# 12

# Computational Quantum Field Theory

## 12.1 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 analytical and numerical techniques. The numerical tools are currently Monte Carlo and Molecular Dynamics computer simulations as well as exact enumeration techniques. The computational approach to theoretical physics is expected to gain more and more importance with the future advances of computer technology, and is likely to become the third cornerstone of physics besides experiment and analytical theory as sketched in Fig. 12.1. 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 University computing centre, and, upon successful grant application at the national supercomputing centres in Jülich, Stuttgart and München on parallel supercomputers. This hierarchy of various platforms gives good training opportunities for the students and offers promising job perspectives in many different fields for their future career.

Our research activities are closely integrated into the Graduate School "BuildMoNa": Leipzig School of Natural Sciences – *Building with Molecules and Nano-objects*, two ESF Junior Research Groups, the International Max Planck Research School

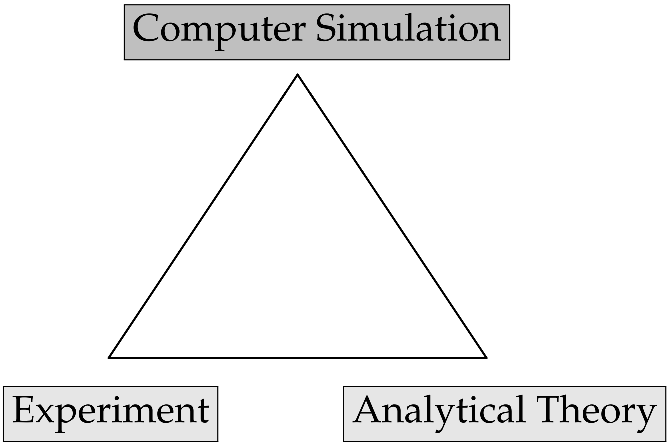


**Figure 12.1:** Sketch of the "triangular" relationship between experiment, analytical theory and computer simulation.

(IMPRS) *Mathematics in the Sciences*, and the International Graduate School *Statistical Physics of Complex Systems* with Université de Lorraine in Nancy, France, supported by the Deutsch-Französische Hochschule (DFH-UFA). In the second funding period 2011–2013, Coventry University in England has been integrated as an associated partner, and in the 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 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*

## 12.2 Effects of bending stiffness on a coarse grained polymer model

M. Marenz, W. Janke

To investigate the generic behavior of polymers and proteins with computer simulations, it is common to use generic models. On the one hand, these models neglect chemical details, which means that one cannot observe any specific behavior. Instead the general behavior for the type of polymer is exposed. However, using these coarse-grained models is the only possibility to investigate the physical system on a large time scale, length scale or parameter range. One of the most common coarse-grained models is the so called bead-stick polymer. The Hamiltonian is given by

$$H = 4\sum_{i=1}^{N-2}\sum_{j=i+2}^{N}\left(\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}}\right) + \kappa\sum_{\theta_i}(1-\cos\theta_i)\ , \tag{12.1}$$

where $r_{ij}$ is the distance between non-adjacent monomers, and $\theta_i$ is the angle of two adjacent bonds. The Hamiltonian allows us to modify the bending stiffness by varying $\kappa$, so that the simulated polymer can be anything between flexible, semi-flexible or stiff.

To simulate the system in the complete $(T, \kappa)$-plane we used two advanced Monte Carlo algorithms. A two-dimensional replica-exchange method, which simulates the system in parallel in the $T$ and $\kappa$ direction, is able to generate well equilibrated canonical mean values. These simulations are supported by the parallel multicanonical algorithm [1] combined with a one-dimensional replica exchange in the $\kappa$ 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 ($N = 14, 28, 42$).

Despite the simplicity of the model, the phase diagram is remarkably rich, see Fig. 12.2. Many of theses phases are comparable to conformations which have been observed for real polymers and proteins. Compared to former work simulating similar coarse-grained models, we observed a novel type of pseudo-phases which are best described by thermodynamically stable knots (noted by $\mathrm{KC}_n$ in Fig. 12.2) [2]. The transitions into these knot phases exhibit some surprising characteristics. Although we observed a clear phase coexistence between the knotted and unknotted phases, the transitions show no latent heat. Instead the two sub-energies, the Lennard-Jones energy and the bending energy, are transformed into each other while the polymer knots itself.

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

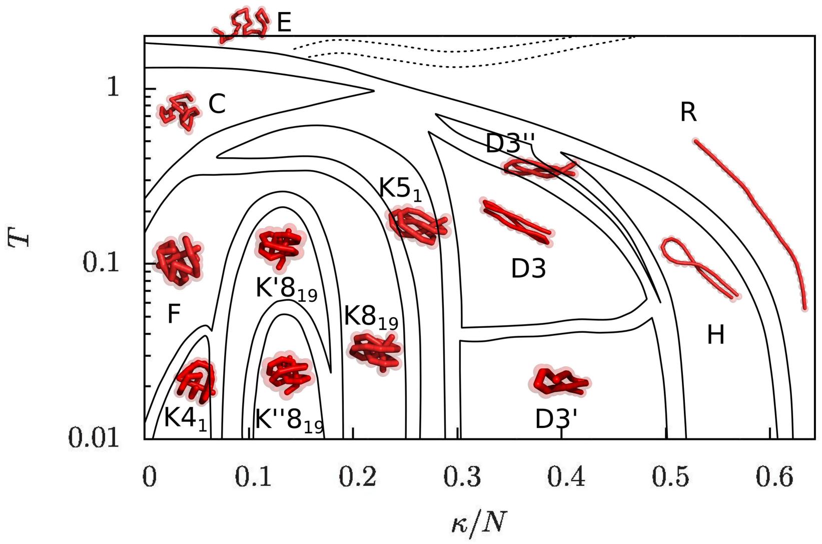


**Figure 12.2:** The pseudo-phase diagram for the bead-stick model with 28 monomers. The different pseudo phases are labeled as follows: E - elongated, R - rod-like, C - collapsed, F - frozen, K$C_n$ - knotted phase with the corresponding knot type, D$N$ - $(N-1)$ times bent polymers, H - hairpin.

[2] M. Marenz, W. Janke: *Knots as topological order parameter for semi-flexible polymers*, Leipzig preprint (May 2015), submitted

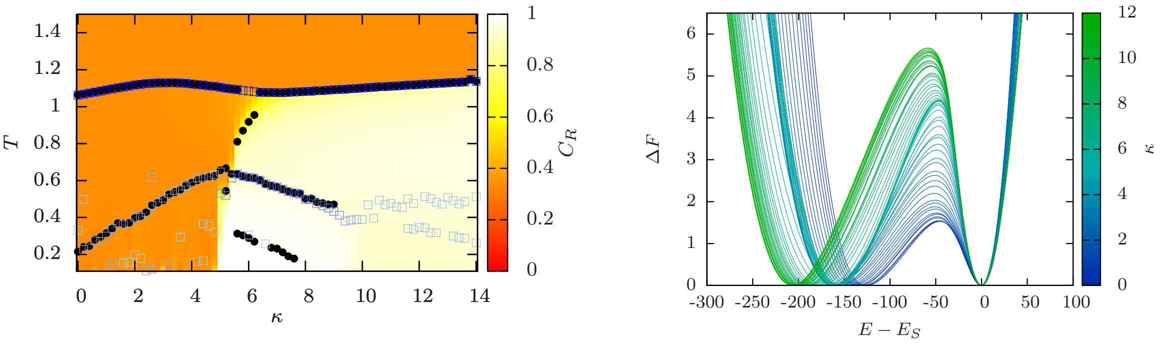
## 12.3 The role of stiffness on structural phases in polymer aggregation

J. Zierenberg, W. Janke

We have investigated the role of stiffness in polymer aggregation leading from amorphous aggregates for rather flexible polymers to polymer bundles for stiffer polymers [1]. Employing parallel multicanonical simulations [2], we were able to map out generic $T$-$\kappa$ structural phase diagrams describing an entire class of coarse-grained semiflexible polymers. Figure 12.3 (a) shows such a diagram for 8 polymers of length $N = 13$, exhibiting 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. A microcanonical analysis supports the first-order like transition characteristics of polymer aggregation, the transition line at higher temperatures.

A first-order (like) transition is usually accompanied by a free-energy barrier. We compared the microcanonical free-energy for the available stiffness range, guided by a recent claim that the free-energy of amorphous aggregation is lower than the formation of ordered structures such as fibrils [3]. Indeed Fig. 12.3 (b) shows that the free-energy barrier (local maximum) increases with increasing stiffness already for a finite system of 8 semiflexible polymers, supporting the previous claim.

The numerical data was generated on the supercomputer JUROPA at Jülich Supercomputing Centre (JSC) under Grant No. HLZ21.



(a)

(b)

**Figure 12.3:** (a) 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). (b) Free-energy barrier of the same system at equal height temperature for several bending-stiffness parameters $\kappa \in [0, 12]$ encoded in the line color. Figures adapted from Ref. [1].

[1] J. Zierenberg, W. Janke: Europhys. Lett. **109**, 28002 (2015)
[2] J. Zierenberg et al.: Comput. Phys. Comm. **184**, 1155 (2013)
[3] Y. Yoshimura et al.: Proc. Natl. Acad. Sci. U. S. A. **109**, 14446 (2012)

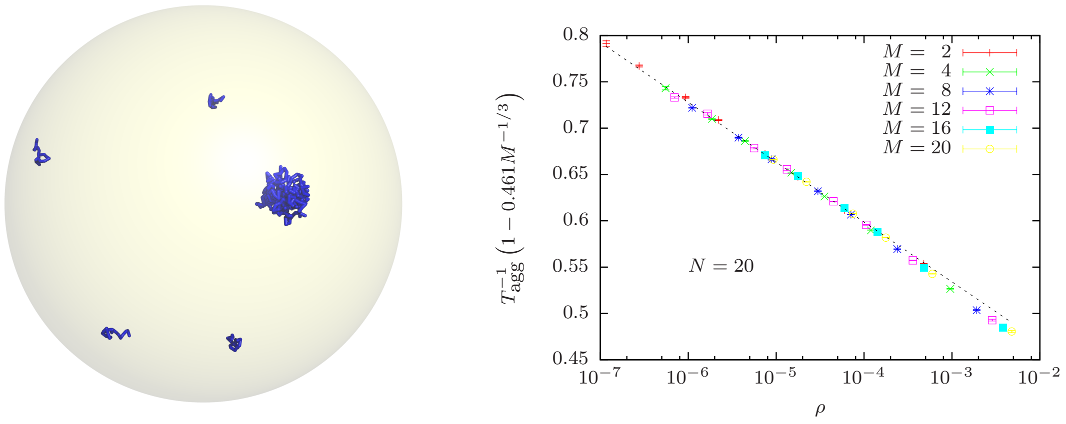
## 12.4 Aggregation of $\theta$-polymers in spherical confinement

J. Zierenberg, M. Mueller, 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, see the left of Fig. 12.4. 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.

With this setup, we are thus able to explore the influence of the density onto the aggregation transition temperature. We simulated this system of $\theta$-polymers (which means they are parametrized by a model that allows a single polymer to undergo a collapse transition) in the multicanonical ensemble. 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



(a) (b)

**Figure 12.4:** (a) We enclose a small number $M$ of polymers in a sphere and vary its radius, 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.

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 then relate the entropy difference of the two regimes to the microcanonical temperature $T_{\mathrm{agg}}$, allowing the derivation of an explicit relation of the inverse transition temperature to the logarithm of the density,

$$1/T_{\mathrm{agg}}(\rho) = \frac{S(E_{\mathrm{sep}}, \rho) - S(E_{\mathrm{agg}}, \rho)}{\Delta E} \sim \frac{S(E_{\mathrm{sep}}, \rho)}{\Delta E} =\sim -\ln \rho + \mathrm{const}\,, \tag{12.2}$$

under the assumption that, for fixed $M$ and $N$, the latent heat $\Delta E = E_{\mathrm{sep}} - E_{\mathrm{agg}} = M\Delta e$ 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. (12.2) 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 in the right of Fig. 12.4.

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 in the aggregate, it becomes smaller for stiffer polymers. 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.: *Probing the effect of density on the aggregation temperature of semi-flexible polymers in spherical confinement*, Leipzig preprint (March 2015), to appear in Physics Procedia (2015), in print

[5] J. Zierenberg, W. Janke: Europhys. Lett. **109**, 28002 (2015)

## 12.5 Polymer adsorption onto a stripe-patterned substrate

M. Möddel[*], M. Bachmann[†], W. Janke

[*]Present address: Blue Yonder GmbH, Karlsruher Str. 88, 76139 Karlsruhe, Germany

[†]Center for Simulational Physics, The University of Georgia, Athens, Georgia 30602, USA

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

The goal was to see the influence on the level of the whole pseudo-phase diagram, where "pseudo" refers to the finiteness of the simulated chain length. Since already the phase diagram of the polymer near the homogeneous substrate is very rich in transitions (cf. Fig. 12.5(a)), to extract any meaningful results the chosen surface heterogeneity needs to be easily controllable and preferably simple.

