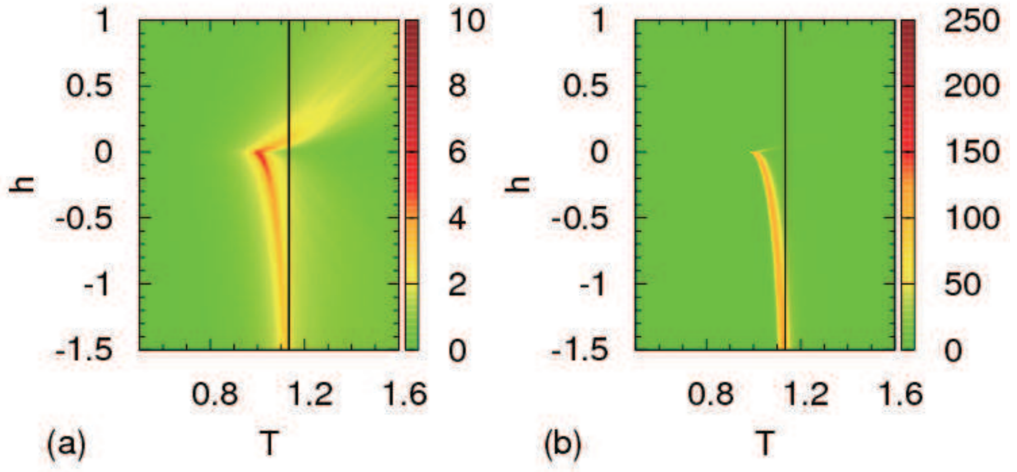

Figure 10.22: (a) Specific heat C/L^2 and (b) magnetic susceptibility χ/L^2 as functions of T and h for $L = 80$. The solid vertical line at $T = 1.1346$ shows the critical temperature of the Ising model (in 2-state Potts model normalization).

into the Ising universality class [6], as expected. For positive magnetic fields, the phase transition disappears altogether.

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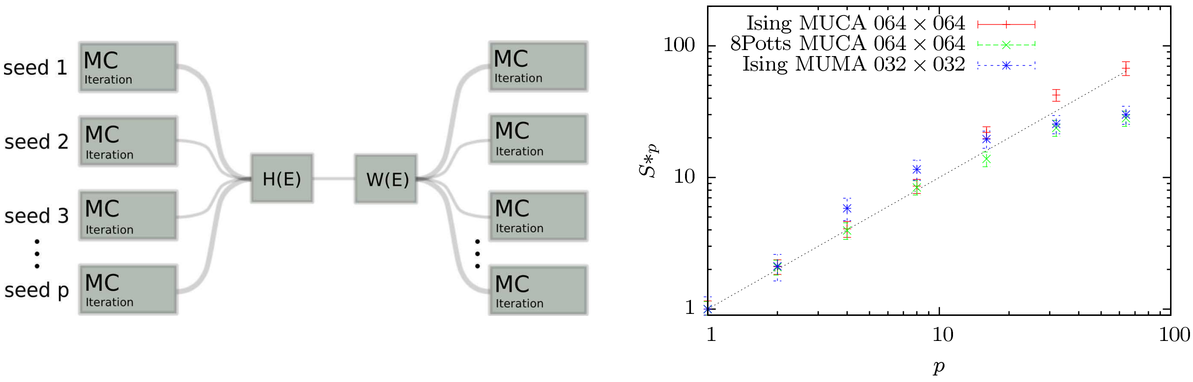
10.21 Scaling Properties of a Parallel Version of the Multicanonical Method

J. Zierenberg, M. Marenz, W. Janke



(a) (b)

Figure 10.23: (a) The working principle of the parallel implementation. After each iteration, the histograms of the independent Markov Chains are merged, the consecutive weight function is determined and distributed again onto the independent processes. (b) Statistical speedup for the multicanonical simulation of the Ising and Potts model as well as the multimagnetic simulation of the Ising model.

At times, with computer performance increasing mainly in terms of parallel processing on multi-core architectures, it is crucial to parallelize the applied algorithm. With this in mind, we extended our Monte Carlo tool box by a parallel implementation of the multicanonical method. The parallelization relies on independent equilibrium simulations that only communicate when the multicanonical weight function is updated. That way, the Markov chains efficiently sample the temporary distributions allowing for good estimations of consecutive weight functions. We discovered that similar approaches have been made in the literature [1, 2], without giving a detailed answer to the performance of this parallelization.

