11

Computational Quantum Field Theory

11.1 Introduction

The Computational Physics Group performs basic research into classical and quantum statistical physics with special emphasis on phase transitions and critical phenomena. In the centre of interest are the physics of spin glasses, diluted magnets and other materials with quenched, random disorder, soft condensed matter physics with focus on fluctuating paths and interfaces, biologically motivated problems such as protein folding, aggregation and adhesion as well as related properties of semiflexible polymers, and the intriguing physics of low-dimensional quantum spin systems. Investigations of a geometrical approach to the statistical physics of topological defects with applications to superconductors and superfluids and research into fluctuating geometries with applications to quantum gravity (e.g., dynamical triangulations) are conducted within a European Research Training Network (RTN) collaboration of 13 teams, and within an Institute Partnership of the Humboldt Foundation the statistical mechanics of complex networks is studied in collaboration with our partner university in Krakow, Poland.

The methodology is a combination of analytical and numerical techniques. The numerical tools are currently mainly Monte Carlo computer simulations and high-temperature series expansions. The computational approach to theoretical physics is expected to gain more and more importance with the future advances of computer technology, and is likely to become the third cornerstone of physics besides experiment and analytical theory. Already now it can help to bridge the gap between experiments and the often necessarily approximate calculations of analytical work. To achieve the desired high efficiency of the numerical studies we develop new algorithms, and to guarantee the flexibility required by basic research all computer codes are implemented by ourselves. The technical tools are Fortran, C, and C++ programs running under Unix or Linux operating systems and computer algebra using Maple or Mathematica. The software is developed and tested at the Institute on a cluster of PCs and workstations, where also most of the numerical analyses are performed. Large-scale simulations requiring vast amounts of computer time are carried out at the Institute on quite powerful compute servers, at the parallel computers of the University computing center, and, upon successful grant application at the national supercomputing centres in Jülich and München on IBM and Hitachi parallel supercomputers. This hierarchy of various

platforms gives good training opportunities for the students and offers promising job perspectives in many different fields for their future career.

Within the University, our research activities are closely integrated into the Graduate School "BuildMoNa": Leipzig School of Natural Sciences – *Building with Molecules and Nano-objects* funded by the German Research Foundation (DFG) within the German Excellence Initiative and the international DFH-UFA Graduate School *Statistical Physics of Complex Systems* with Nancy Université, France, supported by the Deutsch-Französische Hochschule. The two Graduate Schools are both "Classes" of the Research Academy Leipzig (RAL), providing the organizational frame for hosting visiting students, offering language courses and for many other practical matters. At the post-graduate level our research projects are embedded into the "Sächsische DFG-Forschergruppe" FOR877 *From Local Constraints to Macroscopic Transport*, the International Max Planck Research School (IMPRS) *Mathematics in the Sciences* and into two of the top level research areas ("Profilbildende Forschungsbereiche (PbF)") and the Centre for Theoretical Sciences (NTZ) of the University. In particular the latter structures are instrumental for our cooperations with research groups in experimental physics and biochemistry.

On an international scale, our research projets are carried out in a wide net of collaborations funded by the German Academic Exchange Service (DAAD), the Alexander-von-Humboldt Foundation though an Institute Partnership with the Jagellonian University in Krakow, Poland, as well as their Fellowship Programme, and the European Commission through the Research Training Network "ENRAGE": *Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*. From 17.–22. May 2009 an International Network Conference under the title *ENRAGEing Perspectives – Random Geometry and Random Matrices: From Quantum Gravity to Econophysics* has been organized by us at the Max-Planck-Institut für Physik komplexer Systeme in Dresden (`http://www.mpipks-dresden.mpg.de/~enrage09/`). Since 2008 our group is annually hosting the Humboldt Research Prize Winner Professor Bernd A. Berg from Florida State University, Tallahassee, USA, for a few months. Further close contacts and collaborations are established with research groups in Armenia, Austria, China, France, Great Britain, Israel, Italy, Japan, Poland, Russia, Spain, Sweden, Taiwan, Turkey, Ukraine, and the United States. These contacts are refreshed and furthered through topical Workshops and Tutorials and our International Workshop series *CompPhys: New Developments in Computational Physics*, taking annually place at the end of November just before the first advent weekend.

A special event in 2009 was the 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34* with about 120 participants, which we organized together with Prof. S. Trimper (Martin-Luther-Universität Halle-Wittenberg) here in Leipzig in our main department building Linnéstraße 5 from 30. March – 01. April 2009 (`http://www.physik.uni-leipzig.de/~meco34/`).

Wolfhard Janke

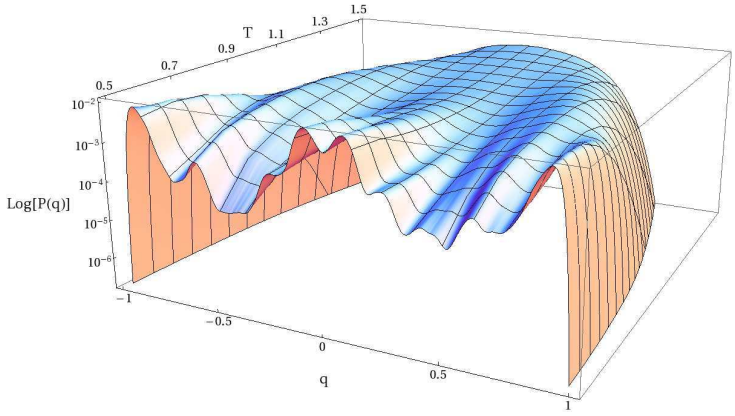

Figure 11.1: The logarithm of the canonical distribution $P(q)$ of the spin-glass overlap parameter q for the 3D Edwards-Anderson model on a moderately large 8^3 lattice as a function of the temperature T for a typical disorder realisation, illustrating how the rugged free-energy landscape develops for low temperatures.

11.2 Edwards-Anderson Ising Spin Glass Model

A. Nußbaumer, E. Bittner, W. Janke

One of the most challenging problems in the statistical physics of disordered systems is the nature of the low-temperature phase of finite-dimensional spin-glass systems. There is a still on-going debate over which of the most prominent theses in the field, Parisi's replica symmetry-breaking theory or the phenomenological droplet scaling picture of Fisher and Huse, describes the nature of the spin-glass phase correctly (for some reviews see Refs. [1–3]). There exist even views according to which neither of the two scenarios alone can capture the intriguing physics of spin glasses completely.

Due to the complexity of the problem, advances in analytical considerations are very limited and also computer simulations are at the verge of what can be achieved presently. The origin of the numerical problems is that, like in the thermodynamic limit of the (infinite-range) mean-field spin glass, the frozen phase of a finite system shows a complicated corrugated structure. As a consequence of the disorder and frustration characterising spin glasses in general, there is a rugged free-energy landscape with probable regions separated by rare event-states [4]. Consequently, conventional Monte Carlo simulations tend to get stuck in local free-energy valleys.

In this project we try to overcome this kind of problem by using a novel update algorithm which combines the parallel tempering method [5] with the multioverlap Monte Carlo algorithm [6]. Extensive large-scale simulations on our local computer cluster as well as on the "JUROPA" capability computer of the Jülich Supercomputing Centre have been performed mainly for the (short-range) Edwards-Anderson Ising spin-glass model [7] and, for comparison and gauging of the analysis methods, also for the Sherrington-Kirkpatrick mean-field limit [8].

The typical outcome for a randomly chosen disorder realisation is shown in Fig. 11.1. To get "physical" results, several thousand different realisations must be averaged, making the vast amount of computer time needed (many CPU years) understandable. A preliminary discussion of our results can be found in Ref. [9].

[1] A.P. Young (ed.): *Spin Glasses and Random Fields* (World Scientific, Singapore 1997)
[2] K.H. Fischer, J.A. Hertz: *Spin Glasses* (Cambridge University Press, Cambridge (England) 1991)
[3] K. Binder, A.P. Young: Rev. Mod. Phys. **58**, 801 (1986)
[4] W. Janke (ed.): *Rugged Free Energy Landscapes: Common Computational Approaches to Spin Glasses, Structural Glasses and Biological Macromolecules*, Lect. Notes Phys. **736** (Springer, Berlin 2008)
[5] K. Hukushima, K. Nemoto: J. Phys. Soc. Jpn. **65**, 1604 (1996)
[6] B.A. Berg, W. Janke: Phys. Rev. Lett. **80**, 4771 (1998)
[7] S.F. Edwards, P.W. Anderson: J. Phys. F: Metal Phys. **5**, 965 (1975)
[8] D. Sherrington, S. Kirkpartick: Phys. Rev. Lett. **35**, 1792 (1975)
[9] E. Bittner et al.: in *NIC Symposium 2008*, ed. by G. Münster et al., NIC Series Vol. **39** (John von Neumann Institute for Computing, Jülich 2008) p 229

11.3 Stretching Polymers in Crowded Environments

V. Blavatska*, W. Janke

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

Long flexible macromolecules in good solvent possess configurational statistics which is perfectly captured by the model of self-avoiding random walks (SAW) on a regular lattice [1]. This corresponds to the *regime of polymer coils* which holds when the temperature T is above the so-called Θ-temperature. In this regime, the mean end-to-end distance of an N-step chain scales as $R_N \sim N^{\nu_{\rm SAW}}$, where $\nu_{\rm SAW}$ is a universal exponent which depends on the dimension d only. When lowering the temperature, the effect of monomer-monomer attraction grows and the polymer radius shrinks. At $T = T_\Theta$ the effective repulsion due to the volume exclusion constraint is exactly balanced by attractive interactions. At this particular temperature, a crossover occurs from high temperature SAW behaviour to Θ-statistics with another critical exponent ν_Θ. The properties of polymers in the vicinity of the Θ-point can be modeled by *self-attracting* SAWs (SASAWs), where a nearest-neighbour attraction between non-covalently bound monomers is included [2]. Below the Θ-temperature, the entropic effects, which make the polymer chain swell, are overcome by interaction energy and a collapse to the *globule regime* characterized by a size exponent $\nu_c = 1/d$ occurs. The coil-globule transition is of second order, in the sense that the density of an infinite globule is zero at $T = T_\Theta$ and increases continuously when T is lowered further; more precisely, it is a tricritical point with the upper critical dimension $d_c = 3$.

New challenges have been raised recently when studying protein folding in the natural cellular environment [3]. Real biological cells can be described as a very crowded environment built of various biochemical species, which occupy a large fraction of the total volume; the “volume exclusion" arises due to the steric repulsion between molecules. In the language of lattice models, the crowded environment with structural obstacles can be considered as a disordered lattice, where some amount of randomly

chosen sites contains defects. Of particular interest is the case, when the concentration p of lattice sites allowed for the SAWs equals the critical concentration p_c and the lattice becomes percolative. Under these conditions, the critical exponents for SAWs take different values [4–6] and the interesting phenomenon of multifractality can be observed [7, 8].

The recent progress in experimental techniques employing optical tweezers, atomic force microscopy and soft microneedles makes it possible to monitor the behaviour of various polymers under tension and stress. In particular, applying a force on an isolated protein, the mechanism of force-driven phase transitions was studied. Of special interest in biophysics is the stretching of a collapsed polymer, i.e., of a polymer in a poor solvent below the Θ-temperature. Unfolding proteins in this way could give important information on their spontaneous folding pathways.

The aim of the present study is to apply state-of-the-art computer simulations based on the pruned-enriched Rosenbluth method (PERM) to analyze the properties of SASAWs on site-diluted lattices at the percolation threshold under applied external stretching force in space dimensions $d = 2$ and 3. We estimate the shift of the Θ-temperature of the globule-coil transition under the influence of stretching and analyze the effect of applied force on the phase transitions between collapsed, extended and stretched phases [9].