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

$$E_{\text{bulk}} = 4\sum_{i=1}^{N-2}\sum_{j=i+2}^{N}\left(r_{ij}^{-12} - r_{ij}^{-6}\right) + \frac{1}{4}\sum_{i=1}^{N-2}(1-\cos\vartheta_i)\ , \tag{12.3}$$

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

$$E_{\text{sur, stripe}}(x,z) = \begin{cases} \left(\frac{2}{15}z^{-9} - z^{-3}\right)\left[\epsilon_s + \epsilon_{\text{stripe}}\cos^2\left(\pi\left(\text{mod}\left(x+\frac{D}{2},D\right)-\frac{D}{2}\right)\right)\right], & \text{if}\left|\text{mod}\left(x+\frac{D}{2},D\right)-\frac{D}{2}\right| \le \frac{1}{2} \\ \left(\frac{2}{15}z^{-9} - z^{-3}\right)\epsilon_s\,, & \text{else}\,. \end{cases} \tag{12.4}$$

The impact of those stripes was described in detail with an emphasis on the onset of the "recognition" transition below which the polymer perfectly adapts the shape of the stripe. Figure 12.5(b) shows that despite some striking differences, many conclusions drawn for the adsorption of a single polymer on a homogeneous substrate remain valid in the more general heterogeneous case [6].

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

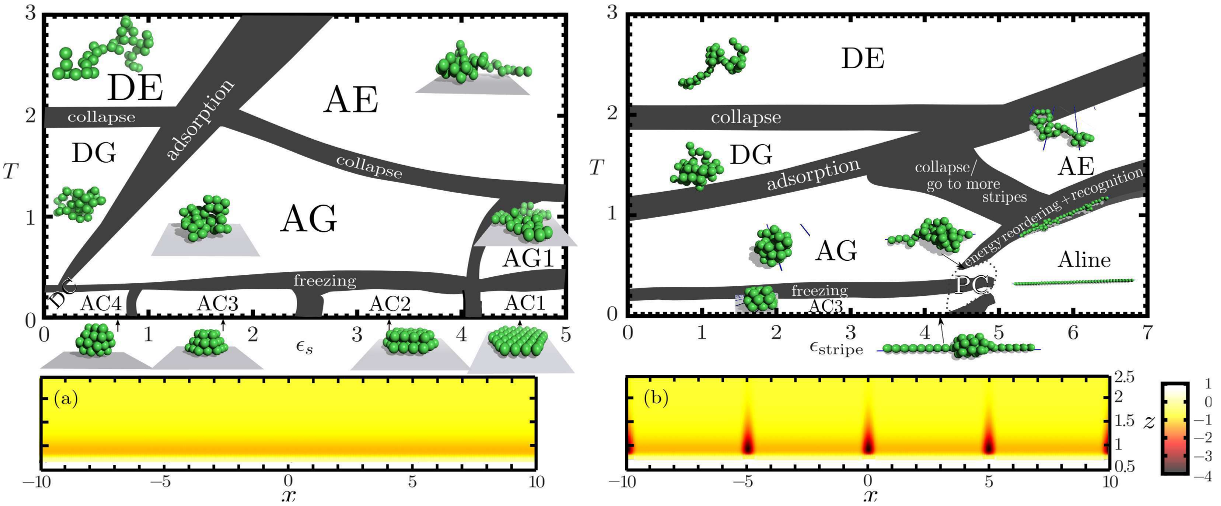


**Figure 12.5:** (a) Pseudo-phase diagram for polymer adsorption to a homogeneous substrate ($\epsilon_{\rm stripe} = 0$) in the temperature ($T$) – surface attraction ($\epsilon_s$) plane and a "heat map" of the substrate potential for $\epsilon_s = 1$. (b) Analogous pseudo-phase diagram for the stripe patterned case in the $T$–$\epsilon_{\rm stripe}$ plane for $\epsilon_s = 1$. Phases with "A/D" are adsorbed/desorbed, while "E", "G", and "C" denote phases with increasing order: expanded, globular, and compact. "PC" stands short for a region with phase coexistence.

[2] M. Möddel et al.: Phys. Chem. Chem. Phys. **12**, 11548 (2010)
[3] M. Möddel et al.: Macromolecules **44**, 9013 (2011)
[4] M. Möddel et al.: Comput. Phys. Comm. **182**, 1961 (2011)
[5] M. Möddel et al.: in Proceedings of the *NIC Symposium 2012*, eds. K. Binder, G. Münster, M. Kremer, John von Neumann Institute for Computing, Jülich, NIC Series, Vol. **45**, p. 277 (2012)
[6] M. Möddel et al.: Phys. Rev. Lett. **112**, 148303 (2014)

## 12.6 Poly(3-hexylthiophene) (P3HT) adsorption on reconstructed Au(001)

M. Ivanov, J. Gross, W. Janke

Regioregular Poly(3-hexylthiophene) (P3HT) is a very well studied conjugated polymer due to its interesting electronic and optical properties [1]. Recently P3HT has attracted attention for the use in donor/acceptor blends for photovoltaic applications [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 the influence of structure formation by polymer self-assembly on ideal surfaces on the electronic properties of oligo- and polythiophenes [5, 6]. Due to the complexity of these macromolecules the experimental findings have not been supported with simulations so far, which in contrast is well-established for studies of small organic molecules. This study reported on an collaborative effort within the DFG SFB/TRR 102 project to combine the experimental

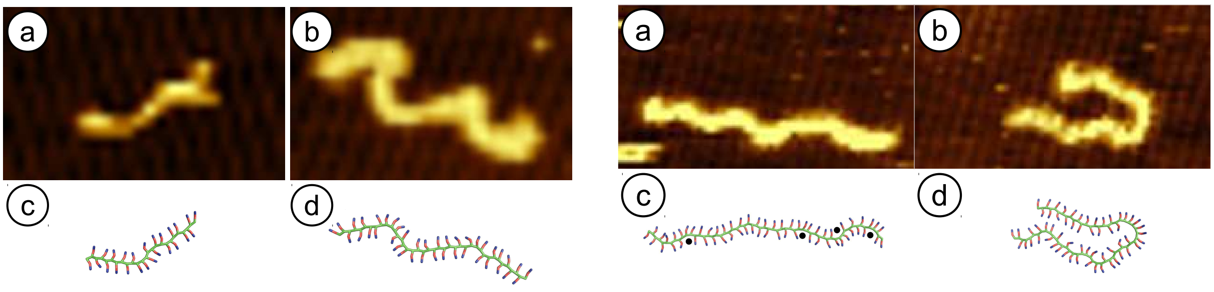


**Figure 12.6:** Left: Typical conformation of P3HT chains with (a, c) 25 and (b, d) 40 monomers observed in experiment (upper row) and simulation (lower row). Right: Similar comparison for (a, c) elongated coil and (b, d) collapsed hairpin conformations of a 60 monomer chain. Flipped side chains are marked with black dots in (c).

observation of polymer chain conformations adsorbed on a metal surface with Monte Carlo simulations of the coarse-grained P3HT model developed by Huang *et al.* [8].

In a previous study it has been shown that two different adsorption behaviours can be observed for in-situ deposited P3HT molecules on an Au(001) surface [7]. The polymer molecules adsorb either as weakly bonded random chains or as stronger interacting entities which locally lift the Au(001) reconstruction. The former random chain conformation is metastable at room temperature. It allows a molecular diffusion on the surface and was in the focus of the present work.

P3HT chains with a maximum length of 60 monomers were simulated in contact with an Au(001) surface. Their shapes were found in qualitative agreement with experimentally obtained chain conformations of in-situ deposited P3HT molecules on Au(001) as observed with scanning tunneling microscopy (STM), cf. Fig. 12.6. For a quantitative comparison the end-to-end distance as well as the radius of gyration of the molecules were determined. The results are published in Ref. [9].

[1] X. Bai, S. Holdcroft: Macromolecules **26**, 4457 (1993); Z. Bao et al.: Appl. Phys. Lett. **69**, 4108 (1996); M.R. Andersson et al.: J. Mater. Chem. **9**, 1933 (1999); B.W. Boudouris et al.: Macromolecules **44**, 6653 (2011)
[2] J.M. Frost et al.: Nano Letters **6**, 1674 (2006)
[3] M. Campoy-Quiles et al.: Nat. Mater. **7**, 158 (2008)
[4] A.M. Ballantyne et al.: Adv. Funct. Mater. **18**, 2373 (2008)
[5] Z.-Y. Yang et al.: ACS Nano **2**, 743 (2008)
[6] Y.-F. Liu et al.: Nanoscale **5**, 7936 (2013)
[7] S. Förster, W. Widdra: J. Chem. Phys. **141**, 054713 (2014)
[8] D.M. Huang et al.: J. Chem. Theory Comput. **6**, 526 (2010)
[9] S. Förster et al.: J. Chem. Phys. **141**, 164701 (2014)

## 12.7 Cluster growth during a polymer collapse

S. Majumder, W. Janke

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

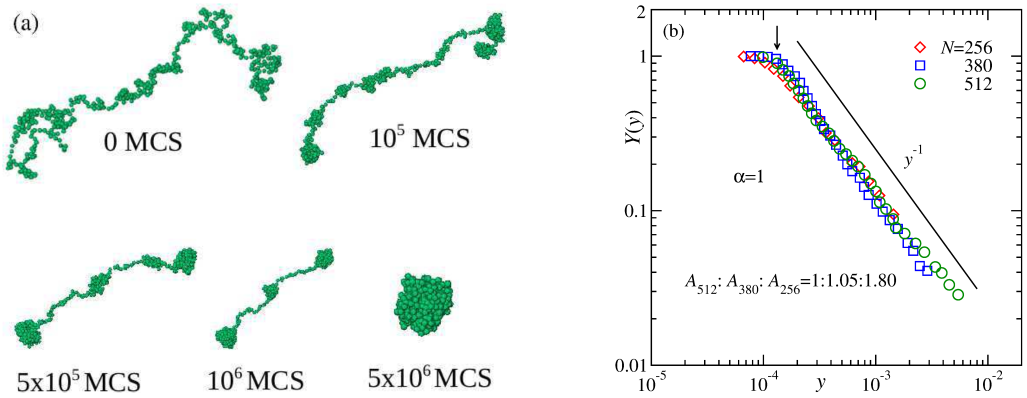


**Figure 12.7:** (a) Snapshots of a flexible polymer at different times showing the sequence of events occurring during the collapse, after being quenched from a high temperature expanded state to temperature below the theta transition [1]. (b) Finite-size scaling plots showing the collapse of data for different chain lengths confirming the linear growth of the average cluster size [1].

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 the formation, growth and subsequent coarsening or coalescence of clusters of monomers to form a single compact globule [2] as shown in Fig. 12.7(a). During this coarsening 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 have been studied in previous works [2], there exist no simulation studies which quantify the growth exponent unambiguously.

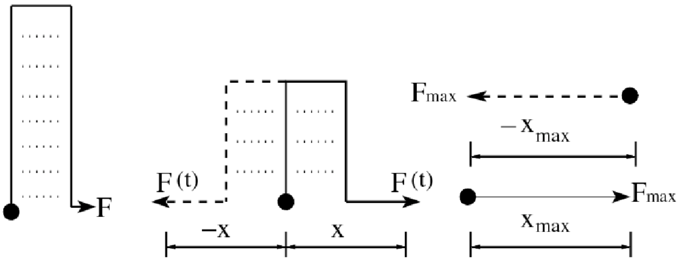
In this work we have addressed this issue from state of the art Monte Carlo simulations of a model polymer with the primary goal of quantifying the growth exponent for the cluster coarsening stage of the collapse. In the light of other coarsening systems we analyze our results via the application of finite-size scaling techniques in the nonequilibrium context [3]. Figure 12.7(b) shows such a scaling plot where the decay of the master curve suggests a linear growth of the average cluster size, confirming the universal Lifshitz-Slyozov mechanism of cluster growth, in contradiction to the previous theoretical and simulation results of Ref. [4].

[1] S. Majumder, W. Janke: *Cluster coarsening during polymer collapse: Finite-size scaling analysis*, Leipzig preprint (February 2015), to appear in Europhys. Lett., in print
[2] A. Halperin, P. Goldbart: Phys. Rev. E **61**, 565 (2000)
[3] S. Majumder, S.K. Das: Phys. Rev. E **81**, 050102(R) (2010); Phys. Rev. E **84**, 021110 (2011)
[4] Yu.A. Kuznetsov et al.: J. Chem. Phys. **103**, 4807 (1995); J. Chem. Phys. **104**, 3338 (1996)

## 12.8 Hysteresis and scaling of periodic driven DNA

S. Kumar*, R. Kumar, W. Janke

*Department of Physics, Banaras Hindu University, Varanasi 221 005, India



(a) Zipped

(b) Partially Zipped

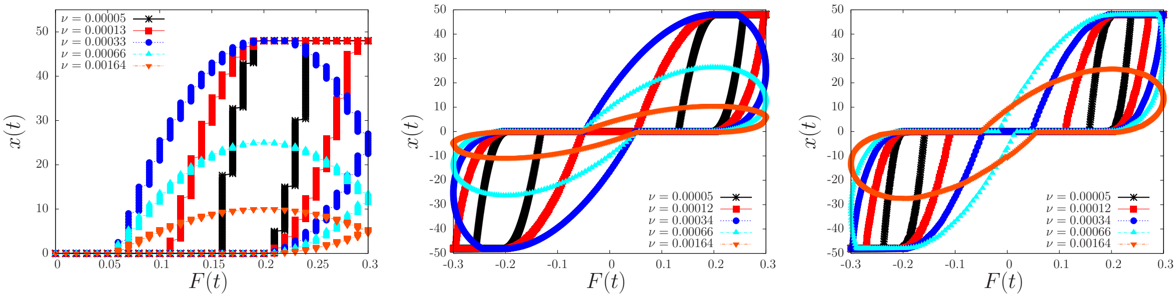
(c) Unzipped

**Figure 12.8:** Schematic representations of DNA: (a) zipped, (b) partially zipped, (c) unzipped state. One end is kept fixed (indicated by the solid circle), while the other end may move.

