10

Computational Quantum Field Theory

10.1 Introduction

The Computational Physics Group performs basic research into classical and quantum statistical physics with special emphasis on phase transitions and critical phenomena. In the centre of interest are 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.

The methodology is a combination of numerical and analytical techniques. The numerical tools are mainly 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. 10.1. Already now it often helps 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, C++, and Python programs running under Unix or Linux operating systems and computer algebra using Maple or Mathematica. The software is developed and tested at the Institute on a cluster of PCs and workstations, where also most of the numerical analyses are performed. Currently we are also exploring the possibilities of the rapidly developing graphics card computing, that is computer simulations on graphics processing units (GPUs) with many cores. Large-scale simulations requiring vast amounts of computer time are carried out at the Institute on quite powerful compute servers, at the parallel computers of the Saxon computing centre in Dresden, and, upon successful grant application, at the national supercomputing centres in Jülich, Stuttgart and München on parallel high-capability computers. This hierarchy of various platforms gives good training and qualification opportunities for the students, which offers promising job perspectives in many different fields for their future careers.

Our research activities are closely integrated into the Graduate School "BuildMoNa": Leipzig School of Natural Sciences – *Building with Molecules and Nano-objects*, the International Max Planck Research School (IMPRS) *Mathematics in the Sci-*

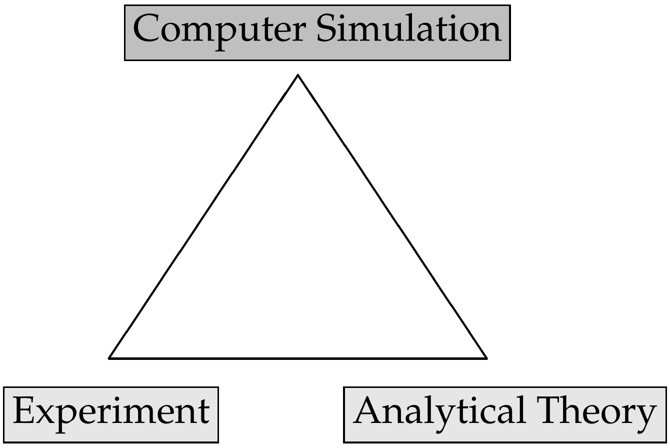


Figure 10.1: Sketch of the "triangular" relationship between experiment, analytical theory and computer simulation.

ences, 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 current third funding period 2014–2016, also the National Academy of Sciences of Ukraine in Lviv has joined as another associated partner institution, offering our PhD students now several interesting options for secondments. For instance, in 2014, one PhD student started a "co-tutelle de thèse" jointly supervised with a colleague from Coventry University. 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.

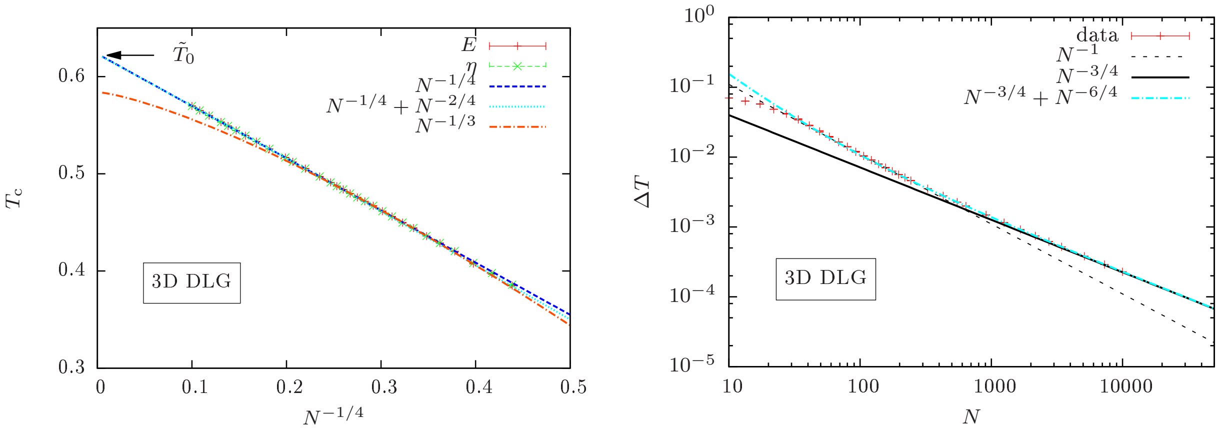
At a more post-graduate level our research projects are embedded into the "Sächsische DFG-Forschergruppe" FOR877 *From Local Constraints to Macroscopic Transport* jointly with the universities in Chemnitz and Dresden, and the Sonderforschungsbereich/Transregio SFB/TRR 102 *Polymers under Multiple Constraints: Restricted and Controlled Molecular Order and Mobility* together with Halle University. Our group also actively contributes to two of the top level research areas ("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 are carried out in a wide net of collaborations which are currently mainly funded by the Alexander von Humboldt Foundation through an Institute Partnership with the National Academy of Sciences in Lviv, Ukraine, on *Polymers in Porous Environments and on Disordered Substrates* and the EU IRSES Network DIONICOS: *Dynamics of and in Complex Systems*, a consortium of 6 European and 12 non-European partners, including sites in England, France and Germany as well as in Armenia, Russia, Ukraine, India, the United States and Venezuela, which commenced work in 2014. Further close contacts and collaborations are established with research groups in Armenia, Austria, China, France, Great Britain, India, 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

10.2 Finite-size scaling of droplet condensation

J. Zierenberg, W. Janke



(a) (b)

Figure 10.2: Finite-size scaling of (a) the transition temperature and (b) the transition rounding of a three-dimensional lattice gas at fixed density $\rho = 10^{-2}$.

We investigated the finite-size scaling behaviour of the droplet condensation-evaporation transition for the two- and three-dimensional Ising lattice gas as well as the three-dimensional Lennard-Jones gas [1]. The lattice models allow to exploit the equivalence to the Ising model, comparing to exact results in two dimensions and low-temperature series expansions in three dimensions. The Lennard-Jones model ensured the generality of our results. Opposed to the consideration at fixed temperature [2], for which leading-order predictions exist [3], we consider an orthogonal setup at fixed density. Applying Taylor expansions around the infinite-system limit, we obtain the same leading-order scaling behaviour for the finite-size transition temperature $T_c(N)$ and rounding ΔT of a D-dimensional system with N particles:

$$T_c(N) - T_0 \propto N^{-1/(D+1)}\,, \tag{10.1}$$

$$\Delta T \propto N^{-d/(D+1)}\,. \tag{10.2}$$

This is not the standard $1/V$ finite-size scaling of a first-order phase transition, because droplet evaporation-condensation describes a transition between a homogenous gas phase and an inhomogeneous or mixed phase where a single droplet is in equilibrium with surrounding vapor. A comparison with our numerical results from parallel multicanonical simulations [4] is shown in Fig. 10.2 for the case of the three-dimensional lattice gas.

For intermediate system sizes, we observe a non-expected scaling regime where the system behaves as for homogeneous phase transitions, i.e., $T_c(N) - T_0 \propto N^{-1/d}$ and $\varDelta T \propto N^{-1}$. For the three-dimensional lattice gas we can compare to low-temperature series expansion estimates of the transition temperature $\tilde{T}_0(\rho)$ and the agreement is very good. With our approach, we were able to reach up to $N = 10\,000$ lattice particles and the finite-size scaling analysis suggests that we are in fact quite close to the asymptotic scaling regime.

[1] J. Zierenberg, W. Janke: Phys. Rev. E **92**, 012134 (2015)
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[3] M. Biskup et al.: Europhys. Lett. **60**, 21 (2002); Commun. Math. Phys. **242**, 137 (2003)
[4] J. Zierenberg et al.: Comput. Phys. Comm. **184**, 1155 (2013)

10.3 Aggregation of θ-polymers in spherical confinement

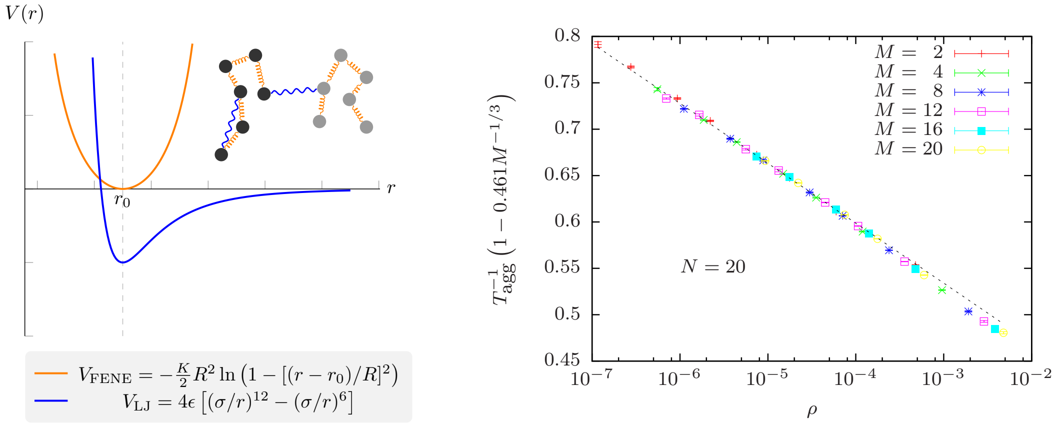
J. Zierenberg, M. Müller, P. Schierz, M. Marenz, W. Janke

This project aims for a better understanding of the influence of external confinement onto the physical properties of a small number of polymers [1]. We therefore investigated the change of the aggregation temperature for few polymers enclosed in a sphere. This enables a systematic variation of the available space by only one parameter, the radius of the sphere. The enclosing sphere is steric, leading at most to an effective repulsion, without introducing technical difficulties with self-interactions imposed by periodic boundaries.

We are thus able to explore the influence of the density onto the aggregation transition temperature of this system of θ-polymers (which means they are parametrized by a model that allows a single polymer to undergo a collapse transition), whose parametrization is summarized in Fig 10.3(a). This allows us to reweight our data to a whole range of different temperatures of the surrounding heat bath, hence the notion of *multi*-canonical simulations. We conducted such simulations in a highly parallelized way [2, 3] for several different radii of the sphere and with that we vary the volume accessible to the system. In the canonical picture we find that the aggregation temperature shifts in dependence of the radii.

To gain a quantitative understanding of this shift, we note that the spatial entropy available to the *aggregate* is in a first approximation independent from the radius of the surrounding sphere. In the separated regime the polymers can be treated similar to an ideal gas. Here, we can thus relate the entropy to the volume of the system, and with that to the radius of the sphere and the system's density. With the Gibbs construction we relate then the entropy difference of the two regimes to the microcanonical temperature T_{agg}, allowing the derivation of an explicit relation of the inverse transition temperature to the logarithm of the density,

$$1/T_{\text{agg}}(\rho) = \frac{S(E_{\text{sep}},\rho) - S(E_{\text{agg}},\rho)}{\varDelta E} \sim \frac{S(E_{\text{sep}},\rho)}{\varDelta E} = \frac{S(E_{\text{sep}},\rho)}{M\varDelta e} \sim -\ln\rho + \text{const}\,, \quad (10.3)$$



(a) (b)

Figure 10.3: (a) The different interaction potentials that characterize a small number M of θ-polymers, which are enclosed in a sphere whose radius is varied, watching closely the aggregation transition temperature. (b) Combining entropic and energetic arguments, and respecting the typical length scale of the aggregate, we find an empirical data collapse of the inverse transitions temperatures over a broad range of densities.

with $\Delta E = E_{\mathrm{sep}} - E_{\mathrm{agg}} = M\Delta e$ under the assumption that, for fixed M and N, the latent heat Δe is almost constant.

For *flexible* polymers, the aggregate of M polymers with N monomers can be approximated by a single polymer with length $M \times N$, and this defines a "typical" length scale $R \sim (NM)^{-1/3}$ of the polymer aggregate, which may be exploited to derive an empirical scaling law for the inverse temperature in Eq. (10.3) in dependence of the *number of polymers*. With this we gain some insight into the nature of the finite-size effects in such a system enabling the empirical data collapse for a broad range of densities for different numbers of polymers shown in Fig. 10.3(b).

For *stiffer* polymers this typical length scale is not as easy to determine. Here, we found interesting structural properties that are already visible in a very intuitive order parameter [4], the so-called phase-separation parameter. This is essentially the average center-of-mass distance of the different polymers, and for the aggregate, it becomes smaller the stiffer the polymers are. This is at first sight counter-intuitive, but can be traced back to the formation of polymer bundles [5] which allow the polymers' center-of-masses to get closer as the polymers align.

[1] J. Zierenberg et al.: J. Chem. Phys. **141**, 114908 (2014)
[2] J. Zierenberg et al.: Comput. Phys. Comm. **184**, 1155 (2013)
[3] J. Zierenberg et al.: in *Computer Simulation Studies in Condensed-Matter Physics XXVI*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, Physics Procedia **53**, 55 (2014)
[4] M. Mueller et al.: in *Computer Simulation Studies in Condensed-Matter Physics XXVIII*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, Physics Procedia **68**, 95 (2015)
[5] J. Zierenberg, W. Janke: Europhys. Lett. **109**, 28002 (2015)

10.4 Aggregation of semiflexible polymers

J. Zierenberg, W. Janke

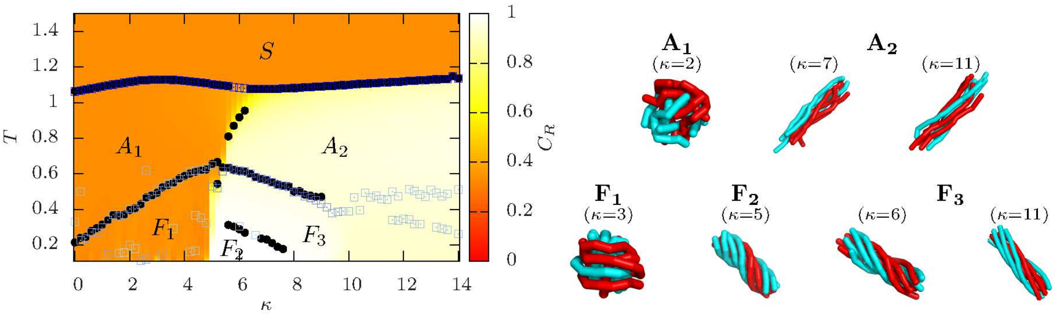


Figure 10.4: Full temperature-stiffness structural phase diagram of 8 polymers with 13 monomers each, combining the surface plot of a correlation parameter (1 = correlated; 1/3 = uncorrelated) with the peak locations of the heat capacity (black) and the thermal derivative of the phase separation parameter (blue). Representative conformations are presented next to the phase diagram. Figure taken from Ref. [2].