[1] P.-G. de Gennes: *Scaling Concepts in Polymer Physics* (Cornell University Press, Ithaca and London 1979)
[2] C. Vanderzande: *Lattice Models of Polymers* (Cambridge University Press, Cambridge (England) 1998)
[3] A. Horwich: Nature **431**, 520 (2004)
[4] V. Blavatska, W. Janke: Europhys. Lett. **82**, 66006 (2008)
[5] V. Blavatska, W. Janke: in Proceedings of the International Conference *Path Integrals – New Trends and Perspectives*, ed. by W. Janke, A. Pelster (World Scientific, Singapore 2008) p 585
[6] V. Blavatska, W. Janke: J. Phys. A **42**, 015001 (2009)
[7] V. Blavatska, W. Janke: Phys. Rev. Lett. **101**, 125701 (2008)
[8] V. Blavatska, W. Janke: in *Computer Simulations in Condensed Matter Physics XXII*, ed. by D.P. Landau et al., Physics Procedia **3**, 1431 (2010)
[9] V. Blavatska, W. Janke: Phys. Rev. E **80**, 051805 (2009)

11.4 Worm Algorithm Applied to Critical Loop Gases

W. Janke, T. Neuhaus*, A.M.J. Schakel

*Jülich Supercomputing Centre, Forschungszentrum Jülich, Germany

The loop gas approach to lattice field theory provides an alternative, geometrical description in terms of fluctuating loops. It derives form the strong-coupling expansion in relativistic quantum field theories formulated on a spacetime lattice, representing the hopping of particles from one lattice site to the next. The standard approach, which is rooted in the functional integral approach to field quantization, involves estimating

observables (expressed in terms of the fields) by sampling a representative set of field configurations. New configurations are typically generated by means of a Monte Carlo technique which uses importance sampling, with each field configuration weighted according to the probability that it occurs. In contrast, the approach based on the strong-coupling, or hopping expansion, which is closely connected to Feynman's spacetime approach to quantum theory [1], involves linelike objects. Physical observables are in this geometrical approach no longer estimated by sampling an ensemble of field configurations, but by sampling a grand canonical ensemble of (mostly closed) world lines, known as a *loop gas*, instead. The weight of a given world-line configuration is typically determined by the total length of the paths, the number of intersections, and the number of loops contained in the tangle. In statistical physics, the strong-coupling expansion is known as the high-temperature series expansion [2]. Lattice field theories studied in this context are typically spin models, such as the O(N) spin model, whose representation in terms of high-temperature (HT) graphs is known as a *loop model*.

About a decade ago, Prokof'ev and Svistunov [3] have introduced a Monte Carlo update algorithm that, although based on local updates, does away with critical slowing down almost completely. The so-called *worm algorithm* generates loop configurations through the motion of the end points of an *open* world line – the "head" and "tail" of a "worm". A loop is generated in this scheme when the head bites the tail, or through a "back bite" where the head erases a piece (bond) of its own body and thereby leaves behind a detached loop and a shortened open chain.

Besides this outstanding technical advantage, the worm algorithm has the additional advantage in the context of statistical physics that the complete set of standard critical exponents can be determined at a stroke. This set is known to split into two, namely the thermal and the magnetic exponents. While the thermal exponents, such as the specific heat exponent α, pertain to closed paths, the magnetic exponents, such as the magnetic susceptibility exponent γ, pertain to open paths in the geometrical approach. By the nature of the worm algorithm, which features an open path between loop updates, data for both sectors are generated on the fly in this scheme. More specifically, the open paths directly sample the spin-spin, or two-point, correlation function.

In this project, which extends previous work by two of us on the subject [4, 5], we describe estimators of physical observables that naturally arise in a loop gas and that allow determining the standard critical exponents. Our approach amalgamates concepts from percolation theory – the paradigm of a geometrical phase transition – and the theory of self-avoiding random walks. We relate this geometrical approach to phase transitions in terms of fluctuating paths to the more familiar field theory approach by considering the O(N) symmetric ϕ^4 theory. To support our arguments we performed Monte Carlo "worm" simulations for the two-dimensional O(1) loop model on a honeycomb lattice [6]. This model serves as a prototype with its various exact results providing a yardstick for our numerical results and also for the feasibility of our approach.

[1] R.P. Feynman: Rev. Mod. Phys. **20**, 367 (1948)
[2] H.E. Stanley: *Introduction to Phase Transitions and Critical Phenomena* (Oxford University Press, New York 1971)
[3] N. Prokof'ev, B. Svistunov: Phys. Rev. Lett. **87**, 160601 (2001)
[4] W. Janke, A.M.J. Schakel: Nucl. Phys. B [FS] **700**, 385 (2004)

[5] W. Janke, A.M.J. Schakel: Phys. Rev. Lett. **95**, 135702 (2005)
[6] W. Janke et al.: Nucl. Phys. B **829**, 573 (2010) [arXiv:0910.5231]

11.5 Partially Asymmetric Exclusion Processes

R.A. Blythe*, W. Janke, D.A. Johnston†, R. Kenna‡

*SUPA, School of Physics and Astronomy, University of Edinburgh, UK
†Department of Mathematics and the Maxwell Institute for Mathematical Sciences, Heriot-Watt University, Edinburgh, UK
‡Applied Mathematics Research Centre, Coventry University, UK

Although the asymmetric exclusion process (ASEP) has been reinvented in various different guises over the years [1], it is only relatively recently that exact solutions have been available. The solution of the ASEP with open boundary conditions in [2] using a matrix-product ansatz was a landmark in the study of driven diffusive systems and this was extended in [3, 4] to the partially asymmetric exclusion process (PASEP), in which backward hops are also admitted. As discussed in a recent review of the matrix product approach to solving for the steady state of nonequilibrium Markov processes [1], there are a range of different methods for analysing the thermodynamic phase behaviour of the simplest versions of the ASEP. By contrast, more general models – collectively known as the partially asymmetric exclusion process (PASEP) – that admit particles to hop in both directions in the bulk, and even more generally to enter and exit at both left and right boundaries (cf. Fig. 11.2), have so far been studied only through a diagonalisation of the matrices appearing in the formalism [3, 4]. In this project, we extended a technique that previously admitted an extremely quick derivation of the ASEP phase behaviour under various updating schemes [5, 6] to these more general models.

The idea is to consider the behaviour of a "grand-canonical partition function" for the model. More precisely, we examine the generating function of the normalization of the nonequilibrium steady-state distribution over an ensemble of different lattice lengths whose mean is controlled by a fugacity. The thermodynamic phase behaviour can then be read off from the singularities of this generating function. Whilst obtaining this generating function is straightforward for the ASEP [5, 6], a convenient closed form for the PASEP had remained elusive.

Here we demonstrate that a representation of the generating function that allows the thermodynamic phase behaviour to be determined with relative ease takes the form of an infinite continued fraction [7]. This we arrive at through an interpretation of the PASEP normalization as the (equilibrium) partition function of lattice paths. We show how to analyse the singularities embedded in the continued fraction representation. We find that the analysis is intimately related to an approach based on finite-dimensional matrix representations [8, 9], exact along special lines in the phase diagram, and that the continued fraction shows how these particular solutions and the general solution are related. We further show that the continued-fraction approach extends to the most general version of the PASEP and that one can access both currents and correlation

Figure 11.2: Typical particle configuration and allowed moves in the PASEP model.

lengths through it. Finally, we return to the lattice path picture to elucidate the equilibrium counterpart of a nonequilibrium phase transition identified in [4] that occurs when the bias on bulk hop rates opposes that imposed by the boundary conditions.

[1] R.A. Blythe, M.R. Evans: J. Phys. A: Math. Theor. **40**, R333 (2004)
[2] B. Derrida et al.: J. Phys. A: Math. Gen. **26**, 1493 (1993)
[3] T. Sasamoto: J. Phys. A: Math. Gen. **32**, 7109 (1999)
[4] R.A. Blythe et al.: Phys. A: Math. Gen. **33**, 2313 (2000)
[5] R.A. Blythe et al.: J. Stat. Mech.: Theor. Exp. P06001 (2004)
[6] R.A. Blythe et al.: J. Stat. Mech.: Theor. Exp. P10007 (2004)
[7] R.A. Blythe et al.: J. Phys. A: Math. Theor. **42**, 325 002 (2009)
[8] K. Mallick, S. Sandow: J. Phys. A: Math. Gen. **30**, 4513 (1997)
[9] F.H. Jafarpour: J. Phys. A: Math. Gen. **33**, 1797 (2000)

11.6 Pair-Factorized Steady States in Stochastic Mass-Transport Models

B. Waclaw, J. Sopik*, W. Janke, H. Meyer-Ortmanns*

*School of Engineering and Science, Jacobs University, Bremen, Germany

A variety of stochastic processes out-of-equilibrium is summarized under the name of stochastic mass transport models, with stochastic transport of some conserved quantity, called "mass". Examples for such processes are traffic flow, ranging from the intracellular to the macroscopic level, force propagation in granular media, aggregation and fragmentation of clusters, and others [1]. We have studied mass transport models which lead to steady states that factorize over the links of arbitrary connected graphs, so-called pair-factorized steady states [2–4].

For systems in one and two dimensions we derive the phase structure from these states, in particular the transition from a liquid phase to a phase with a condensate. Condensation amounts to spontaneous symmetry breaking in these systems where the dynamical rules are symmetric. In one dimension we derive the critical mass density of the transition, analytically predict the shape of the condensate, its scaling with the system size, its fluctuations and the single-site mass distribution. The shape of the condensate is not universal, but can be tuned from an extended to a localized one via the competition of local and ultralocal interactions that are implemented in the hopping rates (cf. Fig. 11.3). The scaling shows features familiar from first- and second-order phase transitions. The system of anisotropic hopping that we considered in two dimensions can be dimensionally reduced to an effective zero-range process in one

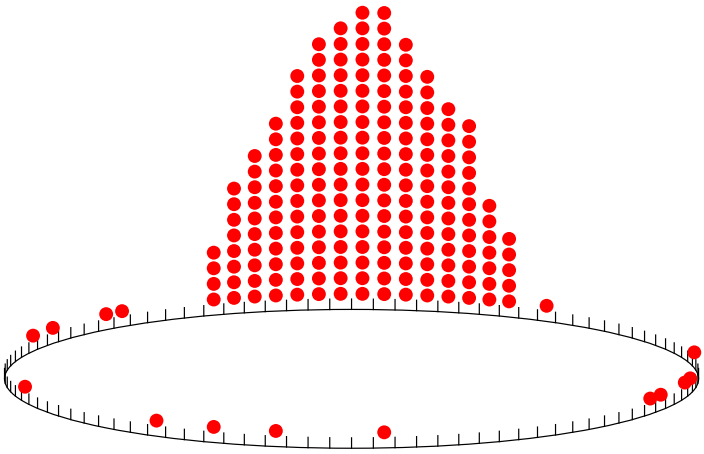

Figure 11.3: Schematic illustration of a condensate of bell shape on a ring.

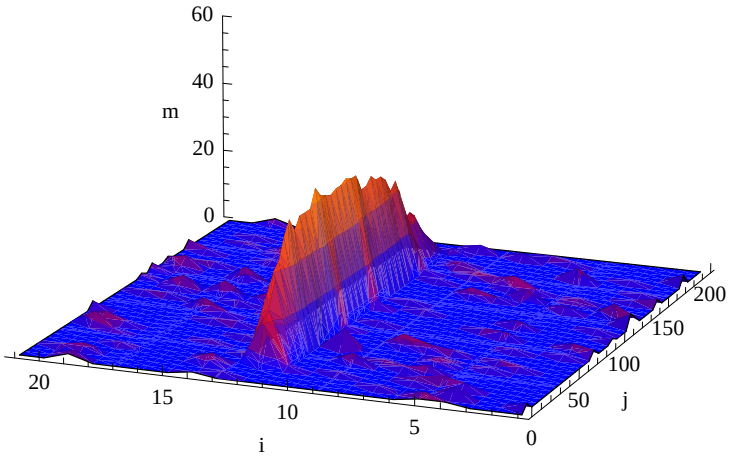

Figure 11.4: Condensate localized in x-direction and extended in y-direction for $\rho_1 < \rho < \rho_2$.

dimension. Here we predict two transitions, in particular in a certain density range the formation of a condensate that is extended in one direction and localized in the other direction, see Fig. 11.4. We also discuss possible extensions on arbitrary graphs [5].

This work is partially supported by an Institute Partnership grant "Krakow-Leipzig" (`http://www.physik.uni-leipzig.de/~waclaw/AvH`) of the Alexander von Humboldt Foundation, the EU Network "ENRAGE", and the Deutsche Forschungsgemeinschaft.