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

In this project, we have shown within a simplified model the existence of a dynamical transition in a system of driven DNA under the influence of an oscillatory force of amplitude $F$ and frequency $\omega$ [6], for a sketch see Fig. 12.8. A detailed comparison of the full Langevin equation with the Langevin equation in the over-damped limit has been performed. This shows that the scaling does not change by applying this approximation. For a chain of finite length, we observe that the area of hysteresis loops shown in Fig. 12.9 scales with the same exponents as proposed in the recent study of a semi-microscopic model [3]. However, in the true thermodynamic limit, we find that the high-frequency scaling regime extends to lower frequencies for larger chain length $L$, and the system has only one scaling regime where the area of the hysteresis loop scales with $\omega^{-1}F^2$. This indicates that a true dynamical transition may not exist in the thermodynamic limit. The scaling properties appear to be independent of temperature. Hence, the model proposed by us is accurate enough to study scaling properties, and at the same time it provides a possibility of analytic studies within certain limits.

[1] B. Alberts et al.: *Molecular Biology of the Cell* (Garland Publishing, New York, 1994)



(a) (b) (c)

**Figure 12.9:** Hysteresis loop for the model with parameters $L = 24$ and $F = 0.3$ for (a) a staircase-like and (b, c) a sinusoidal periodic force. (c) shows the effect of the over-damped limit.

[2] S. Kumar, M.S. Li: Phys. Rep. **486**, 1 (2010)
[3] S. Kumar, G. Mishra: Phys. Rev. Lett. **110**, 258102 (2013)
[4] G. Mishra et al.: Phys. Rev. E **87**, 022718 (2013)
[5] R.K. Mishra et al.: J. Chem. Phys. **138**, 244905 (2013)
[6] S. Kumar et al.: *Driven DNA: Does a dynamical transition exist in the thermodynamic limit?*, Varanasi/Leipzig preprint (May 2015), to be published

## 12.9 Self-avoiding walks on critical percolation clusters

N. Fricke, W. Janke

We investigate self-avoiding walks (SAWs) in the fractal disorder landscape of a diluted lattice at the percolation threshold. This well-established model for flexible polymers in disordered environments [1] poses a formidable challenge that has long eluded efficient numerical treatment.

Recently, we developed an exact enumeration algorithm which makes use of the self-similar, finitely-ramified structure of the system [2]. Through a properly targeted decomposition of the critical clusters, we are able to overcome the exponential complexity that is usually inherent to exact enumeration methods, enabling us to handle SAWs of several thousand steps on critical clusters of arbitrary dimensionality [3].

Enumerating walks of $N = 25$ to $N = 12800$ steps on over $5 \times 10^4$ clusters for each individual length we could precisely determine the exponent $\nu$ describing the asymptotic scaling behavior of the quenched average of the mean squared end-to-end distance via

$$\left[\left\langle R_{\mathrm{ee}}^2 \right\rangle\right] \sim N^{2\nu}. \tag{12.5}$$

This was done for the full incipient percolation clusters and the so-called cluster backbones, substructures without singly-connected dangling ends. As can be seen in Fig. 12.10 for the three-dimensional system, the asymptotic behavior is identical in both cases but only truly reveals itself after about $N = 800$ steps. Previous numerical studies [4, 5] had therefore yielded significantly larger results than our own [6]. Another surprising finding of our investigation concerns the average number of conformations,

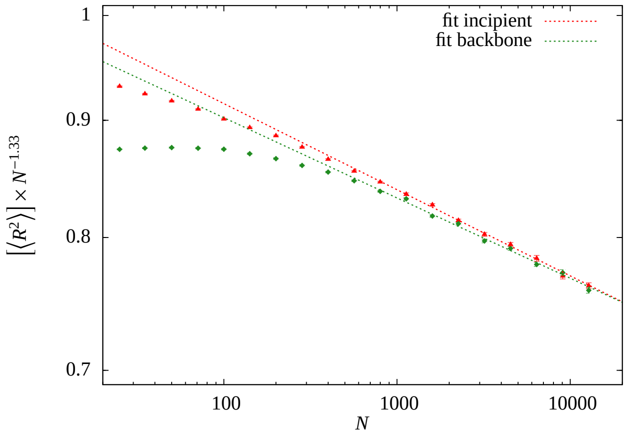


**Figure 12.10:** Mean squared end-to-end distance vs number of steps for SAWs on incipient critical clusters (red) and backbones (green) on a log-log scale. The lines show the results from least-squares fits of Eq. (12.5) over the ranges $N = 800$–$12800$ (incipient) and $N = 1131$–$12800$ (backbone). The factor $N^{-1.33}$ ($\approx N^{-2\nu}$) serves to magnify the differences.

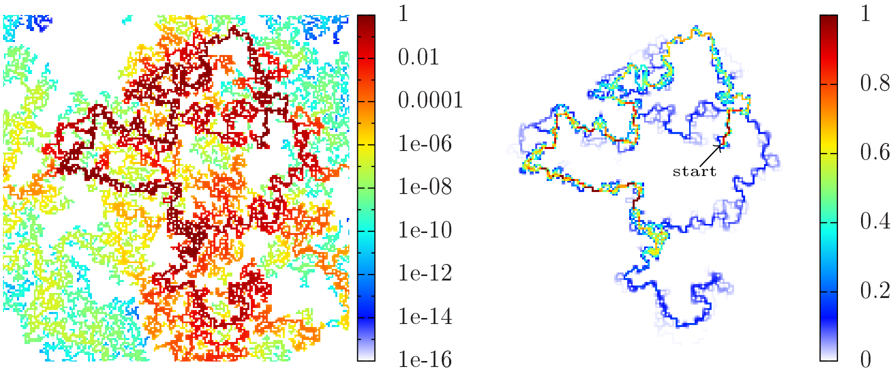


**Figure 12.11:** Fraction of SAW conformations passing through each site of a critical percolation cluster plotted on logarithmic (left) and linear color scale (right). Here the walks originate from the appendage in the upper right region and have a total length of $N = 800$ steps. Most conformations end in the dark red / yellowish region below the center.

which turned out to follow a scaling law of the form $[Z] \sim \mu^{N+bN^{\xi}}$ instead of the widely assumed $[Z] \sim \mu^N N^{\gamma-1}$. This unusual behavior is related to the fact that the entropy on each cluster is typically dominated by only one or two small regions, towards which the vast majority of SAWs of a fixed length gravitate via designated flow channels; see Fig. 12.11.

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[2] N. Fricke, W. Janke: Europhys. Lett. **99**, 56005 (2012)
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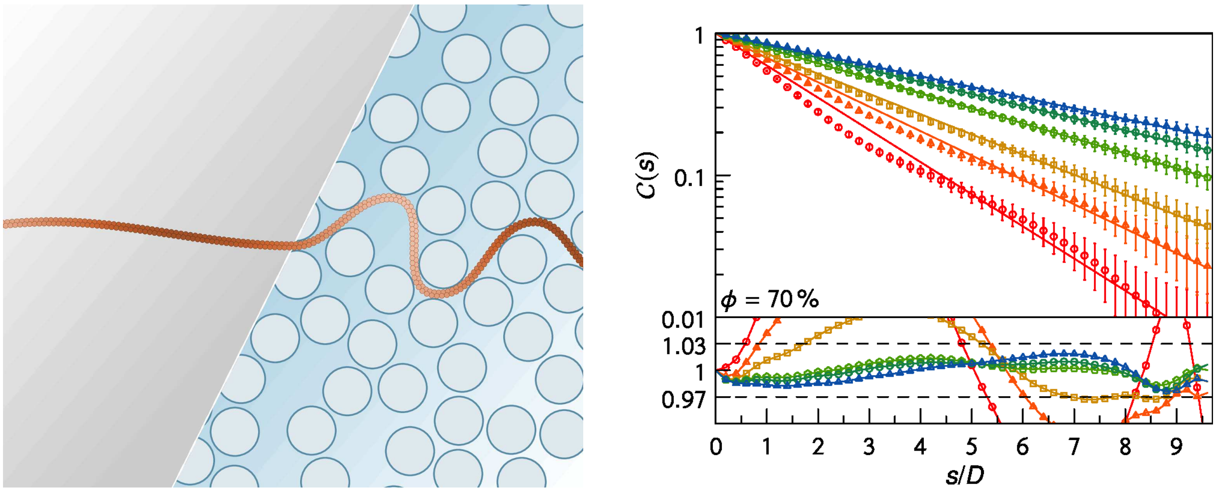
[6] V. Blavatska et al.: Condens. Matter Phys. **17**, 33604 (2014)

## 12.10 Semiflexible polymers in a hard-disk fluid: Persistence-length renormalization

S. Schöbl*, S. Sturm†, W. Janke, K. Kroy†

*Present address: d-fine GmbH, An der Hauptwache 7, 60313 Frankfurt, Germany
†Research Unit "Theory of Condensed Matter (TKM)"



(a) (b)

**Figure 12.12:** (a) Sketch of semiflexible polymers exposed to the quenched environment of a hard-disk fluid. Due to the randomly distributed obstacles the polymers bend more strongly (right) than their unconstrained counterparts in free space (left). (b) The numerically determined tangent-tangent correlations decay exponentially in the limit $\ell_p/D \to \infty$ (here shown for $\ell_p/D = 2, 3, 4, 6, 8, 10$ and a background filling fraction of 70%), and decay more quickly for higher disorder filling fractions $\phi$. The relative deviations of our exponential fits to the data shown in the lower panel nowhere exceed ≈ 3% above $\ell_p = 6D$. Reproduced from Ref. [5].

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 $\ell_p$.

When the same polymer is embedded in a quenched, disordered environment, this property may change quantitatively or even qualitatively. We addressed this problem by performing extensive numerical simulations of semiflexible polymers in a quenched equilibrium hard-disk fluid which represents the (correlated) disordered environment. Only the space between the hard disks 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].

As a main result we find that the wormlike chain statistics apparently still applies to the quenched, disordered environment, albeit with a renormalized persistence length $\ell_p^*$ [5]. For an illustration see Fig. 12.12. We identify a universal form of this disorder renormalization by showing that the observed $\ell_p^*$ fall onto a single master curve $l_p^D$ defined through

$$\frac{1}{\ell_p^*} = \frac{1}{\ell_p} + \frac{1}{\ell_p^D}, \tag{12.6}$$

where the "disorder persistence length" $\ell_p^D$ depends only on the disorder filling fraction. We argue that this novel effect may provide a useful quantitative measure of molecular crowding.

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[5] S. Schöbl et al.: Phys. Rev. Lett. **113**, 238302 (2014)

## 12.11 Random heteropolymer models

V. Blavatska[*], W. Janke

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

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

We studied the conformational transitions of quenched, random heteropolymers within a lattice model containing $N_A$ monomers of type A and $N_B = N - N_A$ monomers of type B. Such a model can describe in particular the sequences of hydrophobic and hydrophilic residues in proteins [1] and polyampholytes with oppositely charged groups [2]. Restricting ourselves only to short-range interactions between any pair of monomers residing on neighboring lattice sites that are not connected by a covalent bond, we considered 5 different parametrizations of this model. In particular, model 1 ($\varepsilon_{AA} = \varepsilon_{BB} = 1, \varepsilon_{AB} = -1$) where like monomers repel and opposite ones attract each other, refers to strongly screened Coulomb interactions [2]. The model 3 ($\varepsilon_{AA} = 1, \varepsilon_{BB} = \varepsilon_{AB} = 0$) is a particular case of model 1 and corresponds to a polymer chain containing charged (A) and neutral (B) monomers. Model 4 ($\varepsilon_{AA} = -1, \varepsilon_{BB} = \varepsilon_{AB} = 0$) refers to the (minimal) HP model [5] with hydrophobic (A) and hydrophilic (B) monomers. Models

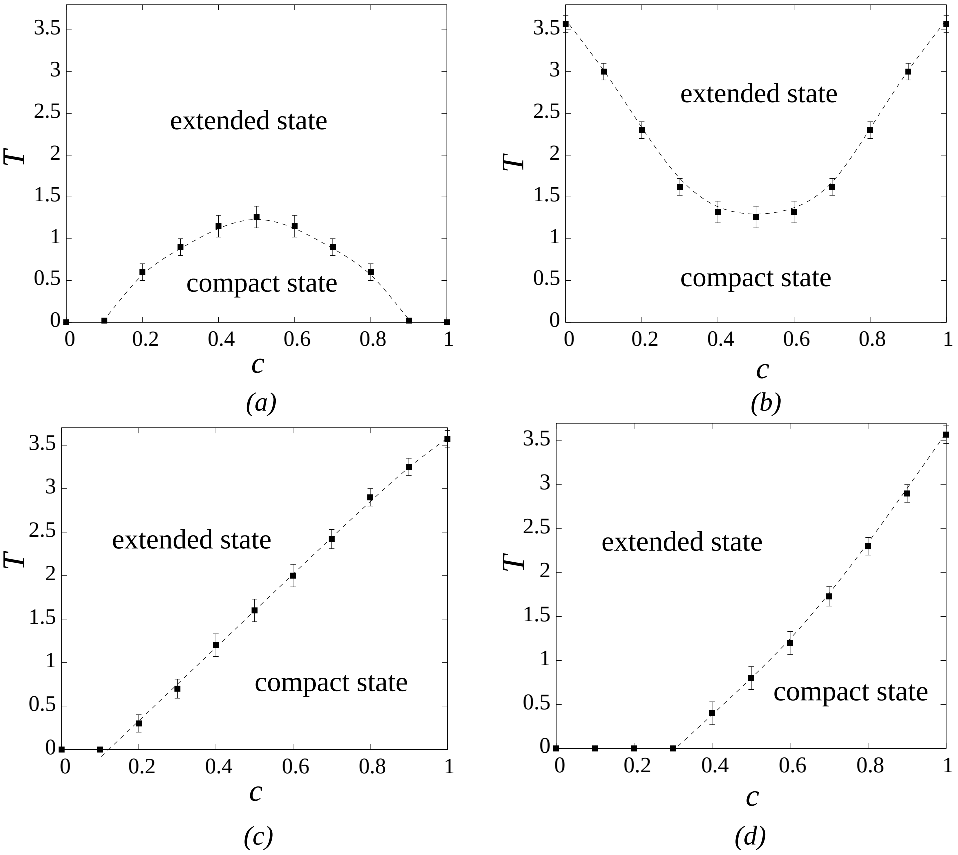

**Figure 12.13:** Phase diagrams of quenched, random heterogeneous polymer chains in $T$-$c$ space. (a) model 1, (b) model 2, (c) model 4, (d) model 5.

