11

Computational Quantum Field Theory

11.1 Introduction

The Computational Physics Group performs basic research into classical and quantum statistical physics with special emphasis on phase transitions and critical phenomena. In the centre of interest are the physics of spin glasses, diluted magnets and other materials with quenched, random disorder, soft condensed matter physics with focus on fluctuating paths and interfaces, biologically motivated problems such as protein folding, aggregation and adsorption as well as related properties of homopolymers, and the intriguing physics of low-dimensional quantum spin systems. Our investigations of a geometrical approach to the statistical physics of topological defects with applications to superconductors and superfluids and research into fluctuating geometries with applications to quantum gravity, e.g., dynamical triangulations, build on the 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 AvH Institute Partnership project with the Institute for Condensed Matter Physics of the National Academy of Sciences in Lviv, Ukraine, on *Polymers in Porous Environments and on Disordered Substrates* commenced its work.

The methodology is a combination of analytical and numerical techniques. The numerical tools are currently Monte Carlo and Molecular Dynamics computer simulations as well as exact enumeration techniques. The computational approach to theoretical physics is expected to gain more and more importance with the future advances of computer technology, and is likely to become the third cornerstone of physics besides experiment and analytical theory as sketched in Fig. 11.1. Already now it can help to bridge the gap between experiments and the often necessarily approximate calculations in analytic approaches. To achieve the desired high efficiency of the numerical studies we develop new algorithms, and to guarantee the flexibility required by basic research all computer codes are implemented by ourselves. The technical tools are Fortran, C, and C++ programs running under Unix or Linux operating systems and computer algebra using Maple or Mathematica. The software is developed and tested at the Institute on a cluster of PCs and workstations, where also most of the numerical analyses are performed. Currently we are also exploring the possibilities of the rapidly developing

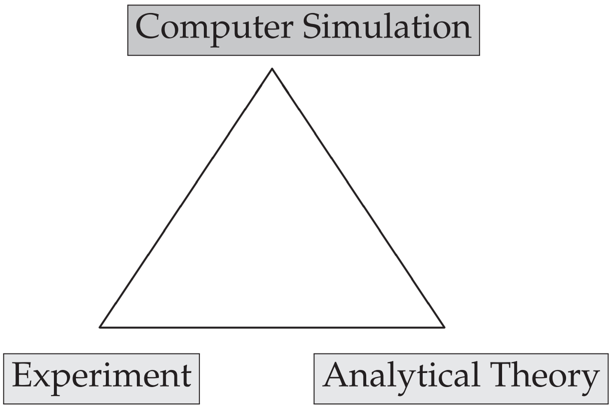

Figure 11.1: Sketch of the "triangular" relationship between experiment, analytical theory and computer simulation.

graphics card computing, that is computer simulations on graphics processing units (GPUs) with many cores. Large-scale simulations requiring vast amounts of computer time are carried out at the Institute on quite powerful compute servers, at the parallel computers of the University computing centre, and, upon successful grant application at the national supercomputing centres in Jülich, 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*, two ESF Junior Research Groups, the International Max Planck Research School (IMPRS) *Mathematics in the Sciences*, and the International Graduate School *Statistical Physics of Complex Systems* with Université de Lorraine in Nancy, France, supported by the Deutsch-Französische Hochschule (DFH-UFA). In the second funding period 2011–2013, Coventry University in England has been integrated as an associated partner, and in the recently approved third funding period 2014–2016, also the Natinonal Academy of Sciences of Ukraine in Lviv has joined as another associated partner institution, offering our PhD students now several interesting options for secondments. 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* jointly with the universities in Chemnitz and Dresden, 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 (previously "Profilbildende Forschungsbereiche (PbF)", currently being reorganized into so-called "Profillinien") 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 which are in part initiated by the European RTN “ENRAGE” and the previous 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 Institute Partnership with the National Academy of Sciences in Lviv, Ukraine, as well as their Fellowship Programmes. 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, Advanced Training Modules and Tutorials, and our International Workshop series *CompPhys: New Developments in Computational Physics*, taking annually place at the end of November just before the first advent weekend.

Wolfhard Janke

11.2 Morphing the energy landscape of spin glasses

S. Schnabel, W. Janke

Among the numerous systems that became accessible for investigation with the introduction of Monte Carlo simulations, spin glasses have proven to be among the most challenging. This becomes apparent when the Edwards-Anderson model [1] is studied. While being closely related to the very thoroughly examined and well-understood Ising model the introduction of disorder,

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} S_i S_j \,,$$

in the form of random couplings J_{ij} leads to an energy landscape that is characterized by an excessive number of local minima separated by energy barriers. This severely hampers Monte Carlo simulations since a random walker has to change frequently between high and low energies in order to sample a representative part of the state space. In consequence both the search for the ground state and the investigation of thermodynamic properties can only be performed for relatively modest system sizes. While for the former new methods keep being introduced, at least in the last two decades progress in the latter has exclusively been achieved due to an increase of computational resources.

We propose a novel technique related to the basin hopping algorithm [2]. In addition to the energy of a given configuration we evaluate the energy of the system after a short energy minimization and attribute this energy to the original configuration as well. Combining these two values it is possible to obtain a variable that retains the minima of the Hamiltonian but alters the shape of the surrounding valleys, thus facilitating the simulation and reducing autocorrelation time.

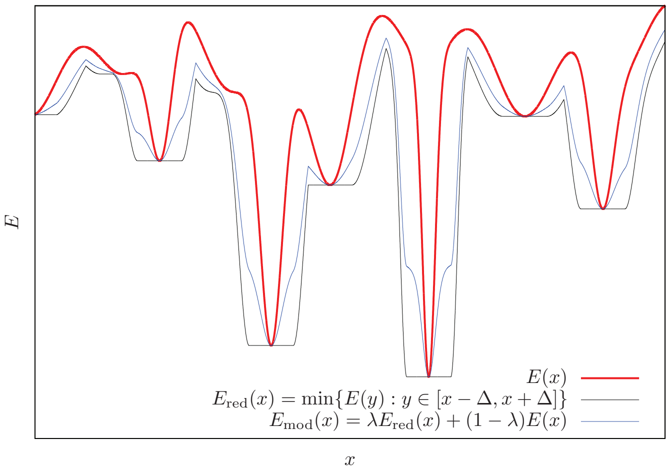

Figure 11.2: This sketch shows how a new variable (blue) with favorable characteristics can be composed from the energy (red) and a minimized energy (black).

We obtain ground-state energies that correspond well with data from the literature. Furthermore, we are able to reach lower energies in balanced simulations than possible before.

[1] S.F. Edwards, P.W. Anderson: J. Phys. F **5**, 965 (1975)
[2] D.J. Wales: J. Phys. Chem. A **101**, 5111 (1997)

11.3 Polymer adsorption onto a stripe-patterned substrate

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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. 11.3(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

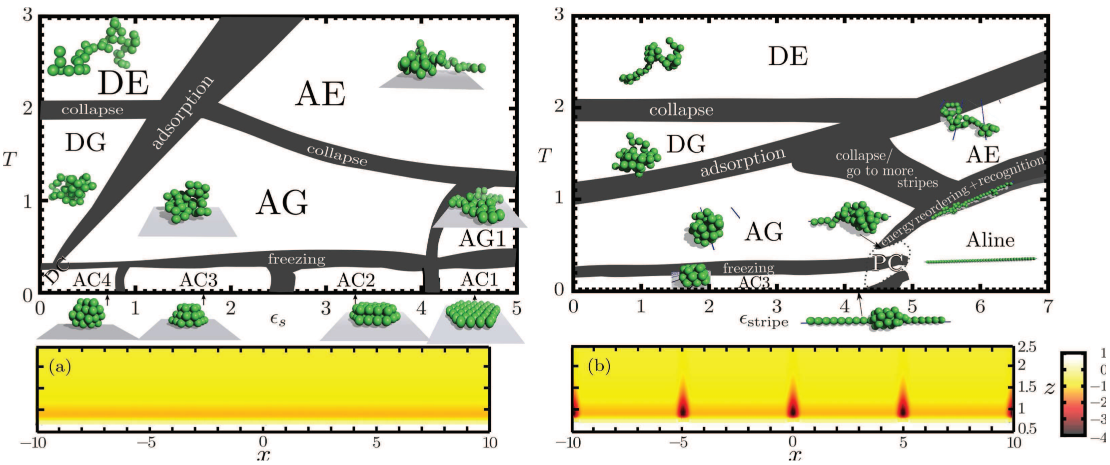

Figure 11.3: (a) Pseudo-phase diagram for polymer adsorption to a homogeneous substrate ($\epsilon_{\text{stripe}} = 0$) in the temperature ($T$) – surface attraction ($\epsilon_s$) plane and a "heat map" of the substrate potential for $\epsilon_s = 1$. (b) Analogous pseudo-phase diagram for the stripe patterned case in the T–ϵ_{stripe} plane for $\epsilon_s = 1$. Phases with "A/D" are adsorbed/desorbed, while "E", "G", and "C" denote phases with increasing order: expanded, globular, and compact. "PC" stands short for a region with phase coexistence.

cosine-square potential of distance $D = 5$ such that the energy of the system in total is

$$E_{\text{bulk}} = 4\sum_{i=1}^{N-2}\sum_{j=i+2}^{N}\left(r_{ij}^{-12} - r_{ij}^{-6}\right) + \frac{1}{4}\sum_{i=1}^{N-2}(1-\cos\vartheta_i)\ , \tag{11.1}$$

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

$$E_{\text{sur, stripe}}(x,z) = \begin{cases} \left(\frac{2}{15}z^{-9} - z^{-3}\right)\left[\epsilon_s + \epsilon_{\text{stripe}}\cos^2\left(\pi\left(\text{mod}\left(x+\frac{D}{2},D\right)-\frac{D}{2}\right)\right)\right], & \text{if}\left|\text{mod}\left(x+\frac{D}{2},D\right)-\frac{D}{2}\right| \le \frac{1}{2} \\ \left(\frac{2}{15}z^{-9} - z^{-3}\right)\epsilon_s, & \text{else.} \end{cases} \tag{11.2}$$

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. Figure 11.3(b) shows that 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].

[1] M. Möddel et al.: J. Phys. Chem. B **113**, 3314 (2009)
[2] M. Möddel et al.: Phys. Chem. Chem. Phys. **12**, 11548 (2010)
[3] M. Möddel et al.: Macromolecules **44**, 9013 (2011)
[4] M. Möddel et al.: Comput. Phys. Commun. **182**, 1961 (2011)
[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)
[6] M. Möddel et al.: Phys. Rev. Lett. **112**, 148303 (2014)

11.4 Structural phases of stiff and flexible polymers

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In order to get a systematic understanding of the structural behaviour of polymers with a varying degree of stiffness we performed extensive simulations for a bead-spring model. The Hamiltonian contains three types of interactions:

- Excluded volume and hydrophobicity are modeled by a Lennard-Jones potential

  $$U_{\mathrm{LJ}}(r_{ij}) = r_{ij}^{-12} - 2r_{ij}^{-6}$$

  with a minimum at $r_{ij} = 1$, acting upon all non-neighbouring monomer pairs.

- Bonds are introduced by a FENE-potential

  $$U_{\mathrm{FENE}}(r_{ii+1}) = -R^2 \ln\left[1 - (r_{ii+1}/R)^2\right],$$

  with the maximum bond length $R = 1.2$. An adjusted Lennard-Jones potential is added in order to match the equilibrium distance to that of the non-bonded pairs.

- The polymer obtains stiffness via a bending energy

  $$U_{\mathrm{bend}}(\Theta_l) = \kappa\,(1 - \cos\Theta_l)$$

  based on the angle between adjacent bonds Θ_l.

Employing advanced generalized-ensemble Monte Carlo techniques we were able to sample the state space for all relevant κ-values in a single simulation [1]. Transition lines were afterwards identified using thermal fluctuations of energy (Fig. 11.4) and radius of gyration.

We did not only focus on the general phases between the limits stiff and flexible but investigated the influence of finite-size effects on structure formation. This is a significant problem as it has become apparent that the structural properties of classes of short semiflexible bio-molecules can significantly deviate from the standard wormlike-chain behavior. The changed structural behavior, therefore, needs to be considered in the understanding of biomolecular processes on short length scales and also in the nanofabrication of molecular devices.

[1] D.T. Seaton et al.: Phys. Rev. Lett. **110**, 028103 (2013)

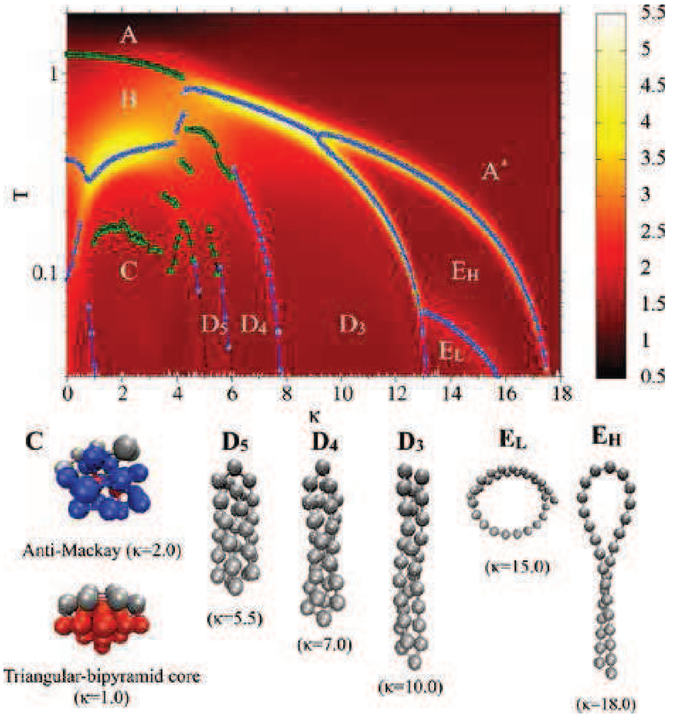

Figure 11.4: Surface plot of the specific heat for classes of polymers with $N = 30$ monomers as a function of temperature T and stiffness κ. Brighter colors correspond to higher thermal activity, signaling structural transitions. For a large number of κ values, locations of peaks and shoulders are emphasized by circles and squares, respectively, for easier identification of transition points. Conformational phases are labeled as follows: A, random coil; A^*, random rodlike; B, liquid globular; C, solid globular; D_m, rodlike bundles with m segments; and E, toroidal.