[1] M.R. Evans et al.: Phys. Rev. Lett. **97**, 010602 (2006)
[2] B. Waclaw et al.: J. Phys. A: Math. Theor. **42**, 315003 (2009)
[3] B. Waclaw et al.: Phys. Rev. Lett. **103**, 080602 (2009)
[4] B. Waclaw et al.: J. Stat. Mech. P10021 (2009)
[5] B. Waclaw et al.: in Proceedings of the *XI Latin American Workshop on Nonlinear Phenomena: LAWNP'09*, Búzios, Brazil, to appear in J. Phys.: Conf. Ser. (in press)

11.7 Ground-States and Thermodynamics of Tubelike Flexible Polymers

T. Vogel, T. Neuhaus*, M. Bachmann†, W. Janke

*Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich, Germany
†Present address: IFF-2 and IAS-2, Forschungszentrum Jülich, Germany

The thickness of tubelike flexible polymers is controlled by a single parameter, the global radius of curvature, which depends on three-body interactions [1]. It is well known that the resulting geometrical constraint tends to enhance secondary structure formation. By means of computer simulations we studied the thermodynamical behaviour of such a tube model for simple homopolymers as well as for an exemplified hydrophobic-polar heteropolymer [2, 3].

After focusing on ground states of homopolymers and their properties in a preceding step [4], we identified dominant structural pseudophases at finite temperatures, i.e., specific-heat landscapes depending on the thickness parameter ρ and temperature T, representing the conformational phase diagram. Independently of the polymer length, we find four major structural phases. These include helices (α), sheetlike planar structures (β), bended rings (γ) and sprawled random coils (δ). The resulting phase diagram in the ρ-T plane is shown in Fig. 11.5 for a 10mer and a 13mer. The different secondary structure phases can thus be assigned to different ranges of the tube thickness. The thickness parameter is therefore suitable for a classification of the structural behaviour of classes of polymers.

Furthermore, we introduced the AB tube model for hydrophobic-polar heteropolymers and obtained results for a specific sequence of monomers, which has extensively been studied before without thickness [5]. We showed that a specific monomer sequence can stabilize the general secondary structures. We find, for example, a very pronounced and stable region of β-sheet structures. We further showed that the additional introduction of a bending stiffness plays a subordinate role. This observation is important to relate our general conclusions to existing results for special systems. We could in particular reproduce simulational results published within the past years for polymer models without explicit thickness as limiting case of our study [3].

[1] O. Gonzalez, J. Maddocks: Proc. Natl. Acad. Sci. USA **96**, 4769 (1999)
[2] T. Vogel et al.: Europhys. Lett. **85**, 10003 (2009)
[3] T. Vogel et al.: Phys. Rev. E **80**, 011802 (2009)
[4] T. Vogel et al.: Eur. Phys. J. E **30**, 7 (2009)
[5] M. Bachmann et al.: Phys. Rev. E **71**, 031906 (2005), and references therein

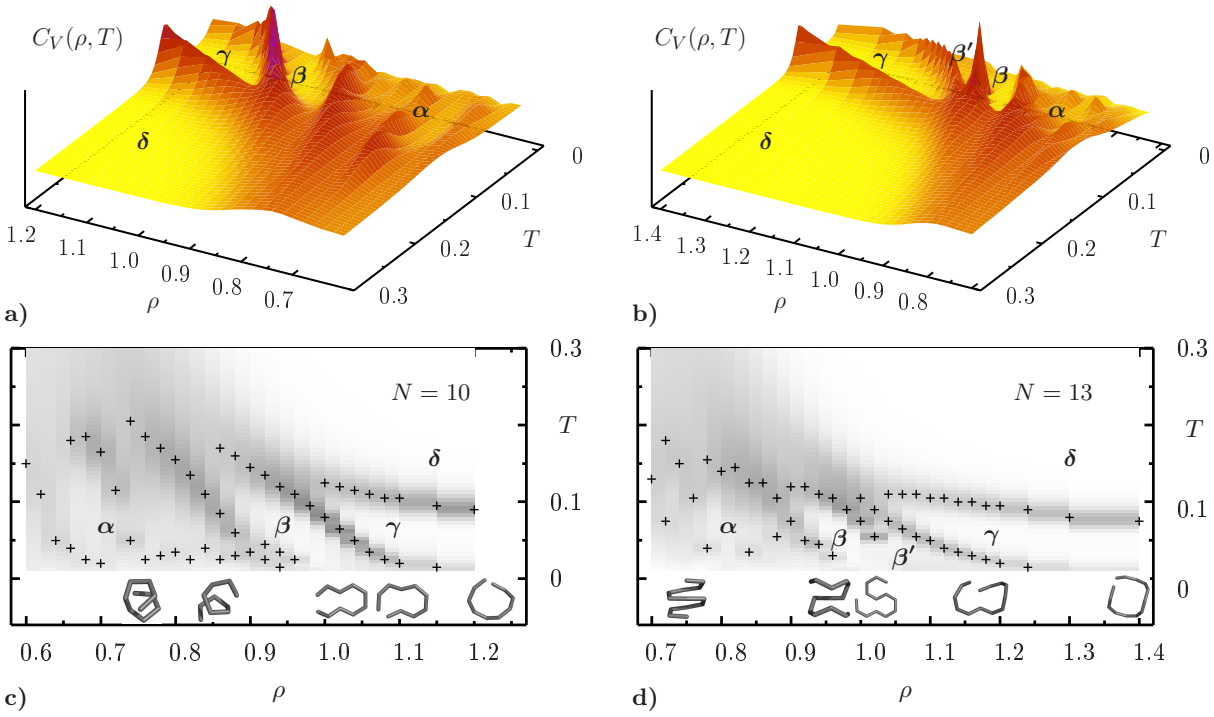

Figure 11.5: Phase diagrams of the homopolymers with $N = 10$ (left) and $N = 13$ (right). The labels α, β, γ, and δ indicate the different pseudophases at finite temperature. The panels **a)** and **b)** show the perspective view of the specific-heat landscape, and in **c)** and **d)**, the top-views are plotted with marked peak positions for various parameters ρ. The specific-heat values are encoded in gray scale. The conformations depicted in the insets in **c)** and **d)** correspond to the ground states obtained in Ref. [4].

11.8 Dominance of Finite-Size Effects in Nucleation Processes

S. Schnabel, T. Vogel, M. Bachmann*, W. Janke

*Present address: IFF-2 and IAS-2, Forschungszentrum Jülich, Germany

Thermodynamic phase transitions are typically analyzed in the thermodynamic limit, i.e., for an idealized infinite system size. This approach is reasonable for inherently large systems, where finite-size effects vanish with increasing system size. However, there are many physical systems where the thermodynamic limit is a nonsensical idealization. A typical scenario is the nucleation of a system and prominent examples for such processes are atomic cluster formation, the freezing of polymers, the aggregation of polymers, and the folding of proteins.

This project is devoted to numerical investigations of the freezing or crystallization transition of single elastic polymers [1, 2]. In the model that we employed the bond length is adaptive in a way that highly symmetric conformations can form in the cystalline phase. In our high-performance Monte Carlo simulations employing generalized ensemble methods we found for all different chain lengths low-energy conformations with basic icosahedral symmetries. The formation of such "discretized spherical" shapes is not surprising. A small system that has to reduce surface contacts

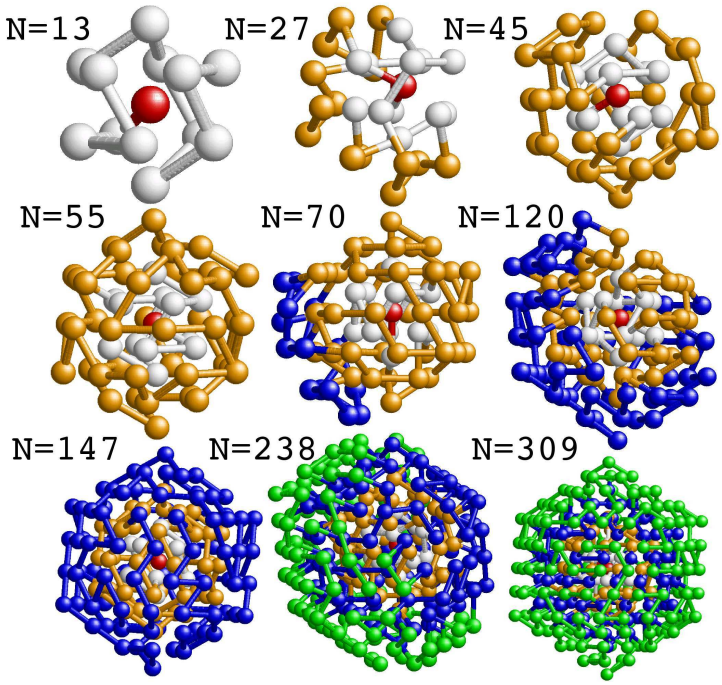

Figure 11.6: Icosahedral or icosahedral-like ground-state state conformations of elastic polymers for different system sizes [2]. Equally colored monomers belong to the same shell.

with its environment and requires stable structures prefers an icosahedral shape. A prominent example are virus capsids enclosing the viral genetic material.

In our study, we also verified the expectation that the thermodynamic crystallization behaviour is different for all system sizes. We identified a nontrivial systematic chain-length dependence that is associated with the type of growth of the nucleus [1, 2]. However, a conventional scaling behaviour has not been found – it simply does not exist. This is also known from atomic clusters [3]. A particularly sharp transition signal from fluctuating quantities, such as the specific heat, is obtained for "magic" chain lengths $N = 13, 55, 147, 309, \ldots$, in which cases almost perfect icosahedra can form (see Fig. 11.6). These shapes are particularly stable and typically represent the core cells in the structure formation of longer chains.

The formation of optimally discretized spherical shapes is required for systems that have to optimize the contact surface to a less attractive environment (for example, a "poor" solvent). The residence of a monomer at this interface is energetically disfavored compared to a position in the interior. In small systems, however, all possible structures, including the most compact ones, have an insufficient surface-to-volume ratio, i.e., a large fraction of particles or monomers reside in the surface layer. Yet for the "magic" 309mer, more monomers are located on the surface (162) than in the bulk (147). Thus, all nucleation processes, even for much larger systems, are still influenced by surface effects. For this reason, quantitative analyses of "first-order-like" nucleation transitions require a treatment different from standard scaling approaches.

[1] S. Schnabel et al.: Chem. Phys. Lett. **476**, 201 (2009)
[2] S. Schnabel et al.: J. Chem. Phys. **131**, 124904 (2009)
[3] J.P.K. Doye, F. Calvo: J. Chem. Phys. **116**, 8307 (2002)

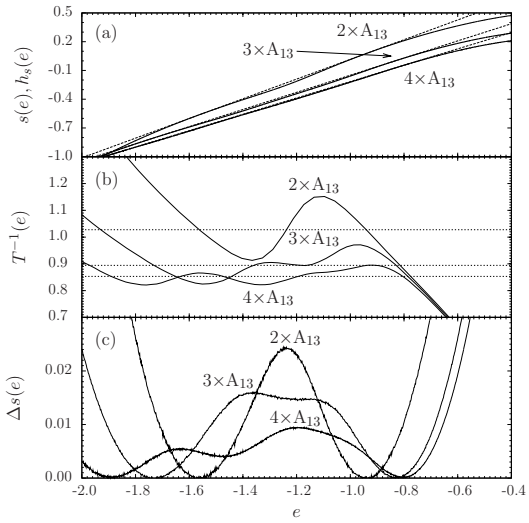

Figure 11.7: (a) Microcanonical entropy per monomer $s(e)$ and the Gibbs constructions $h_s(e)$ (dashed lines) as functions of the energy per monomer $e = E/N$, (b) reciprocal caloric temperatures $T^{-1}(e)$ and Maxwell constructions, and (c) relative surface entropies per monomer Δs_{surf}.

11.9 Microcanonical Analysis of Macromolecule Aggregation

C. Junghans*, M. Bachmann†, W. Janke

*Max-Planck-Institut für Polymerforschung, Mainz, Germany
†Present address: IFF-2 and IAS-2, Forschungszentrum Jülich, Germany

The aggregation of macromolecules may be considered as a special case of the nucleation transition. In biosystems, the formation of peptide plaque can have disastrous consequences. An example is the aggregation of Aβ peptides in the human brain which is associated to the neurodegenerative Alzheimer's disease.