2 ($\varepsilon_{AA} = \varepsilon_{BB} = -1, \varepsilon_{AB} = 1$) and 5 ($\varepsilon_{AA} = -1, \varepsilon_{BB} = 1, \varepsilon_{AB} = 0$) can be considered as generalizations of the two above mentioned cases.

Applying the pruned-enriched Rosenbluth chain-growth algorithm (PERM) [3] we analyzed numerically the transitions from an extended into a compact state as function of the inhomogeneity ratio $c = N_A/N$ for all five heteropolymer chain models [4]. Figure 12.13 shows that in model 3, unlike the other models, the polymer chain expands its size with lowering the temperature due to the repulsion between monomers, and the polymer chain remains in an extended state at any temperature. In model 2, the $\theta$-transition is always present at any value of inhomogeneity ratio $c$, whereas models 1, 4 and 5 remain in an extended state when the concentration of attracting monomers is too small to cause a transition into the compact state. Note also that at small concentration of attractive monomers, the chains can attain the compact state only when they are long enough and have enough attractive nearest-neighbour contacts to overcome the conformational entropy. Models 2, 4 and 5 describe homogeneous polymer chains with nearest-neighbour attractions in the limiting case $c = 1$ (for model 2 also $c = 0$) with known value of the transition temperature $T_\theta = 3.717(3)$ [3].

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## 12.12 Morphing the energy landscape of spin glasses

S. Schnabel, W. Janke

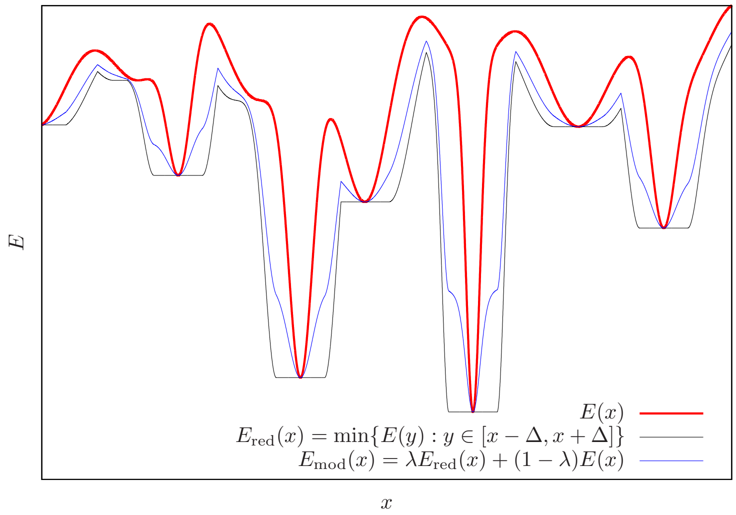

**Figure 12.14:** This sketch shows how a new variable (blue) with favorable characteristics can be composed from the energy (red) and a minimized energy (black).

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

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} S_i S_j \,, \tag{12.7}$$

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

We propose a novel technique related to the basin hopping algorithm [2]. In addition to the energy of a given configuration we evaluate the energy of the system after a short energy minimization and attribute this energy to the original configuration as well.

Combining these two values, it is possible to obtain a variable that retains the minima of the Hamiltonian but alters the shape of the surrounding valleys (see Fig. 12.14), thus facilitating the simulation and reducing autocorrelation time. We obtain ground-state energies that correspond well with data from the literature. Furthermore, we are able to reach lower energies in balanced simulations than possible before.

[1] S.F. Edwards, P.W. Anderson: J. Phys. F **5**, 965 (1975)
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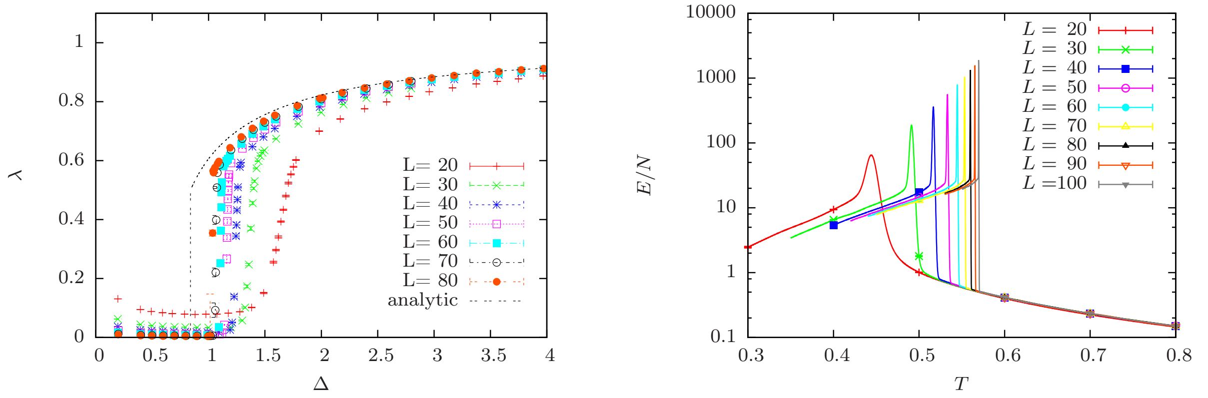
## 12.13 Finite-size scaling of three-dimensional lattice gas

J. Zierenberg, M. Wiedenmann, W. Janke



(a) (b)

**Figure 12.15:** (a) Fraction $\lambda$ of excess particles in the largest cluster versus "dimensionless" density $\Delta$ at fixed temperature $T = 0.5$. (b) Canonical specific-heat curves at fixed density $\rho = 0.01$.

We studied the condensation/evaporation transition of the three-dimensional (3D) lattice gas on a cubic lattice [1, 2]. The lattice gas models particles as occupied sites on the lattice and is equivalent to the Ising model at fixed magnetization. The condensation/evaporation transition is usually discussed and described at fixed temperature, where analytic predictions exist, including rigorous results for the two-dimensional Ising lattice gas [3]. Figure 12.15 (a) shows results for the 3D lattice gas varying a rescaled density compared to analytic predictions. This rescaling already includes the leading-order finite-size corrections and it may be anticipated that in the limit of large system sizes the analytic curve will describe the condensation/evaporation behaviour.

An alternative approach is to consider a fixed density and to identify the condensation transition temperature as the peak of the specific heat in Fig. 12.15 (b). This may be considered as an orthogonal direction, where the finite-size scaling corrections have the same size-dependence but may vary in amplitude [2]. We employed parallel multicanonical simulations [4], which allowed to obtain precise transition point estimates for relatively large system sizes including up to 10 000 particles. For the 3D lattice gas it seems that higher-order finite-size corrections are less pronounced in this approach, such that the largest system sizes were well described by the leading-order scaling predictions [2].

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

## 12.14 Nonstandard finite-size scaling at first-order phase transitions

M. Mueller, W. Janke, D.A. Johnston*

*Department of Mathematics and the Maxwell Institute for Mathematical Sciences,
Heriot-Watt University, Edinburgh, UK

Albeit first-order phase transitions being omnipresent in nature their generic features in numerical studies are rarely discussed compared to the universal aspects of second-order phase transitions. Numerical investigations rely on principle on observations of finite systems due to the finiteness of the memory of computers. Of physical interest, however, are the properties of macroscopic systems. In the limit of infinite system size, first-order phase transitions are characterized by jumps in the order parameter and $\delta$-function like divergences in response functions such as the specific heat or susceptibilities. In finite systems these singularities in observables are rounded and shifted much alike the effects in critical phenomena. These effects are systematic and thus a finite-size scaling theory was developed in the 1980's, which describes how the thermodynamic (many-particle or infinite-size) limit is approached. A rigorous solution for a class of models, including the Potts model under periodic boundary conditions has been found [1].

It is well established that the finite-size corrections at a first-order phase transition under periodic boundary conditions scale with the inverse system *volume*, that is $1/L^3$ for an $L \times L \times L$ lattice in three dimensions. The amplitudes of the correction terms are proportional to the logarithm $\ln q$ of the degeneracy $q$ of the low-temperature phase, which is not particularly important in many standard models, such as the $q$-state Potts model, where that degeneracy is just a constant. However, if the degeneracy $q$ of the low-temperature phase depends on the system size, oblique effects may disturb the traditional scaling ansatz with the inverse volume, leading to potentially wrong transition temperatures, latent heat and other observables.

In an extreme case with a macroscopic degeneracy $q \propto e^L$, the standard $1/L^3$ correction becomes $1/L^2$ [2]. One model with such a feature is the $3d$ plaquette-only gonihedric Ising model [3]. This is a member of a family of Hamiltonians that were originally formulated as a lattice discretization of string-theory actions in high-energy physics, which solely depend on the extrinsic curvature of the worldsheet [4].

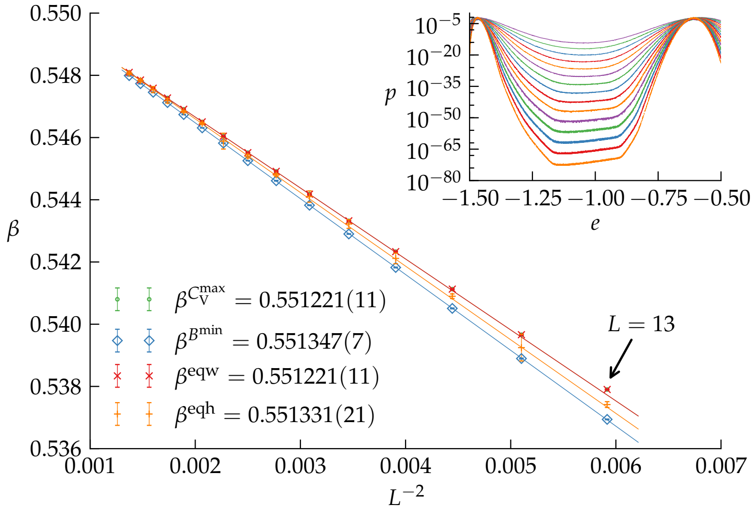

**Figure 12.16:** Fits that show clearly the leading $1/L^2$ scaling behaviour for the transition temperature obtained by different observables for the gonihedric Ising model. The inset shows the typical double-peaked energy probability density near the first-order phase transition temperature for different lattice sizes.

We used multicanonical simulations of this model to generate high-precision data which indeed provides strong confirmation of the nonstandard finite-size scaling law [2], see Fig. 12.16. We checked for consistency in the amplitudes of higher-order corrections [5] and peak values of the specific heat or Binder's energy minimum [6]. The dual to the gonihedric model, which is an anisotropically coupled Ashkin-Teller model [7], has a similar degeneracy and also displays the non-standard scaling law.

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

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[5] M. Mueller et al.: Nucl. Phys. B **888**, 214 (2014)
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## 12.15 Equilibrium properties of the gonihedric plaquette model

M. Mueller, W. Janke, D.A. Johnston*

*Department of Mathematics and the Maxwell Institute for Mathematical Sciences,
Heriot-Watt University, Edinburgh, UK

The plaquette model is a special case of a family of Hamiltonians called gonihedric Ising model, that 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 Hamiltonian of the plaquette-only gonihedric Ising model looks unobtrusive,

$$H = \sum_{[i,j,k,l]} \sigma_i \sigma_j \sigma_k \sigma_l \,, \tag{12.8}$$

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, only very recently we found that the finite-size scaling behaviour for this model is changed due to the exponential degeneracy in the low-temperature phase [3].

Applying the nonstandard finite-size scaling ansatz 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. Furthermore, our high-precision multicanonical simulations allowed the estimation of the interface tension $\sigma = 0.12037(18)$ of the model, along with great consistency in the amplitudes of higher-order corrections [4, 5]. The puzzling effect of obtaining different latent heats for different boundary conditions could be traced back to extraordinary huge boundary effects [6], see Fig. 12.17.

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 nonstandard finite-size effects, as depicted in the right of Fig. 12.17.

With our multicanonical simulations in collaboration 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.