11.5 Ground-state properties of a polymer chain inside an attractive sphere potential

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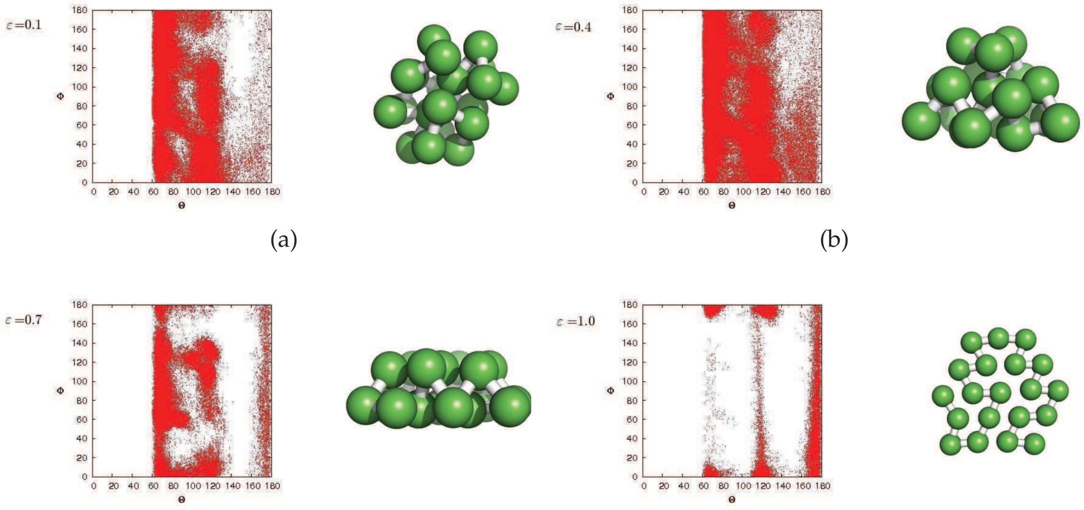
Understanding the basic mechanisms for structure formation of biomolecules at different interfaces is one of the major challenges of modern interdisciplinary research and possible applications in nanotechnology. Knowledge of the origin of structure formation is an important prerequisite for tailoring polymer adhesion to metals and semiconductors [1] and the design of 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



(a) (b)

(c) (d)

Figure 11.5: 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 global minimum energy conformations. The distribution of the torsion angles has reflection symmetry and therefore only the positive interval is shown.

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. 11.5. 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].

[1] M. Bachmann et al.: Angew. Chem. Int. Ed. **49**, 9530 (2010)
[2] E. Nakata et al.: J. Am. Chem. Soc. **126**, 490 (2004)
[3] R.F. Service: Science **270**, 230 (1995)
[4] M. Möddel et al.: J. Phys. Chem. B **113**, 3314 (2009); Phys. Chem. Chem. Phys. **12**, 11548 (2010); Comput. Phys. Commun. **182**, 1961 (2011); Macromolecules **44**, 9013 (2011); in *NIC Symposium 2012*, Proceedings, eds. K. Binder, G. Münster, M. Kremer, John von Neumann Institute for Computing, Jülich, NIC Series, Vol. **45**, 277 (2012); Phys. Rev. Lett. **112**, 148303 (2014)
[5] H. Arkın, W. Janke: Phys. Rev. E **85**, 051802 (2012)
[6] H. Arkın, W. Janke: J. Phys. Chem. B **116**, 10379 (2012)

[7] H. Arkın, W. Janke: Eur. Phys. J. – Special Topics **216**, 181 (2013)

11.6 Polymer shapes in an attractive spherical cage

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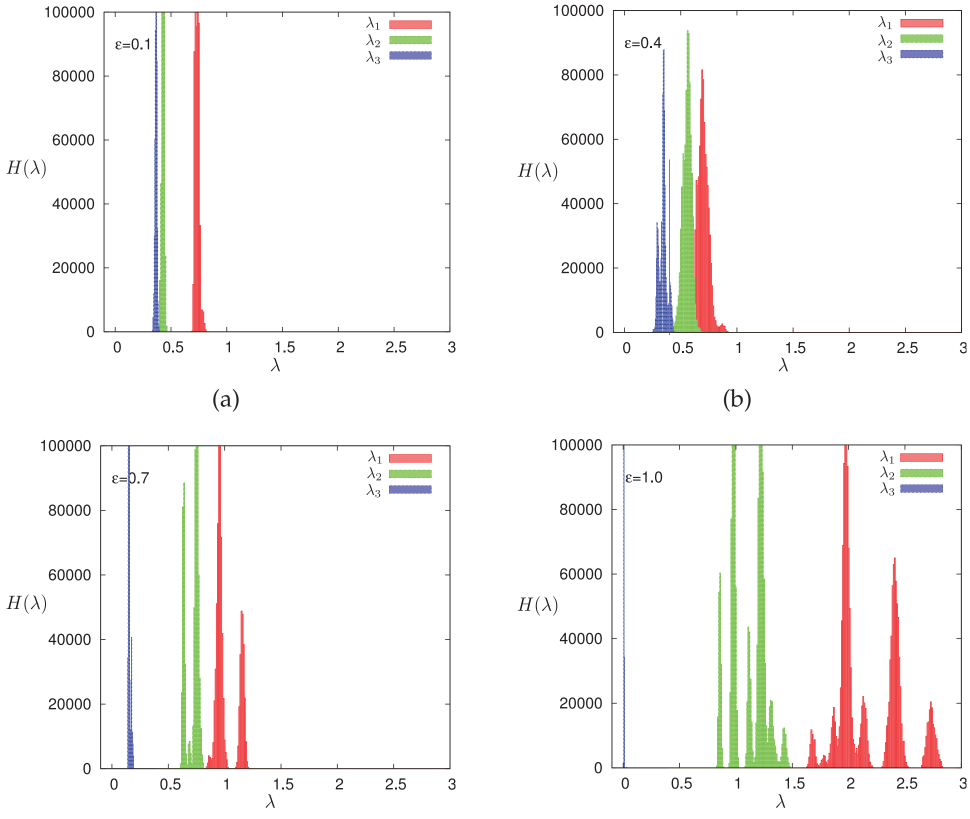
The conformational properties of polymers and proteins confined in cages with different geometries are a subject of great interest in polymer science [1–4], playing an important role both from a physical and chemical perspective. In recent work, we considered a simple off-lattice coarse-grained polymer model inside an attractive sphere, for which we have constructed the finite-temperature phase diagram [5] and investigated the ground-state properties [6]. A careful comparison with results for flat substrates has recently been presented in Ref. [7].

In this work we found highly structured conformations that are of approximately spherical shape or form two-dimensional planar, compact to extended, random coil structures. The observed conformations range from desorbed to partially or even completely adsorbed. In the present study [8], we show that the gyration tensor and related asphericity and shape anisotropy parameters are powerful combinations to characterize the conformational pseudo-phases in detail and to identify the associated typical polymer shapes. In a comparative analysis, a classification of the structures formed in the accompanying adsorption process has been achieved. It is one of the most remarkable results of our study that for different values of the attraction-strength parameter ϵ of the polymer-attractive sphere system, we get conformations that fit perfectly to the inner wall of the sphere with two-dimensional shape.

The eigenvalues of the gyration tensor measure the extensions in the principle axis system and enable us to define several additional, partly universal shape parameters of which information about the system can be extracted that complements the physical picture obtained so far. Some of our results [8] are exemplified in Fig. 11.6, where the distributions of the eigenvalues of the gyration tensor are shown for low-temperature conformations at (a) $\epsilon = 0.1$, (b) $\epsilon = 0.4$, (c) $\epsilon = 0.7$, (d) $\epsilon = 1.0$. For $\epsilon = 0.1$ and 0.4 the eigenvalues are nearly equal to each other. There are no significant differences because these values correspond to almost spherically symmetric shapes or three-layered shapes which are also close to spherical shape. On the other hand, as we know from the T-ϵ phase diagram [5, 7] that for low temperatures the transition point is at $\epsilon \approx 0.6$, the plot for $\epsilon = 0.7$ shows a tendency of increasing values λ_1, λ_2 and decreasing λ_3. For $\epsilon = 1.0$ it can be seen that this tendency becomes more pronounced and λ_3 approaches zero whereas the other two eigenvalues are increasing to higher values. This confirms in a quantitative way that the layering transition at the inner surface of the attractive sphere is a topological transition from 3D to 2D polymer conformations.

[1] F. Takagi et al.: Proc. Natl. Acad. Sci. USA **100**, 11367 (2003)
[2] N. Rathore et al.: Biophys. J. **90**, 1767 (2006)
[3] D. Lu et al.: Biophys. J. **90**, 3224 (2006)



(a) (b)

(c) (d)

Figure 11.6: The eigenvalue distributions of the gyration tensor of low-temperature conformations for surface attraction strength (a) $\epsilon = 0.1$, (b) $\epsilon = 0.4$, (c) $\epsilon = 0.7$, (d) $\epsilon = 1.0$.

[4] M. Marenz et al.: Condens. Matter Phys. **15**, 43008 (2012)
[5] H. Arkın, W. Janke: Phys. Rev. E **85**, 051802 (2012)
[6] H. Arkın, W. Janke: J. Phys. Chem. B **116**, 10379 (2012)
[7] H. Arkın, W. Janke: Eur. Phys. J. – Special Topics **216**, 181 (2013)
[8] H. Arkın, W. Janke: J. Chem. Phys. **138**, 054904 (2013)

11.7 Effects of bending stiffness on a coarse grained polymer model

M. Marenz, W. Janke

To investigate the generic behaviour of polymers and proteins in computer simulations it is common to use generic models. On the one hand, these models neglect chemical details, which means that one cannot observe any specific behaviour. Instead the general behaviour for the type of polymer is exposed. Additionally these coarse-grained models are often the only ones which are treatable with analytical or numerical methods. One of the most used coarse-grained models is the so called bead-stick polymer. For this

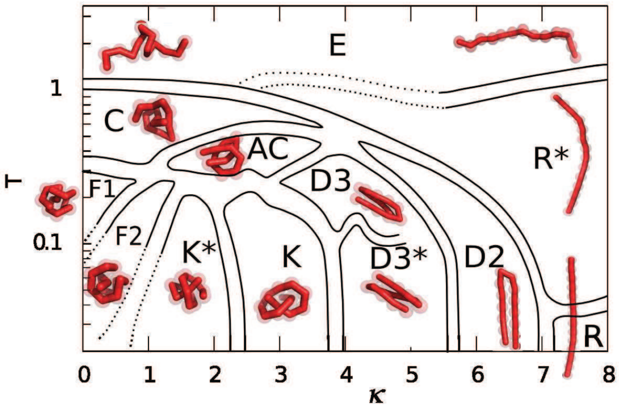


Figure 11.7: Different conformational phases of a hompopolymer consisting of 14 monomers. Black lines indicate pseudo-phase transitions. The different pseudo phases are labeled as follows: E - elongated, R/R* - rod-like, C - collapsed, AC - aligned collapses, F1/F2 - frozen, K/K* knot-like, DN - bended $N-1$ times.

work, we added a bending stiffness to the Hamiltonian of this model, so that we can investigate many different kinds of polymers without reintroducing chemical details. The Hamiltonian of the simulated polymers looks as follows:

$$H = 4\sum_{i=1}^{N-2}\sum_{j=i+2}^{N}\left(\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}}\right) + \kappa\sum_{\theta_i}(1-\cos\theta_i)\,,$$

where r_{ij} denote the distances between non-adjacent monomers and θ_i is the angle of two adjacent bonds.

Now we can adjust the bending stiffness by varying κ, so that the simulated polymer can be anything between flexible, semi-flexible or stiff. To investigate the different conformational phases we need results over a broad temperature range. We therefore used a parallel version of the multicanonical algorithm, which is explained in [1]. This algorithm can produce results over a large temperature range and also overcome problems arising from numerous phase transitions. These phase transitions make it problematic to simulate such models with standard Monte Carlo algorithms. We measured different observables such as the energy $\langle E\rangle$, the squared radius of gyration $\left\langle R_g^2\right\rangle$ or the invariants of the gyration tensor and identified the different (pseudo) phase transitions from peaks in the thermal derivatives.

Despite of the simplicity of the model, the phase diagram is remarkable rich [2], see Fig. 11.7. Many of theses phases are comparable to conformations which have been observed for real polymers and proteins. Similiar but in details different results have recently been observed for a different coase-grained polymer model [3] (cf. Fig. 11.4). For the future we plan to investigate the effect of the polymer length on the different pseudo-phase transitions. Additionally, a finite-size scaling analysis at few selected pseudo-phase transition points could yield a deeper insight into the type and scaling properties of the transitions.

[1] J. Zierenberg et al.: Comput. Phys. Commun. **184**, 1155 (2013)
[2] M. Marenz, W. Janke: Leizpig preprint, to appear in Physics Procedia (2014), in print
[3] D.T. Seaton et al.: Phys. Rev. Lett. **110**, 028103 (2013)

11.8 The role of stiffness on structural phases in polymer aggregation

J. Zierenberg, W. Janke

We have investigated the effect of stiffness on polymer aggregation and were able to show that stiffness plays a crucial role in whether a system forms an amorphous aggregate or a bundle structure [1]. Figure 11.8 shows the temperature-stiffness phase diagram of polymer aggregation for 8 polymers with 13 monomers each. We have performed the same analysis also for 2 and 4 polymers of the same length and were always able to identify a regime of flexible polymers forming uncorrelated aggregates, an intermediate regime and a regime of rather stiff polymers directly forming bundle like structures. With the help of a microcanonical analysis we investigated the intermediate stiffness regime. Here, lowering the temperature for a few polymers the aggregation first forms correlated structures followed by a first-order like transition into the "frozen" states. On the other hand, for an increasing number of polymers, lowering the temperature first drives the system into an uncorrelated aggregate, shortly followed by a second-order like transition into the correlated aggregate.

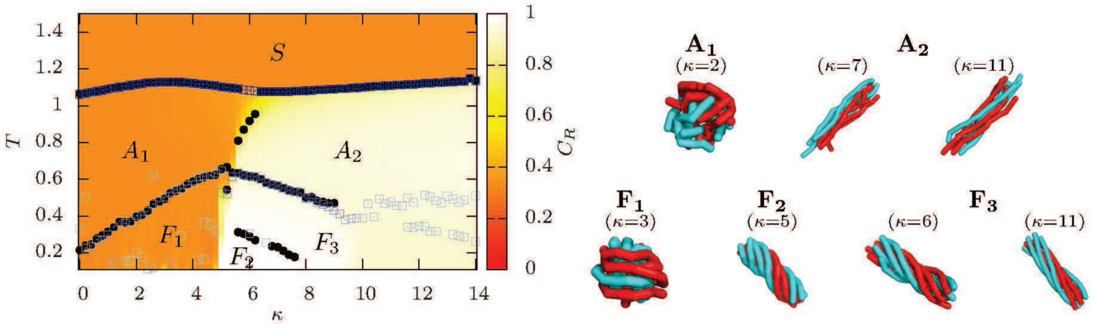


Figure 11.8: Full temperature-stiffness phase diagram of 8 polymers with 13 monomers each. The surface plot shows a correlation order parameter (1 = correlated; 1/3 = uncorrelated) and the black and blue dots represent peaks in the heat capacity and the thermal derivative of the phase separation parameter, respectively [1].