To analyze the aggregation of a few polymers, we proposed in Ref. [1] an approach based on microcanonical statistics. The central quantity in the microcanonical approach is the density of states $g(E)$ which can intuitively be understood as the degeneracy of the energetic states of the system. Then, the microcanonical entropy can be introduced by $S(E) = k_B \ln g(E)$ [2, 3]. In Fig. 11.7(a), it is plotted for systems of two ($2\times A_{13}$), three ($3\times A_{13}$), and four polymer chains with 13 monomers ($4\times A_{13}$). All these entropy curves exhibit a particularly interesting feature: In a certain energy region, they possess *convex* monotony [4]. Consequently, at a certain temperature, the canonical probability density distribution $p(E) \sim g(E) \exp(-E/k_B T_{\text{agg}})$ is bimodal with two peaks of equal height at two energies E_{agg} and E_{frag} that can be associated to phases, where aggregates or fragments dominate, respectively [2]. A minimum at the energy E_{sep} separates the two coexisting phases at the transition temperature T_{agg}. Hence, we conclude that the convex region of the entropy corresponds to the phase separation of the first-order-like aggregation transition. This behaviour is common to all nucleation processes. However, it is a finite-size effect and will vanish in the thermodynamic limit (provided, its definition makes sense at all) [1, 4, 5].

Thus, it is useful to construct the Gibbs hull of the entropy curves in the transition region by connecting the two points $S(E_{\rm agg})$ and $S(E_{\rm frag})$, where the entropy changes its monotony [see Fig. 11.7(a)]. Since the temperature is defined via $T^{-1}(E) = \partial S(E)/\partial E$, the slope of the Gibbs tangent $H_S(E)$ is identical with the reciprocal aggregation transition temperature $T^{-1}_{\rm agg}$. Figure 11.7(b) shows another characteristic feature. The caloric temperature curves $T^{-1}(E)$ bend back in the transition region, i.e., additional energy pumped into the system during the fragmentation process leads to a decrease of the temperature: The melting aggregate becomes first *colder* during the fragmentation transition. This is due to the large entropy deviation from the "expected" Gibbs hull $\Delta S(E)$ plotted in Fig. 11.7(c). The maximum at the separation energy is called "surface entropy" and corresponds to the entropic reduction due to monomer rearrangements at the surface of the aggregate during the melting process. Entropy reduction costs energy. That is why the caloric temperature decreases with increasing energy. In Fig. 11.7(b) we also see that the backbending region becomes flatter with increasing system size (number of chains) and converges to the Maxwell lines, i.e., to the slopes of the Gibbs hulls.

By closer inspection of Fig. 11.7(b), we find for the systems a *hiercharchical substructure* caused by the surface effects. The frequency of oscillations of the curves, increasing with system size, reveals that the aggregation transition is actually a composition of different subprocesses, each of which is an individual phase-separation process. The amplitude of these oscillations decreases with system size showing that these subprocesses have a smaller surface-entropic barrier [4].

[1] C. Junghans et al.: Phys. Rev. Lett. **97**, 218103 (2006)
[2] W. Janke: Nucl. Phys. B (Proc. Suppl.) **63A-C**, 631 (1998)
[3] D.H.E. Gross: *Microcanonical Thermodynamics* (World Scientific, Singapore 2001)
[4] C. Junghans et al.: Europhys. Lett. **87**, 40002 (2009)
[5] C. Junghans et al.: J. Chem. Phys. **128**, 085103 (2008)

11.10 Microcanonical Analyses of Polymer Adsorption Transitions

M. Möddel, M. Bachmann*, W. Janke

*Present address: IFF-2 and IAS-2, Forschungszentrum Jülich, Germany

After we recently derived the complete phase structure of a single polymer near an attractive substrate of varying adsorption strength combining the information of the canonical expectations values of various structural and energetical quantities obtained in multicanonical computer simulations [1], we focused last year on the detailed properties of the adsorption transition using a microcanonical approach [2].

The model applied is a simple bead-stick model with 12-6 Lennard-Jones (LJ) interaction between nonbonded monomers, a bending stiffness and an attraction to a flat substrate at $z = 0$ whose strength is proportional to a parameter ϵ_s. The bond lengths between adjacent monomers are fixed and normalized to unity. For an illustration of

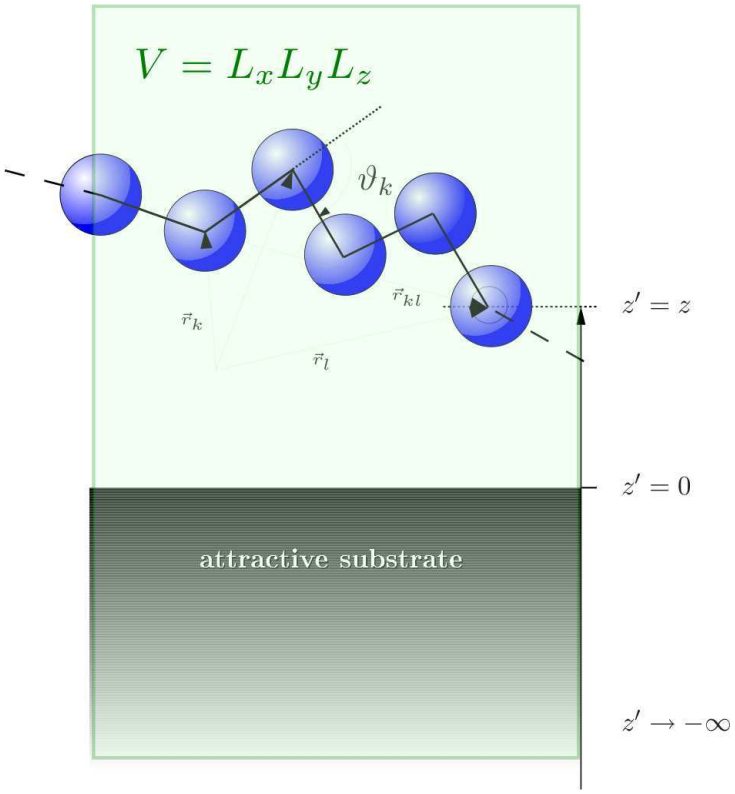

Figure 11.8: The model of the polymer as a Lennard-Jones chain interacting with an attractive substrate at $z = 0$. The distance between two adjacent monomers is fixed to unity. The bending angle at the $(k+1)$th monomer is denoted by ϑ_k and the vector between the kth and lth monomer by $\vec{r}_{kl}$. Each monomer k has a distance to the substrate z_k.

the considered system and the nomenclature, see Fig. 11.8. Altogether, the Hamiltonian of the system reads as

$$E = 4\sum_{i=1}^{N-2}\sum_{j=i+2}^{N}\left(r_{ij}^{-12} - r_{ij}^{-6}\right) + \frac{1}{4}\sum_{i=1}^{N-2}(1-\cos\vartheta_i) + \epsilon_s\sum_{i=1}^{N}\left(\frac{2}{15}z_i^{-9} - z_i^{-3}\right). \tag{11.1}$$

The densities of states necessary for our data analyses were obtained by extensive multicanonical Monte Carlo computer simulations over many orders of magnitude. We used microcanonical analyses because for short chains and strong surface attraction, the microcanonical entropy turns out to be a convex function of energy in the transition regime, see Fig. 11.9. This indicates that surface-entropic effects are relevant. Albeit known to be a continuous transition in the thermodynamic limit of infinitely long chains, the adsorption transition of polymers with finite length thus exhibits a clear signature of a first-order-like transition, with coexisting phases of adsorbed and desorbed conformations. Another remarkable consequence of the convexity of the microcanonical entropy is that the transition is accompanied by a decrease of the microcanonical temperature with increasing energy. Since this is a characteristic physical effect it should not be ignored in analyses of cooperative macrostate transitions in finite systems.

[1] M. Möddel et al.: J. Phys. Chem. B **113**, 3314 (2009)
[2] M. Möddel et al.: e-print arXiv:1002.2000 (cond-mat.stat-mech)

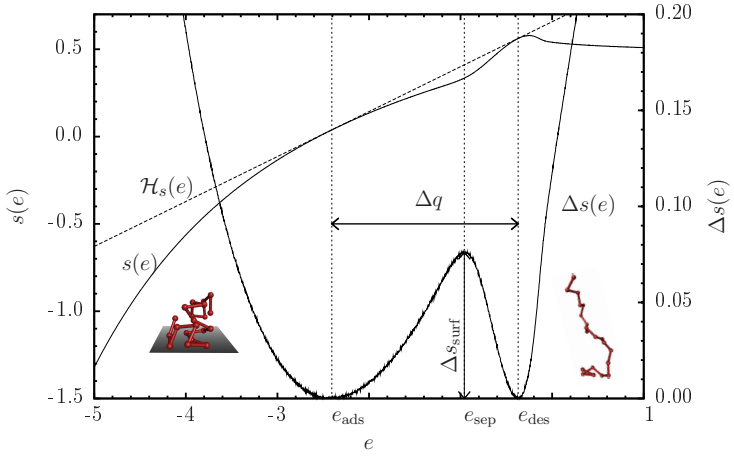

Figure 11.9: Microcanonical entropy $s(e)$ (up to an unimportant constant) for a 20mer at $\epsilon_s = 5$, the Gibbs hull $\mathcal{H}_s(e)$, and their difference $\Delta s(e)$ as functions of the energy per monomer e. The convex adsorption regime is bounded by the energies e_{ads} and e_{des} of the coexisting phases of adsorbed and desorbed conformations at the adsorption temperature T_{ads}, defined via the slope of $\mathcal{H}_s(e)$ [2]. Δs_{surf} denotes the surface entropy per monomer and Δq the latent heat of the first-order-like transition.

11.11 Peptide Adhesion to Semiconductor Substrates: Simulations and Experiments

M. Bachmann*, K. Goede†, A.G. Beck-Sickinger‡, M. Grundmann†, A. Irbäck§, W. Janke

*Present address: IFF-2 and IAS-2, Forschungszentrum Jülich, Germany
†Semiconductor Physics Group, Institut für Experimentelle Physik II
‡Institut für Biochemie
§Computational Biology & Biological Physics Division, Lunds Universitet, Lund, Sweden

In the past few years, the interest in hybrid interfaces formed by "soft" molecular matter and "hard" solid substrates has rapidly grown as such systems promise to be relatively easily accessible candidates for novel biosensors or electronic devices. The enormous progress in high-resolution microscopy and in biochemical engineering of macromolecules is the major prerequisite for studies of hybrid systems and potential applications [1]. One particularly important problem is the self-assembly and adhesion of polymers, proteins, or protein-like synthetic peptides to solid materials such as, e.g., metals [2] and semiconductors [3–5]. Peptide and substrate-specific binding affinity is particularly relevant in pattern recognition processes [6]. Basic theoretical considerations of simplified polymer–substrate and protein–substrate models have predicted complex pseudophase diagrams [7, 8].

In bacteriophage display experiments, only a few peptides out of a library of 10^9 investigated sequences with 12 amino acid residues were found to possess a particularly strong propensity to adhere to (100) gallium-arsenide (GaAs) surfaces [3]. The sequence-specificity of adsorption strength is a remarkable property, but the question remains how it is related to the individual molecular structure of the peptides. We expect that *relevant* mutations of sites in the amino-acid sequence can cause a change of the binding affinity. Indeed, one key aspect of our study is to provide evidence that

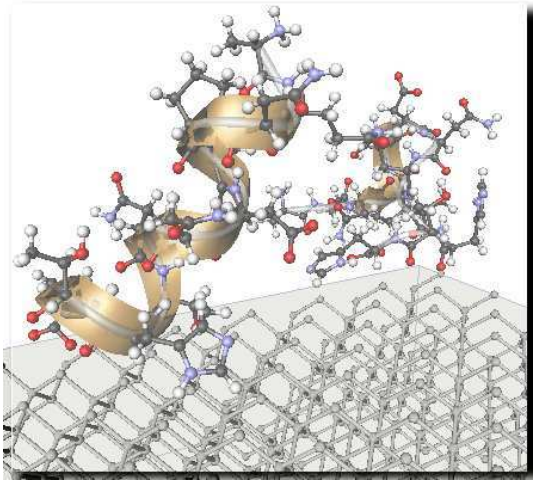

Figure 11.10: The binding properties of a peptide adsorbing at a substrate are influenced by the strongly geometry-dependent, heterogeneous electronic properties of molecule and substrate. The resulting high specificity of adsorption requires a careful force-field parametrization in semiclassical models. The image shows a snapshot from a simulation of two synthetic helical peptides interacting with a de-oxidized silicon (100) surface.

proline is a potential candidate for switching the adsorption propensities to cleaned (100) silicon (Si) substrates.

In this project, we show by means of experimental and computational analyses that the adsorption properties of mutated synthetic peptides at semiconductors exhibit a clear sequence-dependent adhesion specificity. Our simulations of a novel hybrid peptide-substrate model reveal the correspondence between proline mutation and binding affinity to a clean silicon substrate, for a snapshot of typical configurations see Fig. 11.10. After synthesizing the theoretically suggested amino-acid sequences with different binding behaviour, we could confirm the relevance of the selective mutations upon adhesion in our subsequent atomic force microscopy experiments [9].