The effect of solvent salt concentration was shown to influence the dynamics and emerging structures in amyloid fibrils ranging from rapid formation of amorphous structures at high salt concentration to long-time relaxation of amyloid fibrils at low salt concentration [1]. It may be argued that the salt concentration influences the effective stiffness of a coarse-grained description of biopolymers. Therefore, we investigated the role of stiffness on the structural motifs of polymer aggregation, leading from amorphous aggregates for rather flexible polymers to polymer bundles for stiffer polymers [2]. Employing parallel multicanonical simulations [3], we were able to map out generic T-κ structural phase diagrams describing an entire class of coarse-grained semiflexible polymers. In Fig. 10.4 we present such a diagram for 8 polymers of length $N = 13$, including both amorphous aggregates and polymer bundles well described by an end-to-end correlation parameter $C_R \approx 1/3$ and $C_R \approx 1$, respectively. Low-temperature conformations even include twisted bundles known also from biopolymer networks.

The numerical data was generated on the supercomputer JUROPA at Jülich Supercomputing Centre (JSC).

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10.5 Polymer knots as topological order parameter

M. Marenz, W. Janke

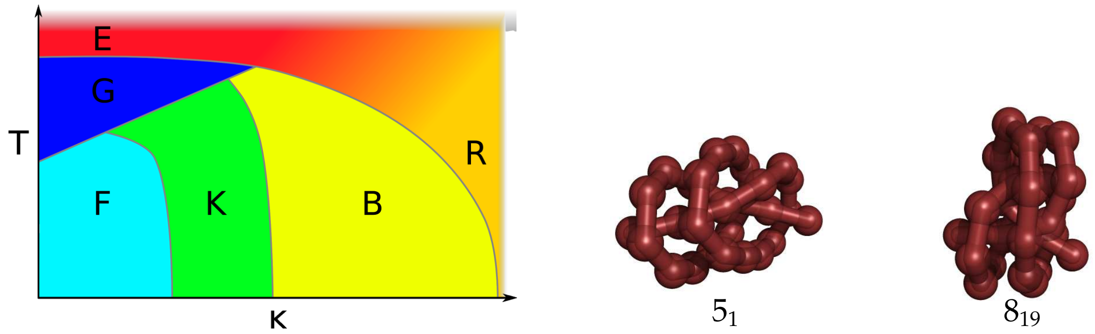

Figure 10.5: Sketch of the phase diagram for a semiflexible bead-stick model exhibiting several phases: E – elongated, R – rod-like, G – globular, F – frozen, K – knotted, B – bent. Next to the phase diagram two typical knots of types 5_1 and 8_{19} for a 28mer are shown.

To investigate the generic behaviour of polymers and proteins with computer simulations, it is common to use minimalistic, coarse-grained models since this is the only possibility to investigate large time scales, length scales or parameter ranges. In this study we used a bead-stick model for a semiflexible polymer defined by the Hamiltonian

$$H = E_{\mathrm{LJ}} + \kappa E_{\mathrm{Bend}} = 4 \sum_{i=1}^{N-2} \sum_{j=i+2}^{N} \left(\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}} \right) + \kappa \sum_{i} (1 - \cos\theta_i) \ , \tag{10.4}$$

where r_{ij} is the distance between non-adjacent monomers, and θ_i is the angle of two adjacent bonds. The parameter κ allows to vary the bending stiffness of the polymer from flexible over semiflexible to stiff.

To simulate the system in the complete (T, κ)-plane we used two advanced Monte Carlo algorithms. A parallel multicanonical algorithm [1] combined with a one-dimensional replica exchange in the κ direction and a two-dimensional replica-exchange method, which simulates the system in parallel in the T and κ direction. Employing both algorithms, we calculated surface plots of various observables (energy, end-to-end distance, radius of gyration, eigenvalues of gyration tensor) to construct the full pseudo-phase diagram for several polymer lengths ($N = 14, 28, 42$) [2, 3].

Despite the simplicity of the model, the phase diagram sketched in Fig. 10.5 is remarkably rich. Compared to former work simulating similar coarse-grained models [4], we observed a novel type of phases labeled by "K", which are characterized by thermodynamically stable knots [5], which may be considered as topological order parameters. The transitions into these knot phases exhibit some intriguing characteristics. Although we observed clear signals of a first-order transition between the knotted and unknotted phases, the transition apparently shows no latent heat [2, 3]. Instead the two sub-energies, the Lennard-Jones energy and the bending energy, are transformed into each other while the polymer knots itself, see Fig. 10.6.

[1] J. Zierenberg et al.: Comput. Phys. Comm. **184**, 1155 (2013)
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[3] M. Marenz, W. Janke: *Stable knots in the phase diagram of semiflexible polymers: A topological order parameter?*, to appear in *Computer Simulation Studies in*

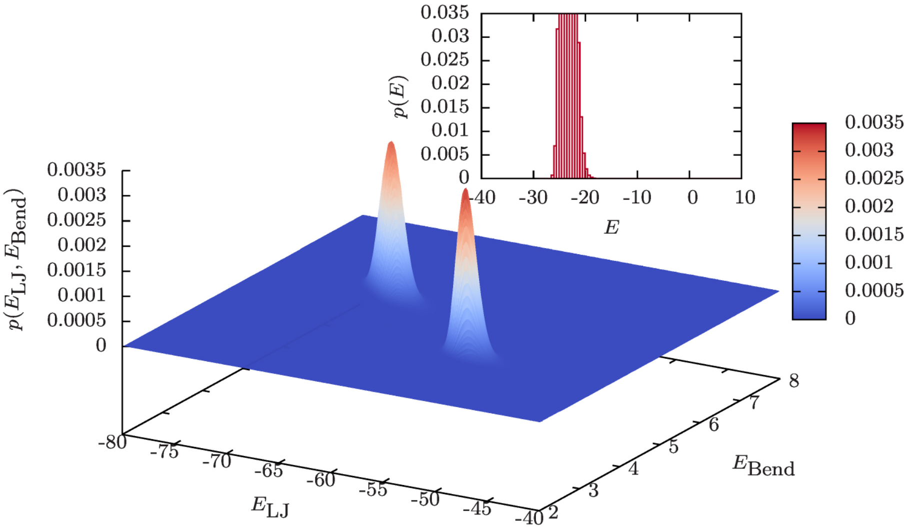

Figure 10.6: Two-dimensional energy histogram $p(E_{\mathrm{LJ}}, E_{\mathrm{Bend}})$ of a 28mer at the transition into the knot phase signaling clear phase coexistence. The inset shows the one-dimensional energy histogram $p(E)$ of the total energy $E = E_{\mathrm{LJ}} + \kappa E_{\mathrm{Bend}}$, which corresponds to a projection along the diagonal of the two-dimensional histogram. In this projection, the two peaks fall on top of each other, so only a single peak is visible in $p(E)$.

Condensed-Matter Physics XXIX, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. (2016), in print
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10.6 Polymer adsorption to a nano-sphere

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The interaction of macromolecules with differently shaped substrates is particularly important for interdisciplinary research and nano-technological applications including, e.g., the fabrication of biosensors and peptide adhesion to metals or semiconductors. The knowledge of structure formation for a variety of interfaces has therefore been a challenging subject of numerous experimental and computational studies.

Recently we have investigated the purely steric confinement effect of a spherical cage enclosing a simple flexible polymer chain to determine its influence on the location of the collapse and freezing transitions [1]. Another hybrid system under consideration was a polymer chain inside an attractive spherical cage for which we have constructed the finite-temperature phase diagram depending on the attraction strength of the sphere inner wall and the temperature [2, 3] and investigated the ground-state properties [4].

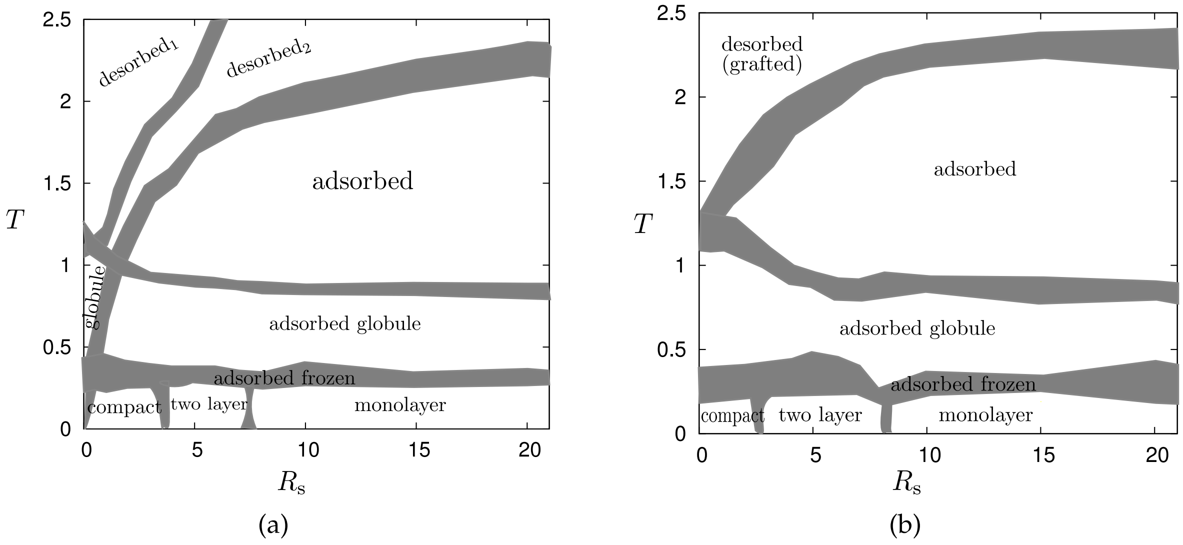

Figure 10.7: The phase diagram of a homopolymer interacting with an attractive spherical surface of radius R_s for (a) a non-grafted and (b) an end-grafted 20mer.

We have also compared the results with the attractive flat surface [5, 6]. These systems exhibit a rich phase behaviour ranging from highly ordered, compact to extended, random coil structures.

Here, we consider the opposite situation: A nano-sphere whose attractive outer spherical surface is the target for the adsorbing polymer. This problem could have practical implications for a broad variety of applications ranging from protein-ligand binding, designing smart sensors to molecular pattern recognition and for the discovery of new drugs that bind to specific receptors. Therefore it is interesting to study the adsorption of macromolecules on different types of substrates and identify the conformational changes that a polymer can experience at the interface.

In this project we investigate a simple coarse-grained polymer model interacting with a spherical surface of varying radius (and consequently curvature) by means of extensive generalized-ensemble Monte Carlo computer simulations [7]. The employed multicanonical method enables us to describe the different phases of the finite chain over a wide range of sphere radius and temperature. In a comparative study, we determined how the structural phase diagram changes with the sphere radius and temperature, both for non-grafted and end-grafted polymer chains. The band widths of the boundaries separating the individual conformational phases in Fig. 10.7 indicate the variation of the peak locations of temperature derivatives of different structural observables which we have analyzed simultaneously [7]. Typical conformation for the case of a non-grafted polymer are shown in Fig. 10.8.

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[5] M. Möddel et al.: J. Phys. Chem. B **113**, 3314 (2009); Phys. Chem. Chem. Phys. **12**, 11548 (2010); Macromolecules **44**, 9013 (2011)

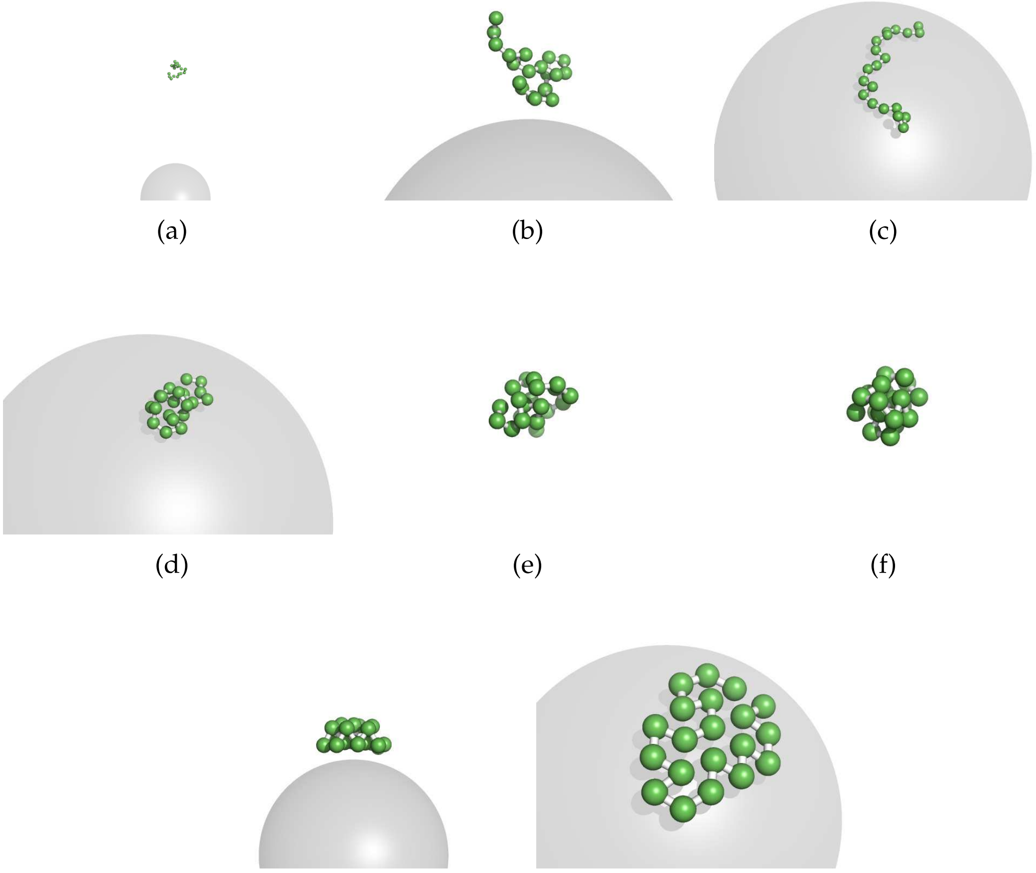
(a) (b) (c) (d) (e) (f) (g) (h)

Figure 10.8: Typical conformations for the regions (a) desorbed$_1$, (b) desorbed$_2$, (c) adsorbed, (d) adsorbed globule, (e) globule, (f) compact, (g) two layer, and (h) monolayer in the phase diagram of a non-grafted polymer.