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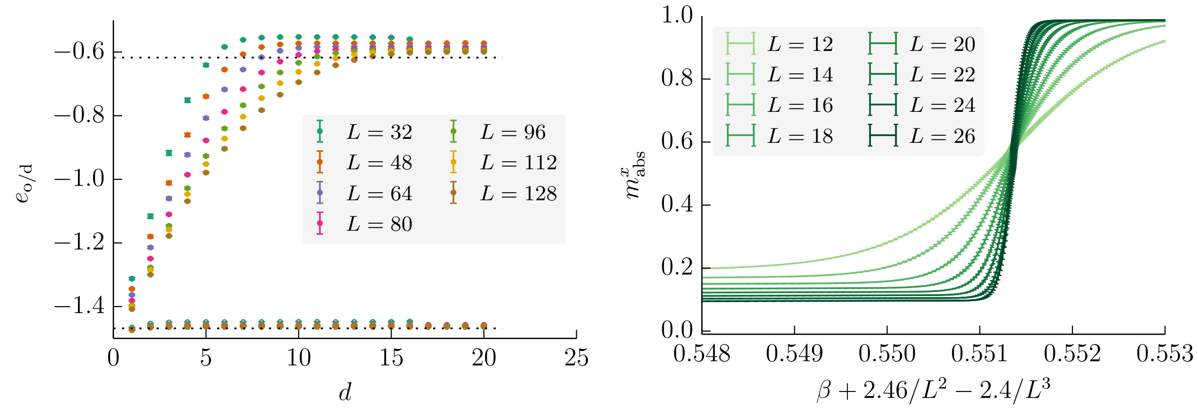

(a) (b)

**Figure 12.17:** (a) The disordered (upper) energies in layers at a distance $d$ to the boundary are severely influenced when applying fixed boundaries, leading to biased latent heats for smaller lattices. This long-range order is also reflected in the definition of the planar order parameter of the model. (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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## 12.16 First-order directional ordering transition in the three-dimensional compass model

M.H. Gerlach*, W. Janke

*Institut für Theoretische Physik, Universität zu Köln, Germany

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

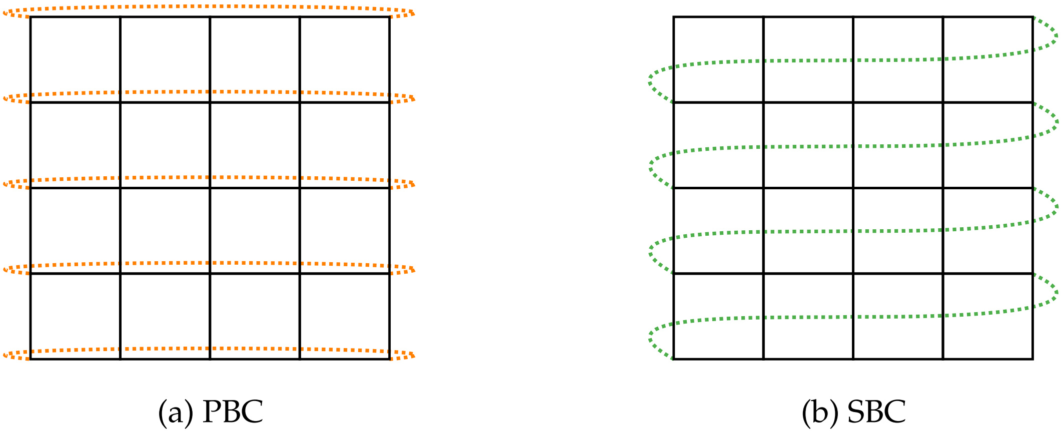

**Figure 12.18:** Sketch of (a) periodic (PBC) and (b) screw-periodic boundary conditions (SBC) along the $x$-axis of a two-dimensional lattice. In the SBC picture the link between the lower right and the upper left corner is not shown. Equivalent boundary conditions are applied to the $y$-direction. Here a screw parameter of $S = 1$ is used.

Hamiltonian

$$\mathcal{H} = J \sum_{i=1}^{N} \left( \sigma_i^x \sigma_{i+e_x}^x + \sigma_i^y \sigma_{i+e_y}^y + \sigma_i^z \sigma_{i+e_z}^z \right), \tag{12.9}$$

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

In recent analyses of high-temperature series expansions of the three-dimensional quantum model (where the classical spins are replaced by Pauli matrices) it was claimed that this model does not exhibit a phase transition at any finite temperature [6]. This motivated us to consider first the three-dimensional classical model and to investigate whether this model exhibits a phase transition [7]. To this end we employed state-of-the-art Monte Carlo computer simulations using Metropolis, cluster, and parallel tempering (PT) techniques. From our previous studies in two dimensions [5] we knew that employing so-called screw-periodic boundary conditions [8] sketched in Fig. 12.18 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. 12.19 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, $\sigma_{\mathrm{od}} \approx 3 \times 10^{-4}$.

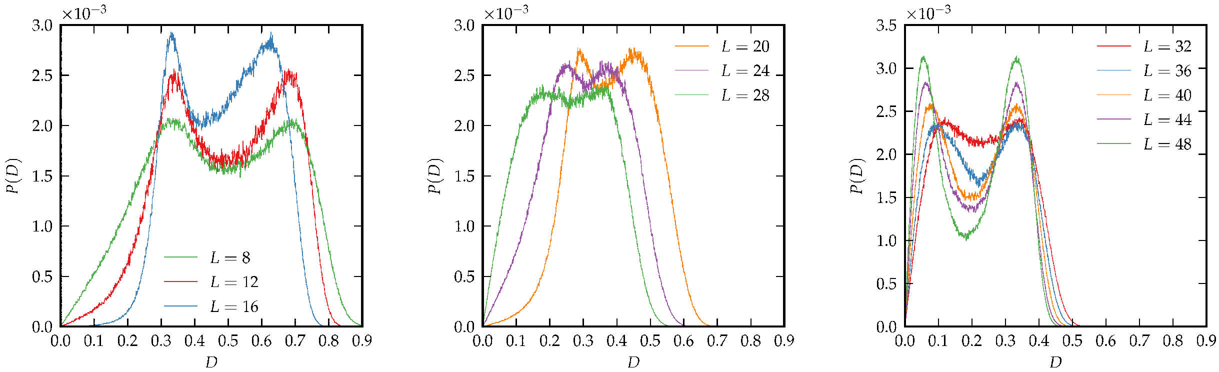

**Figure 12.19:** Histograms of the directional order parameter $D$ in the three-dimensional compass model with screw-periodic boundary conditions for various lattice sizes $L$.

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[9] S. Wenzel, A.M. Läuchli: Phys. Rev. Lett. **106**, 197201 (2011)

## 12.17 Parallel multicanonical study of the three-dimensional Blume-Capel model

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

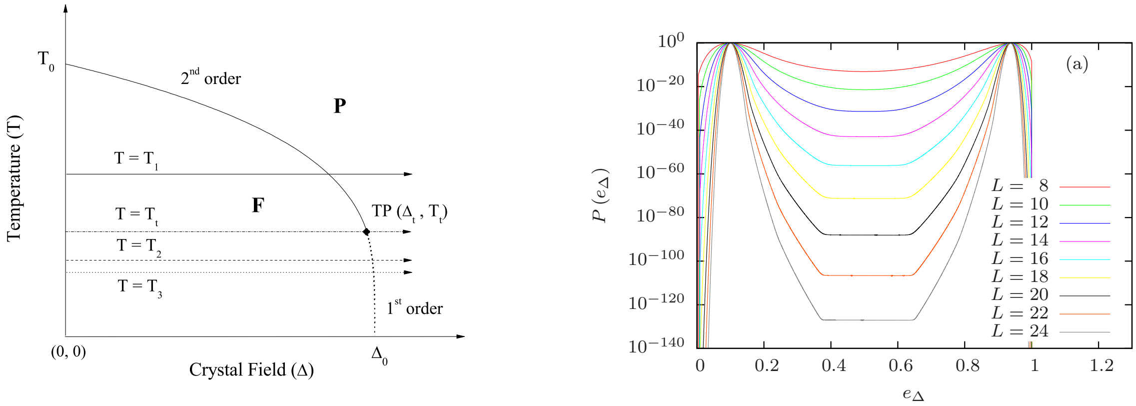
[*] Applied Mathematics Research Centre, Coventry University, UK

We studied the three-dimensional (3D) Blume-Capel model [1, 2] on a cubic lattice, a spin-one Ising model in a crystal field described by the Hamiltonian

$$\mathcal{H} = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j + \Delta\sum_{i}\sigma_i^2 = E_J + \Delta E_\Delta\,. \qquad (12.10)$$

Using a multicanonical based approach, we study the first- and second-order phase transition at fixed temperature along the crystal field axis [3], see Fig. 12.20(a). This exploits the numerical advantage of integer "magnetization" and the systematic advantage of a broad first-order regime over a wide range of temperatures, compared to a fixed-$\Delta$ approach.

Looking at a specific-heat like field-derivative of the spin-spin interaction term, $C(\Delta) = -\beta\big[\langle E_J E_\Delta\rangle - \langle E_J\rangle\langle E_\Delta\rangle\big]$, we performed finite-size scaling analyses in both the



(a) (b)

**Figure 12.20:** (a) Sketch of the 3D Blume-Capel phase diagram in the temperature – crystal field plane showing both a second-order (solid) and first-order (dashed) phase transition between the ferromagnetic (**F**) and paramagnetic (**P**) phase. (b) Fixed-temperature ($T_3 = 0.9$) probability distributions at the transition field $\Delta_{\mathrm{eqh}}$ with respect to $e_\Delta = E_\Delta/V$.

second-order ($T_1 = 2$) and first-order ($T_2 = 1$, $T_3 = 0.9$) regime as well as in the vicinity of a tricritical point estimate $T_t = 1.4182$ [4]. We verified the expected $\sim L^d$ scaling behavior in the first-order regime and the expected Ising universality class in the second-order regime with this orthogonal approach. A feature of this approach is the efficient study of the first-order regime, a tricky numerical task. Using a generalized-ensemble method, where also otherwise suppressed regions are sampled, see Fig. 12.20(b), allowed to even estimate accompanied free-energy like barriers. These may be related to spin-0 droplets/strips and vanish as one approaches the tricritical point. Our results at the tricritical estimate indicated its accuracy and yielded the expected Ising tricritical exponents from extrapolations of effective exponents.

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[4] M. Deserno: Phys. Rev. E **56**, 5204 (1997)

## 12.18 Tunable condensate shapes in a stochastic transport model

H. Nagel, E. Ehrenpreis, W. Janke

Condensation phenomena are observed in a broad range of physical processes on every length scale. While they are originally associated with the transition of matter from gas to some liquid or solid state, they are more generically realizations of nucleation and coarsening phenomena. A versatile approach to study such generic condensation mechanisms is the framework of stochastic transport processes with specific models such as the (asymmetric) simple exclusion process (ASEP), the zero-range process (ZRP)

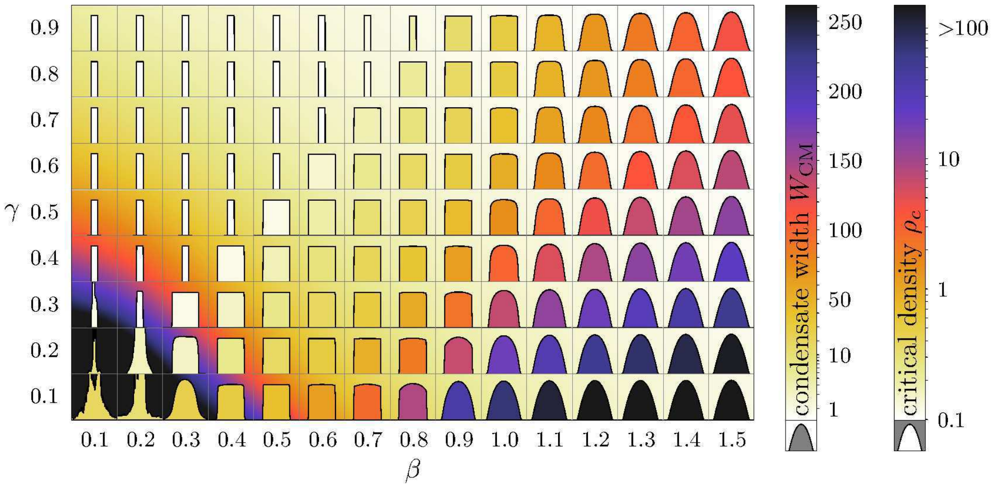

**Figure 12.21:** Numerically determined characteristic condensate shapes for systems of various $\beta$ and $\gamma$ at a condensate volume of about $10^5$ particles. The shapes are formed by rescaling the width and height of all measured condensate sample shapes and only then averaging them. The fill colour inside the condensate shapes encodes the average width while the background colour around the shapes gives the critical density of the condensation. The shapes in the single-site regime are plotted narrowed to give a better distinction to the extended condensate shapes.