[1] M. Sarikaya et al.: Nature Mat. **2**, 577 (2003)
[2] S. Brown: Nature Biotechnol. **15**, 269 (1997)
[3] S.R. Whaley et al.: Nature **405**, 665 (2000)
[4] K. Goede et al.: Nano Lett. **4**, 2115 (2004)
[5] K. Goede et al.: Langmuir **22**, 8104 (2006)
[6] T. Bogner et al.: Phys. Rev. Lett. **93**, 268108 (2004)
[7] M. Bachmann, W. Janke: Phys. Rev. Lett. **95**, 058102 (2005); Phys. Rev. E **73**, 041802 (2006)
[8] M. Bachmann, W. Janke: Phys. Rev. E **73**, 020901(R) (2006)
[9] M. Bachmann et al.: *Microscopic Mechanism of Specific Peptide Adhesion to Semiconductor Substrates*, Leipzig preprint, submitted

11.12 Free-Energy Barrier at Droplet Condensation

A. Nußbaumer, E. Bittner, W. Janke

The precise mechanism for the formation of the first large droplet in condensing systems is one of the fundamental problems in statistical physics. Early analytical studies date back to the 1960s. Over the years this problem has been taken up several times and further advanced both analytically and numerically. Our own simulational study is guided by mathematical considerations of Biskup *et al.* [1, 2], which are based on an equilibrium framework and result in largely model independent scaling predictions for the condensation process in the infinite-volume limit.

In rather elaborate Monte Carlo simulations of the 2D Ising lattice gas model we could verify that the behaviour of droplets which live on a square lattice is compatible with these predictions already for moderately large system sizes [3]. Moreover, recently we have shown that the underlying lattice structure and interaction range are largely irrelevant provided that properly scaled variables are used [4].

Having established the insensitivity of the droplet condensation mechanism to microscopic details, we next turned to exploratory analyses of the coexistence region where the system is either in the condensed phase with a single large droplet that has adsorbed a fraction $\lambda = 2/3$ of the particles (respectively of the excess magnetisation) or in the evaporated phase with many small bubbles ($\lambda = 0$). In Fig. 11.11 the probability distribution of λ is shown which clearly demonstrates the expected two-phase signal. The minimum between the two peaks corresponds to a free-energy barrier. More precisely, according to the theory [5], the ratio of the minimum to the maximum should decrease with system size L as $\exp(-\beta\Delta F) \simeq \exp(-cL^{2/3})$ with $c = 0.1522$ at $T = 1/\beta = 1.5$. If we allow for an additional power-like prefactor $\propto L^{\kappa}$, a least-squares fit through the data points for $L \geq 90$ yields $c = 0.211 \pm 0.003$ with a goodness-of-fit parameter $Q = 0.22$. Even though this estimate is quite far off the expectation, if we fix $c = 0.1522$ and consider the data for $L \geq 170$, we obtain a perfectly compatible fit with a goodness of $Q = 0.16$. For the larger lattice sizes the two fits are hardly distinguishable which makes it so difficult to estimate the parameter c reliably [5].

Alternatively, by measuring the (integrated) autocorrelation time τ_{int} in simulations with the magnetisation fixed directly at the evaporation/condensation point, we also find a compatible asymptotic scaling behaviour, $\tau_{\text{int}} \simeq \exp(c\,L^{2/3})$, with $c = 0.124 \pm 0.008$, but the parameter c is again difficult to estimate reliably with the present data set [5]. Presumably much larger lattices are needed to arrive at a firm estimate.

Note that in multimagnetical simulations with a flat magnetisation distribution, this free-energy barrier is not directly visible when monitoring the magnetisation alone. Rather, it appears as a "hidden" obstacle in an "orthogonal" direction of phase space. However, it is still clearly reflected by a slowing down of the performance of the simulations, which makes it important to understand the scaling properties of this barrier also from a purely algorithmic point of view.

[1] M. Biskup et al.: Europhys. Lett. **60**, 21 (2002)
[2] M. Biskup et al.: Comm. Math. Phys. **242**, 137 (2003)
[3] A. Nußbaumer et al.: Europhys. Lett. **75**, 716 (2006)
[4] A. Nußbaumer et al.: Phys. Rev. E **77**, 041109 (2008)

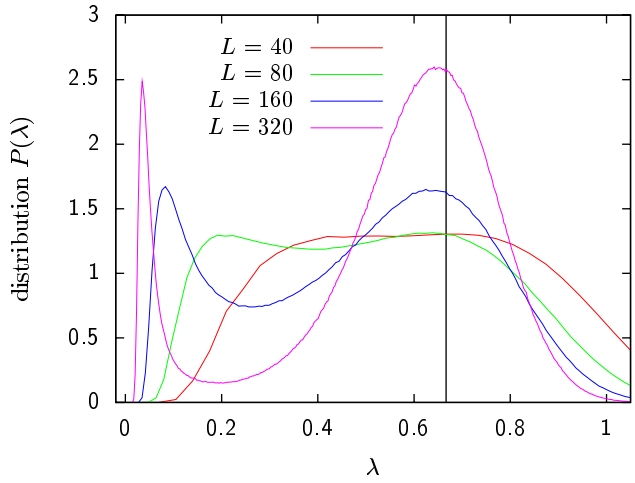

Figure 11.11: Probability distribution of the fraction λ close to the evaporation/condensation transition on 2D square lattices at $T = 1.5$, exhibiting a clear two-phase signal. The minimum between the two peaks corresponds to the free-energy barrier.

[5] A. Nußbaumer et al.: *Free-Energy Barrier at Droplet Condensation*, Prog. Theor. Phys. Suppl. (in press)

11.13 Quantum Critical Points for Mixed Heisenberg Spin Chains

R. Bischof, W. Janke

The main focus of this project is on quantum critical phenomena and low-temperature properties of various versions of the 1D antiferromagnetic quantum Heisenberg model, which is one of the most fundamental models of quantum magnetism and is related to high-temperature superconductors. The low-temperature properties of quantum spin chains depend significantly on the size of spins involved. Uniform chains of half-odd integer spins have no energy gap between the ground state and first excited states (i.e., they are quantum critical), whereas chains with integer spins do show an excitation gap. Above that, spin chains can be driven to and away from criticality by tuning appropriate parameters (such as bond alternation, exchange anisotropy, next-nearest-neighbour interaction, spin-phonon coupling, etc.). While there exists a wide literature about quantum critical phenomena in uniform spin chains, mixed chains have yet rarely been considered.

By means of quantum Monte Carlo (QMC) simulations based on the continuous imaginary time loop algorithm [1, 2] and quantum reweighting methods [3] we have first investigated the uniform $S = 1/2$ Heisenberg spin chain with bond alternation and alternating quantum chains of mixed spins, consisting of two different kinds of spin, $S_a = 1/2$ and $S_b = 1$, that appear alternatingly in pairs ("model A"). For comparison, we recently also started investigations of the cases $S_a = 1/2$ and $S_b = 3/2$ ("model B") as well as $S_a = 1$ and $S_b = 3/2$ ("model C").

If the coupling-constant ratio $\alpha = J'/J$ is varied at fixed anisotropy parameter Δ (multiplying the z-component of the spin-spin scalar product), one observes a second-order phase transition at zero temperature. For the simple Heisenberg model symmetric in spin space ($\Delta = 0$) one has $\alpha_c = 1$ and the critical exponent of the correlation length takes the value $\nu = 2/3$. Due to the self duality of the Heisenberg spin chain, $\alpha_c = 1$ is valid for all $0 \leq \Delta \leq 1$, but ν varies continuously from 2/3 to 1 for $\Delta = 0$. Mixed spin chains do not exhibit self duality and hence also the critical coupling α_c varies with Δ. One of our goals was therefore a precise determination of the phase diagrams in the $\alpha - \Delta$ parameter space. While most data have already been generated, the final analysis will still take some time. In general the scaling behaviour of the correlation length ξ is complicated by multiplicative logarithmic corrections which, in the simplest case, take the form $\xi \sim \alpha^{-2/3} |\ln \alpha|^{1/2}$. Such a behaviour is difficult to analyze numerically and often results in the determination of effective exponents which include or imitate the logarithmic correction term.

The twist order parameter is well suited to signal quantum phase transitions between different valence bond configurations in various 1D quantum spin systems. At non-zero temperature we have found the formation of a plateau in the twist order parameter around the (zero temperature) quantum critical point [4]. We have investigated the possibility that this plateau is related to the quantum critical region that fans out from the quantum critical point. However, up to the present accuracy of our simulations the data does not yet support this conjecture [4]. Alternative one may also consider a disorder parameter for which we have developed a suitable generalization to mixed spin chains. This new observable is currently tested numerically.

[1] B.B. Beard, U.J. Wiese: Phys. Rev. Lett. **77**, 5130 (1996)
[2] H.G. Evertz: Adv. Phys. **52**, 1 (2003)
[3] M. Troyer et al.: Braz. J. Phys. **34**, 377 (2004)
[4] R. Bischof, W. Janke: in Proceedings of the International Conference *Path Integrals – New Trends and Perspectives*, ed. by W. Janke, A. Pelster (World Scientific, Singapore 2008) p 514

11.14 Critical Behaviour of Quantum Compass and Plaquette Orbital Models

S. Wenzel, W. Janke, A. Läuchli*

*Max Planck Institute for the Physics of Complex Systems (MPI PKS), Dresden, Germany

This project deals with a new type of quantum spin models that is currently getting into focus of condensed matter physics. These are systems which look very similar to an ordinary Heisenberg model but lack some of the couplings which are present there. Examples are the famous Kitaev model [1] which has prompted enormous efforts because of a potential realization as a topological quantum computer. In this line of research also a related model, the so-called compass model, was investigated in the literature in connection to interesting physics ranging from orbital order in transition

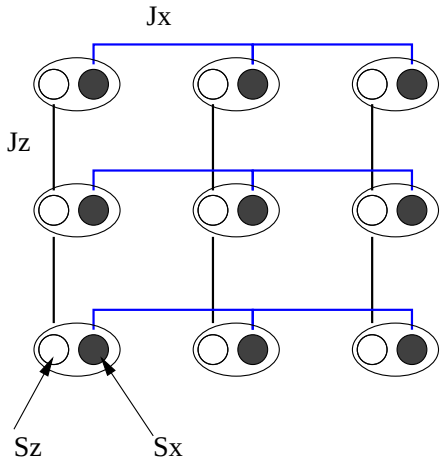

Figure 11.12: Visualization of the quantum compass model. The different components of the spin interact differently and only along specific directions.

metal compounds to topologically protected qbits [2, 3]. The compass model is defined in two dimensions by the following Hamiltonian

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

where σ are the usual Pauli operators, J_x, J_y coupling constants and e_z a unit vector in z direction (cp. Fig. 11.12). Although this is a simple looking Hamiltonian it is rather hard to study. It was actually shown to possess rich physics ranging from highly degenerate ground states, quantum phase transitions to an exciting thermal phase transition. A recent Letter [4] furthermore proposes that directional order in the quantum compass model is rather stable against dilution, which is not the case for the classical model.

To investigate these questions in more detail, we have performed a comprehensive study of the two-dimensional (2D) compass model on square lattices for classical and quantum spin degrees of freedom using classical and quantum Monte Carlo methods [5]. We employed state-of-the-art implementations using Metropolis, stochastic series expansion (SSE) and parallel tempering (PT) techniques to obtain the critical ordering temperatures and critical exponents. In a pre-investigation we reconsidered the classical compass model where we study and contrast the finite-size scaling (FSS) behaviour of ordinary periodic boundary conditions against annealed boundary conditions. We found that periodic boundary conditions suffer from extreme finite-size effects, which might be caused by closed loop excitations on the torus, so that one needs to go to very large lattice sizes to see the asymptotic scaling behaviour. Our numerical results are at odds with recent literature on the subject which we can trace back to neglecting these strong finite-size effects on periodic lattices. Our analysis showed, however, that one arrives at quite different conclusions when these effects are properly taken into account [5, 6]. Our findings for the quantum model might have an impact on previous conclusions concerning the dilution effects on the compass model because a precise estimate of the critical temperature T_c enters crucially into this analysis [6].