We set out to answer this open question for well known simple test systems, namely the two-dimensional Ising model and 8-state Potts model. They exhibit phase transitions of second and first order, respectively. As the parallelization employs independent Markov chains, simulations with different number of cores may not be compared one to one. This demanded a detailed consideration of the involved parameters in order to compare the average optimal performance at each degree of parallelization.

Overall, the parallelization was shown to scale quite well for up to 64 cores [3, 4]. In the case of multicanonical simulations of the 8-state Potts model, the optimal performance is limited due to emerging barriers. The parallelization can be applied also to other flat-histogram simulations, e.g. multimagnetic simulations. It may be pointed out that no greater adjustment to the usual implementation is necessary and that additional modifications may be carried along. This allows a straightforward application of this parallelization to complex systems like (bio) polymers and (spin) glasses.

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with first and second order phase transitions, to appear in Physics Procedia (2013), in print

10.22 Funding

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

Graduate School *Statistical Physics of Complex Systems*
W. Janke (with B. Berche, Nancy)
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W. Janke (Principal Investigator, project P9 in collaboration with K. Kroy)
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W. Janke (Principal Investigator, project B04)
Deutsche Forschungsgemeinschaft (DFG)

Institute Partnership with the Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Lviv, Ukraine, *Polymers in Porous Environments and on Disordered Substrates*
W. Janke (with V. Blavatska, Lviv)
Alexander von Humboldt Foundation

Dynamik und Statik von Spingläsern
W. Janke
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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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W. Janke and M. Möddel
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W. Janke
Alexander von Humboldt Foundation

Host of Buket Taşdizen (Ankara University, Turkey), ERASMUS Fellowship
W. Janke
ERASMUS Programme

10.23 Organizational Duties

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- Director, Institute for Theoretical Physics (ITP), Universität Leipzig
- Director, Naturwissenschaftlich-Theoretisches Zentrum (NTZ), Universität Leipzig
- Member of Department Council ("Fakultätsrat"), Faculty for Physics and Earth Sciences, Universität Leipzig
- Member of the Steering Committee ("Direktorium") of the Graduate Centre *Mathematics/Computer Science and Natural Sciences*, Research Academy Leipzig
- Member Priority Research Area PbF1 *Molecules and Nano-objects*
- Member Priority Research Area PbF2 *Mathematical Sciences*
- Spokesperson of the German-Ukrainian Institute Partnership Leipzig-Lviv of the Alexander von Humboldt Foundation
- Spokesperson of the German-French Graduate College *Statistical Physics of Complex Systems*
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- Member of the Scientific-Technical-Council of the Supervisory Board ("Aufsichtsrat") of the Forschungszentrum Jülich GmbH
- Permanent Member of the "International Advisory Board", *Conference of the Middle European Cooperation in Statistical Physics (MECO)*
- Member of the Programme Committee for the 4th Conference on *Statistical Physics: Modern Trends and Applications*, Lviv, Ukraine, 03.–06. July 2012
- Member of the International Advisory Board for the XXV IUPAP *Conference on Computational Physics* CCP2013, Moscow, Russia, 20.–24. August 2013
- Co-organizer of the "BuildMoNa"Modul *Basic Concepts in Physics* (with P. Esquinazi and J. Haase), Universität Leipzig, 14. February 2012
- Co-organizer of the AvH Kick-Off Workshop *Polymers in Porous Environments and on Disordered Substrates* (with V. Blavatska), Ivan Franko National University, Lviv, Ukraine, 03. July 2012
- Co-organizer of the "BuildMoNa" Module 2012-M10 *Multifunctional Scaffolds* (with F. Kremer, K. Kroy, and T. Pompe), Universität Leipzig, 27.–28. September 2012
- Organizer of the Workshop *CompPhys12* – 13th International NTZ Workshop on *New Developments in Computational Physics*, ITP, Universität Leipzig, 29. November – 01. December 2012

- Organizer of the Workshop *CompPhys13* – 14th International NTZ Workshop on *New Developments in Computational Physics*, ITP, Universität Leipzig, 28.–30. November 2013
- Editor "Computational Physics", Central European Journal of Physics, Krakow, Poland
- Member of Editorial Board, Condens. Matter Phys., Lviv, Ukraine
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- 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, New Journal of Physics, International Journal of Modern Physics C