For increasing numbers of polymers, we can see that the "frozen"(low-temperature) states in Fig. 11.8 show a twisted bundle structure if the stiffness is large enough. This sort of structure has been reported before in the context of material design for specific interactions usually related to proteins. Since our study did not include any specific interactions, but instead a homopolymer with short-range attraction/repulsion with additional bending stiffness, we conclude that specific interactions are not necessary but may stabilize or destabilize those occurring structures.

In order to generate the data, we employed parallel multicanonical simulations [2] with up to 128 cores on the supercomputer JUROPA at Jülich Supercomputing Centre (JSC).

[1] J. Zierenberg, W. Janke: e-print arXiv:1401.3227, submitted
[2] J. Zierenberg et al.: Comput. Phys. Comm. **184**, 1155 (2013)

11.9 Effect of coupling constants on polymer aggregation (ISAWs)

J. Zierenberg, B. Schott, W. Janke

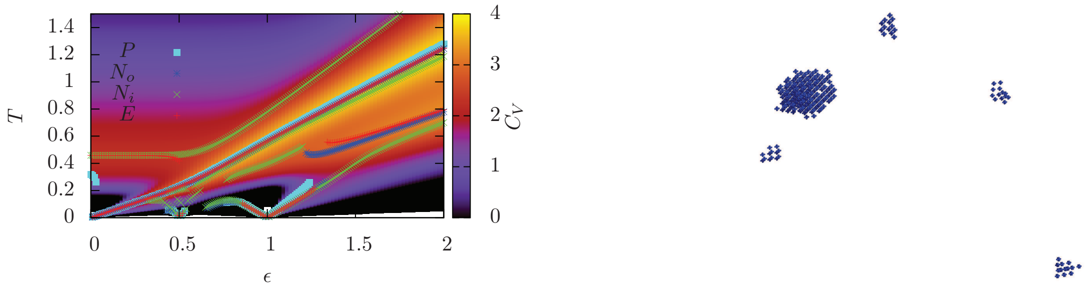
Interacting self-avoiding walks (ISAWs) are a first-order approximation to flexible θ-polymers and a suitable way to study generic effects of aggregation in relatively large systems. The model has been applied to a variety of problems including protein folding and surface adsorption and benefits from a discretized energy with nearest-neighbour interaction only. The Hamiltonian is given by

$$\mathcal{H} = -(\epsilon_i N_i + \epsilon_o N_o) \ , \tag{11.3}$$

where N_i, N_o are the number of contacts of the polymers with themselves and with each other, respectively. Here, we consider a three-dimensional cubic lattice with edge length L. The discretization allows a fast calculation of the system energy and, moreover, allows to enumerate small systems exactly.

Usually, one assumes $\epsilon_i = \epsilon_o$ which leads to competition of the polymer collapse and polymer aggregation [1]. This, we were able to recapture in principle with parallel multicanonical simulations [2] of ISAWs, showing in addition that in equilibrium the polymers homogenously aggregate into one macroscopic aggregate [3] similar to gas condensation. Moreover, the simplified model allows to systematically study the effect of the coupling constants on the occurring transitions. To this end, we introduce the ratio $\epsilon = \epsilon_o/\epsilon_i$, expressing the inter-polymer coupling in terms of the intra-polymer coupling. The result of an exact enumeration of two polymers ($N = 9$, $L = 35$) is shown in Fig. 11.9. Next to the heat capacity, it also shows the maxima and minima of the temperature derivative of the energy (E), the phase separation parameter (P), and the number of intra-(N_i) and inter-(N_o) polymer contacts.

This simple but exact example shows that the collapse and the aggregation only compete in the vicinity of $\epsilon \approx 1$. For small ϵ the two polymers first collapse before aggregating, while for large ϵ the polymers aggregate already at higher temperatures followed by further rearrangement transitions. The exact enumerations are extended



(a) (b)

Figure 11.9: (a) Pseudo-phase diagram of two polymers ($N = 9$) with variable coupling constant $\epsilon = \epsilon_o/\epsilon_i$. (b) 20 polymers ($N = 13$) in the aggregated phase.

by Monte Carlo simulations in order to better characterize the occurring phases also for larger systems, with an increasing number of longer chains.

[1] C. Junghans et al.: Europhys. Lett. **87**, 40002 (2009)
[2] J. Zierenberg et al.: Comput. Phys. Comm. **184**, 1155 (2013)
[3] J. Zierenberg, W. Janke: Leipzig preprint (2013)

11.10 Random heteropolymer models

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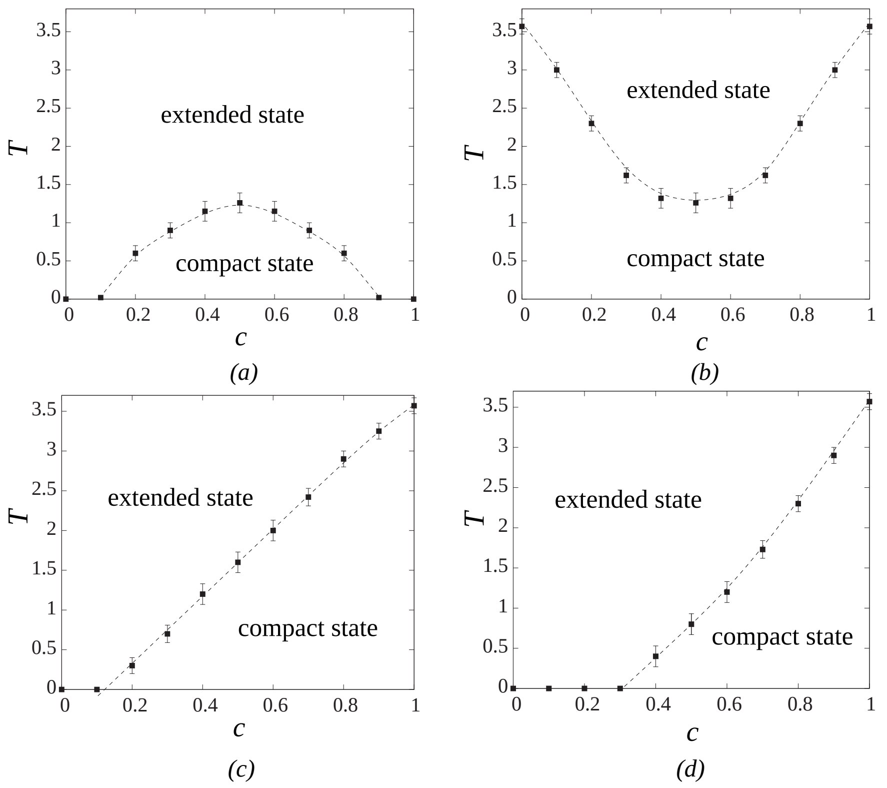
The conformational properties of long heteropolymer chains are a subject of great interest in both chemical and biological physics. Typical examples are proteins, consisting of sequences of amino acid residues connected by peptide bonds. The conformations of individual macromolecules are controlled by 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 a lattice model containing 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 interactions between any pair of monomers residing on neighboring lattice sites that are not connected by a covalent bond, we considered 5



(a) (b) (c) (d)

Figure 11.10: Phase diagrams of heterogeneous polymer chains in T-c space. (a) model 1, (b) model 2, (c) model 4, (d) model 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]. Figure 11.10 shows that 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. In model 2, the θ-transition 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. Models 2, 4 and 5 describe homogeneous polymer chains with nearest-neighbour attractions in the limiting case $c = 1$ (for model 2 also $c = 0$) with known value of the transition temperature $T_\theta = 3.717(3)$ [3].

[1] K.A. Dill: Biochemistry **24**, 1501 (1985); K.F. Lau, K.A. Dill: Macromolecules **22**, 3986 (1989)
[2] Y. Kantor, M. Kardar: Europhys. Lett. **28**, 169 (1994)
[3] P. Grassberger: Phys. Rev. E **56**, 3682 (1997)
[4] V. Blavatska, W. Janke: J. Chem. Phys. **140**, 034904 (2014)

11.11 Hysteresis and scaling of DNA under oscillatory force

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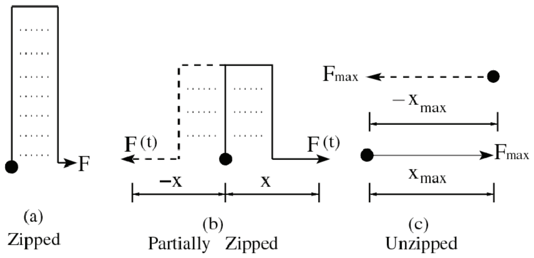
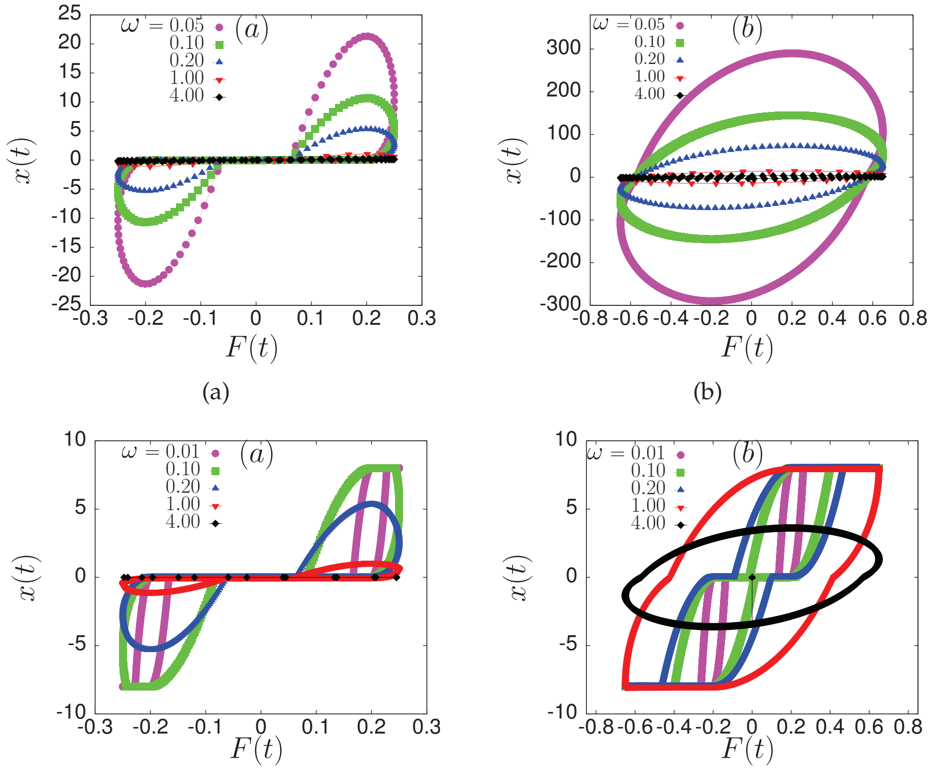


Figure 11.11: Schematic representations of DNA: (a) zipped, (b) partially zipped, and (c) unzipped. One end is kept fixed (indicated by the solid circle), while the other end may move in positive (shown by the solid line) or negative direction (shown by the dashed line), depending on the applied force direction.

Much attention has been paid in recent years to the understanding of biological processes, e.g., transcription and replication of nucleic acids, packing of DNA in a capsid, synthesis and degradation of proteins etc., which are driven by different types of molecular motors *in vivo* [1]. Experiments on biomolecules using single molecule force spectroscopy (SMFS) techniques have enhanced our understanding about these processes [2]. Unlike *in vivo*, where these motors are driven by oscillatory forces resulting from the periodic consumption of ATP to ADP, a constant force or loading rate used in SMFS experiments provides a limited picture of these processes *in vitro*. This has been highlighted in recent studies, where it was suggested that by varying the frequency and amplitude of the applied force, new aspects of a force-driven transition can be introduced [3–5], which otherwise would not be possible in the case of a steady force.

In this project, we have shown within a simplified model the existence of a dynamical transition in a system of driven DNA under the influence of an oscillatory force of amplitude F and frequency ω [6], for a sketch see Fig. 11.11. For a chain of finite length, we observe that the area of hysteresis loops shown in Fig. 11.12 scales with the same exponents as proposed in the recent study [3]. However, in the true thermodynamic



(a)

(b)

(c)

(d)

Figure 11.12: Hysteresis of the end points separation under a periodic force for different frequencies ω and (a) small amplitude ($F = 0.25$) respectively (b) large amplitude ($F = 0.65$) in the infinite chain-length limit $L = \infty$. The lower part (c), (d) of the figure shows the corresponding plots for a chain of finite length $L = 4$ where $|x(t)| \leq 8$.

limit, we find that the high-frequency scaling regime extends to lower frequencies for larger chain length L, and the system has only one scaling regime where the area of the hysteresis loop scales with $\omega^{-1}F^2$. This indicates that a true dynamical transition may not exist in the thermodynamic limit. We also show that the scaling for large but finite L at temperature $T = 0$ and $\neq 0$ remains invariant.

[1] B. Alberts et al.: *Molecular Biology of the Cell* (Garland Publishing, New York, 1994)
[2] S. Kumar, M.S. Li: Phys. Rep. **486**, 1 (2010)
[3] S. Kumar, G. Mishra: Phys. Rev. Lett. **110**, 258102 (2013)
[4] G. Mishra et al.: Phys. Rev. E **87**, 022718 (2013)
[5] R.K. Mishra et al.: J. Chem. Phys. **138**, 244905 (2013)
[6] S. Kumar et al.: Varanasi/Leipzig preprint (2014), to be published

11.12 Exact enumeration of polymers in fractal disorder

N. Fricke, W. Janke

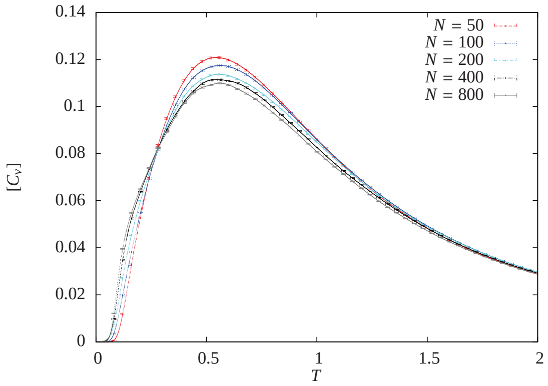


Figure 11.13: Quenched averages of the specific heat for self-attracting self-avoiding walks of varying length on critical percolation clusters.