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10.7 Comparative simulations of poly(3-hexylthiophene) models

J. Gross, M. Ivanov, W. Janke

Regioregular Poly(3-hexylthiophene) (P3HT) is a very interesting conjugated polymer due to its electronic and optical properties [1]. One of its applications is the use as semiconducting layer in organic photovoltaics [2–4]. Studies of P3HT on the microscopic level are of great importance for a fundamental understanding of the tuneability of electronic properties and their dependence on external constraints, e.g. the adsorption on electrode surfaces. Hence a number of experimental studies addressed for example

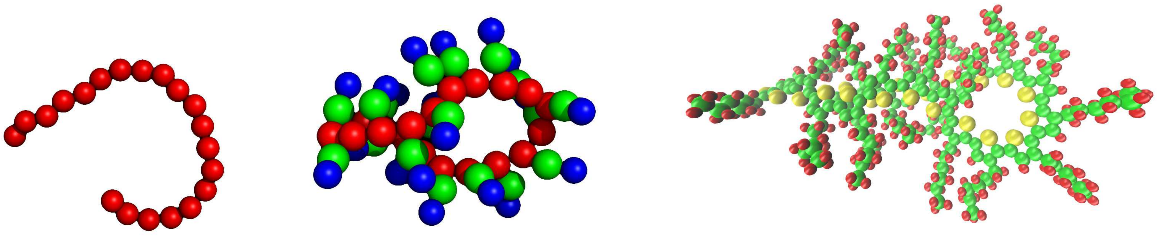

Figure 10.9: Hairpin conformations of Poly(3-hexylthiophene) for a degree of polymerization $DP_n = 20$ in three different models. (Left) One-particle coarse-grained model (one bead per monomer), (middle) three-particle coarse-grained model, and fully atomistic model (right).

the influence of structure formation by polymer self-assembly on ideal surfaces on the electronic properties of oligo- and polythiophenes [5]. Due to the complexity of these macromolecules many of the experimental findings have not been supported with simulations so far, which in contrast is well-established for studies of small organic molecules. Our pervious study [6] reported on an collaborative effort within the DFG SFB/TRR 102 project to combine the experimental observation of polymer chain conformations adsorbed on a metal surface with Monte Carlo simulations of a coarse-grained P3HT model developed by Huang *et al.* [7]. Based on our previous work on a three beads per monomer coarse-grained model, we expanded our studies in two directions. We focused our interest on the polymer itself and, firstly, investigated an even coarser model with one bead per monomer [8] using Monte Carlo simulations. Secondly, we simulated a fully atomistic representation of P3HT using molecular dynamics. We pursue these two routes to gauge the level of detail that is necessary to reproduce experimental findings more accurately. Another interest is the development of our own simplified model by systematically performing the coarse-grain procedure ourselves. For this we looked at the iterative Boltzmann inversion method [9]. The comparative analysis of all three models regarding structural observables, but also computational effort are discussed in Ref. [10].

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10.8 Kinetics of cluster formation and growth during collpase of a polymer

S. Majumder, W. Janke

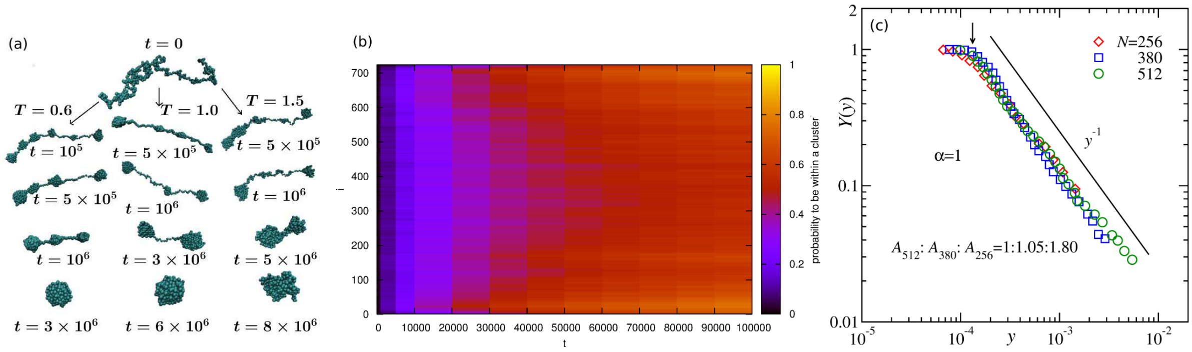

Figure 10.10: (a) Time evolution showing the sequence of events occurring during the collapse of a polymer upon being quenched from an expanded state (at high temperature) into the globular phase (at low temperatures). (b) Probability of formation of clusters at a site *i* along the polymer chain during the nucleation stage of the collapse. (c) Finite-size scaling plots showing the collapse of data for different chain lengths confirming the linear growth of the average cluster size [1].

A polymer undergoes a collapse transition when it is quenched from a high-temperature expanded coil state (or in good solvent) to a low-temperature compact globule (in poor solvent). Understanding the kinetics of the collapse of a polymer is an important physical problem considering its potential connections to many biological phenomena such as protein folding. A polymer collapses via nucleation, growth and subsequent coarsening or coalescence of clusters of monomers to form a single compact globule [2], as shown in Fig. 10.10(a). During the coarsening stage the average cluster size (average number of monomers within a cluster), $C_s(t)$, is expected to follow a power law. In spite of the fact that the relaxation dynamics during the collapse has been studied in previous works [2], there exist no simulation studies which quantify the growth exponent unambiguously.

In this work we have addressed this issue by state-of-the-art Monte Carlo simulations of a model polymer with the aim to understand the kinetics of cluster formation and growth exponent related to the coarsening stage of the collapse. In Fig. 10.10(b) we show the probability of nucleation of clusters at a site *i* during the first stage of the collpase [3]. By drawing analogy with standard coarsening systems we analyze our results via the application of finite-size scaling technique in the nonequilibrium context [4]. Figure 10.10(c) shows such a scaling plot where in contradiction to previous theoretical and simulation results [5], the decay of the master curve shows a linear growth of the average cluster size, as known from the Lifshitz-Slyozov mechanism of cluster growth.

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10.9 Aging and related scaling during collapse of a polymer

S. Majumder, W. Janke

Aging, a phenomenon characterized by faster relaxation of younger systems than older ones is quite popular for systems with slow dynamics, e.g., glasses (both spin glass and structural glass), and especially for ordering kinetics or coarsening the theoretical understanding is richly developed [1, 2]. On the other hand, in spite of phenomenological similarities with standard coarsening systems there have been only few efforts to explore this aging during the collapse of a polymer chain when it is quenched from its extended state in a good solvent (above the collapse transition temperature) to the globular phase in a poor solvent (below the collapse transition temperature). This motivates us to look into aging during the collapse of a polymer seeking the presence of any dynamical scaling.

Aging is probed by multiple time quantities, e.g., the two-time autocorrelation of a microscopic variable (O_i) as

$$C(t, t_w) = \langle O_i(t) O_i(t_w) \rangle - \langle O_i(t) \rangle \langle O_i(t_w) \rangle, \tag{10.5}$$

where t and t_w ($\ll t$) are the observation and waiting times, respectively. Slower decay of $C(t, t_w)$ with an increase of t_w is the signature of aging phenomena. For a nonequilibrium process, $O_i(t)$ is generally a quantity reflecting the time evolution of the system and here we judicially choose this parameter to be ± 1 depending on whether the monomer is inside ($+1$) or outside (-1) a cluster formed during the collapse, thus constructing an analogue to the ususal density-density autocorrelation used in glassy systems or the order-parameter autocorrelation used in coarsening kinetics. In Fig. 10.11(a) we show plots of such autocorrelations which decay slower as the age of the system increases, the signature of aging. In the inset we show the scaling of the autocorrelation as a function of t/t_w [3]. Our data not only shows scaling with respect to t/t_w but also with respect to the ratio of cluster size $C_s(t)/C_s(t_w)$ as

$$C(t, t_w) \sim [C_s(t)/C_s(t_w)]^{-\lambda_c} \tag{10.6}$$

For the exponent λ_c governing the decay, we provide a simple scaling argument to predict a bound (10.7)

$$(\nu d - 1) \leq \lambda_c \leq 2(\nu d - 1) \tag{10.7}$$

in relation to the universal Flory exponent ν. Numerical estimate of λ_c via finite-size scaling analysis gives $\lambda_c = 1.25(5)$ which obeys the predicted bound. In Fig. **??** we show scaling plots of the autocorrelation as a function of $C_s(t)/C_s(t_w)$ for different temperatures

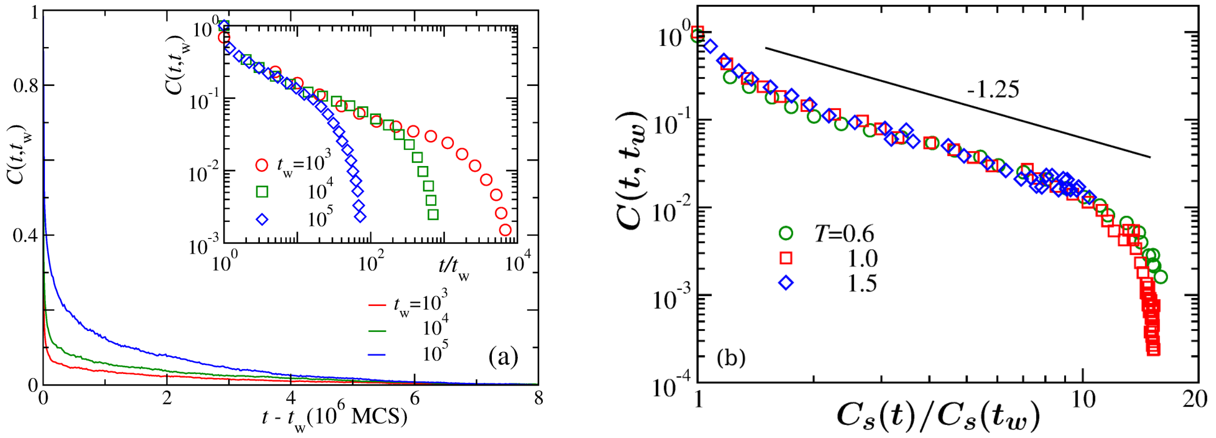

Figure 10.11: (a) Plot of the autocorrelation function $C(t, t_w)$ of a polymer with $N = 724$ for three different values of t_w at $T = 1$. The inset shows the scaling with respect to t/t_w. (b) Scaling plot of $C(t, t_w)$ as a function of $C_s(t)/C_s(t_w)$ for collapse at three different temperatures as indicated in the legend.

[4]. The consistency of our data with the power-law decay having an exponent −1.25 obeying the bound (10.7) confirms that the observed dynamical scaling is independent of temperature.

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10.10 Periodically driven DNA: A comparative study of Langevin and Brownian dynamics

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DNA replication is one of the most important biological processes in living organisms. Under the influence of special enzymes, two strands of the DNA double helix can separate themselves like a zip. The first step in the process of DNA replication is to unzip the double-helix structure of the DNA molecule. Therefore, it is very important to study the unzipping of DNA. There has been some experimental studies at a constant force or loading rate used in SMFS experiments to unzip the DNA *in vitro*. In these experiments one end of the DNA was fixed and a constant force was applied on its other end. However, such processes are driven by different types of molecular motors

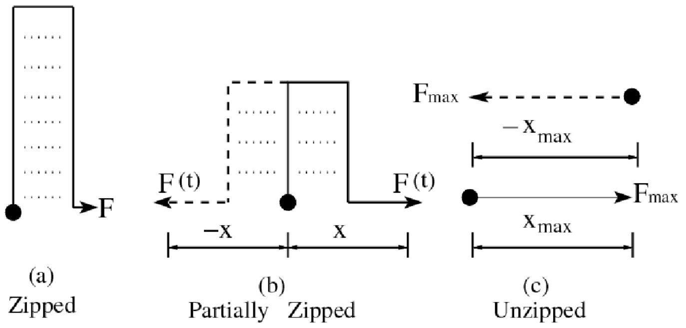
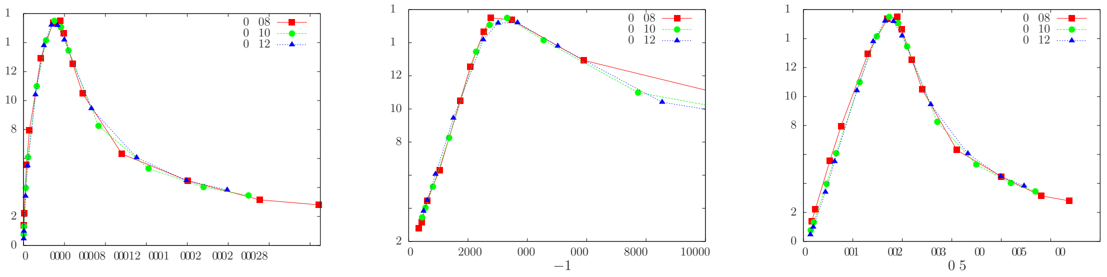


Figure 10.12: Schematic representations of DNA: (a) zipped, (b) partially zipped, and (c) unzipped state. One end is kept fixed (indicated by a solid circle), while the other end may move.



(a) (b) (c)

Figure 10.13: Effect of temperature on the area of the hysteresis loop for the model with parameters $L = 32$, $F = 1.0$, and $\gamma = 0.4$ for (a) A_{loop} vs. ν, (b) area vs. ν^{-1} in the higher frequency regime, and (c) area vs. $\nu^{0.5}$ in the lower frequency regime. Here the x-axis is rescaled in order to show the data collapse for all temperatures.

in vivo [1]. Hence, the picture provided by constant force unzipping is not complete. In some recent theoretical studies it was suggested [2–5] that the application of a periodic force shows a force-driven transition in contrast to the case of a steady force.

This model was further simplified in [6, 7] by reducing the degrees of freedom and studying the overdamped limit using Brownian dynamics. This simplified model was investigated only at zero temperature. Therefore, it became crucial to further investigate how the temperature effects the dynamics of such system using the detailed model described in [2]. Emphasis was placed on the effect of different temperatures on the scaling properties. Moreover, we compared results of the Langevin dynamics for the detailed model and Brownian dynamics for the simplified model. We observed that the temperature and over-damped limit does not effect the scaling exponents. Hence, the model proposed by us is good enough to study the scaling properties and provides a possibility of analytic studies within certain limits.