10.24 External Cooperations

Academic

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- Istituto Nazionale di Fisica Nucleare, Sezione di Milano-Bicocca, Milano, Italy
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  Prof. Dr. David B. Saakian
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  Prof. Dr. Lev N. Shchur
- Banaras Hindu University, Varanasi, India
  Prof. Dr. Sanjay Kumar
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  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

10.25 Publications

Journals

H. Arkın, W. Janke: *Structural Behavior of a Polymer Chain Inside an Attractive Sphere*, Phys. Rev. E **85**, 051802-1–9 (2012)

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S. Schnabel, D.P. Landau: *Fictitious Excitations in the Classical Heisenberg Antiferromagnet on the Kagome Lattice*, Phys. Rev. B **86**, 014413-1–10 (2012)

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N. Fricke, W. Janke: *Self-Avoiding Walks on Strongly Diluted Lattices: Chain-Growth Simulations vs Exact Enumeration*, Eur. Phys. J. – Special Topics **216**, 175–179 (2013) [Fig. 1 selected for the cover page of this volume]

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Talks

H. Arkın: *Structure Formation of a Polymer Chain in an Attractive Sphere*, CECAM Workshop, Paris, France, 21.–23. May 2012

H. Arkın: *Conformational Behavior of a Polymer Chain in an Attractive Spherical Cage*, SFB/TR102 Fall Meeting Miniworkshop, Brehna, Germany 19. October 2012

H. Arkın: *Thermodynamics of a Polymer Chain in a Spherical Cage*, 13th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys12*, Universität Leipzig, Germany, 29. November – 01. December 2012

N. Fricke: *Scale-Free Enumeration of Self-Avoiding Walks on Percolation Clusters*, 25th Annual CSP Workshop "Recent Developments in Computer Simulation Studies in Condensed Matter Physics", The University of Georgia, Athens, Georgia, USA, 20. February 2012

N. Fricke: *How to Enumerate* 10^{1000} *Self-Avoiding Walks on a Critical Percolation Cluster*, AvH Institute Partnership Leipzig-Lviv Kick-Off Workshop *Polymers in Porous Environments and on Disordered Substrates* (Satellite Workshop of the 4th Conference on *Statistical Physics*), Ivan Franko National University, Lviv, Ukraine, 03. July 2012

N. Fricke: *Self-Avoiding Walks on Disordered Lattices*, 5th BuildMoNa Workshop for Doctoral Candidates, Burgstädt, Germany, 24.–25. September 2012

W. Janke: *Monte Carlo Methods in Classical Statistical Physics*, BuildMoNa Module B3 *Basic Concepts in Physics*, Universität Leipzig, Germany, 14. February 2012

W. Janke: *Formation/Dissolution of Equilibrium Droplets*, Statistical Physics Seminar, Virginia Tech, Blacksburg, USA, 16. February 2012

W. Janke: *Polymer Adsorption on a Fractal Substrate*, 25th CSP Workshop on *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, The University of Georgia, Athens, Georgia, USA, 20.–24. February 2012

W. Janke: *Polymer Adsorption to a Fluctuating Membrane*, MECO 37 Conference, Tatranské Matliare, High Tatras, Slovakia, 19.–21. March 2012

W. Janke: *Numerical Study of Polymer Adsorption on a Fractal Substrate*, DPG Frühjahrstagung 2012, TU Berlin, Germany, 25.–30. March 2012

W. Janke: *Polymer Adsorption to a Fluctuating Membrane*, Workshop *Statistical Physics and Low Dimensional Systems – SPLDS*, Pont-à-Mousson, France, 29. May – 01. June 2012

W. Janke: *Transition Trajectory for Equilibrium Droplet Formation*, Workshop on *Computation of Transition Trajectories and Rare Events in Non-Equilibrium Systems*, Centre Blaise Pascal, ENS de Lyon, France, 11.–15. June 2012

W. Janke: *Computer Simulations of Polymers in Disordered Media*, BuildMoNa Module 2012-T6 *Hybrid Systems*, Universität Leipzig, Germany, 27. June 2012

W. Janke: *Football Fever: Self-Affirmation Model for Goal Distributions*, Lange Nacht der Wissenschaften, Universität Leipzig, Germany, 29. June 2012