The asymptotic scaling behaviour of flexible polymers in a good solvent is properly captured by self-avoiding walks (SAWs) on a regular lattice [1]. By including a nearest-neighbour attraction, ϵ, one can account for van-der-Waals forces that will cause a transition to a collapsed state at a certain temperature Θ. These so-called self-attracting self-avoiding walks (SASAWs) or Θ-polymers are characterized by three different sets of exponents: above, at, and below Θ.

To describe polymers in disordered environments such as porous rocks, one often considers quenched averages of (SA)SAWs on critical percolation clusters; see [2]. One interesting aspect there is the fractal nature of the clusters, which have non-integer Hausdorff dimensions. This model is difficult to treat analytically, and previous numerical approaches have proved rather cumbersome.

We developed a new enumeration method to exactly determine the configurational averages on a random sample of critical clusters [3–5]. Our approach makes use of the fractal geometry of the clusters and is thus considerably more efficient than any previous numerical method. The principal idea is to partition the critical cluster into a hierarchy of weakly connected regions, where the walks can be enumerated independently. The method can easily handle 10^4 steps for normal SAWs and about 6×10^3 for SASAWs on three-dimensional clusters at a fixed temperature. For shorter chains (about 800 steps), it can also be used to generate the complete density of states, Ω_E, from which the configurational averages at any temperature can be calculated. For instance, the specific heat, C_V, as a function of temperature, T which is typically studied when investigating thermal phase transitions, is obtained as:

$$C_V = \frac{1}{N k_B T^2}\left(\frac{\sum_E \Omega_E E^2 e^{-\frac{E}{k_B T}}}{Z} - \left(\frac{\sum_E \Omega_E E e^{-\frac{E}{k_B T}}}{Z}\right)^2\right),$$

where E is a walk's total energy, N the number of monomers and Z the partition function.

For single clusters, we found that C_V typically shows sharp peaks, whereas the quenched average only has a cusp at around $T = 0.55\epsilon/k_B$ (Fig. 11.13). We are currently investigating whether this corresponds to a collapse transition.

[1] P.-G. de Gennes: *Scaling Concepts in Polymer Physics* (Cornell University Press, Ithaca, 1976)
[2] B. Barat, B.K. Chakrabarti: Phys. Rep. **258**, 377 (1995)
[3] N. Fricke, W. Janke: Europhys. Lett. **99**, 56005 (2012)
[4] N. Fricke, W. Janke: in *Computer Simulation Studies in Condensed-Matter Physics XXV*, eds. D.P. Landau, H.-B. Schüttler, S.P. Lewis, M. Bachmann, Physics Procedia **34**, 39 (2012)
[5] N. Fricke, W. Janke: Eur. Phys. J. Special Topics **216**, 175 (2013)

11.13 Kinetic growth random walks in fractal disorder

N. Fricke, J. Bock, W. Janke

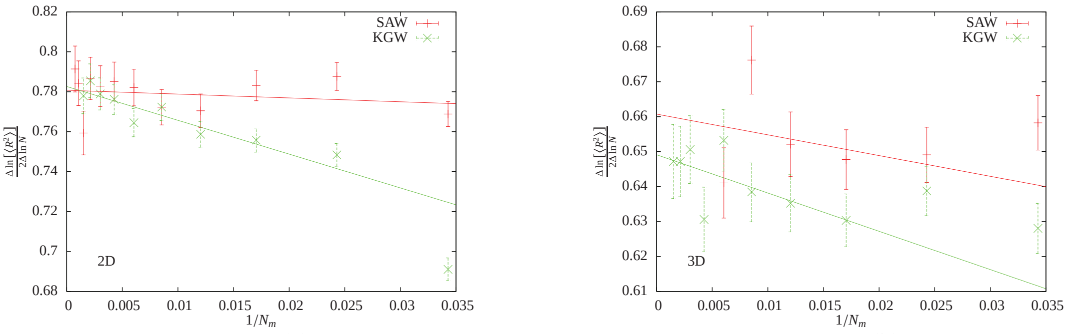
The self-avoiding random walk (SAW) has been a popular model for polymers since the 1950s [1]. Of particular interest is the asymptotic scaling behaviour of its mean squared end-to-end distance with the number of steps, described by a power law with a universal exponent, $\langle R^2 \rangle \sim N^{2\nu}$. The average can be defined in two different ways: For the standard SAW, each trajectory contributes equally, corresponding to equilibrium statistics. The so-called kinetic growth walk (KGW) models a growing polymer; each trajectory contributes to the average according to the probability that it would occur in a self-avoiding growth process. On regular lattices, SAWs and KGWs appear to have different scaling exponents; see [2, 3].

To model polymers in random environments, one often constrains the walks to a critical percolation cluster, the paradigm for a highly disordered medium [4]. Our previous investigations had suggested that here, too, the exponents are different [3]. However, these results were preliminary, the number of steps and the amount of statistics having been rather small. By now we were able to significantly improve our measurements, owing to the use of more efficient algorithms: To simulate the KGWs, we used a modification of the pruned-enriched Rosenbluth method (PERM), which avoids trapping of the walks in dead ends [5]. The standard SAWs were exactly enumerated using a new technique that exploits the fractal nature of the clusters [6]. We were thus able to study SAWs and KGWs of up to 800 steps on a sample of 10^4 randomly generated clusters in two and three dimensions. The closer look revealed that while the behaviours differ initially, they clearly appear to converge when the number of steps is sufficiently increased; see Fig. 11.14. Our estimates for the exponent ν for SAWs and KGWs on critical clusters are given in Table 11.1, alongside the previously obtained full-lattice values.

Based on these findings, we conclude that the asymptotic scaling behavior of SAWs and KGWs on critical percolation clusters is probably identical, contrary to the situation on the full lattice.

Table 11.1: Values the scaling exponent ν.

medium	ν_{2D} (SAW)	ν_{2D} (KGW)	ν_{3D} (SAW)	ν_{3D} (KGW)
full lattice	3/4	0.682(2) [3]	0.587597(7) [7]	0.520(1) [3]
perc. cluster	0.780(5) [5]	0.782(3) [5]	0.66(3) [5]	0.649(4) [5]



(a) (b)

Figure 11.14: Extrapolations of $\frac{1}{2}\frac{\Delta \ln[\langle R^2\rangle]}{\Delta \ln N}$ vs. $1/N$ to estimate the exponent ν on (a) 2D and (b) 3D percolation clusters. Only values where $1/N < 0.02$ were used for the fits. N_m denotes the mean of successive values of N.

[1] P. Flory: *Principles of Polymer Chemistry* (Cornell University Press, Ithaca, 1953)
[2] K. Kremer, J.W. Lyklema: Phys. Rev. Lett. **55**, 2091 (1985)
[3] J. Bock: Master Thesis, Universität Leipzig (2013)
[4] B. Barat, B.K. Chakrabarti: Phys. Rep. **258**, 377 (1995)
[5] N. Fricke et al.: diffusion-fundamentals.org **20**, 111 (2013)
[6] N. Fricke, W. Janke: Europhys. Lett. **99**, 56005 (2012)
[7] N. Clisby: Phys. Rev. Lett. **104**, 055702 (2010)

11.14 Dynamics of the binary frustrated unit: The effect of multiple inherent time scales

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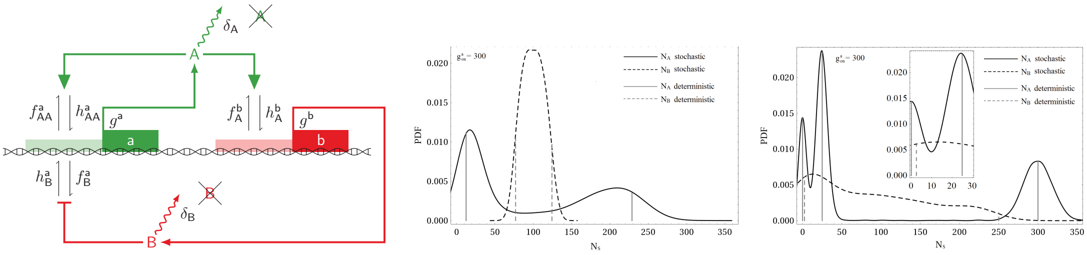
The motif of a self-activating species A that also activates another species B, which in turn represses its activator A, is often found in biological systems, particularly in those featuring inherent oscillatory behaviour. In such biological systems a source of delay in the interaction is essential for 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.

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. 11.15.



(a) (b) (c)

Figure 11.15: (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.

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.

[1] A. Garai et al.: J. Stat. Mech.: Theor. Exp., P01009 (2012)
[2] D. Labavić et al.: Phys. Rev. E **87**, 062706 (2013)

11.15 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 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

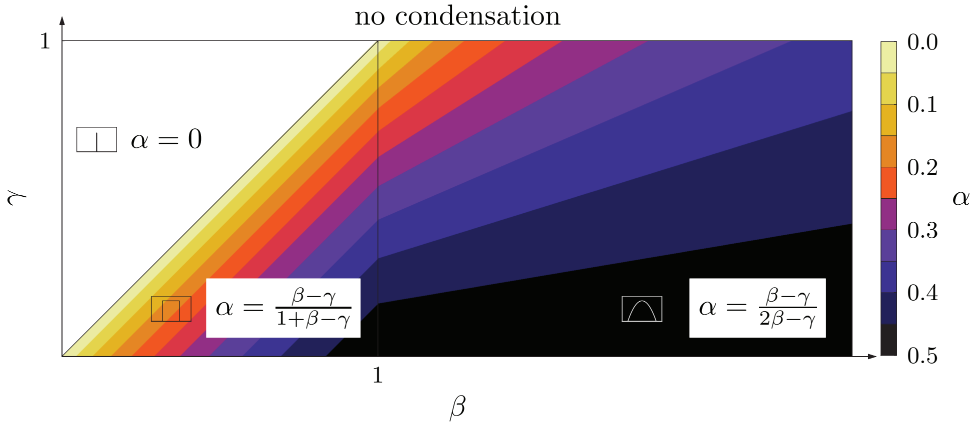


Figure 11.16: Theoretically predicted phase diagram for $K(x) \sim e^{-x^\beta}$ and $p(m) \sim e^{-m^\gamma}$, exhibiting condensed phases with point-like, rectangular and parabolic shapes (from left to right). The predicted value of the exponent α in the scaling law for the condensate extension W with the number M' of condensed particles, $W \simeq M'^\alpha$, is indicated by the color code.

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. 11.16.

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. 11.17 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.

[1] M.R. Evans et al.: Phys. Rev. Lett. **97**, 010602 (2006)
[2] B. Wacław et al.: J. Phys. A: Math. Theor. **42**, 315003 (2009)
[3] B. Wacław et al.: Phys. Rev. Lett. **103**, 080602 (2009)
[4] B. Wacław et al.: J. Stat. Mech. P10021 (2009)
[5] B. Wacław et al.: J. Phys.: Conf. Ser. **246**, 012011 (2010)
[6] E. Ehrenpreis et al.: J. Phys. A: Math. Theor. **47**, 125001 (2014)

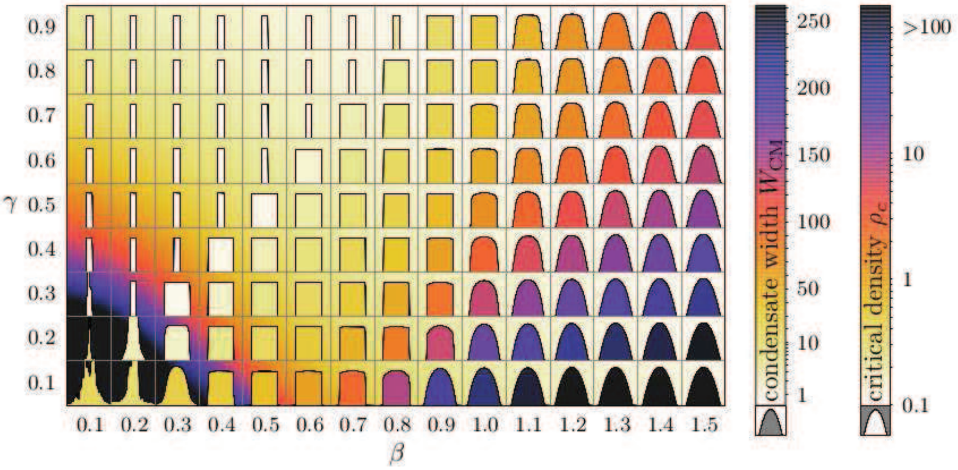


Figure 11.17: Numerically determined characteristic condensate shapes for systems of various β and γ at a condensate volume of about 10^5 masses. The shapes are formed by rescaling the width and height of all measured condensate sample shapes and only then averaging them. The fill colour inside the condensate shapes encodes the respective measured condensate width while the background colour around the shapes gives the critical density of the system. The shapes in the single-site condensate regime are plotted narrowed to give better distinction to extended shapes.

11.16 Transmuted finite-size scaling at first-order phase transitions

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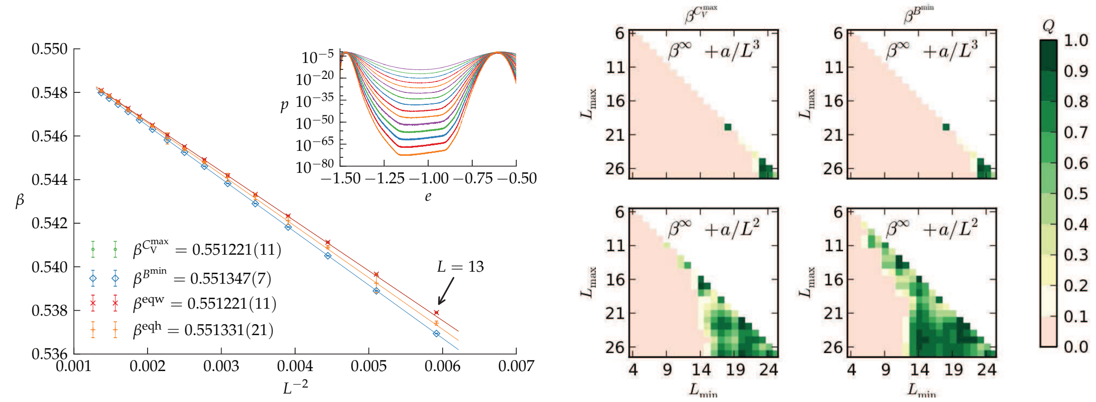
First-order phase transitions are ubiquitous in nature. In the limit of infinite system size they are characterized by jumps in the energy and/or order parameter and δ-function like divergencies in response functions such as the specific heat. Similarly to critical phenomena, in finite systems these singularities are rounded and shifted. It is well established [1] that the finite-size corrections at a first-order phase transition scale with the inverse system volume, i.e., $1/L^3$ for an $L \times L \times L$ lattice in 3D, with the amplitudes of the correction terms being proportional to $\ln q$, where q denotes the degeneracy of the low-temperature phase. In many standard models such as the q-state Potts model, this factor is not particularly important since q is just a constant which does not change with system size.