In the search for other fundamental spin models and to gain further insights into the field around the underlying Kitaev model, we have proposed a different, topolo-

gical modification of the compass model and studied its intriguing physics [7]. Our main result for this "plaquette orbital model" is the establishment of an interesting (topological) order that can be described by a crystallization and modulation of local energy contributions but which lacks conventional magnetic order. We show that our new model falls into the Ising universality class and that it possesses well behaved FSS properties in contrast to the compass model. As a bi-product we can then argue that quantum spins make these orbital models stiff against all kinds of disturbances – geometrical variations and impurities – in contrast to classical fields [6, 7].

The precision of our results for the quantum model was still rather low compared to many other systems of statistical physics. In this respect it was therefore a challenging project to devise and analyze special boundary conditions for the quantum model with improved FSS behaviour compared to periodic boundary conditions. To this end we reconsidered recently the directional-ordering transition in the two-dimensional classical and quantum compass model on the square lattice, obtaining several improvements [8]. First, an improved algorithm is proposed which builds on the Wolff cluster algorithm in one-dimensional subspaces of the configuration space. This improvement allows us now to study much larger classical systems up to $L = 512$. Based on the new algorithm we give evidence for the presence of strongly anomalous scaling for periodic boundary conditions which is much worse than anticipated before. Second, we propose and study alternative boundary conditions for the compass model which do not make use of extended configuration spaces of the annealed boundary schemes and show that they completely remove the problem with finite-size scaling. In particular we apply these boundary conditions to the quantum problem and present a considerably improved estimate for the critical temperature which should be of interest for future studies on the compass model. The origin of the anomalous scaling is also discussed.

Work supported by the Studienstiftung des deutschen Volkes and the Leipzig Graduate School *BuildMoNa*.

[1] A. Kitaev: Ann. Phys. **321**, 2 (2006)
[2] K.I. Kugel, D.I. Khomskii: Sov. Phys. Usp. **25**, 231 (1982)
[3] B. Douçot et al.: Phys. Rev. B **71**, 024505 (2005)
[4] T. Tanaka, S. Ishihara: Phys. Rev. Lett **98**, 256402 (2007)
[5] S. Wenzel, W. Janke: Phys. Rev. B **78**, 064402 (2008); see also "Publisher's Note" in Phys. Rev. B **78**, 099902(E) (2008) [Fig. 1 selected for Phys. Rev. B "Kaleidoscope" August 2008]
[6] S. Wenzel: *Monte Carlo Investigations of Low-Dimensional Classical and Quantum Spin Systems: Unconventional Criticality and Orbital Ordering*, PhD thesis, Universität Leipzig (2009)
[7] S. Wenzel, W. Janke: Phys. Rev. B **80**, 054403 (2009) [Fig. 2(c) selected for Phys. Rev. B "Kaleidoscope" August 2009]
[8] S. Wenzel et al.: Phys. Rev. E **81**, 066702 (2010) [arXiv:1002.3508]

11.15 Universal Amplitude Ratios for the Potts Model

B. Berche*, P. Butera†, W. Janke, L. Shchur‡

*Laboratoire de Physique des Matériaux, Nancy Université, France
†Istituto Nazionale di Fisica Nucleare, Milano, Italy
‡Landau Institute for Theoretical Physics, Chernogolovka, Russia

At a second-order phase transition not only critical exponents are universal but also certain amplitude ratios, i.e., they do not depend on the details of the considered statistical system. A typical example is provided by the scaling relation for the magnetic suceptibility χ which in the vicinity of the critical temperature T_c behaves according to $\chi \sim \Gamma_{\pm}|T/T_c - 1|^{-\gamma}$, where γ is the critical exponent and Γ_+ and Γ_- denote the critical amplitudes in the high- and low-temperature phase, respectively. The ratio Γ_+/Γ_- is then such a universal amplitude ratio.

Values for Γ_+/Γ_- could recently be predicted analytically for the two-dimensional q-state Potts model with $q = 2, 3$ and 4 states [1, 2]. This is one of simplest models which exhibit a phase transition. It is solved exactly at the critical point for any number of spin components q and it is known that for $q \leq 4$ it has a continuous phase transition whereas for $q > 4$ the phase transition is of first order. The model has a great theoretical interest as new theories may be tested in this model. At the same time, these models may have some practical interest as they may be realized in an adsorbate lattice placed onto a clean crystalline surface. The full classification of such systems with continuous transitions is known theoretically and there exist experiments in which some of them realize the 3-state and 4-state Potts models, so that the critical exponents can be experimentally estimated.

While for $q = 2$ and 3 the prediction for the amplitude ratios could subsequently be confirmed with numerical techniques (Monte Carlo simulations and high-temperature series expansions) [3], the situation for $q = 4$ remained controversial. The origin for the disagreement can probably be traced back to relatively strong logarithmic corrections of the leading scaling behaviour [4]. It is a common belief that the $q = 4$ Potts and the Baxter-Wu model (a model with three-spin interaction on a triangular lattice) [5] belong to the same universality class. Still, at the same time, the critical behaviour of the Baxter-Wu model is *not* modified by logarithmic corrections. Our extensive numerical analysis shows that critical amplitude ratios are very close for both models and, therefore, gives support to the hypothesis that the critical behaviour of both systems is governed by the same renormalization group fixed point.

[1] G. Delfino, J.L. Cardy: Nucl. Phys. B [FS] **519**, 551 (1998)
[2] G. Delfino et al.: Nucl. Phys. B **565**, 521 (2000)
[3] L.N. Shchur et al.: Nucl. Phys. B **620**, 579 (2002)
[4] B. Berche et al.: Comp. Phys. Comm. **180**, 493 (2009)
[5] R.J. Baxter, F.Y. Wu: Phys. Rev. Lett. **31**, 1294 (1973); Aust. J. Phys. **27**, 357 (1974)

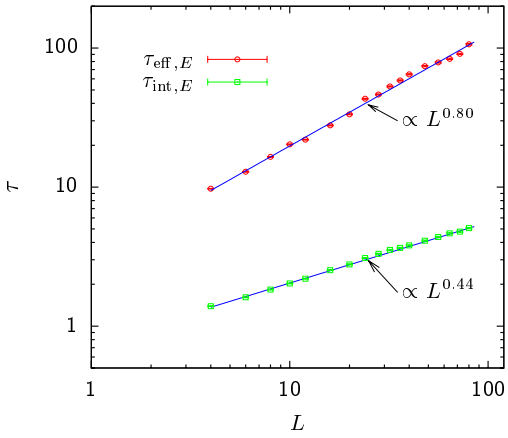

Figure 11.13: Autocorrelation times τ_{int} and τ_{eff} for the energy of the 3D Ising model, where $\tau_{\mathrm{eff}} = N_{\mathrm{rep}}\,\tau_{\mathrm{int}}$ and N_{rep} is the number of replica of the parallel tempering algorithm.

11.16 Parallel Tempering Cluster Algorithm

E. Bittner, W. Janke

While much attention has been paid in the past to simulations of first-order phase transitions and systems with rugged free-energy landscapes in generalized ensembles (umbrella, multicanonical, Wang-Landau, parallel/simulated tempering sampling) [1], the merits of this non-Boltzmann sampling approach also for simulation studies of critical phenomena have been pointed out only recently. In finite-size scaling analyses of Monte Carlo simulations of second-order phase transitions one often needs an extended temperature range around the critical point. In Ref. [2], Berg and one of the authors combined multibondic sampling [3] with the Wang-Landau recursion [4] to cover the complete desired "critical" temperature range in a single simulation for each lattice size, where the "desired" range derives from a careful finite-size scaling (FSS) analysis of all relevant observables. Since the individual reweighting ranges of the involved observables may be quite disparate, this scaling analysis is the second important ingredient of the method.

Here we combine the parallel-tempering algorithm [5] with cluster updates [6] and an improved adaptive routine to find the range of interest [7]. To assess the performance of our method, we measured the integrated autocorrelation time $\tau_{\mathrm{int}}(T_i, L)$ for each temperature and system size. We found that the maximal integrated autocorrelation times $\tau_{\mathrm{int}}(L) = \max_{i=1,N_{\mathrm{rep}}} \tau_{\mathrm{int}}(T_i, L)$ for the energy, squared magnetization and the first structure factor scale only weakly $\propto L^z$ with the system size L, e.g., $z = 0.44(1)$ for the energy of the 3D Ising model. To make a fair comparison with other methods, we also take the computational effort into account and include the number of replica N_{rep} of the parallel tempering algorithm into the definition of an effective autocorrelation time according to $\tau_{\mathrm{eff}} = N_{\mathrm{rep}}\,\tau_{\mathrm{int}} \propto L^{z_{\mathrm{eff}}}$, yielding for the energy an exponent $z_{\mathrm{eff}} = 0.80(1)$, i.e., $N_{\mathrm{rep}} \propto L^{0.36}$, cf. Fig. 11.13.

As a result, we gain two further orders of magnitude in the performance for 2D and 3D Ising models in comparison with the recently proposed Wang-Landau recursion for cluster algorithms based on the multibondic algorithm, which is already a great improvement over the standard multicanonical variant [8, 9].

[1] W. Janke (Ed.): *Rugged Free Energy Landscapes: Common Computational Approaches to Spin Glasses, Structural Glasses and Biological Macromolecules*, Lect. Notes Phys. **736** (Springer, Berlin 2008)
[2] B.A. Berg, W. Janke: Phys. Rev. Lett. **98**, 040602 (2007)
[3] W. Janke, S. Kappler: Phys. Rev. Lett. **74**, 212 (1995)
[4] F. Wang, D.P. Landau: Phys. Rev. Lett. **86**, 2050 (2001)
[5] K. Hukushima, K. Nemoto: J. Phys. Soc. Jpn. **65**, 1604 (1996)
[6] R.H. Swendsen, J.-S. Wang: Phys. Rev. Lett. **58**, 86 (1987)
[7] E. Bittner et al.: Phys. Rev. Lett. **101**, 130603 (2008)
[8] E. Bittner, W. Janke: PoS (LAT2009) 042
[9] E. Bittner, W. Janke: *Parallel Tempering Cluster Algorithm for Computer Simulations of Critical Phenomena*, Leipzig preprint, submitted

11.17 Error Estimation and Reduction with Cross Correlations

M. Weigel*, W. Janke

*Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany

Monte Carlo simulations, and in particular Markov chain based methods, have matured over the last decades into a highly versatile and powerful toolbox for studies of systems in statistical and condensed-matter physics, ranging from classical spin models over soft-matter problems to quantum systems. Their competitiveness with other approaches such as, e.g., field-theoretic expansions for the study of critical phenomena, is largely based on the development and refinement of a number of advanced simulation techniques such as cluster algorithms and generalized-ensemble methods.

Equally important to the generation of simulation data, however, is their correct and optimal analysis. In this field, a number of important advances over the techniques used in the early days have been achieved as well. These include, e.g., the finite-size scaling (FSS) approach, turning the limitation of simulational methods to finite system sizes into a systematic tool for accessing the thermodynamic limit, reweighting techniques, lifting the limitation of numerical techniques to the study of single points in parameter space to allow for continuous functions of estimates to be studied, as well as advanced statistical tools for error estimation such as the jackknife and other resampling schemes of data analysis [1].

Of these techniques, the statistical data analysis appears to have received the least attention. Hence, while FSS analyses, even including correction terms, are quite standard in computer simulation studies, a proper analysis and reduction of statistical errors and bias appears to be much less common. More specifically, data generated by a Monte Carlo (MC) simulation are subject to two types of correlation phenomena, namely (a) autocorrelations or temporal correlations for the case of Markov chain MC (MCMC) simulations, which are directly related to the Markovian nature of the underlying stochastic process and lead to an effective reduction of the number of independently sampled events, and (b) cross correlations between different estimates extracted from the same set of original time series data coming about by the origin of estimates in

the same statistical data pool. The former can be most conveniently taken into account by a determination of the relevant autocorrelation times and a blocking or binning transformation resulting in an effectively uncorrelated auxiliary time series [2, 3]. Such analyses are by now standard at least in seriously conducted simulational studies.