W. Janke: *Polymer Adsorption on a Fractal Substrate*, AvH Institute Partnership Leipzig-Lviv Kick-Off Workshop *Polymers in Porous Environments and on Disordered Substrates* (Satellite Workshop of the 4th Conference on *Statistical Physics*), Ivan Franko National University, Lviv, Ukraine, 03. July 2012

W. Janke: *Polymer Statistics in an Attractive Sphere*, 4th Conference on *Statistical Physics: Modern Trends and Applications*, Ivan Franko National University, Lviv, Ukraine, 03.–06. July 2012

W. Janke: *Computer Simulations of Polymer Adsorption*, IGER International Symposium on *Science of Molecular Assembly and Biomolecular Systems 2012*, Nagoya University, Japan, 04.–05. September 2012

W. Janke: *Computer Simulations of Equilibrium Droplet Formation*, Physics Seminar, Tokyo Metropolitan University, Tokyo, Japan, 07. September 2012

W. Janke: *Generalized Ensemble Simulations of Polymer Adsorption*, International Workshop *Statistical Mechanics: Interplay of Theory and Computer Simulations*, Universität Mainz, Germany, 19.–21. September 2012

W. Janke: *Simulating Polymer Systems on GPU*, MPI-PKS Dresden IMPRS School 2012 *GPU Computing Methods and Applications in the Natural Sciences*, Wroclaw, Poland, 29. October – 02. November 2012

M. Marenz: *Framework for Off-Lattice Monte Carlo Simulations*, 5th BuildMoNa Workshop for Doctoral Candidates, Burgstädt, Germany, 24.–25. September 2012

M. Müller: *Multicanonical Analysis of the Gonihedric Ising Model*, Seminar of the cdfa-dfdk, Université Lorraine, Nancy, France, 07. November 2012

M. Möddel: *Grafted and Nongrafted Adsorption of Polymers on Different Substrates*, Retreat of the SFB/TRR 102, Bad Blankenburg, Germany, 14.–16. March 2012

M. Möddel: *Influence of Striped Surface-Inhomogeneities on the Conformations of a Single Self-Interacting Polymer near an Attractive Substrate*, DPG Frühjahrstagung 2012, TU Berlin, Germany, 30. March 2012

J. Zierenberg: *Simulating Flexible Polymers in Hard Disk Background Potentials*, Seminar of the cdfa-dfdk, Coventry University, England, 22. February 2012

J. Zierenberg: *Scaling Properties of a Parallel Implementation of the Multicanonical Algorithm*, Seminar of the cdfa-dfdk, Université Lorraine, Nancy, France, 07. November 2012

J. Zierenberg: *Scaling Properties of a Parallel Implementation of the Multicanonical Algorithm*, 13th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys12*, Universität Leipzig, Germany, 30. November 2012

Posters

H. Arkın, W. Janke: *Polymer Chain Inside Confinement*, Network Meeting, Alexander von Humboldt Foundation, Kiel, Germany, 08.–10. February 2012

H. Arkın, W. Janke: *Conformational Phase Diagram of a Polymer Chain Inside an Attractive Sphere*, Conference *Career in Polymers 2012*, Prag, Czech Republic, 28.–30. June 2012

H. Arkın, W. Janke: *Polymer Chain in an Attractive Spherical Confinement*, International Workshop *Statistical Mechanics: Interplay of Theory and Computer Simulations*, Mainz, Germany, 19.–21. September 2012

N. Fricke: *Scale-Free Enumeration of Self-Avoiding Walks on Critical Percolation Clusters*, 5th Scientific Symposium of the Graduate School BuildMoNa, Helmholtz Centre for Environmental Research, Leipzig, Germany, 12. March 2012

N. Fricke, W. Janke: *Scale-Free Enumeration of Self-Avoiding Walks on Percolation Clusters*, Conference of the Middle European Cooperation in Statistical Physics "MECO37", Tatranské Matliare, High Tatras, Slovakia, 19.–21. March 2012

N. Fricke, W. Janke: *Self-Avoiding Walks on Critical Percolation Clusters*, 4th Conference on *Statistical Physics: Modern Trends and Applications*, Ivan Franko National University, Lviv, Ukraine, 03.–06. July 2012