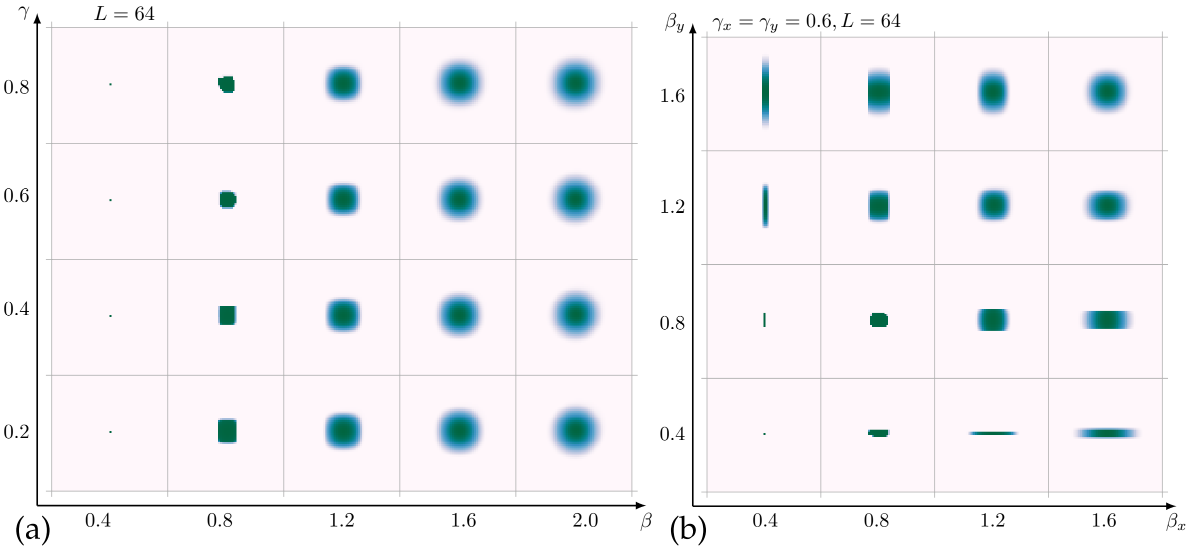

**Figure 12.22:** Mean condensate shapes for various values of the coupling constants $\beta$ and $\gamma$ of the considered condensation model in two dimensions for (a) isotropic and (b) anisotropic couplings (with $\gamma = 0.6$).

or the pair-factorized steady states (PFSS) transport model as a generalization of the ZRP with short-range interactions [1]. In this work, we consider a generic stochastic transport process with tunable nearest-neighbour interactions

$$g(m,n) = \exp[-|m-n|^{\beta} - 1/2(|m|^{\gamma} + |n|^{\gamma})]\,, \tag{12.11}$$

with the coupling constants $\beta$ and $\gamma$ for short-range and zero-range interactions, respectively. As predicted in previous analytical work [2, 3], these interactions lead to a steady state that features the formation of spatially extended particle condensates of various shapes and sizes for strengths of the zero-range coupling in the range $0 < \gamma < 1$. Single site condensates with properties similar to those of the ZRP are observed for weak nearest-neighbour couplings $\beta < \gamma$. Extended condensates are observed with rectangular shape for $\gamma < \beta < 1$ and with smooth parabolic shape for $\beta > 1$. Using Monte Carlo simulations we validated the predictions concerning characteristic shapes (see Fig. 12.21) and scaling laws of the condensate size of the emerging condensates in most parts of the $\beta$-$\gamma$ plane with very good agreement to the predicted scaling exponent $\alpha$ [4]. To simulate the technically challenging regime of rectangular condensates we proposed and successfully used a collective update method to overcome large barriers in the state space in between. Finally we extended the model to a two-dimensional system to systematically check how the mean condensate shape and the scaling of the its size is affected under change of the the coupling constants $\beta$ and $\gamma$, see Fig. 12.22.

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## 12.19 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 studied and understood on an abstract level is the emergence of generic condensates. In this project we systematically studied the phase diagram of such a transport process under driven particle exchange through open boundaries. While boundary drive induced phase transitions are long known for the ASEP, the research for the ZRP with condensation dynamics is more recent [1].

We considered a transport process 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.

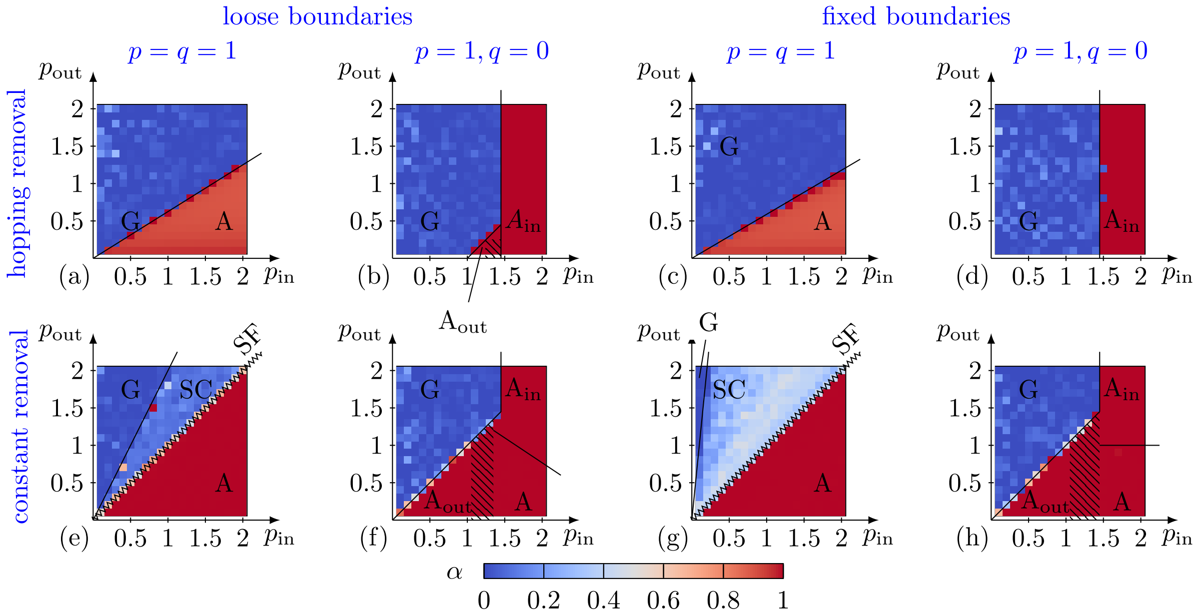

**Figure 12.23:** Phases induced by driven particle exchange through open boundary conditions of the system. With respect to the specific implementation of the interaction at the boundary, different phase diagrams are observed.

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]. The main phases, as shown in Fig. 12.23, 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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## 12.20 A simple non-equilibrium model for Stranski-Krastanov growth

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

[*]Marian Smoluchowski Institute of Physics and Mark Kac Complex Systems Research Center, Kraków, Poland
[†]School of Physics and Astronomy, University of Edinburgh, Scotland, UK

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

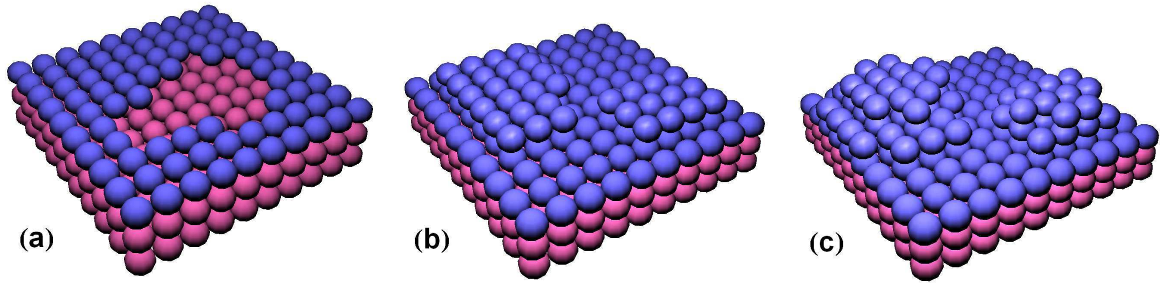

**Figure 12.24:** Schematic stages of Stranski-Krastanov growth. (a) The substrate (purple spheres) is covered with an increasing number of adatoms (blue spheres), starting from an incomplete monolayer. (b) As the density of adatoms increases, the adatoms form a complete monolayer and a partially filled 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.

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.

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[7] E. Ehrenpreis et al.: J. Phys. A: Math. Theor. **47**, 125001 (2014)

## 12.21 NVE-WHAM and the bridge between molecular dynamics and Monte Carlo simulations for liquid-gas like phase transitions

P. Schierz, J. Zierenberg, W. Janke

Molecular dynamics (MD) and Monte Carlo (MC) simulations are starting from two distinct physical points of views. While MD numerically integrates Newton's equations of motion, MC samples according to known ensemble probabilities from statistical physics. The foundation of statistical physics states that both approaches should give the same results in equilibrium.

MD simulations are normally considered to sample the NVE ensemble which is not entirely correct. Here $N$ stands for the particle number, $V$ denotes the volume, and $E = E_{\mathrm{kin}} + E_{\mathrm{pot}}$ is the total energy of the system. Since MD simulations without a thermostat encounter total linear and total angular momentum conservation, the available phase space for an MD simulation is restricted in comparison to the microcanonical ensemble. This results in a deviating behaviour of MD simulation data in comparison to NVE MC [1, 2] simulations for a small number of degrees of freedom. The simulation of a liquid-gas like phase transition becomes especially complicated with an MD simulation with periodic boundary conditions (PBC). For the gas phase the PBC will lead to a nonconserved angular momentum where the ensemble is described by: particle number, volume, total energy and total linear momentum $P$ (NVEP ensemble [4]). For the liquid phase the PBC will not change the total angular momentum $J$ which results in an ensemble where the angular momentum is additionally conserved (NVEPJ ensemble [5]).

Nonetheless it was possible to develop a method which allows to estimate the density of states of the simulated systems for the relevant potential energies of the liquid-gas like transitions [6]. For an illustration, see Fig. 12.25. This method was adapted from the known "Weighted Histogram Analysis Method" (WHAM) for the canonical ensemble [3]. The canonical weight in the WHAM method is replaced by the appropriate ensemble weights of the NVEP and NVEPJ ensemble. Therefore it is possible to estimate the density of states.

The density of states can be used to calculate the behaviour in the NVT ensemble and therefore to investigate phase transitions with varying temperature. Since the NVE ensemble shows very good sampling in the potential energy range of canonical first-order phase transitions it seems possible to estimate the NVT phase-transition behaviour by performing many NVE simulations at various total energies. In this way it is possible to distribute the computational effort to many computer cores. 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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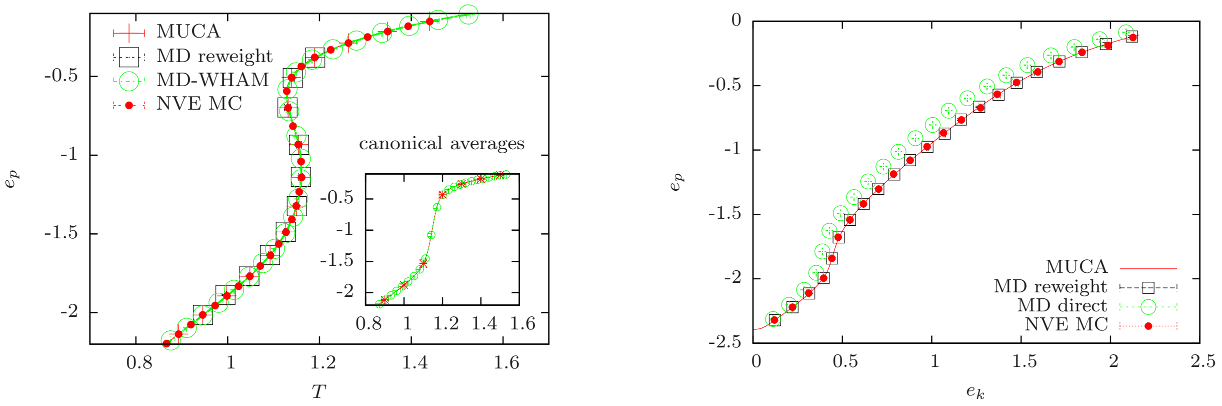


(a)

(b)

**Figure 12.25:** (a) The potential energy vs. temperature for 8 polymers with 13 monomers each, simulated with two Monte Carlo techniques and MD. (b) The potential energy vs kinetic energy for a single polymer with 13 monomers. The MD data is once evaluated directly (NVEPJ ensemble) and once reweighted to the NVE ensemble.

[6] P. Schierz et al.: *Molecular Dynamics and Monte Carlo simulations in the microcanonical ensemble: Quantitative comparison and reweighting techniques*, Leipzig preprint (May 2015), to be published

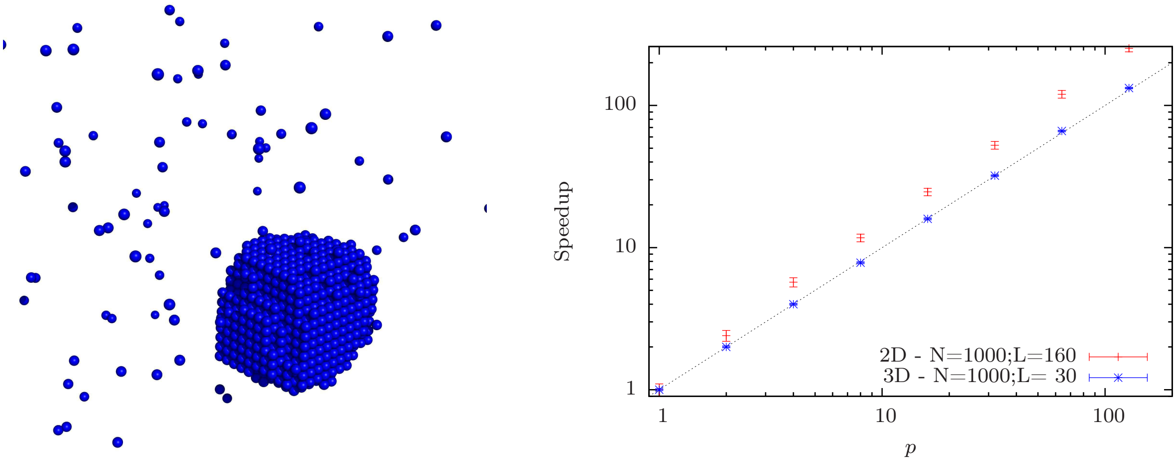
## 12.22 Application of the parallel multicanonical method to a broad range of problems

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

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

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

For any real-life application, we continue to consider a fixed number of sweeps per multicanonical iteration that is distributed onto the number of cores. This is the only possibility to assess larger or more complicated systems and shows the expected scaling also for first-order transitions like gas condensation in two and three dimensions, see Fig. 12.26 [3]. With this method, we were able to show that in three dimensions lattice gas condensation shows an unexpected deviation from the analytic predictions which may be explained by finite-size effects but needs additional investigations.