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

[1] B. Efron, R.J. Tibshirani: *An Introduction to the Bootstrap* (Chapman and Hall, Boca Raton 1998)
[2] H. Flyvbjerg, H.G. Petersen: J. Chem. Phys. **91**, 461 (1989)
[3] W. Janke: Lect. Notes Phys. **739**, 79 (2008)
[4] H.G. Ballesteros et al.: Phys. Lett. B **387**, 125 (1996)
[5] W. Janke, T. Sauer: J. Chem. Phys. **107**, 5821 (1997)
[6] M. Weigel, W. Janke: Phys. Rev. B **62**, 6343 (2000)
[7] M. Weigel, W. Janke: Phys. Rev. Lett. **102**, 100601 (2009)
[8] L.A. Fernández, V. Martín-Mayor: Phys. Rev. E **79**, 051109 (2009)
[9] M. Weigel, W. Janke: Phys. Rev. E **81**, 066701 (2010) [arXiv:1002.4517]

11.18 Funding

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

Forschergruppe 877: From Local Constraints to Macroscopic Transport
W. Janke (Principal Investigator)
Deutsche Forschungsgemeinschaft (DFG)

Research Training Network (RTN) "ENRAGE": Random Geometry and Random Matrices: From Quantum Gravity to Econophysics
W. Janke (Principal Investigator)
EU, Grant No. MRTN-CT-2004-005616

Statistical Mechanics of Complex Networks
W. Janke (with Z. Burda, Krakau)
Alexander von Humboldt Foundation, "Institutspartnerschaft" with the Jagiellonian University, Krakow, Poland, Grant No. 3.4-Fokoop-DEU/1117877

Statistical Physics of Complex Systems
W. Janke (with B. Berche, Nancy)
Deutsch-Französische Hochschule, "Deutsch-Französisches Doktorandenkollegium (DFDK)" with "Co-tutelle de Thèse", jointly with Nancy Université, France, Grant No. CDFA-02-07

Θ-Polymers in Porous Media Under Applied Force
W. Janke
Alexander von Humboldt Foundation, Host of Humboldt Fellowship for Dr. Viktoria Blavatska, Lviv, Ukraine, Grant No. 3.3-UKR/11207567 STP-2

Host of *Alexander von Humboldt Research Prize Winner Bernd A. Berg (Florida State University, Tallahassee, USA)*
W. Janke
Alexander von Humboldt Foundation

Dynamik und Statik von Spingläsern
W. Janke
Deutsche Forschungsgemeinschaft (DFG), Grant No. JA483/22-1

Phasenübergänge in Systemen mit einschränkender Geometrie
W. Janke
Deutsche Forschungsgemeinschaft (DFG), Grant Nos. JA483/23-1 and 2

Investigation of Thermodynamic Properties of Lattice and Off-Lattice Models for Proteins and Polymers
M. Bachmann and W. Janke
Deutsche Forschungsgemeinschaft (DFG), Grant Nos. JA483/24-1 and 2

Molecular Conformation Mechanics of Proteins and Polymers
W. Janke
Deutsche Forschungsgemeinschaft (DFG), Grant No. JA483/24-3

Mass Transport Models on Networks
W. Janke (twin project with H. Meyer-Ortmanns, Jacobs University Bremen)
Deutsche Forschungsgemeinschaft (DFG), Grant No. JA483/27-1

Monte Carlo Simulationen der Statik und Dynamik von Spingläsern
E. Bittner and W. Janke
NIC Jülich (computer time grant for "JUROPA"), Grant No. hlz10

Statistical Mechanics of Protein and Polymer Structure Formation Processes
M. Bachmann and W. Janke
NIC Jülich (computer time grant for "JUROPA"), Grant No. hlz11

Quantum Monte Carlo Simulations of Quantum Spin Models
W. Janke
NIC Jülich (computer time grant for "JUROPA"), Grant No. hlz12

Grant for support of the Conference *MECO34*, 29. March – 01. April 2009
W. Janke (Organizer, together with S. Trimper, Universität Halle)
Deutsche Forschungsgemeinschaft (DFG), Grant No. JA 483/26-1

Grant for support of the Conference *MECO34*, 29. March – 01. April 2009
W. Janke (Organizer, together with S. Trimper, Universität Halle)
SMWK, Grant No. 4-7531.50-05-09/4

Grant for support of students participating in the Conference *MECO34*, 29. March – 01. April 2009
W. Janke (Organizer, together with S. Trimper, Universität Halle)
Wilhelm und Else Heraeus-Stiftung

Grant for full support of 75 participants of the *International Conference ENRAGEing Perspectives – Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*, 17.–22. May 2009
W. Janke (Organizer)
Max-Planck-Institut für Physik komplexer Systeme, Dresden

Grant for support of the Workshop *Simulations on GPU*, 11.-12. June 2009
W. Janke (Organizer, together with M. Bordag, Abt. QFG)
Deutsche Forschungsgemeinschaft (DFG), Grant No. BO1112/17-1

Quanten Monte Carlo Simulationen von (ungeordneten) Quantenspinsystemen
R. Bischof
Landesgraduiertenstipendium

Dimerized Heisenberg Models
S. Wenzel
Studienstiftung des deutschen Volkes

11.19 Organizational Duties

Michael Bachmann

- Referee for Physical Review Letters, Journal of the American Chemical Society, IEEE/ACM Transactions on Computational Biology and Bioinformatics, Physical Review A, Physical Review E, Journal of Physics A, European Journal of Physics D, Biophysical Reviews and Letters, Computer Physics Communications, Journal of Computational Chemistry, Macromolecules, PhysChemChemPhys
- External Reviewer for Engineering and Physical Sciences Research Council (EPSRC), Great Britain; National Science Foundation (NSF), USA

Elmar Bittner

- Scientific Secretary of the 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34*, Universität Leipzig, 29. March – 01. April 2009
- Scientific Secretary of the Workshop *Simulations on GPU*, ITP, Universität Leipzig, 11.–12. June 2009

- Co-organizer of the contribution *Fußball-Fieber wissenschaftlich betrachtet*, Wissenschaftsmesse *Studieren in Mitteldeutschland* (with W. Janke, A. Nußbaumer), Neue Messe Leipzig, 5. September 2009
- Scientific Secretary of the Workshop *CompPhys09 – 10th International NTZ-Workshop on New Developments in Computational Physics*, ITP, Universität Leipzig, 26.–29. November 2009
- Scientific Secretary of the Workshop *CompPhys10 – 11th International NTZ-Workshop on New Developments in Computational Physics*, ITP, Universität Leipzig, 25.–27. November 2010
- Referee for Physical Review Letters, Physical Review E, Journal of Physics A, European Journal of Physics B, Computer Physics Communications

Wolfhard Janke

- Director, Naturwissenschaftlich-Theoretisches Zentrum (NTZ), Universität Leipzig
- Chairperson of the Programme Committee "Scientific Computing" of Forschungszentrum Jülich
- Member of the Scientific-Technical-Council of the Supervisory Board ("Aufsichtsrat") of the Forschungszentrum Jülich GmbH
- External Member of the Jagiellonian University Graduate School *International Ph.D. Studies in Physics of Complex Systems*, Krakow, Poland
- Specialist Editor, Computer Physics Communications (CPC), Elsevier, Amsterdam, The Netherlands
- Editor "Computational Sciences", Lecture Notes of Physics, Springer, Berlin, Heidelberg, Germany
- Editor "Computational Physics", Central European Journal of Physics, Krakow, Poland
- Member of Editorial Board, Condens. Matter Phys., Lviv, Ukraine
- Permanent Member of the "International Advisory Board", *Conference of the Middle European Cooperation in Statistical Physics (MECO)*
- Organizer of the *Symposium der Sächsischen Forschergruppe FOR877* (with K. Kroy, Abt. TKM), Fakultät für Physik und Geowissenschaften, Universität Leipzig, 27. January 2009
- Organizer of the 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34* (with S. Trimper, Martin-Luther-Universität Halle-Wittenberg), Universität Leipzig, 29. March – 01. April 2009
- Organizer of the International Conference *ENRAGEing Perspectives – Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*, Max-Planck-Institut für Physik komplexer Systeme in Dresden, 17.–22. May 2009
- Organizer of the contribution of the DFH-UFA German-French Graduate College *Physics of Complex Systems* at the International Science Fair *Research*, FU Berlin, 28. May 2009
- Organizer of the Workshop *Simulations on GPU* (with M. Bordag, Abt. QFG), ITP, Universität Leipzig, 11.–12. June 2009
- Organizer of the Workshop and Tutorial *Modeling and Simulating Macromolecules*, ITP, Universität Leipzig, 9.–10. July 2009
- Co-organizer of the contribution *Fußball-Fieber wissenschaftlich betrachtet*, Wissenschaftsmesse *Studieren in Mitteldeutschland* (with E. Bittner, A. Nußbaumer), Neue

Messe Leipzig, 5. September 2009
- Organizer of the Workshop *CompPhys09 – 10th International NTZ-Workshop on New Developments in Computational Physics*, ITP, Universität Leipzig, 26.–29. November 2009
- Member of International Organization Committee of the 10th International Conference *Path Integrals* (with L.S. Schulman (USA), M. Gutzwiller (USA), A. Inomata (USA), J.R. Klauder (USA), D. Fujikawa (Japan) und Chookyu Lee (South Korea)), Washington DC, USA, 11.–16. July 2010
- Organizer of the Workshop *CompPhys10 – 11th International NTZ-Workshop on New Developments in Computational Physics*, ITP, Universität Leipzig, 25.–27. November 2010
- External Reviewer for Humboldt-Stiftung; Deutsche Forschungsgemeinschaft; Studienstiftung des deutschen Volkes; the Jeffress Memorial Trust, Bank of America, Virginia, USA; "Fond zur Förderung der wissenschaftlichen Forschung (FWF)", Österreich; "The Royal Society", Great Britain; The "Engineering and Physical Sciences Research Council (EPSRC)", Great Britain; The University of Warwick, England, Great Britain; Coventry University, England, Great Britain; CECAM, Lyon, France; National Science Foundation (NSF), USA; Israel Science Foundation, Israel
- Referee for Physical Review Letters, Physical Review B, Physical Review E, Journal of Chemical Physics, Europhysics Letters, Physics Letters A, Physics Letters B, The European Physical Journal B, Physica A, Proceedings of the Royal Physical Society, Journal of Physics A, Computer Physics Communications, JSTAT, New Journal of Physics, International Journal of Modern Physics C

Andreas Nußbaumer
- Scientific Secretary of the 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34*, Universität Leipzig, 29. March – 01. April 2009
- Co-organizer of the contribution *Fußball-Fieber wissenschaftlich betrachtet*, Wissenschaftsmesse *Studieren in Mitteldeutschland* (with E. Bittner, W. Janke), Neue Messe Leipzig, 5. September 2009

11.20 External Cooperations

Academic

- EU RTN "ENRAGE" – *Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*
  Research Training Network of 13 teams throughout Europe
- Dept. of Physics, Florida State University, Tallahassee, USA
  Prof. Dr. Bernd A. Berg
- CEA/Saclay, Service de Physique Théorique, France
  Dr. Alain Billoire
- Laboratoire de Physique des Matériaux (UMR CNRS No 7556), Nancy Université, France
  Prof. Dr. Bertrand Berche, Dr. Christophe Chatelain, Dr. Olivier Collet, Prof. Dr. Malte Henkel, Dr. Dragi Karevski

- Groupe de Physique des Matériaux (UMR CNRS No 6634), Université de Rouen, France
  Dr. Pierre-Emmanuel Berche
- Department of Mathematics and the Maxwell Institute for Mathematical Sciences, Heriot-Watt University, Edinburgh, Scotland, UK
  Prof. Dr. Desmond A. Johnston
- SUPA, School of Physics and Astronomy, University of Edinburgh, Scotland, UK
  Dr. Richard A. Blythe, Prof. Dr. Martin Evans
- Applied Mathematics Research Centre, Coventry University, England, UK
  Dr. Ralph Kenna, PD Dr. Christian von Ferber
- Applied Mathematics, Universitat Pompeu Fabra, Barcelona, Spain
  Dr. Ramon Villanova
- Engineering of Physics, Ankara University, Turkey
  Prof. Dr. Handan Arkin (Olgar)
- Dept. of Physics, Hacettepe University, Ankara, Turkey
  Prof. Dr. Tarik Çelik, Gökhan Gökoğlu
- Institute for Condensed Matter Physics, National Academy of Sciences, Lviv, Ukraine
  Dr. Viktoria Blavatska, Prof. Dr. Yurij Holovatch
- Complex Systems Division, Department of Theoretical Physics, Lund University, Lund, Sweden
  Prof. Dr. Anders Irbäck, Simon Mitternacht
- Dept. of Physics, Michigan Technological University, Houghton, USA
  Prof. Dr. Ulrich H.E. Hansmann
- Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich
  Prof. Dr. Peter Grassberger, PD Dr. Thomas Neuhaus
- Institut für Physik, Universität Mainz
  Prof. Dr. Kurt Binder, Dr. Hsiao-Ping Hsu, Dr. Martin Weigel
- Atominstitut, TU Wien, Austria
  Prof. Dr. Harald Markum, Dr. Rainer Pullirsch
- Istituto Nazionale di Fisica Nucleare, Sezione di Milano-Bicocca, Milano, Italy
  Prof. Dr. Pablo Butera
- Banaras Hindu University, Varanasi, India
  Prof. Dr. Sanjay Kumar
- Brunel Univ. of West London, England, UK
  Dr. Gernot Akemann
- Inst. für Theoretische Physik, FU Berlin
  Prof. Dr. Hagen Kleinert
- IAC-1, Universität Stuttgart
  Prof. Dr. Rudolf Hilfer, Anjan Prasad Gantapara
- Inst. für Theoretische Physik, Universität Duisburg-Essen
  PD Dr. Axel Pelster