However, if the degeneracy q of the low-temperature phase depends exponentially on the system size, say $q \propto e^L$, the usual $1/L^3$ would be modified to $1/L^2$. In [2] we noted that one model with precisely this feature is a 3D plaquette (4-spin) interaction Ising model on a cubic lattice where $q = 2^{3L}$ on an L^3 lattice [3]. This is a member of a family of so-called gonihedric Ising models [4] whose Hamiltonians contain, in general, nearest, next-to-nearest, and plaquette interactions. These were originally formulated as a lattice discretization of string-theory actions in high-energy physics which depend



(a) (b)

Figure 11.18: (a) Best fits using the leading $1/L^2$ scaling behaviour for the gonihedric model. (b) Plot of the goodness-of-fit parameter Q for fits on the extremal locations of the specific heat, $\beta^{C_V^{\max}}$, and Binder's energy cumulant, $\beta^{B^{\min}}$, of the original model for different fitting ranges $L_{\min} - L_{\max}$. Large values of Q (green color) indicate acceptable fits. Upper row: Standard $1/L^3$ finite-size scaling ansatz. Lower row: Transmuted $1/L^2$ finite-size scaling.

solely on the extrinsic curvature of the string worldsheet [5].

We used multicanonical simulations of this model to generate high-precision data which indeed provides strong confirmation of the non-standard finite-size scaling law [2, 6], see Fig. 11.18. The dual to the gonihedric model, which is an anisotropically coupled Ashkin-Teller model [7], has a similar degeneracy and also displays the non-standard scaling [2, 6].

Our observation for the gonihedric model and its dual applies generically to any models which have a low-temperature phase degeneracy that depends exponentially on the system size. Examples range from ANNNI models to topological "orbital" models in the context of quantum computing. Numerous other systems, such as the Ising antiferromagnet on a 3D FCC lattice, have an exponentially degenerate number of ground states but a small number of true low-temperature phases. Nonetheless, they do possess an exponentially degenerate number of low-energy excitations so, depending on the nature of the growth of energy barriers with system size, an *effective* modified scaling could still be seen at a first-order transition for the lattice sizes accessible in typical simulations.

[1] C. Borgs et al.: J. Stat. Phys. **62**, 529 (1991); W. Janke: Phys. Rev. B **47**, 14757 (1993)
[2] M. Mueller et al.: Phys. Rev. Lett. **112**, 200601 (2014)
[3] R. Pietig, F. Wegner: Nucl. Phys. B **466**, 513 (1996); *ibid.* **525**, 549 (1998)
[4] G.K. Savvidy, F.J. Wegner: Nucl. Phys. B **413**, 605 (1994); D.A. Johnston, R.K.P.C. Malmini: Phys. Lett. B **378**, 87 (1996)
[5] R.V. Ambartzumian et al.: Phys. Lett. B **275**, 99 (1992); G.K. Savvidy, K.G. Savvidy: Int. J. Mod. Phys. A **8**, 3393 (1993); Mod. Phys. Lett. A **8**, 2963 (1993)
[6] M. Mueller et al.: Leipzig preprint (2014), to be published
[7] D.A. Johnston, R.P.K.C.M. Ranasinghe: J. Phys. A: Math. Theor. **44**, 295004 (2011)

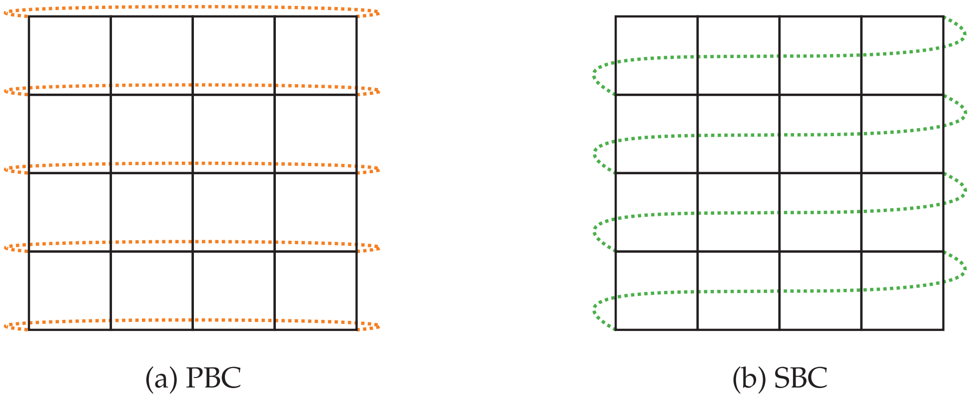

(a) PBC (b) SBC

Figure 11.19: Sketch of (a) periodic (PBC) and (b) screw-periodic boundary conditions (SBC) along the x-axis of a two-dimensional lattice. In the SBC picture the link between the lower right and the upper left corner is not shown. Equivalent boundary conditions are applied to the y-direction. Here a screw parameter of $S = 1$ is used.

11.17 First-order directional ordering transition in the three-dimensional compass model

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Both the classical and the quantum version of the compass model have recently attracted much interest in the literature. The resaon is its connection to interesting quantum phenomena ranging from orbital order in transition metal compounds to topologically protected qbits [1–3]. In three dimensions the classical model is defined by the Hamiltonian

$$\mathcal{H} = J \sum_{i=1}^{N} \left(\sigma_i^x \sigma_{i+e_x}^x + \sigma_i^y \sigma_{i+e_y}^y + \sigma_i^z \sigma_{i+e_z}^z \right) , \tag{11.4}$$

where $\sigma = (\sigma^x, \sigma^y, \sigma^z)$ are three-dimensional unit spin vectors, e_x, e_y, and e_z are unit vectors in x, y, and z direction, and J is a coupling constant. Although simple looking at first sight, surprisingly little is known about this model in three dimensions. Most studies so far focused on the two-dimensional analogue which still turned out to be rather hard to study numerically. It was shown to possess rich physics ranging from highly degenerate ground states to quantum phase transitions to an exciting thermal phase transition [4, 5].

In recent analyses of high-temperature series expansions of the three-dimensional quantum model (where the classical spins are replaced by Pauli matrices) it was claimed that this model does not exhibit a phase transition at any finite temperature [6]. This motivated us to consider first the three-dimensional classical model and to investigate whether this model exhibits a phase transition [7]. To this end we employed state-of-the-art Monte Carlo computer simulations using Metropolis, cluster, and parallel tempering (PT) techniques. From our previous studies in two dimensions [5] we knew

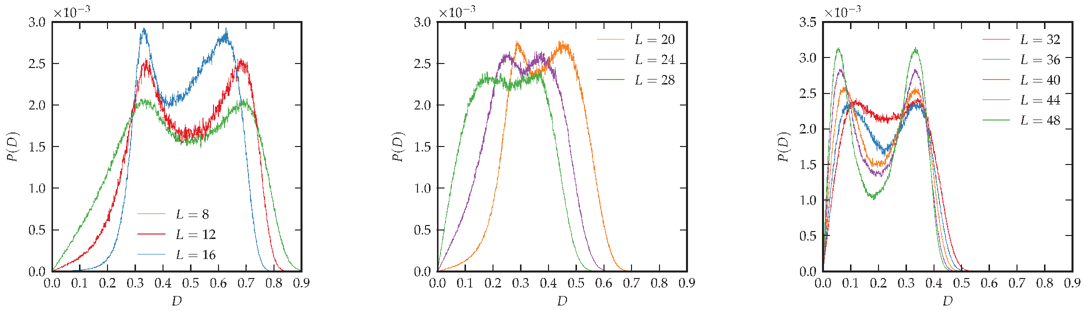


Figure 11.20: Histograms of the directional order parameter D in the three-dimensional compass model with screw-periodic boundary conditions for various lattice sizes L.

that employing so-called screw-periodic boundary conditions [8] sketched in Fig. 11.19 considerably improves the finite-size scaling behaviour of this model. As a result we obtained convincing numerical evidence for a phase transition of first-order at the temperature $T_0 = 0.098328 \pm 0.000003$. This value is in good agreement with a brief remark in Ref. [9]. The nature of the phase transition can be read off from the histograms of the directional order parameter D of the model in Fig. 11.20 which exhibit for large lattice sizes L a characteristic double-peak structure. Note the nonmonotonic behaviour as function of lattice size: Initially, the double peak becomes *less* pronounced until $L \approx 28-32$, and only from then on it becomes more pronounced with further increasing L. By analyzing the ratio of peak maximum to peak minimum, we arrive at a definitely nonzero, albeit small value for associated interface tension, $\sigma_{\mathrm{od}} \approx 3 \times 10^{-4}$.

[1] K.I. Kugel, D.I. Khomskii: Sov. Phys. Usp. **25**, 231 (1982)
[2] B. Douçot et al.: Phys. Rev. B **71**, 024505 (2005)
[3] A. Kitaev: Ann. Phys. **321**, 2 (2006)
[4] S. Wenzel, W. Janke: Phys. Rev. B **78**, 064402 (2008); see also "Publisher's Note" in Phys. Rev. B **78**, 099902(E) (2008) [Fig. 1 selected for Phys. Rev. B "Kaleidoscope" August 2008]
[5] S. Wenzel et al.: Phys. Rev. E **81**, 066702 (2010) [arXiv:1002.3508]
[6] J. Oitmaa, C.J. Hamer: Phys. Rev. B **83**, 094437 (2011)
[7] M.H. Gerlach, W. Janke: *First-order directional ordering transition in the three-dimensional compass model*, e-print arXiv:1406.1750 (cond-mat.stat-mech), submitted
[8] E. Bittner et al.: Nucl. Phys. B **820**, 694 (2009)
[9] S. Wenzel, A.M. Läuchli: Phys. Rev. Lett. **106**, 197201 (2011)

11.18 Status of our framework for programming Monte Carlo simulation (βMC)

M. Marenz, J. Zierenberg, W. Janke

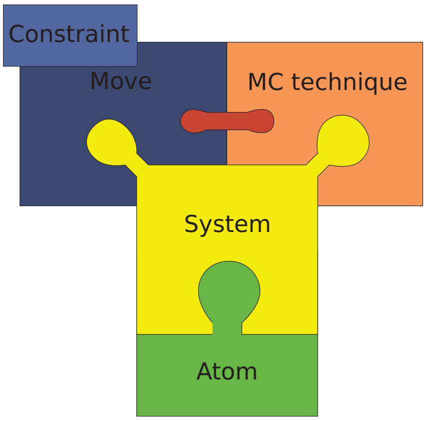


Figure 11.21: The 5 basic building blocks.

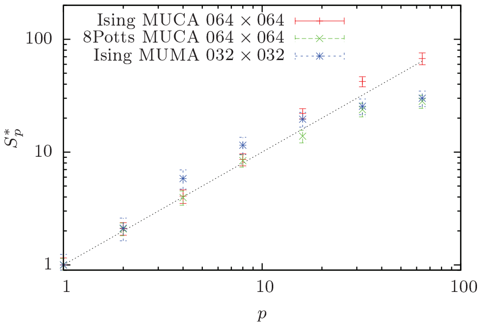


Figure 11.22: Scaling properties of the parallel multicanonical algorithm as a function of the number of processors p.

Monte Carlo (MC) computer simulations are a very powerful tool for investigating and understanding the thermodynamical behaviour of a wide variety of physical systems. These systems range from such simple ones like the Ising spin model to complex ones like the adsorption properties of proteins on surfaces [1]. In contrast to Molecular Dynamics (MD) simulations, the other important class of algorithm to simulate microscopical systems, MC simulations are not suitable to investigate dynamical properties. On the other hand, the ability of modern MC methods to explore effectively the phase space of physical systems, especially those with a phase transition, makes them a very powerful and indispensable tool.

Another difference to MD simulations is the lack of a widely used program package for generic MC simulations. One reason for this lack is the versatility of modern MC algorithms – there are various different algorithm and many different possibilities to adjust a MC simulation to a specific problem.

This was the starting point for the development of our framework for advanced MC algorithms. The aim of the framework is to enable the programmer to implement specific simulations in an easy and efficient way, without the need to implement all the tricky details for every new problem. The framework is implemented in the C++ programming language and is designed such that it separates basics parts of a MC algorithm in separate building blocks. These building blocks can be used by the programmer to implement a specific simulation.

There are 5 basic building blocks as illustrated in Fig. 11.21: The first one is the "system", which defines the Hamiltonian and the structure of the physical system. This means that the "system" building block encapsulates the energy calculation and the structure of the considered physical problem. For off-lattice system this block contains a smaller subpart, the "atom" block, which encodes the geometry of the system (e.g., boundary conditions). As systems we have implemented so far different kinds of coarse-grained homopolymers, the Lennard-Jones gas, the TIP4P water model, lattice polymers and the Potts model in different dimensions. On top of the "system" are the last two other building blocks, the "move" and the "MC technique". A "move" defines a single update proposal, propagating the system from the current state to the next one. Additionally a "constraint" can be added to every "move" in order to simulate efficiently systems with geometrical confinements. The "MC technique" implements the

Monte Carlo algorithm itself. At the moment we have implemented various algorithms such as Metropolis MC, parallel tempering, multicanonical MC, multimagnetic MC and the Wang-Landau MC algorithm. One of the most advanced MC algorithms we have implemented is a parallel version of the multicanonical algorithm [2], see Fig. 11.22.

The boundaries between these blocks are well defined, so that one can easily exchange one of them. For example one can use two different algorithm to simulate a specific system without implementing a completely new program. The framework is already in practical use for different studies, for example the investigation of the influence of bending stiffness on a coarse-grained homopolymer, the influence of a spherical confinement to pseudo-phase transitions of homopolymers, the study of polymer aggregation of several polymers for a large set of parameters (temperature, bending stiffness). Thus the framework is very useful and has let already to the publication of several papers [2–5].