M. Marenz, J. Zierenberg, H. Arkın, W. Janke: *Simple Polymer in a Spherical Cage*, 4th Conference on *Statistical Physics: Modern Trends and Applications*, Ivan Franko National University, Lviv, Ukraine, 03.–06. July 2012

M. Marenz, J. Zierenberg, H. Arkın, W. Janke: *Simple Polymer in a Spherical Cage*, 13th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys12*, Universität Leipzig, Germany, 29. November – 01. December 2012

M. Müller, D.A. Johnston, W. Janke: *Multicanonical Analysis of the Gonihedric Ising Model*, 13th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys12*, Universität Leipzig, Germany, 29. November – 01. December 2012

M. Möddel, W. Janke, M. Bachmann: *Comparison of Grafted and Non-Grafted Polymer Adsorption in Different Ensembles*, Conference of the Middle European Cooperation in Statistical Physics "MECO37", Tatranské Matliare, High Tatras, Slovakia, 19.–21. March 2012

M. Möddel, M. Bachmann, W. Janke: *Comparison of Grafted and Non-Grafted Polymer Adsorption in Different Ensembles*, NIC Symposium 2012, Forschungszentrum Jülich, Germany 07.–08. February 2012

H. Nagel, D. Labaviç, H. Meyer-Ortmanns, W. Janke: *Stochastic Description of a Bistable Frustrated Unit* DPG Frühjahrstagung 2012, TU Berlin, Germany, 26.–30. March 2012

H. Nagel, D. Labaviç, H. Meyer-Ortmanns, W. Janke: *Stochastic Description of a Bistable Frustrated Unit* 13th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys12*, Universität Leipzig, Germany, 29. November – 01. December 2012

E. Ehrenpreis, H. Nagel, W. Janke: *Numerical Survey of the Tunable Condensate Shape and Scaling Laws in Pair-Factorized Steady States* 13th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys12*, Universität Leipzig, Germany, 29. November – 01. December 2012

S. Schöbl, J. Zierenberg, K. Kroy, W. Janke: *Broadscale Examination of the Influence of Disorder on Semiflexible Polymers*, 13th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys12*, Universität Leipzig, Germany, 29. November – 01. December 2012

S. Schöbl, J. Zierenberg, W. Janke: *Simulating Flexible Polymers in a Potential of Randomly Distributed Hard Disks*, Conference of the Middle European Cooperation in Statistical Physics "MECO37", Tatranské Matliare, High Tatras, Slovakia, 19.–21. March 2012

S. Schöbl, J. Zierenberg, W. Janke: *Simulating Flexible Polymers in a Potential of Randomly Distributed Hard Disks*, DPG Frühjahrstagung 2012, TU Berlin, Germany, 26.–30. March 2012

10.26 Graduations

Doctorate

- Monika Möddel
  Statistical Equilibrium Behaviour of Finite Polymers Near Attractive Substrates
  20. June 2012

Diploma

- Max Henner Gerlach
  Directional Ordering in the Classical Compass Model in Two and Three Dimesions
  24. February 2012
- Arnd Tretbar
  Polymer Aggregation on a Simple Cubic Lattice
  03. September 2012

- Thomas Peschel
  Exakte Auszählung von Selbst-Avoiding-Walks auf n-dimensionalen einfach kubischen Gittern
  02. October 2012

Master

- Eugen Ehrenpreis
  Mass Condensation in Driven Stochastic Transport Processes – Interaction- and Potential-Driven Condensation Phenomena
  10. May 2012
- Momchil Ivanov
  Polymer Adsorption onto a Stripe-Patterned Surface
  25. October 2012

10.27 Guests

- Buket Taşdizen
  Ankara University, Turkey
  ERASMUS Programme
  01. December 2011 – 29. February 2012
- Prof. Dr. Sanjay Kumar
  Department of Physics, Banaras Hindu University, Varanasi, India
  NTZ/FOR877 Colloquium
  DNA under Periodic Force: Scaling and Phase Diagram
  07. June 2012
- Tetsuro Nagai
  Nagoya University, Japan
  NTZ Colloquium (12. July 2012)
  The Simulated Tempering and Magnetizing Algorithm 01. May - 31. August 2012