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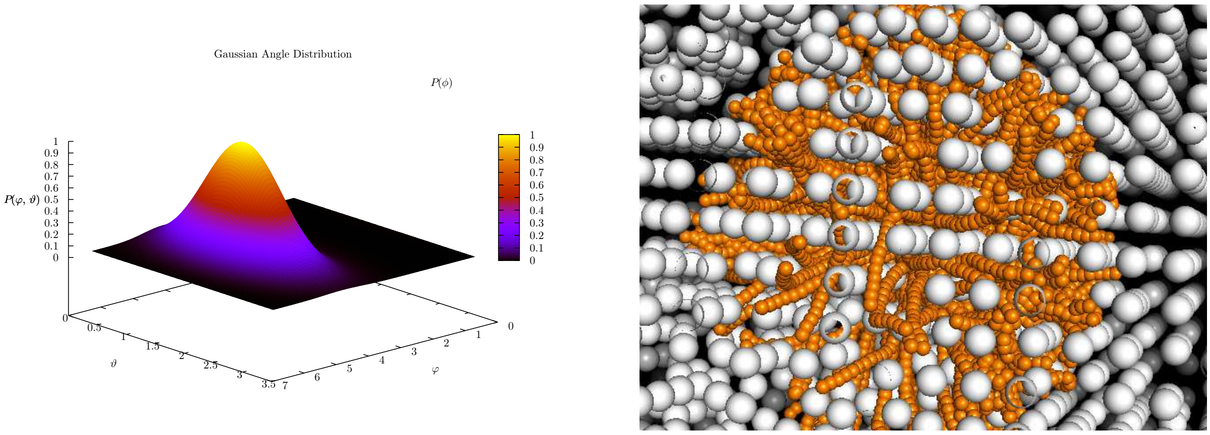
10.11 Computer simulations of semiflexible polymers

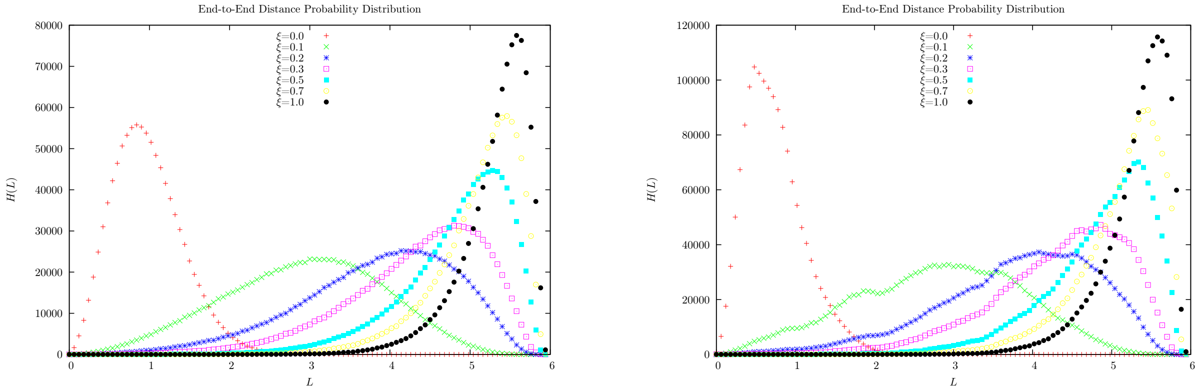
J. Bock, W. Janke



(a) Weighting histogram (b) Semiflexible polymer in 3D disorder

Figure 10.14: (a) Histogram used for the guiding field in 3D and (b) an examplary configuration of a polymer with $N = 30$ and $\xi = 1$.

Single-molecule experiments have established the wormlike chain (WLC) as a standard model for semiflexible polymers [1]. Exploiting the analogy of the WLC with a one-dimensional Heisenberg ferromagnet, it can be shown that the equilibrium tangent-tangent correlation function decays exponentially. The decay rate defines the thermal persistence length l_p. When the same polymer is embedded in a quenched, disordered environment in three dimensions, this property may change quantitatively or even qualitatively. We addressed this problem by performing extensive numerical simulations of semiflexible polymers in a simple lattice disorder and in a gaseous disorder constructed by microcanonical Lennard-Jones gas simulation which represents the disordered environment. Further plans are to simulate the polymers in algebraically correlated disorder. Only the space between the spheres is accessible to the polymer. The extreme strength and density of the environmental constraints are a great challenge to conventional Monte Carlo simulation schemes, which we found hard to overcome even with a sophisticated multicanonical histogram reweighting procedure [2]. We have therefore adopted a breadth-first chain-growth algorithm [3] that resolves this difficulty by circumventing energy barriers instead of trying to cross them [2, 4], see examples in Fig. 10.14. Therefore the already existing procedures were expanded to the third dimension to investigate the behaviour of the tangent-tangent correlation length, the mean square end-to-end distance and the end-to-end probability distribution function, see Fig. 10.15. A difference in behaviour is clear and the task now is to check wether the differences scale similarly as in two dimensions, where the disorder renormalization is



(a) Free polymers (b) Polymers in disorder

Figure 10.15: End-to-end distance distributions for (a) free polymers and (b) polymers in gaseous disorder, both in 3D.

stated to be [5]:

$$\frac{1}{l_p^*} = \frac{1}{l_p} + \frac{1}{l_p^D},$$

with l_p^* the renormalized persistence length, l_p the persistence length given as simulation parameter and l_p^D the measured disorder persistence length.

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10.12 Low-temperature behaviour of polymers in fractal disorder

N. Fricke, W. Janke

The asymptotic scaling behaviour of flexible polymers with short-range interactions is well described by the model of discrete self-avoiding walks with nearest-neighbor attractions, see [1]. For these so-called self-attracting self-avoiding walks (SASAWs), the canonical average of an observable such as the squared end-to-end distance, $\langle R^2 \rangle$, is given by

$$\langle R^2 \rangle_T = \frac{\sum_\omega R_\omega^2 e^{-m_\omega \epsilon/(k_B T)}}{\sum_\omega e^{-m_\omega \epsilon/(k_B T)}}, \tag{10.8}$$

where the sums go over all possible chain conformations ω, m_ω is the number of neighboring monomer pairs, ϵ gives the strength of attraction (set to $\epsilon = k_B$ for convenience),

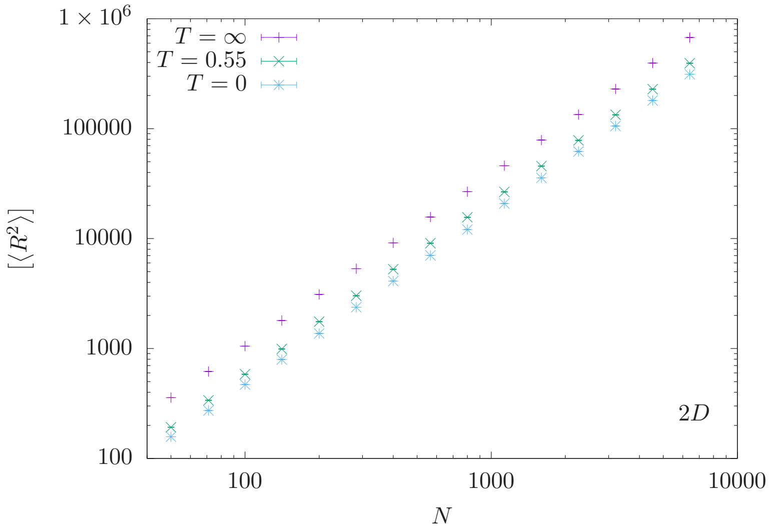

Figure 10.16: Quenched averages of the mean-squared end-to-and distances vs. number of steps for self-attracting self-avoiding walks on critical percolation clusters at different temperatures. Each data point was obtained by averaging over all walk conformations on 10^4 randomly generated clusters.

and T denotes the temperature. On regular lattices, this system undergoes a phase transition from an entropy-dominated *coiled* phase to an energy-dominated *globular* phase when the temperature is lowered. This so-called Θ-transition manifests itself through a change of the exponent describing the scaling of the average end-to-end distance with the number of steps, $\langle R^2 \rangle \sim N^{2\nu_T}$: above the transition temperature the value of ν_T is the same as for non-interacting self-avoiding walks, while below it is given by the inverse of the system's dimension.

We investigated SASAWs in the presence of fractal disorder. Specifically, we looked at the quenched averages on critical percolation clusters for square and cubic lattices. This has been considered in several previous studies where evidence for a Θ-transition had been reported [2, 3]. However, these works had relied on numerical methods that only allowed for rather small systems, so that the conclusiveness of the results was limited. We could study the system in much greater detail thanks to a new exact enumeration technique [4, 5], which makes use of the system's fractal geometry and can thus easily handle walks of several thousand steps. This revealed that the asymptotic scaling behaviour of SASAWs on critical percolation clusters is actually independent of the temperature as can be seen in Fig. 10.16 where the quenched averages of $\langle R^2 \rangle$ for SASAWs at different temperatures are plotted against the number of steps N. Indeed, our estimates for the exponents ν_T all agree within the errors of the fits. This unusual absence of a temperature-driven collapse transition might be explained by the fact that –unlike for the undiluted system– energy and entropy do not compete: At both high and low temperatures, the average on a critical percolation cluster is dominated by a few highly interconnected cluster regions, which are entropically favorable while at the same time allowing for most nearest-neighbor contacts.

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10.13 Dynamical greedy algorithm for the Edwards-Anderson model

S. Schnabel, W. Janke

One of the most intuitive and natural approaches to optimization problems is realized by the so-called greedy algorithms. These methods create trajectories in the space of possible solution by always choosing the next step such that the energy is maximally reduced (or a fitness function maximally increased). Naturally, this will usually not find the global optimum, just as starting at a random spot and always walking uphill will usually not lead a wanderer to the summit of Mt. Everest. Therefore, in practice many attempts with randomly created starting points are made and if the problem is not too difficult the global optimum may be found this way.

On the other hand, there is practically no chance of success if the energy landscape is as complicated and possesses as many local minima as in the case of the Edwards-Anderson spin-glass model [1], whose Hamiltonian is given by

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

where the spins can take two values $S_i \in \{-1, 1\}$ and adjacent spins interact via normally distributed random couplings J_{ij}. If such a model on a three-dimensional cubic lattice of 1000 spins is considered, about 10^{30} attempts were necessary in order to find the ground state this way.

However, the greedy algorithm can still be a very helpful tool, since it is a comparatively simple and reliable method to reach states of low energy. We devised a method to efficiently update the greedy algorithm, i.e., to reuse the data created during a minimization from a configuration $\mathbf{S}$ to the configuration $\mathbf{S}_{\mathrm{min}}$ to obtain the result $\mathbf{S}'_{\mathrm{min}}$ of the minimization from a configuration $\mathbf{S}'$ which differs from $\mathbf{S}$ only in the values of one or very few spins. If furthermore, both, the terminal configuration, delivered by the greedy algorithm, and its energy are understood as attributes of the starting configuration, it is possible to use the energy of the minimized configurations $\mathbf{S}_{\mathrm{min},t}$ to steer a path in the space of starting configurations $\mathbf{S}_t$.

A simple application is to apply the greedy algorithm again: It is tested which alteration (e.g which single spin flip) of the starting configuration will reduce the energy of the *minimized* configuration by the largest amount and this locally optimal step is performed. Repeating this simple procedure as long as viable as a “second order greedy algorithm” will lead to much lower energies albeit not the ground state.

Alternatively, the energy of the minimized configuration can be used as argument for the occupation probability for a generalized ensemble [2]:

$$P(\mathbf{S}) = P(\mathbf{S}_{\mathrm{min}}),$$

which can then be sampled using Monte Carlo techniques. All states in the same "valley" in the energy landscape, i.e., all configuration which minimize to the same local energy minimum, now occur with the same probability and the barriers of high energy which greatly hamper standard Monte Carlo simulations simply vanish. In consequence, the configuration space is sampled much more easily and the performance of ground-state search is greatly improved.

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10.14 Spin glasses with variable frustration

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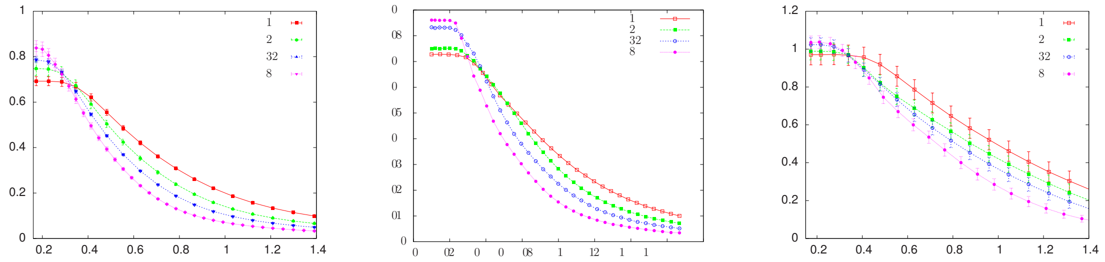

(a) (b) (c)

Figure 10.17: Correlation length as a function of temperature for (a) stochastic frustrated system, (b) a system with 46% frustration, and (c) a system with 20% frustration.

Together with randomness, frustration is believed to be a crucial prerequisite for the occurrence of glassy behaviour in spin systems. The degree of frustration is normally the result of a chosen distribution of exchange couplings in combination with the structure of the lattice under consideration. Here, however, we discuss a process for tuning the frustration content of the Edwards-Anderson model on arbitrary lattices. With the help of extensive parallel-tempering Monte Carlo simulations we study such systems on the square lattice and compare the outcomes to the predictions of a recent study employing the Migdal-Kadanoff real-space renormalization procedure [1]. We use a cluster algorithm proposed in [2] in order to reduce the equilibration time. The phase transition studies are done by looking at the divergence of the correlation length, see Fig. 10.17. The results are benchmarked by comparing to the stochastic case described in [3].

We find that the divergence of the correlation length occurs at non-zero finite temperature for the 2D Ising spin glass. This gives hints of a phase transition, but such transitions have to be studied carefully in order to fully understand the phases [4].

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10.15 Equilibrium properties of the plaquette model

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A family of Hamiltonians, called gonihedric Ising model, originates from high-energy physics as a possible discretization of the area swept out by a string worldsheet moving through spacetime. The name comprises the greek words gonia (angle) and hedra (face) as a reminder of the origin, see [1] for a review.

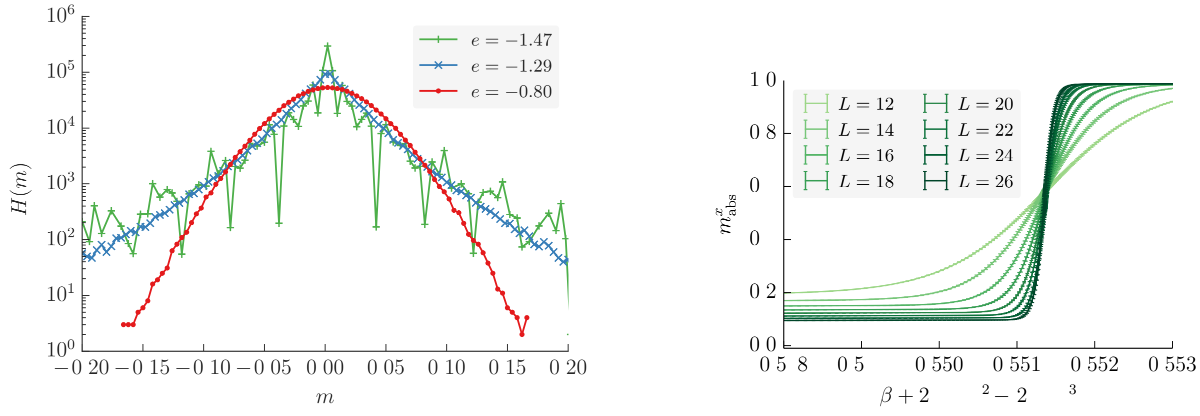
The plaquette model is a special case of this gonihedric Ising model which looks unobtrusive,

$$H = \sum_{[i,j,k,l]} \sigma_i \sigma_j \sigma_k \sigma_l \,, \tag{10.9}$$

but features very interesting properties. The first-order phase transition apparent in the system [2] is a very strong one and thus canonical simulations get easily trapped in one of the phases, potentially spoiling estimators for the transition temperature and latent heat. In addition, we found that the finite-size scaling behaviour for this model is changed due to the exponential degeneracy in the low-temperature phase [3]. Taking that into account, we found an overall consistent inverse transition temperature of the infinite system $\beta = 0.551\,334(8)$ that incorporates estimators from both periodic and fixed boundary simulations as well as an estimator coming from a dual representation of the model [4, 5]. The puzzling effect of obtaining different latent heats for different boundary conditions could be traced back to extraordinary huge boundary effects [6].