[1] M. Bachmann et al.: Angew. Chem. Int. Ed. **49**, 9530 (2010) [Ang. Chem. **122**, 9721 (2010), in German]
[2] J. Zierenberg et al.: Comput. Phys. Comm. **184**, 1155 (2013)
[3] M. Marenz et al.: Condens. Matter Phys. **15**, 43008 (2012)
[4] J. Zierenberg et al.: J. Phys.: Conf. Ser. **510**, 012017 (2014)
[5] J. Zierenberg, W. Janke: e-print arXiv:1401.3227, submitted

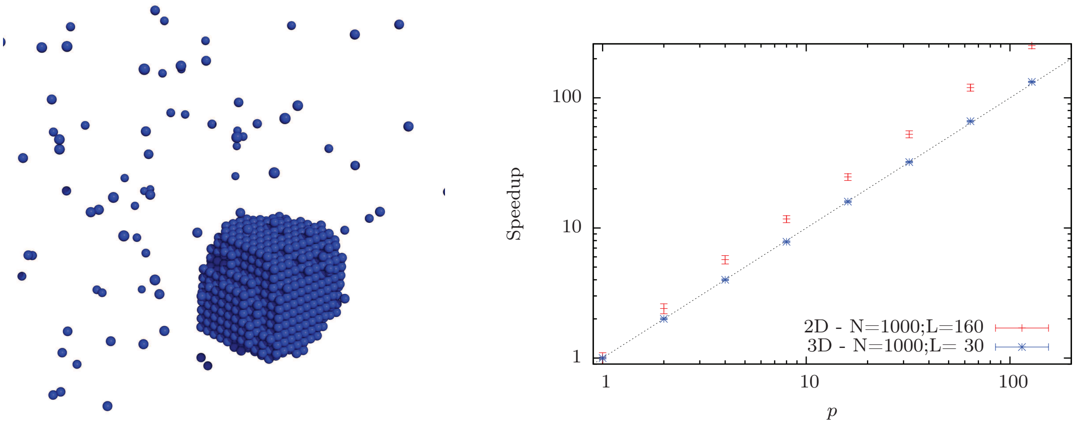
11.19 Application of the parallel multicanonical method to a broad range of problems

J. Zierenberg, M. Wiedemann, M. Marenz, W. Janke

We applied our recently refined parallel multicanonical method [1] to a broad range of problems and investigated the scaling properties including the Ising spin model, the q-state Potts model and bead-spring polymers [2], as well as the lattice gas model [3]. In all cases, we find a close to linear scaling with slope one for up to 128 cores used. This means, that doubling the number of involved processors would reduce the wall-clock time necessary by a factor of two. Moreover, it is a straightforward and simple implementation especially if wrapped around an existing multicanonical simulation.

A detailed analysis of optimized parameters per degree of parallelization for the q-state Potts model in the range $q = \{2, 8\}$ suggests that there exists a limit depending on emerging barriers and associated increasing integrated autocorrelation times [1, 2].

For any real-life application, we continue to consider a fixed number of sweeps per multicanonical iteration that is distributed onto the number of cores. This is the only possibility to assess larger or more complicated systems and shows the expected scaling also for first-order transitions like gas condensation in two and three dimensions, see Fig. 11.23 [3]. With this method, we were able to show that in three dimensions lattice gas condensation shows an unexpected deviation from the analytic predictions which may be explained by finite-size effects but needs additional investigations.



(a) (b)

Figure 11.23: (a) Lattice gas in the droplet phase as an example for (b) the speedup in a day-to-day application.

Altogether, this demonstrates the broad range of application of this parallel version of multicanonical simulations to problems in hard and soft condensed matter in any parameter that occurs linear in the Hamiltonian (temperature, field, etc.).

[1] J. Zierenberg et al.: Comput. Phys. Comm. **184**, 1155 (2013)
[2] J. Zierenberg et al.: e-print `arXiv:1312.2213`, to appear in Physics Procedia, in print
[3] J. Zierenberg et al.: J. Phys.: Conf. Ser. **510**, 012017 (2014)

11.20 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. 11.24), 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

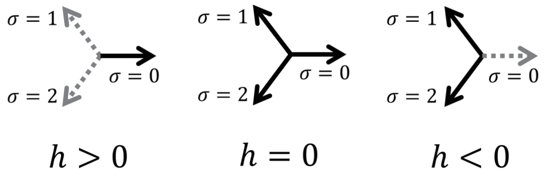

Figure 11.24: Schematic sketch illustrating the behaviour of the spins of the three-state Potts model in an external magnetic field h.

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

[1] F.Y. Wu: Rev. Mod. Phys. **54**, 235 (1982)

[2] W. Janke: Physica A **254**, 164 (1998); U.H.E. Hansmann, Y. Okamoto: in *Annual Reviews of Computational Physics VI*, ed. D. Stauffer (World Scientific, Singapore, 1999), p. 129; W. Janke (ed.): *Rugged Free Energy Landscapes: Common Computational Approaches to Spin Glasses, Structural Glasses and Biological Macromolecules*, Lect. Notes Phys. **736** (Springer, Berlin, 2008)

[3] A. Mitsutake, Y. Okamoto: Phys. Rev. E **79**, 047701 (2009); J. Chem. Phys. **130**, 214105 (2009)

[4] T. Nagai, Y. Okamoto: Phys. Rev. E **86**, 056705 (2012); Physics Procedia **34**, 100 (2012)

[5] A.P. Lyubartsev et al.: J. Chem. Phys. **96**, 1776 (1992); E. Marinari, G. Parisi: Europhys. Lett. **19**, 451 (1992)

[6] T. Nagai et al.: J. Stat. Mech.: Theor. Exp., P02039 (2013); Condens. Matter Phys. **16**, 23605 (2013)

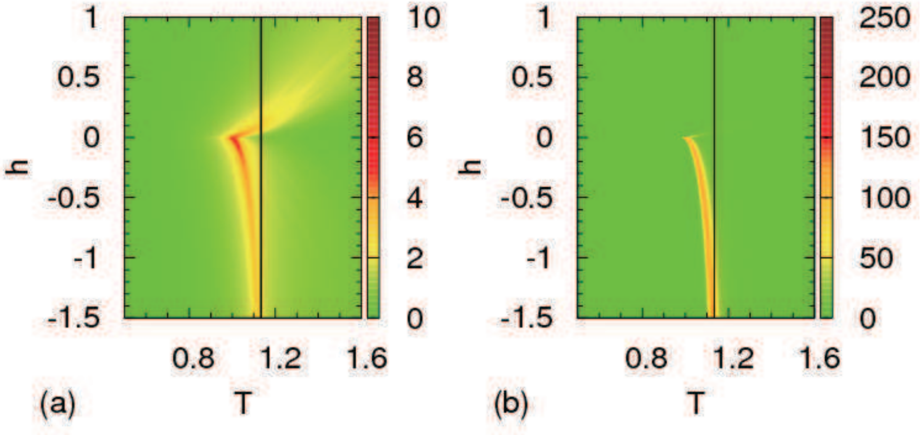

Figure 11.25: (a) Specific heat C/L^2 and (b) magnetic susceptibility χ/L^2 as functions of T and h for $L = 80$. The solid vertical line at $T = 1.1346$ shows the critical temperature of the Ising model (in 2-state Potts model normalization).

11.21 Finding the bridge between Molecular Dynamics and Monte Carlo simulations

P. Schierz, J. Zierenberg, W. Janke

Molecular Dynamics (MD) and Monte Carlo (MC) simulations are two powerful and widely used tools for the investigation of polymer properties. While MD follows the time evolution of the system by integrating Newton's equations of motion, MC simulations are based on statistical mechanics.

The starting question was to which extent we can expect the same results for both simulation techniques when we study polymer aggregation. Simulations for a many polymer system showed deviations between the results from multicanonical (MUCA) MC simulations [1] analysed in the NVE ensemble and MD (see Fig. 11.26(a)), where N is the number of polymers, V the volume, and E the total energy.

In order to find the reason for the observed deviations, similar simulations have been performed for a simpler Lennard-Jones gas. It turned out that the assumption that MD samples the NVE ensemble is not entirely correct. The NVE ensemble would allow all momenta for one configuration which are consistent with the given total energy. In MD, however, we have, for a system without boundary conditions, conservation laws for the total momentum P and total angular momentum J which leads to a restriction of the available phase space and therefore to the NVEPJ ensemble [2].

The knowledge of this ensemble allows the attempt to reweight from the MD data in the NVEPJ ensemble to the NVE ensemble. For a single homopolymer, boundary conditions are not necessary since it will remain at the starting point in an MD simulation.

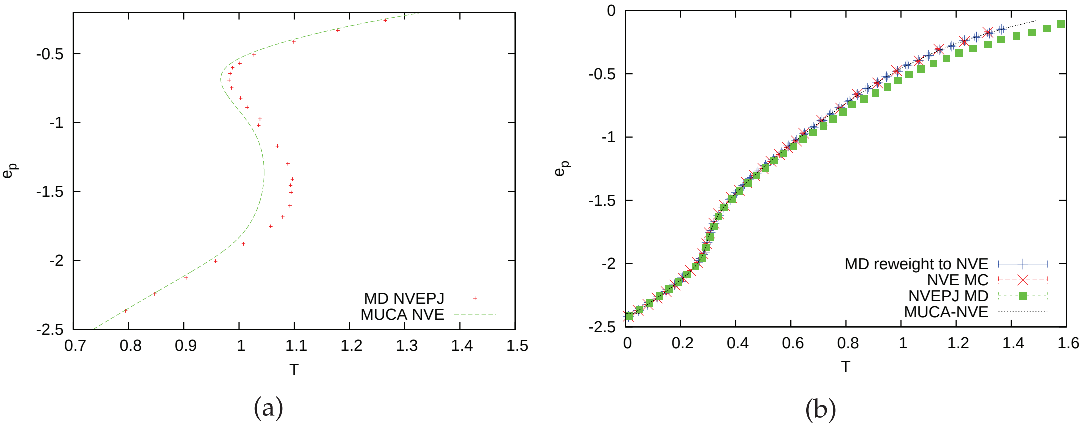

Figure 11.26: (a) Comparison of the energy as function of temperature for 8 polymers with 13 monomers each, simulated with MUCA MC and MD. (b) The energy for a single polymer with 13 monomers simulated by MUCA MC, NVE MC, simple MD, and reweighted MD.

In this case the reweighting technique worked for the whole coil-globule transition, see Fig. 11.26(b). For the Lennard-Jones gas, the boundary conditions are only negligible for the condensed phase with a zero total momentum. As soon as the condensate brakes apart the periodic boundary conditions will break the angular momentum conservation and the NVEPJ ensemble is no longer valid.

[1] B.A. Berg, T. Neuhaus: Phys. Lett. B **267**, 249 (1991); Phys. Rev. Lett. **68**, 9 (1992)
[2] F. Calvo et al.: J. Chem. Phys. **112**, 22 (2000)

11.22 Funding

Graduate School *"BuildMoNa": Leipzig School of Natural Sciences – Building with Molecules and Nano-objects*
W. Janke (Principal Investigator)
Deutsche Forschungsgemeinschaft (DFG), Excellence Initiative Grant GSC185

Graduate School *Statistical Physics of Complex Systems*
W. Janke (with B. Berche, Nancy)
Deutsch-Französisches Doktorandenkollegium (DFDK) with "Co-tutelle de Thèse", jointly with Université de Lorraine, Nancy, France, and Coventry University, UK, and National Academy of Sciences of Ukraine, Lviv, Ukraine, as associated partner
Deutsch-Französische Hochschule (DFH-UFA), Grant No. CDFA-02-07

International Max Planck Research School (IMPRS) *Mathematics in the Sciences*
W. Janke (Scientific Member)
Max Planck Society and Klaus Tschira Foundation

Forschergruppe 877 *From Local Constraints to Macroscopic Transport*
W. Janke (Principal Investigator, project P9 in collaboration with K. Kroy)
Deutsche Forschungsgemeinschaft (DFG), Grant No. JA 483/29-1

Sonderforschungsbereich/Transregio SFB/TRR 102 *Polymers under Multiple Constraints: Restricted and Controlled Molecular Order and Mobility*
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 (AvH)

Molecular Conformation Mechanics of Proteins and Polymers
W. Janke
Deutsche Forschungsgemeinschaft (DFG), Grant No. JA 483/24-3

Mass Transport Models on Networks
W. Janke (twin project with H. Meyer-Ortmanns, Jacobs University Bremen)
Deutsche Forschungsgemeinschaft (DFG), Grant No. JA 483/27-1

Aggregation and Collapse of Polymers in Confinement
W. Janke, M. Marenz, J. Zierenberg
NIC Jülich (computer time grant for "JUROPA"), Grant No. HLZ21

11.23 Organizational Duties

Wolfhard Janke

- 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
- Principal Investigator of the Graduate School "BuildMoNa"
- Scientific Member of the International Max Planck Research School (IMPRS) *Mathematics in the Sciences*
- Principal Investigator of the DFG Sonderforschungsbereich/Transregio SFB/TRR 102 *Polymers under Multiple Constraints: Restricted and Controlled Molecular Order and Mobility*
- Principal Investigator of the DFG Forschergruppe FOR877 *From Local Constraints to Macroscopic Transport*
- Member of the Priority Research Area PbF1 *Molecules and Nano-objects*, Universität Leipzig
- Member ot the Priority Research Area PbF2 *Mathematical Sciences*, Universität Leipzig
- Chairperson of the Programme Committee "Scientific Computing" of Forschungszentrum Jülich
- Member of the Scientific-Technical-Council of the Supervisory Board ("Aufsichtsrat") of the Forschungszentrum Jülich GmbH