- Jeremi Ochab
  Jagiellonian University, Krakow, Poland
  01. August – 30. September 2012
- Dr. Viktoria Blavatska
  Institute for Condensed Matter Physics, Lviv, Ukraine
  Alexander von Humboldt Foundation Institute Partnership Programme
  Conformational Transitions in Random Heteropolymer Models
  01. September – 30. November 2012
- Kristine Haydukivska
  Institute for Condensed Matter Physics, Lviv, Ukraine
  Alexander von Humboldt Foundation Institute Partnership Programme
  01. – 30. November 2012

- Jeremi Ochab
  Jagiellonian University, Krakow, Poland
  Maximal-Entropy Random Walk, Centrality Measures and Communities
  01. November – 20. December 2012

- Prof. Dr. Peter Young
  University of California, Santa Cruz, USA
  NTZ/DFH-UFA/RALeipzig Colloquium
  Mind the Gap: Solving Optimization Problems on a Quantum Computer
  08. November 2012

- Dr. Nathan Clisby
  University of Melbourne, Australia
  NTZ/FOR877 Colloquium
  There are $7 \times 10^{26\,018\,276}$ *self-avoiding walks of* 38 797 311 *steps on* Z^3
  09. November 2012

- Prof. Dr. Bo Zheng
  Zhejiang University, Hangzhou, China
  NTZ/DFH-UFA/RALeipzig Colloquium
  Physics at Zhejiang University
  09. November 2012

- Prof. Dr. Kurt Binder
  Universität Mainz, Germany
  NTZ-Colloquium
  Contact Angles, Wetting Transition, and Macrosopic Interfacial Fluctuations
  28. – 30. November 2012

- Dr. Lev Barash
  Landau Institute, Chernogolovka, Russia
  Parallel Streams of Pseudorandom Numbers for Monte Carlo Simulations: Using most Reliable Algorithms and Applying Parallelism of Modern CPUs and GPUs
  28. November – 02. December 2012

- Dr. Martin Weigel
  Coventry University, England, UK
  Spin Glasses with Many Components
  27. November – 01. December 2012

- Dr. David Yllanes
  "La Sapienza" Rome, Italy
  Finite-Size Scaling Analysis of the Distributions of Pseudo-Critical Temperatures in Spin Glasses
  28. November – 01. December 2012

- Prof. Dr. Juan J. Ruiz-Lorenzo
  Universidad Extremadura, Badajoz, Spain
  Numerical Test of the Cardy-Jacobsen Conjecture in the Site-Diluted Potts Model in Three Dimensions
  28. November – 01. December 2012

- Prof. Dr. Yu-Cheng Lin
  Chengchi University, Taipei, Taiwan
  Correlated Valence-Bond States
  29. November – 01. December 2012
- Prof. Dr. Alexander Hartmann
  Universität Oldenburg, Germany
  Efficient Simulation of Fractional Brownian Motion for Several Values of the Hurst Exponent
  28.–30. November 2012
- Dr. Hsiao-Ping Hsu
  Universität Mainz, Germany
  Scattering Function of Semiflexible Polymer Chains under Good Solvent Conditions
  28. November – 01. December 2012
- Prof. Dr. Malte Henkel
  Nancy Université, France
  Some Exact Results in Systems of Immobile Interacting Particles
  28. November – 01. December 2012
- Prof. Dr. Ferenc Iglói
  Institute of Theoretical Physics, Research Institute for Solid State Physics and Optics, Budapest, Hungary
  Corner Contribution to Percolation Cluster Numbers
  28. November – 02. December 2012
- Tetsuro Nagai
  Nagoya University, Japan
  Simulated Tempering and Magnetizing Simulations of a Potts Model
  27. November – 07. December 2012
- Marcin Zagórski
  Jagiellonian University, Krakow, Poland
  Emergence of Gene Regulatory Networks under Functional Constraints
  28. November – 02. December 2012
- Dr. Elmar Bittner
  Universität Heidelberg, Germany
  Replica-Exchange Cluster Algorithm
  28. November – 01. December 2012
- PD Dr. Thomas Neuhaus
  Jülich Supercomputing Centre, Forschungszentrum Jülich, Germany
  Spin Correlations in the 3D Ising Model on Infinite Cuboids
  28. November – 06. December 2012
- Dr. Artur Barasiński
  Univ. Zielona Góra, Poland
  NTZ/DFH-UFA/RALeipzig Colloquium (06. December 2012)
  Magnetization-Based Assessment of Correlation Energy in Canted Single-Chain Magnets
  28. November – 07. December 2012