To gain a deeper understanding of the properties of the transition, we investigated a recent suggestion in [7, 8] for a candidate order parameter coming from an anisotropic limit of the model. Indeed, we found that this planar order parameter is well suited to distinguish between the different phases [9]. Also, this parameter is subject to the non-standard finite-size effects, as depicted in Fig. 10.18(b). We also showed that the order parameter like behaviour of the susceptibility seen earlier in Metropolis simulations was an artefact of the algorithm failing to explore the phase space of the macroscopic degenerate low-temperature phase. Our multicanonical simulations were able to alleviate this to some extent, but we suggest to incorporate non-local plane-flips into simulations to improve ergodicity properties and measurements of (standard) magnetic properties.

With our multicanonical simulations combined with the nonstandard finite-size scaling, the equilibrium properties of both energetic and magnetic quantities of the 3*D* plaquette gonihedric Ising model are now under good numerical control and the order parameter has been clearly identified. The *non*-equilibrium properties, in particular earlier suggestions that the model might serve as a generic example of glassy behaviour, even in the absence of quenched disorder, still pose open questions.



(a) (b)

Figure 10.18: (a) Conducting 10^6 random plane-flips in three configurations that are fixed in the different phases reveals the symmetry of the magnetic probability density. The ensemble average of the magnetization is equal to zero for both phases. (b) One of the planar order-parameters as a function of inverse temperature, showing a sharp jump at the phase transition point.

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10.16 Boundary conditions and non-local constraints in plaquette models

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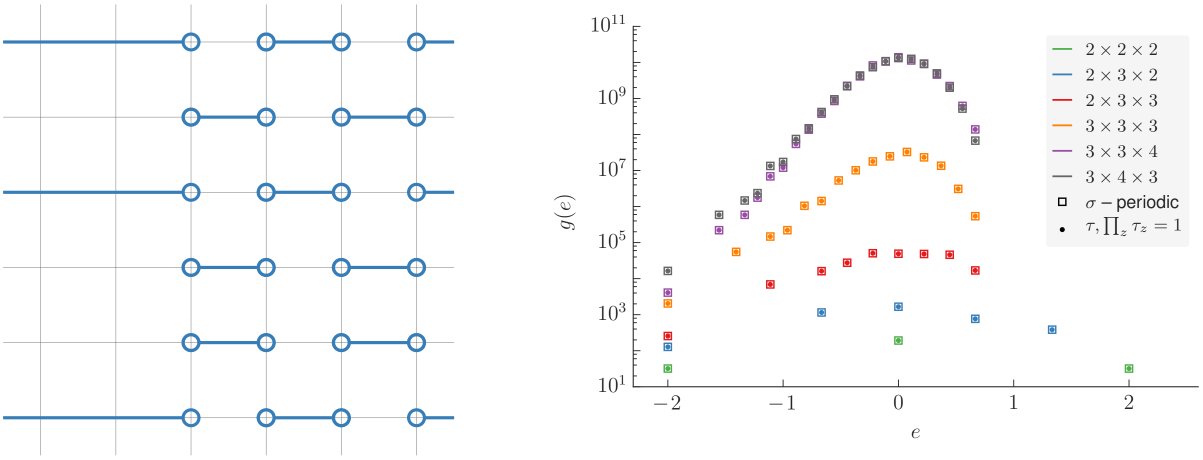
An anisotropic limit of the 3*D* plaquette Ising model, in which the plaquette couplings in one direction were set to zero, was solved for free boundary conditions by Suzuki [1], who later dubbed it the fuki-nuke, or “no-ceiling”, model. Defining new



(a) (b)

Figure 10.19: (a) Graphical dimer-representation of one term that contributes to the partition function in the 2*D* plaquette models. (b) Using exact enumerations to get the number of states $g(E)$ with given energy E, we ensure that no trivial errors enter the calculation of the partition function in the product-spin representation that leads to non-local constraints.

spin variables as the product of nearest-neighbour spins transforms the Hamiltonian into that of a stack of (standard) 2*D* Ising models and reveals the planar nature of the magnetic order, which is also present in the fully isotropic 3*D* plaquette model [2]. More recently, the solution of the fuki-nuke model was discussed for periodic boundary conditions applied to the spin lattice, which require a slightly different approach to defining the product spin transformation, by Castelnovo *et al.* [3].

We find that the essential features of the differences between free and periodic boundary conditions when using a product spin transformation are already present in the 1*D* Ising model [4], which thus provides an illuminating test case for its use in solving plaquette spin models and an alternative method for solving the 1*D* Ising model with periodic boundary conditions.

We clarify the exact relation between partition functions expressed in terms of the original and product spin variables for the 1*D* Ising model, 2*D* plaquette and 3*D* fuki-nuke models with free and periodic boundary conditions. Representing graphically the combinatorial factors that contribute to the partition function, we are able to solve the 2*D* plaquette model with free, periodic and helical boundary conditions and various combination of these in *x*- and *y*-directions, see Fig. 10.19. The various exactly solved examples illustrate how correlations can be induced in finite systems as a consequence of the choice of boundary conditions.

The similarities between the 2*D* plaquette model with periodic boundaries, when expressed in terms of the product spin variables and a "ladder" of interaction-free 1*D* Ising models that are coupled by non-local constraints is subject to further studies and might give even deeper (pedagogical) insight into the interplay between boundary conditions and non-local constraints that directly influence correlations between spins.

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

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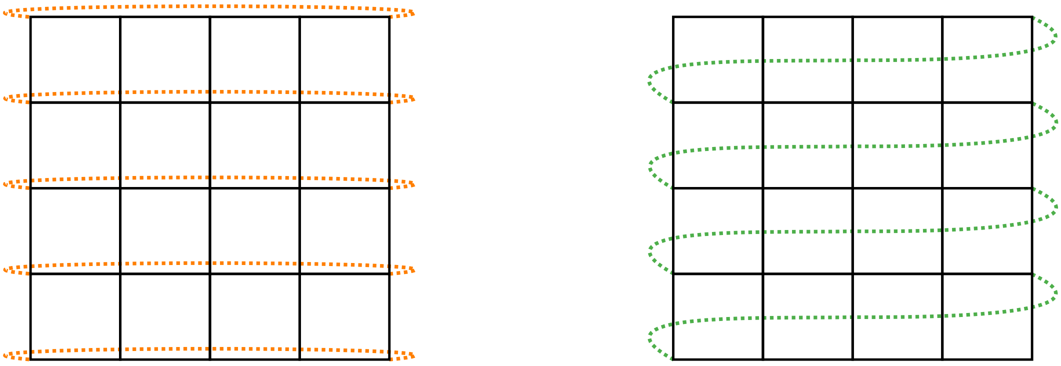

(a) PBC (b) SBC

Figure 10.20: 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.

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

$$\mathcal{H} = J \sum_{i=1}^{N} \left(\sigma_i^x \sigma_{i+e_x}^x + \sigma_i^y \sigma_{i+e_y}^y + \sigma_i^z \sigma_{i+e_z}^z \right), \tag{10.10}$$

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].

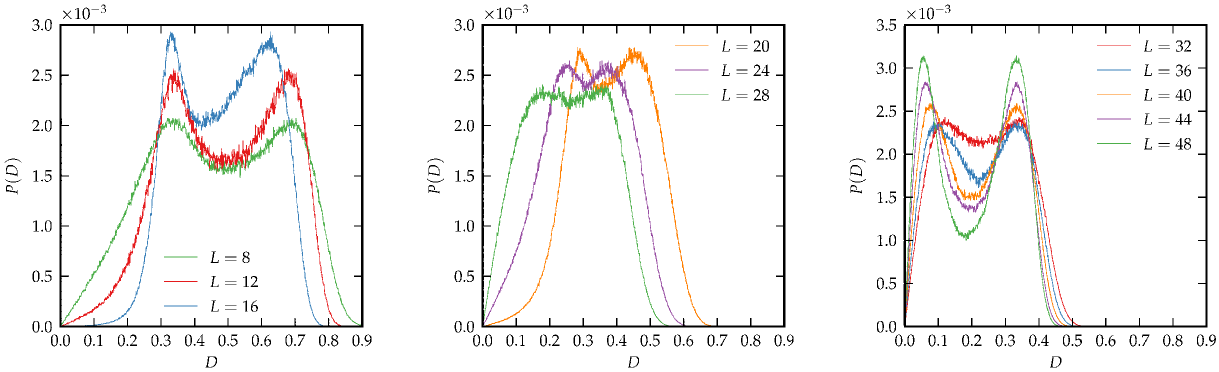

Figure 10.21: Histograms of the directional order parameter D in the three-dimensional compass model with screw-periodic boundary conditions for various lattice sizes L.

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 that employing so-called screw-periodic boundary conditions [8] sketched in Fig. 10.20 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. 10.21 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, $\sigma_{\mathrm{od}} \approx 3 \times 10^{-4}$.

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10.18 Transition barriers in the three-dimensional Blume-Capel model

J. Zierenberg, N.G. Fytas*, W. Janke

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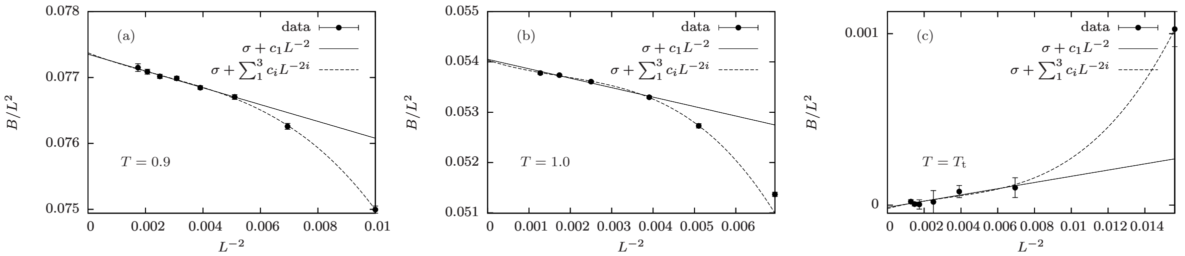

(a) (b) (c)

Figure 10.22: Finite-size scaling of the transition barrier in the 3D Blume-Capel model at fixed temperature under variation of the crystal field for (a) $T = 0.9$, (b) $T = 1.0$, and (c) $T = 1.4182$ (close to the tricritical point).

The Blume-Capel model [1, 2] is a perfect test-model for studies of phase transitions. We consider this spin-one Ising model in a crystal field on a cubic lattice in three dimension (3D), described by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j + \Delta \sum_i \sigma_i^2 = E_J + \Delta E_\Delta \,. \qquad (10.11)$$

Using a multicanonical based approach, we study the first- and second-order phase transitions at fixed temperature along the crystal field axis [3]. This allows us to directly estimate the barrier associated with the suppression of states during a first-order phase transition as

$$B = \frac{1}{2\beta\Delta} \ln \left(\frac{P_{\mathrm{max}}}{P_{\mathrm{min}}} \right)_{\mathrm{eqh}} , \qquad (10.12)$$

where P_{max} and P_{min} are the maximum and the local minimum of the distribution $P(E_\Delta)$, respectively. The resulting barrier connects a spin-0 dominated regime (E_Δ small) and a spin-±1 dominated regime (E_Δ large), which may be associated with condensation and strip formation of spin-0 clusters and thus shows analogies to Ising (lattice gas) droplet/strip transitions [4, 5]. Consequently, we expect a scaling behaviour in three dimensions as $B/L^2 = \sigma + c_1/L^2 + \mathcal{O}\left(1/L^4\right)$, see Fig. 10.22. A higher-order fit yields $\sigma_3 = 0.0774(1)$ and $\sigma_2 = 0.0540(2)$ for $T_3 = 0.9$ and $T_2 = 1.0$, respectively. In the vicinity of the tricritial point [6], at $T_t = 1.4182$, the extrapolation yields $\sigma \approx 0$, indicating as expected that the interface tension vanishes in the thermodynamic limit.

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10.19 Boundary drive induced phase transitions in stochastic transport condensation models

H. Nagel, H. Christiansen, W. Janke

Stochastic mass transport processes such as the asymmetric simple exclusion process (ASEP) or the zero-range process (ZRP) are simple transport models for particle hopping aiming to improve the understanding of basic phenomena in the dynamics of particles in driven diffusive systems. An important class of such phenomena that can be studied and understood on an abstract level is the emergence of generic condensates. In this project we considered such a transport processes under driven particle exchange through open boundaries and systematically studied the emerging phase diagrams. While boundary drive induced phase transitions are known since long for the ASEP, the research for the ZRP with condensation dynamics is more recent [1].

More precisely we investigated transport processes with tunable weights [2] as well as various types of interactions at the boundaries to study these effects on a much broader scale. The tunable model allowed us to effectively interpolate between ZRP-type as well as strong short-range interactions. At the boundaries we considered the existence of fixed versus loose couplings as well as different approaches to particle injection and removal rates. For the generated cases we produced the phase diagrams under differing strengths of the driven particle exchange at the boundaries for symmetric and totally asymmetric dynamics [3–5]. The main phases, as shown in Fig. 10.23, are: a thin particle gas (G), formation of aggregate condensates (A) and the spanning bulk condensate (SC). While the phase diagrams with vanishing as well as stronger short-range interactions are very similar except for the SC phase, we observed a qualitatively different mechanism for aggregate condensate formation with short-range interactions.