- Spokesperson of the German-French Graduate College *Statistical Physics of Complex Systems* with Nancy (France), Coventry (England, UK) and Lviv (Ukraine) of the Deutsch-Französische Hochschule (DFH-UFA)
- Spokesperson of the German-Ukrainian Institute Partnership Leipzig-Lviv of the Alexander von Humboldt Foundation (AvH)
- External Member of the Jagiellonian University Graduate School *International Ph.D. Studies in Physics of Complex Systems*, Krakow, Poland
- *International Visiting Professor* of Coventry University, England, UK
- Permanent Member of the International Advisory Board for the Annual *Conference of the Middle European Cooperation in Statistical Physics (MECO)*
- Co-organizer of the SFB/TRR 102 Advanced Training Module *Introduction to Monte Carlo and Molecular Dynamics Simulation of Polymers* (with W. Paul, Universität Halle), Universität Halle, 07. February 2013 & Universität Leipzig, 08. February 2013
- Co-organizer of the "BuildMoNa" Modul 2013-B3 *Basic Concepts in Physics* (with P. Esquinazi and J. Haase), Universität Leipzig, 12./14. February 2013
- Co-organizer of the "BuildMoNa" Module 2013-T2 *Multifunctional Scaffolds: Modeling and Simulating Macromolecules* (with F. Kremer), Universität Leipzig, 20.–21. June 2013
- Member of the International Advisory Board for the XXV IUPAP *Conference on Computational Physics* CCP2013, Moscow, Russia, 20.–24. August 2013
- Organizer of the Workshop *CompPhys13* – 14th International NTZ Workshop on *New Developments in Computational Physics*, ITP, Universität Leipzig, 28.–30. November 2013
- Organizer of the Workshop *DEC13 – Droplet Evaporation/Condensation*, ITP, Universität Leipzig, 12./13. December 2013
- Member of the International Scientific Committee for the *Humboldt Kolleg: German-Turkish Cooperation in Physics: New Challenges in Science*, Ankara University, Ankara, Turkey, 11.–13. June 2014
- Chair of the Program Committee *Classical Statistical Mechanics and Complex Systems* of the XXVI IUPAP *Conference on Computational Physics* CCP2014, Boston, USA, 11.–14. August 2014
- Organizer of the Workshop *CompPhys14* – 15th International NTZ Workshop on *New Developments in Computational Physics*, ITP, Universität Leipzig, 27.–29. November 2014
- Guest Editor for the Special Issue of Condens. Matter Phys.: *Self-Organization and Collective Behaviour in Complex Systems*
- Editor "Computational Physics", Central European Journal of Physics, Krakow, Poland
- Member of Editorial Board, Condens. Matter Phys., Lviv, Ukraine
- External Reviewer for Deutsche Forschungsgemeinschaft (DFG), Humboldt-Stiftung (AvH), Studienstiftung des deutschen Volkes, Fond zur Förderung der wissenschaftlichen Forschung (FWF), Österreich, The Royal Society, UK, The Engineering and Physical Sciences Research Council (EPSRC), UK, Israel Science Foundation, Israel, National Science Foundation (NSF), USA, Natural Sciences and Engineering Research Council of Canada (NSERC), Canada, The Jeffress Memorial Trust, Bank of America, Virginia, USA, Universität Mainz, Germany, The University of Warwick, England, UK, Coventry University, England, UK, CECAM, Lyon, France

- 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, Condens. Matter Phys., PLOS ONE, New Journal of Physics, International Journal of Modern Physics C

11.24 External Cooperations

Academic

- Institute of Physics, Jagiellonian University, Kraków, Poland
  Prof. Dr. Piotr Białas, Dr. Leszek Bogacz, Prof. Dr. Zdzisław Burda
- CEA/Saclay, Service de Physique Théorique, France
  Dr. Alain Billoire
- Institut für Physik, Universität Mainz, Germany
  Prof. Dr. Kurt Binder, Dr. Hsiao-Ping Hsu, Andreas Nußbaumer, Prof. Dr. Friderike Schmid
- Institut für Theoretische Physik, Universität Heidelberg, Germany
  Dr. Elmar Bittner
- Laboratoire de Physique des Matériaux (UMR CNRS No 7556), Université de Lorraine, Nancy, France
  Prof. Dr. Bertrand Berche, Dr. Christophe Chatelain, Dr. Olivier Collet, Prof. Dr. Malte Henkel, Prof. Dr. Dragi Karevski
- Groupe de Physique des Matériaux (UMR CNRS No 6634), Université de Rouen, France
  Dr. Pierre-Emmanuel Berche
- SUPA, School of Physics and Astronomy, University of Edinburgh, Scotland, UK
  Dr. Richard A. Blythe, Prof. Dr. Martin R. Evans, Dr. Bartłomiej Wacław
- Istituto Nazionale di Fisica Nucleare, Sezione di Milano-Bicocca, Milano, Italy
  Prof. Dr. Pablo Butera
- Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich, Germany
  Prof. Dr. Peter Grassberger, PD Dr. Thomas Neuhaus
- IAC-1, Universität Stuttgart
  Prof. Dr. Rudolf Hilfer, Anjan Prasad Gantapara
- Complex Systems Division, Department of Theoretical Physics, Lunds Universitet, Lund, Sweden
  Prof. Dr. Anders Irbäck, Simon Mitternacht
- Department of Mathematics and the Maxwell Institute for Mathematical Sciences, Heriot-Watt University, Edinburgh, Scotland, UK
  Prof. Dr. Desmond A. Johnston

- Applied Mathematics Research Centre, Coventry University, England, UK
  Dr. Ralph Kenna, PD Dr. Christian von Ferber, Dr. Martin Weigel
- Inst. für Theoretische Physik, FU Berlin, Germany
  Prof. Dr. Hagen Kleinert
- Atominstitut, TU Wien, Austria
  Prof. Dr. Harald Markum, Dr. Rainer Pullirsch
- Jacobs Universität Bremen, Germany
  Prof. Dr. Hildegard Meyer-Ortmanns, Darka Labavić
- Applied Mathematics, Universitat Pompeu Fabra, Barcelona, Spain
  Dr. Ramon Villanova
- CERN (PH-SFT), Geneva, Switzerland
  Dr. Sandro Wenzel
- Department of Engineering of Physics, Ankara University, Turkey
  Prof. Dr. Handan Arkın (Olgar), Mustafa Bilsel, Buket Taşdizen
- Dept. of Physics, Hacettepe University, Ankara, Turkey
  Prof. Dr. Tarik Çelik, Gökhan Gökoğlu
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  Dr. Viktoria Blavatska, Prof. Dr. Yurij Holovatch
- Yerevan Physics Institute, Yerevan, Armenia
  Prof. Dr. David B. Saakian
- Landau Institute for Theoretical Physics, Chernogolovka, Russia
  Prof. Dr. Lev N. Shchur
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  Dr. Christoph Junghans, Dr. Thomas Vogel
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  Prof. Dr. Chin-Kun Hu

- The University of Tokyo, Japan
  Prof. Dr. Nobuyasu Ito
- Banaras Hindu University, Varanasi, India
  Prof. Dr. Sanjay Kumar
- Nagoya University, Japan
  Dr. Tetsuro Nagai, Prof. Dr. Yuko Okamoto
- Zhejiang Institute of Modern Physics, Zhejiang University, Hangzhou, P.R. China
  Prof. Dr. He-Ping Ying, Prof. Dr. Bo Zheng

11.25 Publications

Journals

H. Arkın, W. Janke: *Polymer-Attractive Spherical Cage System*, Eur. Phys. J. – Special Topics **216**, 181–190 (2013)

H. Arkın, W. Janke: *Gyration Tensor Based Analysis of the Shapes of Polymer Chains in an Attractive Spherical Cage*, J. Chem. Phys. **138**, 054904-1–8 (2013)

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]

N. Fricke, J. Bock, W. Janke: *Diffusion and Polymers in Fractal, Disordered Environments*, diffusion-fundamentals.org **20**, 111-1–10 (2013)

D. Labavić, H. Nagel, W. Janke, H. Meyer-Ortmanns: *Caveats in Modeling a Common Motif in Genetic Circuits*, Phys. Rev. E **87**, 062706-1–11 (2013)

T. Nagai, Y. Okamoto, W. Janke: *Application of Simulated Tempering and Magnetizing to a Two-Dimensional Potts Model*, J. Stat. Mech.: Theor. Exp., P02039-1–21 (2013)

T. Nagai, Y. Okamoto, W. Janke: *Crossover Scaling in the Two-Dimensional Three-State Potts Model*, Condens. Matter Phys. **16**, 23605-1–8 (2013)

D.T. Seaton, S. Schnabel, D.P. Landau, M. Bachmann: *From Flexible to Stiff: Systematic Analysis of Structural Phases for Single Semiflexible Polymers*, Phys. Rev. Lett. **110**, 028103-1–5 (2013)

J. Zierenberg, M. Marenz, W. Janke: *Scaling Properties of a Parallel Implementation of the Multicanonical Algorithm*, Comput. Phys. Comm. **184**, 1155–1160 (2013)

Books

in press

V. Blavatska, W. Janke: *Conformational Transitions in Random Heteropolymer Models*, J. Chem. Phys. **140**, 034904-1–7 (2014)

T. Chokbunpiam, R. Chanajaree, T. Remsungnen, O. Saengsawang, S. Fritzsche, C. Chmelik, J. Caro, W. Janke, S. Hannongbua: *N_2 in ZIF-8: Sorbate Induced Structural Changes and Self-Diffusion*, Micropor. Mesopor. Mater. **187**, 1–6 (2014)

E. Ehrenpreis, H. Nagel, W. Janke: *Numerical Survey of the Tunable Condensate Shape and Scaling Laws in Pair-Factorized Steady States*, J. Phys. A: Math. Theor. **47**, 125001-1–16 (2014)

M. Möddel, W. Janke, M. Bachmann: *Adsorption and Pattern Recognition of Polymers at Complex Surfaces with Attractive Stripe-like Motifs*, Phys. Rev. Lett. **112**, 148303-1–5 (2014)

M. Mueller, W. Janke, D.A. Johnston: *Nonstandard Finite-Size Scaling at First-Order Phase Transitions*, Phys. Rev. Lett. **112**, 200601-1–5 (2014)

J. Zierenberg, M. Wiedenmann, W. Janke: *Application of the Parallel Multicanonical Method to Lattice Gas Condensation*, J. Phys.: Conf. Ser. **510**, 012017-1–8 (2014)

M. Marenz, W. Janke: *Effect of Bending Stiffness on a Homopolymer Inside a Spherical Cage*, to appear in: *Computer Simulation Studies in Condensed-Matter Physics XXVII*, eds. D.P. Landau, H.-B. Schüttler, S.P. Lewis, M. Bachmann, Physics Procedia (2014), in print

M. Mueller, W. Janke, D.A. Johnston: *Transmuted Finite-Size Scaling at First-Order Phase Transitions*, to appear in: *Computer Simulation Studies in Condensed-Matter Physics XXVII*, eds. D.P. Landau, H.-B. Schüttler, S.P. Lewis, M. Bachmann, Physics Procedia (2014), in print

H. Nagel, D. Labavić, H. Meyer-Ortmanns, W. Janke: *Open Boundary Conditions in Stochastic Transport Processes with Pair-Factorized Steady States*, to appear in: *Computer Simulation Studies in Condensed-Matter Physics XXVII*, eds. D.P. Landau, H.-B. Schüttler, S.P. Lewis, M. Bachmann, Physics Procedia (2014), in print

J. Zierenberg, M. Marenz, W. Janke: *Application of Parallel Multicanonical Simulations to Systems with First and Second Order Phase Transition*, e-print `arXiv:1312.2213` (physics.comp-ph), in appear in: *Computer Simulation Studies in Condensed-Matter Physics XXVI*, eds. D.P. Landau, H.-B. Schüttler, S.P. Lewis, M. Bachmann, Physics Procedia (2014), in print

Talks

N. Fricke: *Self-Avoiding Walks on Critical Percolation Clusters*, SFG Workshop, Chemnitz, Germany, 09. April 2013

N. Fricke: *Scale-Free Enumeration of Self-Avoiding Walks on Critical Percolation Clusters*, XXV IUPAP International Conference on Statistical Physics, Seoul, South Korea, 22.–26. July 2013

N. Fricke: *Scale-Free Enumeration of Self-Avoiding Walks on Critical Percolation Clusters*, 14th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys13*, Universität Leipzig, Germany, 28.–30. November 2013

J. Gross: *Interaction Range Dependency of Flexible Polymer Structural Phases*, 26th Annual CSP Workshop *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, The University of Georgia, Athens, USA, 27. February 2013

J. Gross, T. Vogel, M. Bachmann: *Adsorption of a Coarse-Grained Flexible Polymer on Nanocylinders – A Monte Carlo Study*, 14th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys13*, Universität Leipzig, Germany, 28.–30. November 2013

M. Ivanov, W. Janke: *Polymer Adsorption onto a Stripe-Patterned Surface*, Retreat of SFB/TRR 102: Polymers under Multiple Constraints, Bad Blankenburg, Germany, 06.–08. March 2013

M. Ivanov: *Computer Simulations of Polymers*, SFB/TRR 102: Doctoral Students Seminar, Universität Leipzig, Germany, 13. August 2013

W. Janke: *Monte Carlo Methods in Classical Statistical Physics*, BuildMoNa Module B3 *Basic Concepts in Physics*, Universität Leipzig, Germany, 12. February 2013

W. Janke: *Scaling Properties of a Parallel Implementation of the Multicanonical Algorithm*, 26th CSP Workshop on *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, The University of Georgia, Athens, USA, 25. February – 01. March 2013

W. Janke: *Polymer Statistics in an Attractive Sphere*, DPG Frühjahrstagung, Universität Regensburg, Germany, 10.–15. March 2013

W. Janke: *Polymer Statistics in an Attractive Sphere*, Conference *MECO 38*, ICTP Trieste, Trieste, Italy, 25.–27. March 2013

W. Janke: *Exploring Critical Loop Gases with Worms*, Physics Seminar, Applied Mathematics Research Center (AMRC), Coventry University, England, UK, 25. April 2013

W. Janke: *Simulated Tempering and Magnetizing Study of Crossover Scaling in the 2d 3-State Potts Model*, invited talk, Workshop *Statistical Physics and Low Dimensional Systems – SPLDS*, Pont-à-Mousson, France, 15.–17. May 2013

W. Janke: *Constrained Polymer Statistics Inside a Spherical Cavity*, StatPhys25 Conference, Seoul, South Korea, 22.–26. July 2013

W. Janke: *Generalized Ensemble Simulations of Polymer Adsorption in an Attractive Spherical Cage*, invited talk, XXV IUPAP *Conference on Computational Physics CCP2013*, Moscow, Russia, 20.–24. August 2013

W. Janke: *Simulated Tempering and Magnetizing: Application to Crossover Scaling in the 2d 3-State Potts Model*, Statistical Physics Seminar, Applied Mathematics Research Centre (AMRC), Coventry University, England, UK, 24. September 2013

M. Marenz, W. Janke: *Effect of Bending Stiffness on a Homopolymer Inside a Spherical Cage*, 14th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys13*, Universität Leipzig, Germany, 28.–30. November 2013

M. Marenz, W. Janke: *Effect of Bending Stiffness on a Homopolymer Inside a Spherical Cage*, Seminar of the cdfa-dfdk, Coventry, England, UK, 03. December 2013

M. Müller: *Transmuted Finite-Size Scaling at First-Order Phase Transitions with Exponential Degeneracy of Ordered States*, Seminar of the cdfa-dfdk, Coventry, England, Uk, 03. December 2013

M. Müller, M. Ivanov: *Statistical Data Analysis*, SFB/TRR 102: iRTG Workshop, Wittenberg, Germany, 11. September 2013

P. Schierz: *A GPU Accelerated Metropolis-Hastings Algorithm for Particle Simulations*, 2nd International Symposium *Computer Simulations on GPU – SimGpu2013*, Freudenstadt, Germany, 28. May 2013

P. Schierz: *GPU Computing for Molecular Dynamics – and Monte Carlo Simulations*, Seminar of the cdfa-dfdk, Nancy, France, 12. September 2013