(a) (b)

**Figure 12.26:** (a) Lattice gas in the droplet phase as an example for (b) the speedup in a day-to-day application.

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

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[2] J. Zierenberg et al.: Physics Procedia **53**, 55 (2014)
[3] J. Zierenberg et al.: J. Phys.: Conf. Ser. **510**, 012017 (2014)

## 12.23 Status of our framework for programming Monte Carlo simulation ($\beta$MC).

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.

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

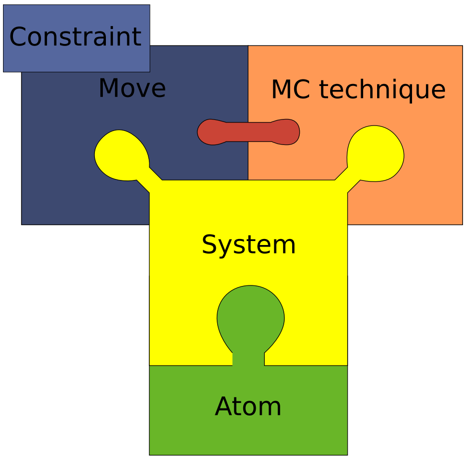

**Figure 12.27:** The 5 basic building blocks.

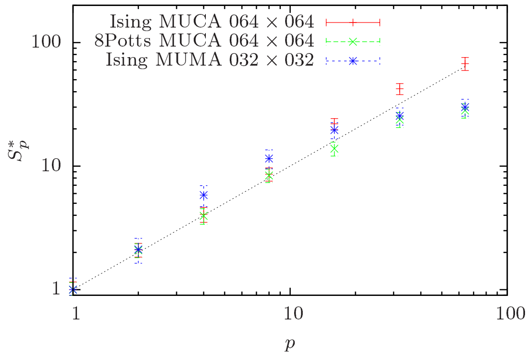

**Figure 12.28:** Scaling properties of the parallel multicanonical algorithm as a function of the number of processors $p$.

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. 12.27: 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. 12.28.

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 let already to the publication of several papers [2–6].

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## 12.24 Funding

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W. Janke (with B. Berche, Nancy)
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W. Janke (Scientific Member)
Max Planck Society and Klaus Tschira Foundation

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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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Sonderforschungsbereich/Transregio SFB/TRR 102 *Polymers under Multiple Constraints: Restricted and Controlled Molecular Order and Mobility*
W. Janke (Principal Investigator, project B04)
Deutsche Forschungsgemeinschaft (DFG)

Junior Research Group ("Nachwuchsforschergruppe") *Werkzeuge und Technologien für die rationale Wirkstoffentwicklung*
J. Bock, W. Janke
Europäischer Sozialfond (ESF)

Junior Research Group ("Nachwuchsforschergruppe") *Funktion durch Selbstorganisation: Emergente Eigenschaften von Atom- und Molekülaggregaten*
P. Schierz, W. Janke
Europäischer Sozialfond (ESF)

*Molecular Conformation Mechanics of Proteins and Polymers*
W. Janke
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W. Janke (twin project with H. Meyer-Ortmanns, Jacobs University Bremen)
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W. Janke (with V. Blavatska, Lviv)
Alexander von Humboldt Foundation (AvH)

Marie Curie IRSES Network *DIONICOS: Dynamics of and in Complex Systems*
W. Janke (Principal Investigator, head of Leipzig node)
European Union (EU)

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

## 12.25 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

- Permanent Member of the International Advisory Board for the Annual *Conference of the Middle European Cooperation in Statistical Physics (MECO)*
- Co-organizer of the "BuildMoNa" Modul 2014-B3 *Basic Concepts in Physics* (with F. Cichos and P. Esquinazi), Universität Leipzig, 7./14./15. May 2014
- Member of the International Scientific Committee for the *Humboldt Kolleg: German-Turkish Cooperation in Physics: New Challenges in Science*, Ankara University, Ankara, Turkey, 11.–13. June 2014
- Chair of Program Committee *Classical Statistical Mechanics and Complex Systems* of the XXVI IUPAP *Conference on Computational Physics* CCP2014, Boston, Massachusetts, USA, 11.–14. August 2014
- Organizer of the Workshop *CompPhys14* – 15th International NTZ Workshop on *New Developments in Computational Physics*, ITP, Universität Leipzig, 27.–29. November 2014
- Organizer of the Workshop *CompPhys15* – 16th International NTZ Workshop on *New Developments in Computational Physics*, ITP, Universität Leipzig, 26.–28. November 2015
- Guest Editor (with Y. Holovatch (Lviv, Ukraine) and S. Turner (Vienna, Austria)) for the Special Issue of Condens. Matter Phys.: *Self-Organization and Collective Behaviour in Complex Systems*
- Editor "Computational Physics", Central European Journal of Physics, Krakow, Poland
- Member of Editorial Board, Condens. Matter Phys., Lviv, Ukraine
- External Reviewer for Deutsche Forschungsgemeinschaft (DFG), Humboldt-Stiftung (AvH), Studienstiftung des deutschen Volkes, Fond zur Förderung der wissenschaftlichen Forschung (FWF), Österreich, The Royal Society, UK, The Engineering and Physical Sciences Research Council (EPSRC), UK, Israel Science Foundation, Israel, National Science Foundation (NSF), USA, Natural Sciences and Engineering Research Council of Canada (NSERC), Canada, The Jeffress Memorial Trust, Bank of America, Virginia, USA, Universität Mainz, Germany, The University of Warwick, England, UK, Coventry University, England, UK, CECAM, Lyon, France
- Referee for Physical Review Letters, Physical Review B, Physical Review E, Journal of Chemical Physics, Europhysics Letters, Physics Letters A, Physics Letters B, The European Physical Journal B, Physica A, Proceedings of the Royal Physical Society, Journal of Physics A, Computer Physics Communications, JSTAT, Condens. Matter Phys., PLOS ONE, New Journal of Physics, International Journal of Modern Physics C

## 12.26 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, Simon Mitternacht
- Department of Mathematics and the Maxwell Institute for Mathematical Sciences, Heriot-Watt University, Edinburgh, Scotland, UK
  Prof. Dr. Desmond A. Johnston
- Applied Mathematics Research Centre, Coventry University, England, UK
  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, Turkey
  Prof. Dr. Handan Arkın (Olgar), Mustafa Bilsel, Buket Taşdizen

- Dept. of Physics, Hacettepe University, Ankara, Turkey
  Prof. Dr. Tarik Çelik, Gökhan Gökoğlu
- Institute for Condensed Matter Physics, National Academy of Sciences, Lviv, Ukraine
  Dr. Viktoria Blavatska, Prof. Dr. Yurij Holovatch
- Yerevan Physics Institute, Yerevan, Armenia
  Prof. Dr. David B. Saakian
- Landau Institute for Theoretical Physics, Chernogolovka, Russia
  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, Dr. Thomas Vogel
- 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
- 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
- Laboratory of Statistical and Computational Physics, Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan
  Prof. Dr. Chin-Kun Hu
- The University of Tokyo, Japan
  Prof. Dr. Nobuyasu Ito
- Banaras Hindu University, Varanasi, India
  Prof. Dr. Sanjay Kumar
- Nagoya University, Japan
  Dr. Tetsuro Nagai, Prof. Dr. Yuko Okamoto
- Zhejiang Institute of Modern Physics, Zhejiang University, Hangzhou, P.R. China
  Prof. Dr. He-Ping Ying, Prof. Dr. Bo Zheng

## 12.27 Publications

**Journals**

V. Blavatska, N. Fricke, W. Janke: *Polymers in Disordered Environments*, Condens. Matter Phys. **17**, 33604-1–11 (2014)

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

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

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

S. Förster, E. Kohl, M. Ivanov, J. Gross, W. Widdra, W. Janke: *Polymer Adsorption on Reconstructed Au(001): A Statistical Description of P3HT by Scanning Tunneling Microscopy and Coarse-Grained Monte Carlo Simulations*, J. Chem. Phys. **141**, 164701-1–8 (2014)

N. Fricke, W. Janke: *Asymptotic Scaling Behavior of Self-Avoiding Walks on Critical Percolation Clusters*, Phys. Rev. Lett. **113**, 255701-1–5 (2014)

J. Gross, T. Neuhaus, T. Vogel, M. Bachmann: *Statistical Analysis of the Influence of Interaction Ranges on Structural Phases of Flexible Polymers*, in: *Computer Simulation Studies in Condensed-Matter Physics XXVI*, eds. D.P. Landau, M. Bachmann, S.P. Lewis, H.-B. Schüttler, Physics Procedia **53**, 50–54 (2014)

M. Marenz, W. Janke: *Effect of Bending Stiffness on a Homopolymer Inside a Spherical Cage*, in: *Computer Simulation Studies in Condensed-Matter Physics XXVII*, eds. H.-B. Schüttler, S. Lewis, M. Bachmann, D.P. Landau, Physics Procedia **57**, 53–57 (2014)

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

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

M. Mueller, W. Janke, D.A. Johnston: *Transmuted Finite-Size Scaling at First-Order Phase Transitions*, in: *Computer Simulation Studies in Condensed-Matter Physics XXVII*, eds. H.-B. Schüttler, S. Lewis, M. Bachmann, D.P. Landau, Physics Procedia **57**, 68–72 (2014)

M. Mueller, D.A. Johnston, W. Janke: *Multicanonical Analysis of the Plaquette-Only Gonihedric Ising Model and its Dual*, Nucl. Phys. B **888**, 214–235 (2014)

H. Nagel, D. Labavić, H. Meyer-Ortmanns, W. Janke: *Open Boundary Conditions in Stochastic Transport Processes with Pair-Factorized Steady States*, in: *Computer Simulation Studies in Condensed-Matter Physics XXVII*, eds. H.-B. Schüttler, S. Lewis, M. Bachmann, D.P. Landau, Physics Procedia **57**, 77–81 (2014)

J.C.S. Rocha, S. Schnabel, D.P. Landau, M. Bachmann: *Identifying Transitions in Finite Systems by Means of Partition Function Zeros and Microcanonical Inflection-Point Analysis: A Comparison for Elastic Flexible Polymers*, Phys. Rev. E **90**, 022601-1–10 (2014)

J.C.S. Rocha, S. Schnabel, D.P. Landau, M. Bachmann: *Leading Fisher Partition Function Zeros as Indicators of Structural Transitions in Macromolecules*, in: *Computer Simulation Studies in Condensed-Matter Physics XXVII*, eds. H.-B. Schüttler, S. Lewis, M. Bachmann, D.P. Landau, Physics Procedia **57**, 94–98 (2014)

S. Schöbl, S. Sturm, W. Janke, K. Kroy: *Persistence-Length Renormalization of Polymers in a Crowded Environment of Hard Disks*, Phys. Rev. Lett. **113**, 238302-1–5 (2014)

J. Zierenberg, M. Marenz, W. Janke: *Scaling Properties of Parallelized Multicanonical Simulations*, in: *Computer Simulation Studies in Condensed-Matter Physics XXVI*, eds. D.P. Landau, M. Bachmann, S.P. Lewis, H.-B. Schüttler, Physics Procedia **53**, 55–59 (2014)

J. Zierenberg, M. Mueller, P. Schierz, M. Marenz, W. Janke: *Aggregation of Theta-Polymers in Spherical Confinement*, J. Chem. Phys. **141**, 114908-1–9 (2014)

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

### Books

Y. Holovatch, W. Janke, S. Thurner (Editors): *Self-Organization and Collective Behaviour in Complex Systems*, Special issue in memory of Professor Alexandr Olemskoi, Condens. Matter Phys., Vol. **17**, No. 3, 2014

### in press

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

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

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

N. Fricke, S. Sturm, M. Lämmel, S. Schöbl, K. Kroy, W. Janke: *Polymers in Disordered Environments*, to appear in Diff. Fundam. (2015), in print

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

W. Janke, M. Mueller, D.A. Johnston: *Finite-Size Scaling and Latent Heat at the Gonihedric First-Order Phase Transition*, to appear in J. Phys.: Conf. Ser. (2015), in print

D.A. Johnston, M. Mueller, W. Janke: *Macroscopic Degeneracy and Order in the 3$d$ Plaquette Ising Model*, to appear in Mod. Phys. Lett. B (2015), in print

S. Majumder, W. Janke: *Cluster Coarsening During Polymer Collapse: Finite-Size Scaling Analysis*, to appear in Europhys. Lett. (2015), in print

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*, to appear in: *Computer Simulation Studies in Condensed-Matter Physics XXVIII*, eds. H.-B. Schüttler, S.P. Lewis, M. Bachmann, D.P. Landau, to appear in Physics Procedia (2015), in print