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10.20 A simple non-equilibrium model for Stranski-Krastanov growth

J.K. Ochab[*], H. Nagel, W. Janke, B. Wacław[†]

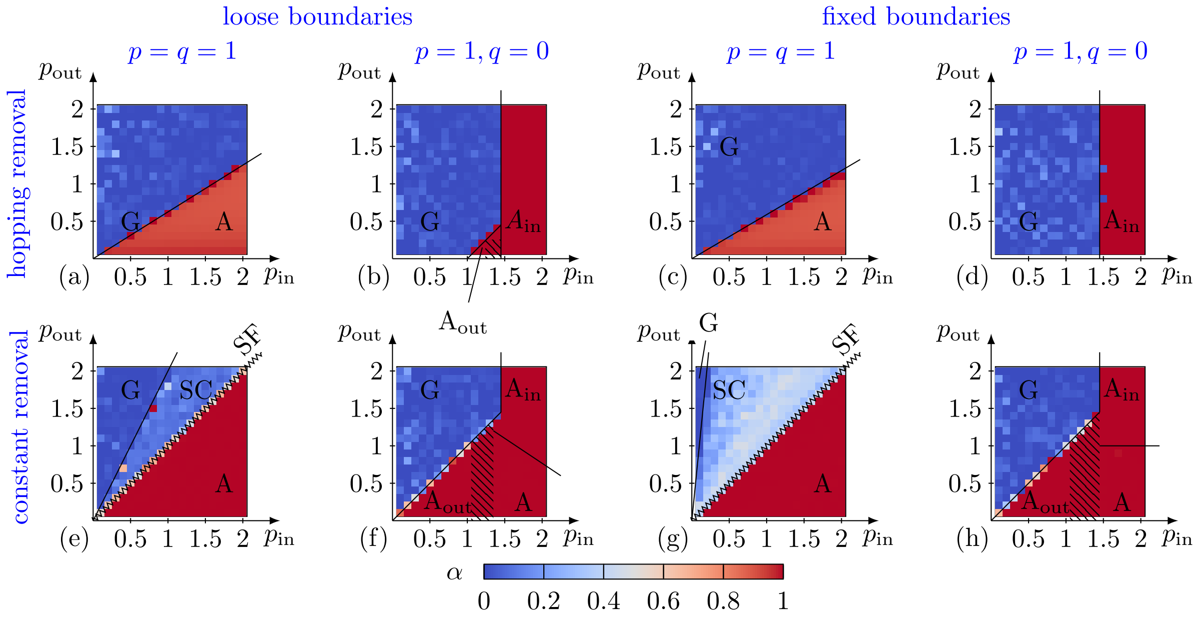

Figure 10.23: Phases induced by driven particle exchange through open boundary conditions of the system [5]. With respect to the specific implementation of the interaction at the boundary, different phase diagrams are observed.

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We consider a simple non-equilibrium model of mass condensation with Lennard-Jones interactions between particles and a substrate. This model is an extension of the zero-range process to nearest-neighbour interactions, similar to that of Refs. [1–3], where particles interact when they are at the same site or at neighbouring sites. Although the model can be driven far from equilibrium, it is closely related to the equilibrium solid-on-solid (SOS) model [4]. A remarkable feature of this stochastic process is that the steady state factorises over pairs of neighbouring sites, also in dimensions higher than one, and thus it is called the pair-factorised steady state (PFSS) process. This property facilitates analytical calculations in the one-dimensional version of the model and, in certain cases, also in more than one dimension [5].

We show that when some number of particles is deposited onto the surface and the system is left to equilibrate, particles condense into an island if the density of particles becomes higher than some critical density [6]. We illustrate this with numerically obtained phase diagrams for (2+1)-dimensional systems. We also solve a (1+1)-dimensional counterpart of this model analytically and show that not only the phase diagram but also the shape of the cross-sections of (2+1)-dimensional condensates qualitatively matches the (1+1)-dimensional predictions [2, 3, 7]. Furthermore, when particles are being deposited with a constant rate, we demonstrate that the system has two phases: a single condensate for low deposition rates, and multiple condensates for fast deposition [6]. The behaviour of our model is thus similar to that of thin film growth processes, and in particular to Stranski-Krastanov growth.

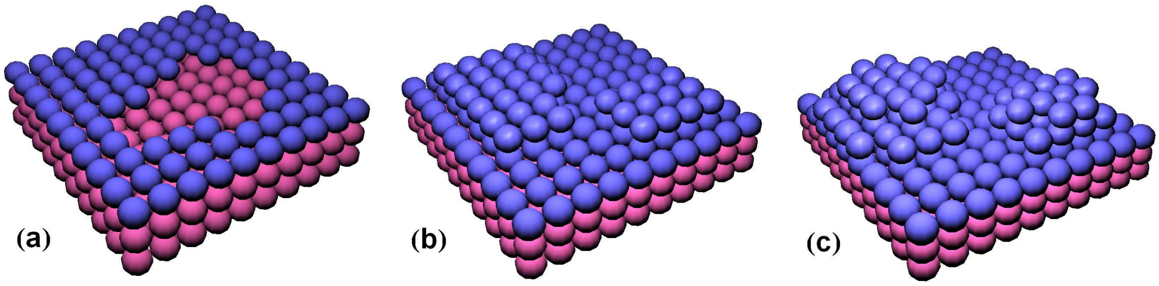

Figure 10.24: Schematic stages of Stranski-Krastanov growth. (a) The substrate (purple spheres) is covered with an increasing number of adatoms (blue spheres), starting from an incomplete monolayer. (b) As the density of adatoms increases, the adatoms form a complete monolayer and a partially filled second layer. (c) Upon further density increase, islands of variable height begin to form on the monolayer. Here the critical density of adatoms above which islands occur equals one adatom per one substrate site.

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10.21 Molecular dynamics simulations of hydrogen diffusion in ZIF-11

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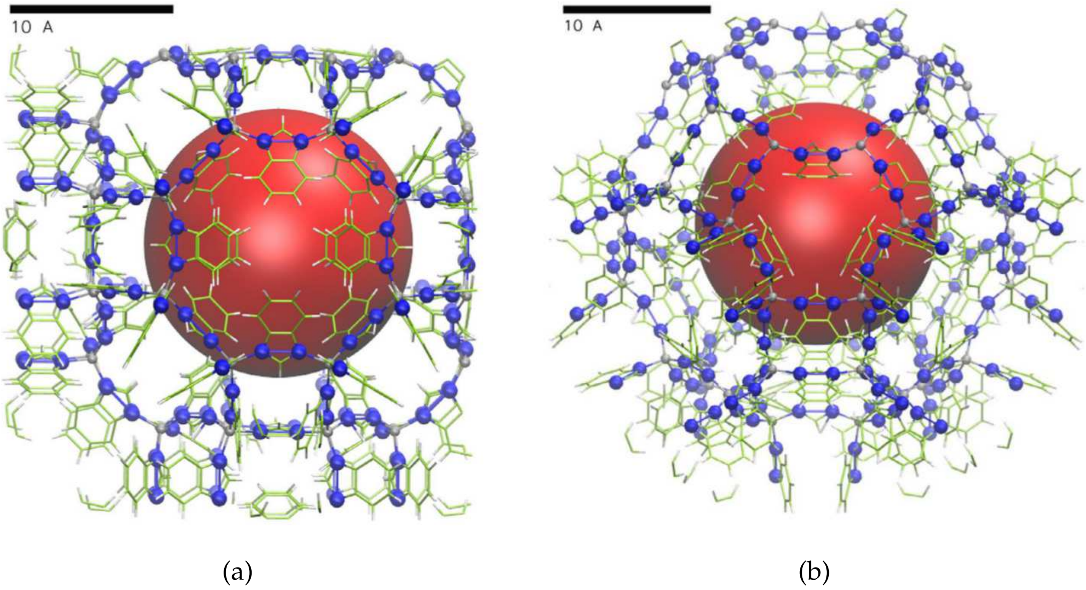
The properties of porous materials have become a topic of great interest for basic research as well as for practical applications. Two of the most common aims are to improve selectivity and storage properties for sorbent applications. In recent years, metal organic frameworks (MOFs) have become porous materials of great interest because of their promising properties and because of the big variety of structures that can be obtained from the combinations of metal knots and organic linkers [1]. ZIFs (zeolitic imidazolate frameworks), as one subgroup of MOFs, have attracted attention due to their exceptional chemical and thermal stability [2].

In this project [3] the crystallographic structure of ZIF-11 was investigated with the conclusion that different linkers should be described with different MD parameters to reproduce the structure as it was determined by X-ray diffraction, see Fig. 10.25.



(a) (b)

Figure 10.25: ZIF-11 structure viewed (a) through the 8-membered ring and (b) through the 6-membered ring window.

It turned out that in ZIF-11, up to room temperature, there is essentially only one type of connections between adjacent cavities. The crystallographic structure of ZIF-11 was reproduced with a high accuracy and the lattice parameters (physical dimension of the unit cell) were shown to be reproduced in NPT test simulations. The force field presented in this work leads to good agreement with the complete experimental adsorption isotherm of hydrogen in ZIF-11, by fitting only the hydrogen-hydrogen Lennard-Jones parameters. For this type of material it is therefore possible to describe experimental values with the used type of force field for at least one temperature. This is encouraging since the used types of force fields are, in some cases, rather simple. The flexibility of the lattice had a small, but noticeable, influence on the adsorption data. To get full accuracy it is advisable to take account of the lattice flexibility of ZIF-11. The good agreement obtained between the simulated and measured adsorption properties is referred to the high accuracy of the ZIF-11 structure ensured in our simulations.

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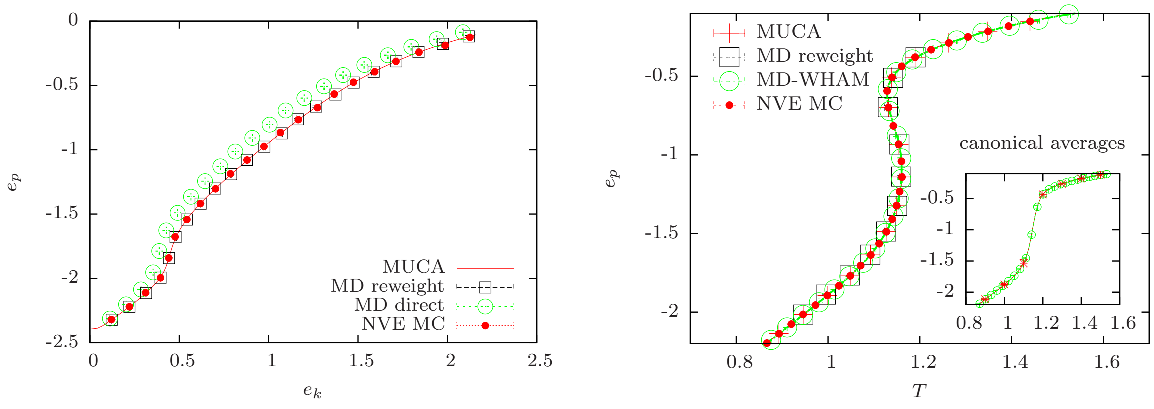
10.22 The NVE ensemble as the bridge between molecular dynamics and Monte Carlo simulations for liquid-gas like phase transitions

P. Schierz, J. Zierenberg, W. Janke



(a) (b)

Figure 10.26: (a) The potential energy e_p vs kinetic energy e_k for a single polymer with 13 monomers. The MD data is once evaluated directly (NVEPJ ensemble) and once reweighted to the NVE ensemble. (b) The potential energy vs. temperature for 8 polymers with 13 monomers each, simulated with two MC techniques and MD.

Molecular dynamics (MD) and Monte Carlo (MC) simulations are starting from two distinct physical points of view. While MD numerically integrates Newton's equations of motion, MC samples according to known ensemble probabilities from statistical physics. The ergodic hypothesis states that both approaches should give the same results in equilibrium, which is the basis for the formulation of the microcanonical ensemble. Energy conserving MD simulations are normally considered to sample the NVE ensemble which is, as we recover, not entirely correct [4]. Since energy conserving MD simulations encounter total angular momentum J and total linear momentum P conservation, the available phase space for an MD simulation is restricted. The resulting ensemble is either the NVEPJ or NVEP ensemble depending on the conserved quantities. Hence we obtain in Fig. 10.26(a) a deviating behaviour in comparison to simulations in the pure NVE ensemble which were obtained with Monte Carlo techniques [2, 3] for a small number of degrees of freedom. MD simulations for a liquid-gas like phase transition encounter a transition between NVEPJ and NVEP ensemble behaviour. The reason are the periodic boundary conditions which lead to a violation of angular momentum conservations whenever they are used. If a system stays within a droplet phase it will not be influenced by the boundaries and hence the angular momentum remains conserved (NVEPJ behaviour [6]). For the gas phase, however, the angular momentum fluctuates and we encounter NVEP behaviour.

With the exact knowledge of the ensemble which is sampled by MD it was possible to develop a method which allows to estimate the density of states of the simulated systems. In a first step we reweighted the obtained data from MD to the NVE ensemble. For the NVE ensemble we adapted the known "Weighted Histogram Analysis Method" (WHAM) [4], which allows one to estimate the density of states.

Afterwards, the density of states can be used to calculate the behaviour in the NVT ensemble [see Fig. 10.26(b)] and therefore to investigate phase transitions with varying temperature without the use of any thermostat in MD. Since the NVE ensemble shows very good sampling behaviour in the potential-energy range of canonical first-order phase transitions it is possible to estimate NVT phase transition behaviour by performing many NVE simulations at various total energies. Since this method estimates the density of states it is also a promising approach for the estimation of free-energy barriers for first-order phase transitions with MD.

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10.23 The real microcanonical ensemble and its advantageous behaviour for first-order phase transitions

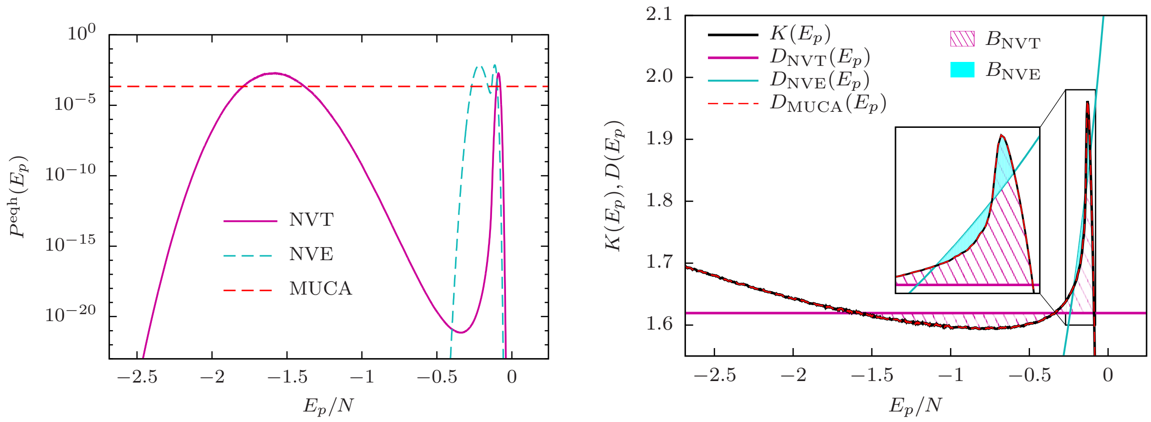
P. Schierz, J. Zierenberg, W. Janke

The microcanonical ensemble can be found in any standard text book on statistical physics. In almost all cases this ensemble is quickly dismissed in favor of the canonical ensemble since it is quite unrealistic for most physical systems in a laboratory. In the literature on phase transitions, however, this ensemble gained some interest also due to the development of the generalized ensemble methods MUCA [1, 2] and Wang-Landau [3]. Here, however, one refers to the microcanonical ensemble at constant potential energy while the “real” microcanonical ensemble was originally defined at constant total energy. We previously investigated the behavior of molecular dynamics and Monte Carlo simulations within this ensemble and made the interesting observation that a Monte Carlo simulation in this ensemble sampled the first-order aggregation transition in a very efficient way [4]. We found that this behavior was previously described by Martin-Mayor [5] for the temperature-driven first-order phase transition for the Potts model. We further investigated this simulation technique in the real microcanonical ensemble for a continuous Lennard-Jones system and found the same sampling advantage. We reached the same amount of particle with these simulations as for the sophisticated MUCA simulation technique.