P. Schierz: *Computer Simulations Study of Polymer Aggregation*, ESF-Nachwuchsforschergruppe *Funktion durch Selbstorganisation: Emergente Eigenschaften von Atom- und Molekülaggregaten*, Leipzig, Germany, 02. December 2013

S. Schnabel, W. Janke: *Microcanonical Flat-Histogram Sampling*, 26th Annual CSP Workshop *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, Athens, Georgia, USA, 27. February 2013

S. Schnabel, D.P. Landau: *Fictitious Spin Waves in a Frustrated Classical Antiferromagnet*, Cambridge, England, UK, 06. March 2013

S. Schnabel, D.P. Landau: *Fictitious Excitations in the Classical Heisenberg Antiferromagnet on the Kagome Lattice*, DPG Frühjahrstagung, Regensburg, Germany, 14. March 2013

B. Schott: *Physical Annealing in the Microcanonical Ensemble*, Guest Student Programme on Scientific Computing, Jülich Supercomputing Centre (JSC), FZ Jülich, Germany, 29. September 2013

J. Zierenberg: *Simulations of Aggregation in Homopolymer Systems*, 6th Annual BuildMoNa Conference, Leipzig, Germany, 05. March 2013

J. Zierenberg: *Simulations of Aggregation in Homopolymer Systems*, DPG Frühjahrstagung, Regensburg, Germany, 11. March 2013

J. Zierenberg: *Condensation of Lattice Gas and Aggregation of Lattice Polymers*, Seminar of the cdfa-dfdk, Coventry, England, UK, 03. July 2013

J. Zierenberg: *Application of the Parallel Multicanonical Method to Lattice Gas Condensation*, XXV IUPAP *Conference on Computational Physics CCP2013*, Moscow, Russia, 21. August 2013

J. Zierenberg: *Polymer Aggregation vs. Particle Condensation*, Workshop on *Droplet Evaporation/Condensation – DEC13*, Leipzig, Germany, 12. December 2013

Posters

U. Arsawang, S. Fritzsche, W. Janke, J. Caro, T. Remsungnen, S. Hannongbua: *Structural and Transport Properties of Hydrogen in ZIF-22*, International Conference *Diffusion Fundamentals V – Basic Principles of Diffusion Theory, Experiment and Application*, Universität Leipzig, Germany, 26.–28. August 2013

J. Bock, N. Fricke, W. Janke: *Kinetic Growth Random Walks*, XXV IUPAP *Conference on Computational Physics CCP2013*, Moscow, Russia, 20.–24. August 2013

T. Chokbunpiam, R. Chanajaree, O. Saengsawang, S. Fritzsche, C. Chmelik, W. Janke, J. Caro, T. Remsungnen, S. Hannongbua: *Diffusion and Adsorption of N_2 and C_2H_6 in ZIF-8 MD and MC Simulations*, International Conference *Diffusion Fundamentals V – Basic Principles of Diffusion Theory, Experiment and Application*, Universität Leipzig, Germany, 26.–28. August 2013

T. Chokbunpiam, R. Chanajaree, O. Saengsawang, S. Fritzsche, C. Chmelik, W. Janke, J. Caro, T. Remsungnen, S. Hannongbua: *N_2 and C_2H_6 in ZIF-8: Guest Induced Structural Changes*, 2013 International Workshop on *Frontiers of Theoretical and Computational Physics and Chemistry*, Ampur Mueng, Cholburi, Thailand, 09.-12. December 2013

E. Ehrenpreis, H. Nagel, W. Janke: *Numerical Survey of the Tunable Condensate Shape and Scaling Laws in Pair-Factorized Steady States* DPG Frühjahrstagung, Universität Regensburg, Germany, 10.–15. March 2013

N. Fricke, J. Bock, W. Janke: *Diffusion and Polymers in Fractal, Disordered Environments*, International Conference *Diffusion Fundamentals V – Basic Principles of Diffusion Theory, Experiment and Application*, Universität Leipzig, Germany, 26.–28. August 2013

N. Fricke, W. Janke: *Self-Avoiding Walks on Critical Percolation Clusters in 2–7 Dimensions*, DPG Frühjahrstagung, Universität Regensburg, Germany, 10.–15. March 2013

N. Fricke, W. Janke: *Diffusion and Self-Avoiding Walks on Percolation Clusters*, International Conference *Diffusion Fundamentals V – Basic Principles of Diffusion Theory, Experiment and Application*, Universität Leipzig, Germany, 26.–28. August 2013

S. Fritzsche, P. Schierz, W. Janke, S. Hannongbua, O. Saengsawang, C. Chmelik: *Diffusion Investigation for Hydrogen Guest Molecules in an Adapted Force Field for ZIF-11*, International Conference *Diffusion Fundamentals V – Basic Principles of Diffusion Theory, Experiment and Application*, Universität Leipzig, Germany, 26.–28. August 2013

M. Ivanov, M. Möddel, W. Janke: *Polymer Adsorption onto a Stripe-Patterned Surface*, XXV IUPAP *Conference on Computational Physics CCP2013*, Moscow, Russia, 20.–24. August 2013

M. Ivanov, W. Janke: *Polymer Adsorption onto a Stripe-Patterned Surface*, SFB/TRR 102: Miniworkshop, Schkeuditz, Germany, 08. November 2013

M. Ivanov, M. Möddel, W. Janke: *Polymer Adsorption onto a Stripe-Patterned Surface*, 14th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys13*, Universität Leipzig, Germany, 28.–30. November 2013

M. Marenz, J. Zierenberg, W. Janke: *Simple Polymer in a Spherical Cage*, DPG Frühjahrstagung, Universität Regensburg, Germany, 10.–15. March 2013

M. Müller, D.A. Johnston, W. Janke: *Multicanonical Analysis of the Gonihedric Ising Model*, 14th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys13*, Universität Leipzig, Germany, 28.–30. November 2013

M. Müller, D.A. Johnston, W. Janke: *Multicanonical Analysis of the Gonihedric Ising Model*, DPG Frühjahrstagung, Universität Regensburg, Germany, 10.–15. March 2013

H. Nagel, J. Vollmer, W. Janke: *Application of a Steady States Transport Model to Condensation of Water Droplets on a Substrate*, International Conference *Diffusion Fundamentals V – Basic Principles of Diffusion Theory, Experiment and Application*, Universität Leipzig, Germany, 26.–28. August 2013

H. Nagel, J. Vollmer, W. Janke: *Application of a Steady States Transport Model to Condensation of Water Droplets on a Substrate*, 14th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys13*, Universität Leipzig, Germany, 28.–30. November 2013

P. Pilvar, S. Fritzsche, J. Caro, W. Janke: *Molecular Dynamics Investigation of the Transport of Hydrogen in ZIF-7*, International Conference *Diffusion Fundamentals V – Basic Principles of Diffusion Theory, Experiment and Application*, Universität Leipzig, Germany, 26.–28. August 2013

P. Schierz, S. Fritzsche, W. Janke, S. Hannongbua, O. Saengsawang, C. Chmelik: *Adsorption and Diffusion of Hydrogen Guest Molecules in the Metal-Organic Framework ZIF-11*, International MOF Symposium 2013, Dresden, Germany, 16.–17. September 2013

P. Schierz, J. Zierenberg, W. Janke: *Microcanonical Molecular Dynamics meets (Multi) Canonical Monte Carlo*, 14th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys13*, Universität Leipzig, Germany, 28.–30. November 2013

J. Zierenberg, M. Marenz, W. Janke: *Scaling Properties of a Parallel Implementation of the Multicanonical Algorithm*, DPG Frühjahrstagung, Universität Regensburg, Germany, 10.–15. March 2013

J. Zierenberg, M. Wiedenmann, W. Janke: *Condensation of a Lattice Gas in Three Dimensions*, International Conference *Diffusion Fundamentals V – Basic Principles of Diffusion Theory, Experiment and Application*, Universität Leipzig, Germany, 26.–28. August 2013

11.26 Graduations

Doctorate

- Rainer Bischof
  Gaussian Critical Line in Anisotropic Mixed Quantum Spin Chains
  06. February 2013
- Sebastian Schoebl
  Macromolecules in Disordered Environments: From Flexible to Semiflexible Polymers
  22. February 2013

Diploma

- Christoph Vogelsberg
  The 2-Dimensional Ising Model with Minus Boundary Condition
  29. January 2013

Master

- Johannes Bock
  Kinetisch wachsende Zufallsläufe
  16. January 2013

Bachelor

- Andreas Wagner
  Kondensatbildung eines Transportprozesses im Steady State – Exemplarische Überprüfung von Kondensatsformen
  15. March 2013

11.27 Guests

- PD Dr. Thomas Neuhaus
  Jülich Supercomputing Centre, Forschungszentrum Jülich, Germany
  15. January – 15. February 2013
- Prof. Dr. Sanjay Kumar
  Department of Physics, Banaras Hindu University, Varanasi, India
  (Bio)polymers under Mechanical Force I and II
  27. May – 07. July 2013
- Dr. Hsiao-Ping Hsu
  Universität Mainz, Germany
  Polymer Simulations with PERM I and II
  19. – 22. June 2013

- Dr. Stefan Förster
  Universität Halle, Germany
  Single Polymer Deposition
  20. – 21. June 2013
- Prof. Dr. Kurt Kremer
  MPI für Polymerforschung, Mainz, Germany
  Multiscale Modeling I and II
  21. – 22. June 2013
- Dr. Viktoria Blavatska
  Institute for Condensed Matter Physics, Lviv, Ukraine
  Alexander von Humboldt Foundation Institute Partnership Programme
  July – August 2013
- M.Sc. Marjana Krasnytska
  National Academy of Sciences of Ukraine, Lviv, Ukraine
  NTZ/DFH-UFA/RALeipzig Colloquium (07. November 2013)
  Critical Behavior for the Potts Model on Uncorrelated Scale-Free Networks: Phase Diagram, Critical Exponents, Scaling Functions and Amplitude Ratios
  20. October – 09. November 2013
- M.Sc. Nicolas Allegra
  Université de Lorraine, Nancy, France
  Boundary Crossover in Non-Equilibrium Interfaces Growth Processes
  17. – 30. November 2013
- Dr. Nikolay Izmailyan
  Yerevan Physics Institute, Yerevan, Armenia
  NTZ Colloquium (05. December 2013)
  Universal Amplitude Ratios in $c = 1/2$ *and* $c = -2$ *Universality Classes*
  27. November – 07. December 2013
- Dr. Christophe Chatelain
  Université de Lorraine, Nancy, France
  Griffiths Phase in a Potts Model with Correlated Disorder
  27. – 30. November 2013
- Dr. Stefan Falkner
  Emory University, Atlanta, USA
  Renormalization Group for Quantum Walks
  27. – 30. November 2013
- Dr. Hsiao-Ping Hsu
  Universität Mainz, Germany
  Confined Semiflexible Chains in a Good Solvent: A Monte Carlo Test of Scaling Concepts
  27. – 30. November 2013
- PD Dr. Thomas Neuhaus
  Jülich Supercomputing Centre, Forschungszentrum Jülich, Germany
  Simulated Quantum Annealing for General Ising Models
  27. – 30. November 2013

- Dr. Francesco Parisen Toldin
  Universität Würzburg, Germany
  Critical Casimir Forces Between Homogeneous and Chemically Striped Surfaces
  27. – 30. November 2013
- Dr. Sergio Perez-Gaviro
  BIFI, University Zaragoza, Spain
  The Janus Family: A Special Purpose Computer Generation Devoted to Spin Glasses
  27. – 30. November 2013
- Prof. Dr. Bengt Petersson
  Humboldt Universität zu Berlin, Germany
  Magnetic Catalysis in 2 Color QCD at Finite Temperature
  27. – 30. November 2013
- Prof. Dr. Mark Taylor
  Hiram College, USA
  Partition Function Zeros and Finite-Size Scaling for Polymer Adsorption
  27. – 30. November 2013
- Dr. Andreas Tröster
  TU Wien, Österreich
  Fourier MC Simulation of Criticality in Solid and Hexatic Membranes
  27. – 30. November 2013
- Dr. Martin Weigel
  Coventry University, England, UK
  Corner Contribution to Cluster Numbers in the Potts Model
  27. – 30. November 2013
- M.Sc. Pierre Wendenbaum
  Université de Lorraine, Nancy, France
  Disentanglement of Two Qubits Coupled to an Ising Chain: Sudden Quench Dynamics
  27. – 30. November 2013
- Dr. David Yllanes
  "La Sapienza" Rome, Italy
  Numerical Study of the Branching Tree of States in Spin Glasses
  27. – 30. November 2013
- Prof. Dr. Michael Allen
  University of Warwick, Coventry, England, UK
  NTZ-Colloquium
  Computer Simulation of Peptide Adsorption
  27. November – 01. December 2013
- Dr. Elmar Bittner
  Universität Heidelberg, Germany
  MuCa vs WL: A Tight Race
  27. November – 01. December 2013
- Prof. Dr. Malte Henkel
  Université de Lorraine, Nancy, France

Statistical Mechanics of the Coagulation-Diffusion Process with a Stochastic Reset
27. November – 01. December 2013

- Prof. Dr. Ferenc Iglói
  Institute of Theoretical Physics, Research Institute for Solid State Physics and Optics, Budapest, Hungary
  Random Quantum Magnets in $d > 2$ *Dimensions: Critical Behavior and Entanglement Entropy*
  27. November – 01. December 2013
- Prof. Dr. Desmond A. Johnston
  Heriot-Watt University, Edinburgh, Scotland, UK
  Potts Models with Invisible States
  27. November – 01. December 2013
- M.Sc. Kai Qi
  Center for Simulational Physics, The University of Georgia, Athens, USA
  Autocorrelation Study for a Coarse-Grained Polymer Model
  27. November – 01. December 2013
- Dr. Christian von Ferber
  Coventry University, England, UK
  Environmental Impact on DNA Denaturation
  28. – 29. November 2013
- Prof. Dr. Michael Bachmann
  Center for Simulational Physics, The University of Georgia, Athens, USA
  Transitions in Small Systems
  28. – 30. November 2013
- Dr. Elmar Bittner
  Universität Heidelberg, Germany
  Muca vs WL in Droplet Models
  11. – 14. December 2013
- Dipl.-Phys. Andreas Nußbaumer
  Universität Mainz, Germany
  Gibbs-Thomson Effect in the 2D Ising Model
  11. – 14. December 2013
- PD Dr. Thomas Neuhaus
  Jülich Supercomputing Centre, Forschungszentrum Jülich, Germany
  Theory of Droplet/Evaporation Transition
  11. – 15. December 2013