**Talks**

N. Fricke, W. Janke: *Self-Avoiding Walks and Θ-Polymers on Critical Percolation Clusters*, DPG Frühjahrstagung, Dresden, Germany, 31. March – 04. April 2014

N. Fricke, W. Janke: *True Asymptotics of Self-Avoiding Walks on 3D Percolation Clusters*, 15th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys14*, Leipzig, Germany, 27.–29. November 2014

J. Gross, M. Bachmann: *Monte Carlo Study of Polymer Adsorption on Nanocylinders*, DPG Frühjahrstagung, Dresden, Germany, 31. March – 04. April 2014

J. Gross, M. Ivanov, W. Janke: *Poly(3-hexylthiophene) Adsorption on Au(001)*, 15th International NTZ-Workshop on *New Developments in Computational Physics – Comp Phys14*, Leipzig, Germany, 27.–29. November 2014

W. Janke: *Monte Carlo Simulations of Polymer Adsorption and Aggregation in Generalized Ensembles*, invited talk, VI International Conference BIFI2014 *Exploring the Role of Computation in Science: From Biology to Physics*, Zaragoza, Spain, 22.–24. January 2014

W. Janke: *Transmuted Finite-Size Scaling at First-Order Phase Transitions with Extensive Low-T Degeneracies*, 27th CSP Workshop on *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, The University of Georgia, Athens, Georgia, USA, 24.–28. February 2014

W. Janke: *Simulated Tempering and Magnetizing Monte Carlo Study of Crossover Scaling in the 2d 3-State Potts Model*, DPG Frühjahrstagung, TU Dresden, Germany, 30. March – 04. April 2014

W. Janke: *Scaling Properties of a Parallel Implementation of the Multicanonical Algorithm*, Physics Seminar, TU Chemnitz, Germany, 23. April 2014

W. Janke: *Introduction to Basic Concepts of Statistical Physics, Thermodynamics, and Computer Simulations*, BuildMoNa Scientific Module 2014-B3 *Basic Concepts in Physics*, Universität Leipzig, Germany, 07. May 2014

W. Janke: *Non-Standard Finite-Size Scaling at First-Order Phase Transitions*, Workshop *Statistical Physics and Low Dimensional Systems – SPLDS*, Pont-à-Mousson, France, 21.–23. May 2014

W. Janke: *Computer Simulation Studies of Polymers – Adsorption and Aggregation from Flexible to Stiff*, invited talk, Humboldt Kolleg 2014 *German-Turkish Cooperation in Physics: New Challenges in Science*, Ankara University, Turkey, 11.–13. June 2014

W. Janke: *Non-Standard Finite-Size Scaling at a First-Order Phase Transition*, XXVI IUPAP *Conference on Computational Physics CCP2014*, Boston University, Massachusetts, USA, 10.–14. August 2014

R. Kumar, S. Kumar, W. Janke: *Dynamical Transition in Driven DNA Under Oscillatory Force: Hysteresis and Scaling*, Seminar of the cdfa-dfdk, Coventry University, England, UK, 15. October 2014

M. Marenz, W. Janke: *Effect of Bending Stiffness on a Homopolymer Inside a Spherical Cage*, 27th CSP Workshop on *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, The University of Georgia, Athens, Georgia, USA, 25. February 2014

M. Mueller: *Pedantic Fitting and Why it Matters*, Seminar of the cdfa-dfdk, Leipzig, Germany, 23. January 2014

M. Mueller, D.A. Johnston, W. Janke: *Macroscopic Degeneracy Influences the Finite-Size Scaling at First-Order Phase Transitions*, 15th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys14*, Leipzig, Germany, 27.–29. November 2014

H. Nagel, D. Labavic, H. Meyer-Ortmanns, W. Janke: *Open Boundary Conditions in Stochastic Transport Processes with Pair-Factorized Steady States*, 27th Annual Workshop of the Center for Simulational Physics, Athens, Georgia, USA, 25. February 2014

P. Schierz, J. Zierenberg, W. Janke: *Comparison of Microcanonical MD and MC Simulations for Liquid-Gas Like Phase Transitions*, 15th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys14*, Leipzig, Germany, 27.–29. November 2014

S. Schnabel, W. Janke: *Trying to Flip the Right Spins in the Edwards-Anderson Model*, Seminar talk at Texas A&M, College Station, Texas, USA, 09. September 2014

J. Zierenberg, W. Janke: *Exploring Different Regimes in Finite-Size Scaling of the Droplet Condensation/Evaporation Transition*, Seminar of the cdfa-dfdk, Coventry University, England, UK, 15. October 2014

J. Zierenberg, M. Mueller, P. Schierz, M. Marenz, W. Janke: *Aggregation of Semiflexible Polymers Under Constraints*, 15th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys14*, Leipzig, Germany, 27.–29. November 2014

**Posters**

E. Bittner, W. Janke: *MuCa vs WL: A Tight Race*, Conference MECO 39, Coventry University, England, UK, 08.–10. April 2014

J. Bock, N. Fricke, W. Janke: *Kinetic Growth Random Walks*, DPG Frühjahrstagung, Dresden, Germany, 31. March – 04. April 2014

J. Bock, W. Janke: *Computer Simulations of Semiflexible Polymers in Disordered Media*, XXVI IUPAP *Conference on Computational Physics CCP2014*, Boston University, Massachusetts, USA, 11.–14. August 2014

J. Bock, W. Janke: *Computer Simulations of Semiflexible Polymers in Disordered Media*, 15th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys14*, Leipzig, Germany, 27.–29. November 2014

M. Ivanov, J. Gross, M. Mueller, W. Janke: *Polymers Interacting with Substrates*, SFB/TRR 102, 3rd Retreat, Wittenberg, Germany, 17. March 2014

M. Ivanov, J. Gross, W. Janke: *P3HT Molecules Interacting with Au(001) Substrates*, SFB/TRR 102, Satellite Meeting Makro 2014, Jena, Germany, 16. September 2014

M. Ivanov, J. Gross, W. Janke: *P3HT Molecules Interacting with Au(001) Substrates*, 15th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys14*, Leipzig, Germany, 27.–29. November 2014

M. Ivanov, M. Möddel, W. Janke: *Polymer Adsorption onto a Stripe-Patterned Surface*, DPG Frühjahrstagung, Dresden, Germany, 31. March – 04. April 2014

W. Janke, J. Zierenberg: *From Amorphous Aggregates to Polymer Bundles: The Role of Stiffness on Structural Phases in Polymer Aggregation*, Conference MECO 39, Coventry University, England, UK, 08.–10. April 2014

M. Marenz, J. Zierenberg, W. Janke: *Semiflexible Polymer in a Spherical Cage*, NIC Symposium, Forschungszentrum Jülich, Germany, 12.–13. February 2014

M. Marenz, N. Fricke, J. Zierenberg, W. Janke: *Revisiting Percolation on Power-Law Correlated Disorder*, 15th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys14*, Leipzig, Germany, 27.–29. November 2014

M. Mueller, W. Janke, D.A. Johnston: *Transmuted Finite-Size Scaling at First-Order Phase Transitions with Exponential Degeneracy of Ordered States*, DPG Frühjahrstagung, Dresden, Germany, 31. March – 04. April 2014

H. Nagel, D. Labavic, H. Meyer-Ortmanns, W. Janke: *Open Boundary Conditions in Stochastic Transport Processes with Tunable Short-Range Interaction*, 15th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys14*, Leipzig, Germany, 27.–29. November 2014

P. Schierz, J. Zierenberg, W. Janke: *A Comparison of Molecular Dynamics and Multicanonical Simulations in the NVE Ensemble*, 7th Annual BuildMoNa Conference, Leipzig, Germany, 03.–04. March 2014

P. Schierz, W. Janke: *3D-Visualisierung von Polymeren - oder wie verkleben Spaghetti*, Lange Nacht der Wissenschaften, Leipzig, Germany, 27. June 2014

S. Schnabel, W. Janke: *Sampling Low-Energy States of the Edwards-Anderson Model*, Conference MECO 39, Coventry University, England, UK, 08.–10. April 2014

J. Zierenberg, M. Mueller, P. Schierz, M. Marenz, W. Janke: *Aggregation of Theta-Polymers in Spherical Confinement*, Biannual Meeting of the GDCh-Division of Macromolecular Chemistry *Polymers and Energy – Synthesis, Engineering, Characterisation and Applications*, Jena, Germany, 14.–16. September 2014

J. Zierenberg, M. Mueller, P. Schierz, M. Marenz, W. Janke: *Aggregation of Theta-Polymers in Spherical Confinement*, Satellite Meeting of the SFB Transregio 102 "Polymers under multiple constraints" *Self-Assembly in Synthetic and Biological Polymers: Similarities and Differences*, Jena, Germany, 15.–16. September 2014

## 12.28 Graduations

### Doctorate

### Diploma

### Master

**Bachelor**

- Dorian Nothaaß
  *Algorithmen für Spindynamik Simulationen*
  28. July 2014
- Henrik Christiansen
  *Stochastic Transport Processes with Open Boundaries*
  11. August 2014
- Karl Horn
  *Exact Enumeration of Lattice Polymers in Geometric Confinement*
  22. September 2014
- David Oberthür
  *Metropolis-Simulationen von Gitterheteropolymeren mit korrelierter Struktur, die einem langreichweitigen Potenzgesetz folgt*
  22. September 2014
- Franz Paul Spitzner
  *Generating Long-range Power-law Correlated Disorder*
  07. October 2014

## 12.29 Guests

- Prof. Dr. Subir K. Das
  Jawaharlal Nehru Centre for Advanced Scientific Research, India
  NTZ/DFH-UFA Colloquium (05. May 2014)
  *Kinetics of Phase Separation in Fluids*
  04.-06. May 2014
- Dr. Viktoria Blavatska
  Institute for Condensed Matter Physics, Lviv, Ukraine
  Alexander von Humboldt Foundation Institute Partnership Programme
  NTZ/DFH-UFA Colloquium (30. October 2014)
  *Conformational Properties of Complex Polymers: Rosette vs. Star-Like Structures*
  October – November 2014
- Prof. Dr. A. Peter Young
  University of California, Santa Cruz, USA
  Physics Colloquium (04. November 2014)
  *Numerical Studies of the Quantum Adiabatic Algorithm*
  04. November 2014
- Prof. Dr. Anastasios Malakis
  University of Athens, Greece
  *Anistropic Spin-Glass Models*
  25. November – 01. December 2014
- Dr. Francesco Parisen Toldin
  Universität Würzburg, Germany

*Fermionic Quantum Criticality in Honeycomb and $\pi$-Flux Hubbard Lattice Models*
26.–28. November 2014

- Dr. Andreas Tröster
  TU Wien, Austria
  *Fourier Monte Carlo Renormalization Group Approach to Crystalline Membranes*
  26.–28. November 2014
- Prof. Dr. Michael Bachmann
  Center for Simulational Physics, The University of Georgia, Athens, USA
  Physics Colloquium (27. November 2014)
  *A 20th Century Physics No-No Problem: The Reasons of us Being*
  26.–29. November 2014
- Prof. Dr. Bertrand Berche
  Université de Lorraine, Nancy, France
  *Subtleties of Gauge Theory in Aharonov-Bohm Rings*
  26.–29. November 2014
- Dr. Hsiao-Ping Hsu
  MPI für Polymerforschung, Mainz, Germany
  *Lattice Monte Carlo Simulations of Polymer Melts*
  26.–29. November 2014
- M.Sc. Tomas Koci
  Center for Simulational Physics, The University of Georgia, Athens, USA
  *Effects of the Bond Elasticity on the Structural Transitions of a Flexible Polymer*
  26.–29. November 2014
- M.Sc. Marjana Krasnytska
  National Academy of Sciences of Ukraine, Lviv, Ukraine
  *Lee-Yang-Fisher Zeros for the Ising Model on Complex Network*
  26.–29. November 2014
- M.Sc. Matthew Williams
  Center for Simulational Physics, The University of Georgia, Athens, USA
  *Structural Transitions in Helical Polymers*
  26.–29. November 2014
- Dr. Nikolaos Fytas
  Coventry University, England, UK
  *Universality in the Three-Dimensional Random-Field Ising Model*
  26.–30. November 2014
- Prof. Dr. Malte Henkel
  Université de Lorraine, Nancy, France
  *Spherical Models of Interface Growth*
  26.–30. November 2014
- Prof. Dr. Ferenc Iglói
  Institute of Theoretical Physics, Research Institute for Solid State Physics and Optics, Budapest, Hungary
  *Random Transverse-Field Ising Chain with Long-Range Interactions*
  26.–30. November 2014

- Dr. Nikolay Izmailyan
  Yerevan Physics Institute, Yerevan, Armenia
  *Corner Contribution to Free Energy for 2D Dimer Model*
  26.–30. November 2014
- Prof. Dr. Desmond A. Johnston
  Heriot-Watt University, Edinburgh, Scotland, UK
  *(Z2) Lattice Gerbe Theory*
  26.–30. November 2014
- Dr. Martin Weigel
  Coventry University, England, UK
  *Fragmentation of Fractal Random Structures*
  26.–30. November 2014
- Prof. Dr. Lev Shchur
  Landau Institute, Chernogolovka, Moscow Region, Russia
  *On the Accuracy of the Wang-Landau Algorithm*
  26. November – 03. December 2014
- PD Dr. Thomas Neuhaus
  Jülich Supercomputing Centre, Forschungszentrum Jülich, Germany
  27.–29. November 2014
- Dr. Elmar Bittner
  Universität Heidelberg, Germany
  27.–29. November 2014