In Ref. [6] we were able to develop a framework based on the generalization of the equal-area rule which allowed us to explain the obtained simulation behaviour of the real microcanonical ensemble. For comparisons we introduced the transition barrier of an ensemble as

$$B = \ln\left[P^{\mathrm{eqh}}\left(E_p^{\pm}\right)/P^{\mathrm{eqh}}\left(E_p^{0}\right)\right], \tag{10.13}$$

where $P^{\mathrm{eqh}}\left(E_p^{\pm}/E_p^{0}\right)$ denotes the equal-height histogram emerging due to phase coexistence, $E_p^{\pm}$ the positions of the two maxima and E_p^{0} the position of the minimum. This quantity hence allows one to evaluate how “hard” the first-order transition between two phases is within an ensemble. This framework allowed the conclusion that the barrier in the canonical ensemble is always larger than in the microcanonical ensemble



(a) (b)

Figure 10.27: (a) The potential-energy histogram at equal height for three different ensembles for the $N = 2048$ Lennard-Jones system [6]. (b) The system dependent quantity $K(E_p)$ and the ensemble dependent $D(E_p)$ for the considered ensembles as defined in [6].

$B_{\mathrm{NVT}} > B_{\mathrm{NVE}}$. In the microcanonical ensemble the transition barrier can even vanish as it was observed in [4] for polymer aggregation and by reproducing the data from Ref. [5]. For the example of the Lennard-Jones system with $N = 2048$ particles we discovered that the sampling with the microcanonical ensemble is of the order of $\exp(B_{\mathrm{NVT}} - B_{\mathrm{NVE}}) \approx 10^{16}$ more efficient than simulations in the canonical ensemble due to the difference of the barriers.

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10.24 Framework for programming Monte Carlo simulations (βMC)

M. Marenz, J. Zierenberg, W. Janke

Monte Carlo (MC) computer simulations are a very powerful tool for investigating and understanding the thermodynamic 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 microscopic 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.

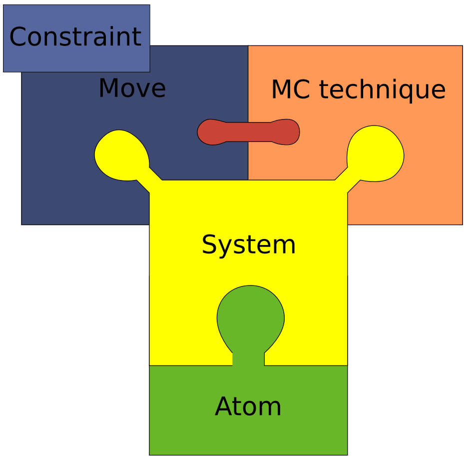

Figure 10.28: The 5 basic building blocks.

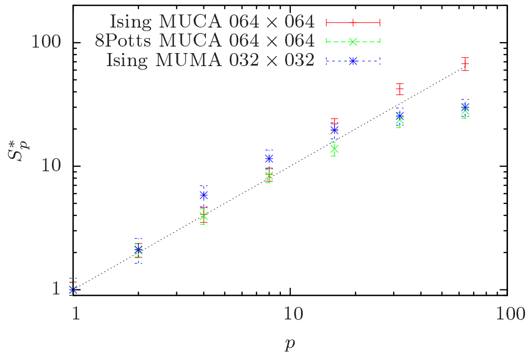

Figure 10.29: Scaling properties of the parallel multicanonical algorithm as a function of the number of processors p.

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. 10.28: 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. 10.29.

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, and 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 led already to several publications [2–8].

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W. Janke (Principal Investigator)

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W. Janke (Principal Investigator, project P9 in collaboration with K. Kroy, Research Unit "Theory of Condensed Matter (TKM)")
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W. Janke (Principal Investigator, project B04)
Deutsche Forschungsgemeinschaft (DFG)

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W. Janke
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W. Janke
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W. Janke
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Free-Energy Landscapes of Semiflexible Polymer Aggregation
W. Janke, J. Zierenberg
NIC Jülich (computer time grant for "JURECA"), Grant No. HLZ24

10.26 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*

- Principal Investigator of "Profillinie" *Complex Matter*, Universität Leipzig
- Principal Investigator of "Profillinie" *Mathematical and Computational Sciences*, Universität Leipzig
- Spokesperson of the German-French Graduate College *Statistical Physics of Complex Systems* with Nancy (France), and associated partners in 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
- *Adjunct Professor* of The University of Georgia, Athens, Georgia, USA
- Permanent Member of the International Advisory Board for the Annual *Conference of the Middle European Cooperation in Statistical Physics (MECO)*
- Member of the Program Committee of the *International Conference on Computer Simulation in Physics and beyond*, Moscow, Russia, September 06.–10. September 2015
- Organizer of the Workshop *CompPhys15* – 16th International NTZ Workshop on *New Developments in Computational Physics*, ITP, Universität Leipzig, 26.–28. November 2015
- Organizer of the Workshop *CompPhys16* – 17th International NTZ Workshop on *New Developments in Computational Physics*, ITP, Universität Leipzig, 24.–26. November 2016
- 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

10.27 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, Andreas Nußbaumer, Prof. Dr. Friderike Schmid
- Max Planck Institute for Polymer Research, Mainz, Germany
  Dr. Hsiao-Ping Hsu, Prof. Dr. Kurt Kremer
- 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, Germany
  Prof. Dr. Rudolf Hilfer, Prof. Dr. Christian Holm
- Complex Systems Division, Department of Theoretical Physics, Lunds Universitet, Lund, Sweden
  Prof. Dr. Anders Irbäck
- 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
  PD Dr. Christian von Ferber, Dr. Nikolaos G. Fytas, Prof. Dr. Ralph Kenna, Dr. Thierry Platini, Dr. Martin Weigel
- Inst. für Theoretische Physik, FU Berlin, Germany
  Prof. Dr. Hagen Kleinert
- Atominstitut, TU Wien, Austria
  Prof. Dr. Harald Markum
- 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, Ankara, Turkey
  Prof. Dr. Handan Arkın (Olgar), Mustafa Bilsel, Buket Taşdizen
- Dept. of Physics, Hacettepe University, Ankara, Turkey
  Prof. Dr. Tarik Çelik, Gökhan Gökoğlu
- Dept. of Physics Engineering, Hacettepe University, Ankara, Turkey
  Prof. Dr. Fatih Yaşar
- Institute for Condensed Matter Physics, National Academy of Sciences, Lviv, Ukraine
  Dr. Viktoria Blavatska, Prof. Dr. Yurij Holovatch
- Yerevan Physics Institute, Yerevan, Armenia
  Prof. Dr. David B. Saakian
- Alikhanyan National Science Laboratory, Yerevan, Armenia
  Prof. Dr. Nerses Ananikyan, Dr. Nikolay Izmailyan
- Landau Institute for Theoretical Physics, Chernogolovka, Russia
  Dr. Lev Barash, Prof. Dr. Lev N. Shchur
- Center for Simulational Physics, The University of Georgia, Athens, USA
  Prof. Dr. Michael Bachmann, Prof. Dr. David P. Landau
- Dept. of Physics, Florida State University, Tallahassee, USA
  Prof. Dr. Bernd A. Berg
- Dept. of Chemistry and Biochemistry, University of Oklahoma, Norman, USA
  Prof. Dr. Ulrich H.E. Hansmann
- Los Alamos National Laboratory, Los Alamos, USA
  Dr. Christoph Junghans
- Dept. of Physics and Astronomy, Texas A&M, College Station, USA
  Prof. Dr. Helmut G. Katzgraber
- Dept. of Physics, Virginia Tech, Blacksburg, USA
  Prof. Dr. Michel Pleimling, Prof. Dr. Royce K.P. Zia
- Physics Department, Carnegie Mellon University, Pittsburgh, USA
  Prof. Dr. Robert H. Swendsen
- Stetson University, DeLand, USA
  Dr. Thomas Vogel
- Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Jakkur, India
  Prof. Dr. Subir K. Das
- Computational Chemistry Unit Cell (CCUC), Department of Chemistry, Chulalongkorn University, Bangkok, Thailand
  Prof. Dr. Supot Hannongbua, Dr. Oraphan Saengsawang
- Ramkhamhaeng University, Department of Chemistry, Faculty of Science, Bangkok, Thailand
  Dr. Tatiya Chokbunpiam

- Laboratory of Statistical and Computational Physics, Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan
  Prof. Dr. Chin-Kun Hu
- The University of Tokyo, Tokyo, Japan
  Prof. Dr. Nobuyasu Ito
- Banaras Hindu University, Varanasi, India
  Prof. Dr. Sanjay Kumar
- Nagoya University, Nagoya, 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

10.28 Publications

Journals

N. Fricke, S. Sturm, M. Lämmel, S. Schöbl, K. Kroy, W. Janke: *Polymers in Disordered Environments*, Diff. Fundam. (diffusion-fundamentals.org) **23**, 7-1–12 (2015)

M.H. Gerlach, W. Janke: *First-Order Directional Ordering Transition in the Three-Dimensional Compass Model*, Phys. Rev. B **91**, 045119-1–8 (2015)

J. Gross, T. Vogel, M. Bachmann: *Structural Phases of Adsorption for Flexible Polymers on Nanocylinder Surfaces*, Phys. Chem. Chem. Phys. **17**, 30702–30711 (2015)

W. Janke: *Computer Simulation Studies of Polymer Adsorption and Aggregation – From Flexible to Stiff*, in *Computer Simulation Studies in Condensed-Matter Physics XXVIII*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, Physics Procedia **68**, 69–79 (2015)

W. Janke, M. Mueller, D.A. Johnston: *Finite-Size Scaling and Latent Heat at the Gonihedric First-Order Phase Transition*, J. Phys.: Conf. Ser. **640**, 012002-1–6 (2015)

D.A. Johnston, M. Mueller, W. Janke: *Macroscopic Degeneracy and Order in the 3d Plaquette Ising Model*, Mod. Phys. Lett. B **29**, 1550109-1–10 (2015)

S. Majumder, W. Janke: *Cluster Coarsening During Polymer Collapse: Finite-Size Scaling Analysis*, Europhys. Lett. **110**, 58001-1–6 (2015)

M. Mueller, W. Janke, D.A. Johnston: *Planar Ordering in the Plaquette-Only Gonihedric Ising Model*, Nucl. Phys. B **894**, 1–14 (2015)

M. Mueller, J. Zierenberg, M. Marenz, P. Schierz, W. Janke: *Probing the Effect of Density on the Aggregation Temperature of Semi-Flexible Polymers in Spherical Confinement*, in *Computer Simulation Studies in Condensed-Matter Physics XXVIII*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, Physics Procedia **68**, 95–99 (2015)

H. Nagel, H. Meyer-Ortmanns, W. Janke: *Boundary Drive Induced Formation of Aggregate Condensates in Stochastic Transport with Short-Range Interactions*, Europhys. Lett. **111**, 30001-1–6 (2015)

J.K. Ochab, H. Nagel, W. Janke, B. Wacław: *A Simple Non-Equilibrium, Statistical-Physics Toy Model of Thin-Film Growth*, J. Stat. Mech.: Theor. Exp., P09013-1–25 (2015)

P. Schierz, S. Fritzsche, W. Janke, S. Hannongbua, O. Saengsawang, C. Chmelik, J. Kärger: *MD Simulations of Hydrogen Diffusion in ZIF-11 with a Force Field Fitted to Experimental Adsorption Data*, Microporous Mesoporous Mater. **203**, 132–138 (2015)

P. Schierz, J. Zierenberg, W. Janke: *Molecular Dynamics and Monte Carlo Simulations in the Microcanonical Ensemble: Quantitative Comparison and Reweighting Techniques*, J. Chem. Phys. **143**, 134114-1–11 (2015)

T. Vogel, J. Gross, M. Bachmann: *Thermodynamics of the Adsorption of Flexible Polymers on Nanowires*, J. Chem. Phys. **142**, 104901-1–8 (2015)

J. Zierenberg, N.G. Fytas, W. Janke: *Parallel Multicanonical Study of the Three-Dimensional Blume-Capel Model*, Phys. Rev. E **91**, 032126-1–8 (2015)

J. Zierenberg, W. Janke: *From Amorphous Aggregates to Polymer Bundles: The Role of Stiffness on Structural Phases in Polymer Aggregation*, Europhys. Lett. **109**, 28002-1–6 (2015)

J. Zierenberg, W. Janke: *Exploring Different Regimes in Finite-Size Scaling of the Droplet Condensation-Evaporation Transition*, Phys. Rev. E **92**, 012134-1–11 (2015)

in press

T. Chokbunpiam, S. Fritzsche, C. Chmelik, J. Caro, W. Janke, S. Hannongbua: *Gate Opening Effect for Carbon Dioxide in ZIF-8 by Molecular Dynamics – Confirmed, but at High* CO_2 *Pressure*, Chem. Phys. Lett. **648**, 178–181 (2016)

W. Janke, W. Paul: *Thermodynamics and Structure of Macromolecules from Flat-Histogram Monte Carlo Simulations*, invited review, Soft Matter **12**, 642–657 (2016)

S. Kumar, R. Kumar, W. Janke: *Periodically Driven DNA: Theory and Simulation*, Phys. Rev. E **93**, 010402(R)-1–5 (2016)

S. Majumder, W. Janke: *Evidence of Aging and Dynamic Scaling in Collapse of a Polymer*, Phys. Rev. E **93**, 032506-1–6 (2016)

M. Marenz, W. Janke: *Knots as a Topological Order Parameter for Semiflexible Polymers*, Phys. Rev. Lett. **116**, 128301-1–6 (2016)

H. Nagel, W. Janke: *Emergence of Dynamic Phases in the Presence of Different Kinds of Open Boundaries in Stochastic Transport with Short-Range Interactions*, J. Stat. Mech.: Theor. Exp., 013207-1–19 (2016)

H. Nagel, W. Janke: *Dynamics of Condensate Formation in Stochastic Transport with Pair-Factorized Steady States: Nucleation and Coarsening Time Scales*, Phys. Rev. E **93**, 052112-1–12 (2016)

Z. Zhu, A.J. Ochoa, S. Schnabel, F. Hamze, H.G. Katzgraber: *Best-Case Performance of Quantum Annealers on Native Spin-Glass Benchmarks: How Chaos can Affect Success Probabilities*, Phys. Rev. A **93**, 012317-1–8 (2016)

J. Gross, M. Ivanov, W. Janke: *Comparing Atomistic and Coarse-Grained Simulations of P3HT*, to appear in *Computer Simulation Studies in Condensed-Matter Physics XXIX*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. (2016), in print

W. Janke, M. Marenz: *Stable Knots in the Phase Diagram of Semiflexible Polymers: A Topological Order Parameter?*, to appear in *Computer Simulation Studies in Condensed-Matter Physics XXIX*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. (2016), in print

S. Majumder, W. Janke: *Aging and Related Scaling During the Collapse of a Polymer*, to appear in *Computer Simulation Studies in Condensed-Matter Physics XXIX*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. (2016), in print

A. Nußbaumer, J. Zierenberg, E. Bittner, W. Janke: *Numerical Test of Finite-Size Scaling Predictions for the Droplet Condensation-Evaporation Transition*, invited talk, Conference Proceedings *CCP2015*, 2 – 5 December 2015, IIT Guwahati, India, to appear in J. Phys.: Conf. Ser. (2016), in print

J. Zierenberg, W. Janke: *Finite-Size Scaling of Lennard-Jones Droplet Formation at Fixed Density*, to appear in *Computer Simulation Studies in Condensed-Matter Physics XXIX*, eds. D.P. Landau, H.-B. Schüttler, S. Lewis, M. Bachmann, J. Phys.: Conf. Ser. (2016), in print

Talks

J. Gross, M. Ivanov, W. Janke: *Comparing Atomistic and Coarse-Grained Simulations of P3HT*, 16th International NTZ-Workshop on New Developments in Computational Physics – CompPhys15, Leipzig, Germany, 26. November 2015

W. Janke: *Computer Simulation Studies of Polymer Adsorption and Aggregation – From Flexible to Stiff*, invited talk, Departmental Colloquium and 28th Annual CSP Workshop on *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, The University of Georgia, Athens, USA, 23.–27. February 2015

W. Janke: *Nonstandard Finite-Size Scaling at First-Order Phase Transitions*, APS March Meeting 2015, San Antonio, Texas, USA, 02.–06. March 2015

W. Janke: *Nonstandard Finite-Size Scaling at First-Order Phase Transitions with Macroscopic Low-Temperature Phase Degeneracy*, DPG Frühjahrstagung 2015, TU Berlin, Germany, 15.–20. March 2015

W. Janke: *Asymptotic Scaling Behavior of Self-Avoiding Walks on Critical Percolation Clusters*, MECO 40 Conference, Esztergom, Hungary, 23.–25. March 2015

W. Janke: *Asymptotic Scaling Behavior of Self-Avoiding Walks on Critical Percolation Clusters*, Workshop *Statistical Physics and Low Dimensional Systems – SPLDS*, Abbaye des Prémontrés, Pont-à-Mousson, France, 20.–22. May 2015

W. Janke: *Computersimulationen in der statistischen Physik*, DPG Schülertagung 2015, Max-Planck-Institut für *Mathematik in den Naturwissenschaften*, Leipzig, Germany, 25. June 2015

W. Janke: *Self-Avoiding Walks on Critical Percolation Clusters – A Paradigm for Polymers in Disordered Environments*, invited talk, 4th International Workshop on *Theory and Computer Simulations of Polymers: New Developments*, Martin-Luther Universität Halle (Saale), Germany, 28. June – 01. July 2015

W. Janke: *Computer Simulation Studies of Polymer Adsorption and Aggregation*, invited plenary talk, International Conference on *Computer Simulation in Physics and Beyond*, Moscow, Russia, 06.–10. September 2015

W. Janke: *Stable Knot Phases of Semiflexible Polymers*, Conference *shape up 2015 – Exercises in Materials Geometry and Topology*, TU Berlin, Germany, 14.–18. September 2015

W. Janke: *Finite-Size Scaling of Particle and Polymer Nucleation*, invited talk, International Conference on *Growing Length Scale Phenomena in Condensed Matter Physics*, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India, 08.–10. October 2015

W. Janke: *Finite-Size Scaling of Particle and Polymer Nucleation*, invited talk, XXVII IUPAP Conference on *Computational Physics – CCP2015*, Indian Institute of Technology, Guwahati, Assam, India 02.–05. December 2015

S. Majumder, W. Janke: *Nonequilibrium Dynamics in Polymer Collapse* Conference on *Growing Length Scale Phenomena in Condensed Matter Physics*, Bangalore, India, 08. October 2015

S. Majumder, W. Janke: *Evidence of Aging and Dynamical Scaling During Collapse of a Polymer*, 16th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys15*, Leipzig, Germany, 26. November 2015

M. Mueller: *Aggregation of Flexible Polymers under Spherical Constraints*, 28th Workshop on *Computer Simulation Studies in Condensed Matter Physics (CSP2015)*, Athens, Georgia, USA, 23. February 2015

H. Nagel, W. Janke: *Boundary Induced Phase Transitions in Stochastic Transport with Short-Range Interactions*, 16th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys15*, Leipzig, Germany, 27. November 2015

P. Schierz, J. Zierenberg, W. Janke: *Computational Investigation of Polymers*, Seminar of the cdfa-dfdk, Coventry, England, UK, 04. February 2015

P. Schierz, J. Zierenberg, W. Janke: *Interesting Properties of the Microcanonical Ensemble with Constant Total Energy*, Seminar of the cdfa-dfdk, Nancy, France, 16. September 2015

P. Schierz, J. Zierenberg, W. Janke: *First-Order Phase Transitions in the Advantageous Full Microcanonical Ensemble*, 16th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys15*, Leipzig, Germany, 26. November 2015

S. Schnabel, W. Janke: *Where to go in a Rough Free-Energy Landscape?*, Annual Conference of the German Physical Society (DPG), TU Berlin, Germany, 15.–20. March 2015

S. Schnabel, W. Janke: *Greedy Monte Carlo for Spin Glass Ground-State Search*, 16th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys15*, Leipzig, Germany, 26.–28. November 2015

J. Zierenberg, W. Janke: *The Role of Stiffness in Polymer Aggregation: Leading from Amorphous Aggregates to Polymer Bundles*, DPG Frühjahrstagung, TU Berlin, Germany, 18. March 2015

J. Zierenberg: *From Particle Condensation to Polymer Aggregation: Phase Transitions and Structural Phases in Mesoscopic Systems*, Seminar of the cdfa-dfdk, Coventry, England, UK, 22. October 2015

J. Zierenberg, W. Janke: *Exploring Different Regimes in Finite-Size Scaling of the Droplet Condensation-Evaporation Transition*, 16th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys15*, Leipzig, Germany, 26. November 2015

J. Zierenberg, M. Mueller, M. Marenz, P. Schierz, W. Janke: *Aggregation of Flexible Polymers under Spherical Constraints*, DPG Frühjahrstagung, Berlin, Germany, 18. March 2015

Posters

J. Bock, W. Janke: *Computer Simulations of Semiflexible Polymers in Disordered Media*, 79th Annual Meeting of the DPG and DPG Spring Meeting, TU Berlin, Germany, 15.–20. March 2015

J. Bock, W. Janke: *Computer Simulations of Semiflexible Polymers in Disordered Media*, 16th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys15*, Leipzig, Germany, 26.–28. November 2015

M. Ivanov, J. Gross, W. Janke: *Poly(3-hexylthiophene) (P3HT) Molecules Interacting with Au(001) Substrates*, 79th Annual Meeting of the DPG and DPG Spring Meeting, TU Berlin, Germany, 15.–20. March 2015

M. Ivanov, J. Gross, W. Janke: *Poly(3-hexylthiophene) (P3HT) Molecules Interacting with Au(001) Substrates*, 4th International Workshop on *Theory and Computer Simulations of Polymers: New Developments*, Martin-Luther Universität Halle (Saale), Germany, 29. June – 01. July 2015

M. Ivanov, J. Gross, M. Mueller, W. Janke: *Computer Simulations of P3HT*, SFB TRR/102 3rd Mini-Workshop, Martin-Luther Universität Halle (Saale), Germany, 02. October 2015

M. Ivanov, P. Schierz, J. Gross, W. Janke: *Boltzmann Inversion of Harmonic Oscillators*, 16th International NTZ-Workshop on New Developments in Computational Physics – CompPhys15, Leipzig, Germany, 26.–28. November 2015

R. Kumar, S. Kumar, W. Janke: *Driven DNA: Does Dynamic Transition Exist in the Thermodynamic Limit?* Bad Honnef Physics School on *Computational Physics of Complex and Disordered Systems*, Physikzentrum Bad Honnef, Germany, 20.–25. September 2015

R. Kumar, S. Kumar, W. Janke: *Driven DNA: Does Dynamic Transition Exist in the Thermodynamic Limit?* 16th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys15*, Leipzig, Germany, 26.–28. November 2015

S. Majumder, W. Janke: *Cluster Growth During a Polymer Collapse*, 4th International Workshop on *Theory and Computer Simulations of Polymers: New Developments*, Martin-Luther Universität Halle (Saale), Germany, 29. June – 01. July 2015

M. Mueller, D.A. Johnston, W. Janke: *Planar ("Fuki-Nuke") Ordering and Finite-Size Effects for a Model with Four-Spin Interactions*, 16th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys15*, Leipzig, Germany, 26.–28. November 2015

H. Nagel, W. Janke: *Boundary Induced Phase Transitions in Stochastic Transport with Short-Range Interactions*, Conference of the Middle European Cooperation in Statistical Physics, Esztergom, Hungary, 23.–25. March 2015

P. Schierz, J. Zierenberg, W. Janke: *Comparability of Microcanonical Data sampled by Molecular Dynamics and Monte Carlo Simulations*, 79th Annual Meeting of the DPG and DPG Spring Meeting, TU Berlin, Germany, 15.–20. March 2015

P. Schierz, J. Zierenberg, W. Janke: *Theta-Polymers in Spherical Confinement: Investigation of the Aggregation Behaviour*, Annual BuildMoNa Conference, Leipzig, Germany, 23.–24. March 2015

P. Schierz, J. Zierenberg, W. Janke: *3D-Visualisierung von Polymeren – oder wie verkleben Spaghetti*, Dies Academicus, Leipzig, Germany, 02. Dezember 2015

J. Zierenberg, W. Janke: *Aggregation of Semiflexible Polymers*, 4th International Workshop on *Theory and Computer Simulations of Polymers: New Developments*, Martin-Luther Universität Halle (Saale), Germany, 29. June – 01. July 2015

10.29 Graduations

Doctorate

- Johannes Zierenberg
  From Particle Condensation to Polymer Aggregation: Phase Transitions and Structural Phases in Mesoscopic Systems
  17. December 2015

Master

- Kieran Austin
  Adsorption and Stiffness of a Grafted Polymer
  23. September 2015

Bachelor

- Simon Schneider
  Stochastic Approximation Monte Carlo Simulations: Applications and Performance Test for the Ising Model
  29. April 2015
- Felix Neduck
  Population Annealing für Spinsysteme
  28. Juli 2015

10.30 Guests

- M.Sc. Hamid Khoshbakht
  Coventry University, England, UK
  DFH-UFA Colloquium (10. February 2015)
  On the Uniform Sampling of Ground States in the 2D $\pm J$ *Ising Spin-Glass Model*
  02.–15. February 2015
- M.Sc. Eren Metin Elçi
  Coventry University, England, UK
  DFH-UFA Colloquium (12. March 2015)
  Perfect Sampling, Relaxation and Extreme Value Theory – An Intriguing Interplay
  13. February – 16. March 2015
- Prof. Dr. Sanjay Kumar
  Banaras Hindu University, Varanasi, India
  SFB/TRR 102 Colloquium (07. May 2015)
  DNA under Force: New Insights from Simulations
  27. April – 20. May 2015

- Dr. Lev Barash
  Landau Institute, Chernogolovka, Russia
  NTZ/DFH-UFA and DIONICOS Colloquium (28. May 2015)
  Population Annealing on GPUs
  26. May – 25. June 2015
- Prof. Dr. Ulrich H.E. Hansmann
  University of Oklahoma, Norman, USA
  SFB/TRR 102 Polymer and Soft-Matter Seminar (02. June 2015)
  Simulations of Folding and Aggregation of Proteins
  28. May – 11. June 2015
- Dr. Christoph Junghans
  Los Alamos National Laboratory, New Mexico, USA
  02. July 2015
- Prof. Dr. Subir K. Das
  Jawaharlal Nehru Centre for Advanced Scientific Research, India
  TKM/DFH-UFA and DIONICOS Colloquium (03. July 2015)
  Aging in Kinetics of Phase Transitions
  02.–04. July 2015
- M.Sc. Ati Moncef
  University of Sciences and Technology of Oran, Algeria
  13. October – 12. November 2015
- Dr. Nikolaos G. Fytas
  Coventry University, England, UK
  DFH-UFA Colloquium (03. December 2015)
  Critical Phenomena in Disordered Systems
  24. November – 04. December 2015
- Prof. Dr. Michael Bachmann
  Center for Simulational Physics, The University of Georgia, Athens, USA
  Stabilization of Helical Structures by Bending Restraints
  25.–27. November 2015
- Prof. Dr. Alexander Hartmann
  Univ. Oldenburg, Germany
  Distribution of Convex Hulls for Single and Multiple Random Walks
  25.–27. November 2015
- Dr. Martin Thomas Horsch
  TU Kaiserslautern, Germany
  Multicriteria Optimization of Molecular Force Field Models
  25.–27. November 2015
- Dr. Francesco Parisen Toldin
  Universität Würzburg, Germany
  Line Contribution to the Critical Casimir Force between a Homogeneous and a Chemically Stepped Surface
  25.–27. November 2015

- Dr. Hsiao-Ping Hsu
  MPI für Polymerforschung, Mainz, Germany
  Static and Dynamic Properties of Large Polymer Melts in Equilibrium
  25.–28. November 2015
- Miriam Klopotek
  Institut für Angewandte Physik, Universität Tübingen, Germany
  Monolayer Growth in a Hard-Rod Lattice Model
  25.–28. November 2015
- Prof. Dr. Ezequiel Albano
  IFLYSIB, La Plata, Argentina
  Multicriticality in Confined Ferromagnets with Impurities
  25.–29. November 2015
- Dr. Ewa Gajda-Zagórska
  AGH University, Krakow, Poland
  Multi-Objective Solver for Inverse Parametric Problems
  25.–29. November 2015
- Prof. Dr. Dennis C. Rapaport
  Bar-Ilan University, Ramat-Gan, Israel
  Joint NTZ–SFB/TRR 102 Colloquium (26. November 2015)
  Simulating Emergent Phenomena (with GPU-based Molecular Dynamics)
  25.–29. November 2015
- Prof. Dr. George Savvidy
  Demokritos NRC, Athens, Greece
  Kolmogorov-Anosov C-Systems and MIXMAX Random Number Generator
  25.–29. November 2015
- Prof. Dr. Lev Shchur
  Landau Institute, Chernogolovka, Moscow Region, Russia
  Current State-of-the-Art in Kinetic Monte Carlo Simulations
  25.–29. November 2015
- Dr. Martin Weigel
  Coventry University, England, UK
  Regular Packings on Periodic Lattices
  25.–29. November 2015
- Dr. Marcin Zagórski
  IST Klosterneuburg/Wien, Austria
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  MPI Dynamik und Selbstorganisation, Göttingen, Germany
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  Emory University, Atlanta, USA
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