- Inst. für Theoretische Physik, Universität Bielefeld
  Prof. Dr. Friderike Schmid
- Jacobs Universität Bremen
  Prof. Dr. Hildegard Meyer-Ortmanns
- Institute of Physics, Jagiellonian University, Kraków, Poland
  Prof. Dr. Piotr Białas, Dr. Leszek Bogacz, Prof. Dr. Zdzisław Burda
- Landau Institute for Theoretical Physics, Chernogolovka, Russia
  Prof. Dr. Lev N. Shchur
- Yerevan Physics Institute, Yerevan, Armenia
  Prof. Dr. David B. Saakian
- Zhejiang Institute of Modern Physics, Zhejiang University, Hangzhou, P.R. China
  Prof. Dr. He-Ping Ying, Prof. Dr. Bo Zheng

11.21 Publications

Journals

G. Akemann, E. Bittner, M.J. Philips, L. Shifrin: *A Wigner Surmise for Hermitian and Non-Hermitian Chiral Random Matrices*, Phys. Rev. E **80**, 065201(R)-1–4 (2009)

B. Berche, P. Butera, W. Janke, L. Shchur: *Universal Ratios of Critical Amplitudes in the Potts Model Universality Class*, Comp. Phys. Comm. **180**, 493–496 (2009)

E. Bittner, A. Nußbaumer, W. Janke: *Anisotropy of the Interface Tension of the Three-Dimensional Ising Model*, Nucl. Phys. B **820**, 694–706 (2009)

E. Bittner, A. Nußbaumer, W. Janke: *Tune the Autocorrelation Time and Unleash the Full Power of the Parallel Tempering Algorithm*, PoS (LAT2009) 027-1–7 (2009)

E. Bittner, A. Nußbaumer, W. Janke, M. Weigel: *Football Fever: Goal Distributions and Non-Gaussian Statistics*, Eur. Phys. J. B **67**, 459–471 (2009) [discussed in Nature News Feature article *Goal Beget Goals*, Nature **441**, 793 (2006)]

V. Blavatska, W. Janke: *Walking on Fractals: Diffusion and Self-Avoiding Walks on Percolation Clusters*, J. Phys. A: Math. Theor. **42**, 015001-1–18 (2009)

V. Blavatska, W. Janke: *Polymers in Crowded Environment Under Stretching Force: Globule-Coil Transitions*, Phys. Rev. E **80**, 051805-1–10 (2009)

R.A. Blythe, W. Janke, D.A. Johnston, R. Kenna: *Continued Fractions and the Partially Asymmetric Exclusion Process*, J. Phys. A: Math. Theor. **42**, 325002-1–21 (2009)

M. Hasenbusch: *The Kosterlitz-Thouless Transition in Thin Films: A Monte Carlo Study of Three-Dimensional Lattice Models*, J. Stat. Mech.: Theor. Exp. P02005-1–34 (2009)

M. Hasenbusch, F. Parisen Toldin, A. Pelissetto, E. Vicari: *Critical and Multicritical Behavior of the ±J Ising Model in Two and Three Dimensions*, J. Phys.: Conf. Ser. **145**, 012055-1–4 (2009)

W. Janke, E. Bittner: *Replica-Exchange Cluster Algorithm*, PoS (LAT2009) 042-1–7 (2009)

W. Janke, E. Bittner, A. Nußbaumer, M. Weigel: *Football Fever: Self-Affirmation Model for Goal Distributions*, Condens. Matter Phys. **12**, 739–752 (2009)

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

C. Junghans, M. Bachmann, W. Janke: *Statistical Mechanics of Aggregation and Crystallization for Semiflexible Polymers*, Europhys. Lett. **87**, 40002-1–5 (2009)

M. Möddel, M. Bachmann, W. Janke: *Conformational Mechanics of Polymer Adsorption Transitions at Attractive Substrates*, J. Phys. Chem. B **113**, 3314–3323 (2009)

S. Schnabel, M. Bachmann, W. Janke: *Elastic Lennard-Jones Polymers meet Clusters – Differences and Similarities*, J. Chem. Phys. **131**, 124904-1–9 (2009)

S. Schnabel, T. Vogel, M. Bachmann, W. Janke: *Surface Effects in the Crystallization Process of Elastic Flexible Polymers*, Chem. Phys. Lett. **476**, 201–204 (2009)

T. Vogel, T. Neuhaus, M. Bachmann, W. Janke: *Thickness-Dependent Secondary Structure Formation of Tubelike Polymers*, Europhys. Lett. **85**, 10003-1–5 (2009)

T. Vogel, T. Neuhaus, M. Bachmann, W. Janke: *Thermodynamics of Tubelike Flexible Polymers*, Phys. Rev. E **80**, 011802-1–8 (2009)

T. Vogel, T. Neuhaus, M. Bachmann, W. Janke: *Ground-State Properties of Tubelike Flexible Polymers*, Eur. Phys. J. E **30**, 7–18 (2009)

B. Wacław, J. Sopik, W. Janke, H. Meyer-Ortmanns: *Pair-Factorized Steady States on Arbitrary Graphs*, J. Phys. A: Math. Theor. **42**, 315003-1–8 (2009) [Selected by the Editors for the special IoP Select collection (July 2009)]

B. Wacław, J. Sopik, W. Janke, H. Meyer-Ortmanns: *Tuning the Shape of the Condensate in Spontaneous Symmetry Breaking*, Phys. Rev. Lett. **103**, 080602-1–4 (2009)

B. Wacław, J. Sopik, W. Janke, H. Meyer-Ortmanns: *Mass Condensation in One Dimension with Pair-Factorized Steady States*, J. Stat. Mech.: Theor. Exp. P10021-1–29 (2009)

S. Wenzel, W. Janke: *Comprehensive Quantum Monte Carlo Study of the Quantum Critical Points in Planar Dimerized/Quadrumerized Heisenberg Models*, Phys. Rev. B **79**, 014410-1–11 (2009)

S. Wenzel, W. Janke: *Finite-Temperature Néel Ordering of Fluctuations in a Plaquette Orbital Model*, Phys. Rev. B **80**, 054403-1–6 (2009) [Fig. 2(c) selected for Phys. Rev. B "Kaleidoscope" August 2009]

M. Weigel, W. Janke: *Cross Correlations in Scaling Analyses of Phase Transitions*, Phys. Rev. Lett. **102**, 100601-1–4 (2009) [selected for Phys. Rev. Lett. *Highlights Synopsis* of April 13, 2009, by Yonko Millev]

Books

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

in press

B.A. Berg, W. Janke: *Wang-Landau Multibondic Cluster Approach to Simulations of Second-Order Transitions*, in *Computer Simulations in Condensed Matter Physics XX*, ed. by D.P. Landau, S.P. Lewis, H.-B. Schüttler (Springer, Heidelberg 2010) (in press)

A. Nußbaumer, E. Bittner, W. Janke: *Free-Energy Barrier at Droplet Condensation*, Prog. Theor. Phys. Suppl. (in press)

A. Nußbaumer, E. Bittner, T. Neuhaus, W. Janke: *Universality of the Evaporation/ Condensation Transition*, in *Computer Simulations in Condensed Matter Physics XX*, ed. by D.P. Landau, S.P. Lewis, H.-B. Schüttler (Springer, Heidelberg 2010) (in press)

B. Wacław, J. Sopik, W. Janke, H. Meyer-Ortmanns: *Mass Condensation on Networks*, in *XI Latin American Workshop on Nonlinear Phenomena – LAWNP'09*, Búzios, Brazil, J. Phys.: Conf. Ser. (in press)

Talks

M. Bachmann: *Conformational Mechanics of Molecular Structure Formation Processes*, Seminar talk, Universität zu Köln, 20. January 2009

M. Bachmann: *Conformational Mechanics of Molecular Structure Formation Processes*, invited talk, 22nd Annual Workshop on *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, Athens, Georgia, USA, 23.–27. February 2009

M. Bachmann: *Modeling and Simulation of Peptide Adsorption at Silicon Substrates*, invited talk, SimBioMa Workshop *Challenges in Modelling the Interface between Biomolecules and Inorganic Surfaces*, Schloss Waldthausen, Mainz, 18.–20. March 2009

M. Bachmann: *Modeling and Simulation of Macromolecule Adsorption to Substrates* Workshop *ProSurf – Protein Surface Interaction*, Sestri Levante, Italy, 04.–06. July 2009

M. Bachmann: *Challenges in Computational Biology*, NTZ Colloquium talk, Universität Leipzig, 09. July 2009

M. Bachmann: *Modeling and Simulation of Macromolecule Adsorption to Substrates*, invited talk, Symposium *Simulation of Molecules and Nanotubes*, Technion, Haifa, Israel, 13. October 2009

M. Bachmann: *Challenges in Computational Biology*, Colloquium talk, Forschungszentrum Jülich, 06. November 2009

M. Bachmann, G. Schröder: Presentation of the *Computational Biology Cluster Jülich*, Workshop *Theoretical Biology*, Universität zu Köln, 09. December 2009

R. Bischof: *QMC of Spin Chains: Order Parameter, Improved Estimators, Reweighting*, Workshop *Simulations on GPU*, Universität Leipzig, 11.–12. June 2009

E. Bittner: *Droplet Condensation at First-Order Phase Transitions*, invited talk, Conference *ENRAGEing Perspectives – Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*, MPI PKS, Dresden, 18.–22. May 2009

E. Bittner: *Make Life Simple: Unleash the Full power of the Parallel Tempering Algorithm*, *The XXVII International Symposium on Lattice Field Theory – Lattice 2009*, Peking University, Beijing, China, 26.–31. July 2009

E. Bittner: *Football Fever: Goal Distributions and Non-Gaussian Statistics*, invited talk, *Österreichische Statistiktage 2009*, WU Wien, Wien, Österreich, 21.–23. September 2009

W. Janke: *Fractals Meet Fractals – Random Walks on Percolation Clusters*, *SFG FOR877 Symposium*, Universität Leipzig, 27. January 2009

W. Janke: *Fractals Meet Fractals – Self-Avoiding Random Walks on Percolation Clusters*, 22th Annual Workshop on *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, University of Georgia, Athens, USA, 23.–27. February 2009

W. Janke: *Aggregation and Crystallization of Semiflexible Polymers*, invited talk, SimBioMa Workshop *Challenges in Modelling the Interface Between Biomolecules and Inorganic Surfaces*, Schloss Waldthausen, Mainz, 18.–20. March 2009

W. Janke: *Computational Statistical Physics*, invited talk ("Hauptvortrag"), Focused Session *50 years DY: Trends in Dynamics and Statistical Physics*, DPG Frühjahrstagung 2009, TU Dresden, 23.–27. March 2009

W. Janke: *Fractals Meet Fractals – Self-Avoiding Random Walks on Percolation Clusters*, invited talk, Atelier Nancy *Statistical Physics and Low Dimensional Systems 2009*, Nancy Université, France, 13.–15. May 2009

W. Janke: *Monte Carlo Sampling of Rare Event States*, invited talk, *Mainz Materials Simulation Days*, Max-Planck-Institut für Polymerforschung, Mainz, 03.–05. June 2009

W. Janke: *Football Fever: Self-Affirmation Model for Goal Distributions*, invited plenary talk, 3rd Conference on *Statistical Physics: Modern Trends and Applications – Stat Phys 09*, Lviv, Ukraine, 23.–25. June 2009

W. Janke: *Universal Aspects of the Condensation/Evaporation Transition of Ising Droplets*, invited talk, Workshop on *Frontiers in Nonequilibrium Physics*, Kyoto, Japan, 21. July – 21. August 2009

W. Janke: *Modeling and Simulating Macromolecules*, Physikalisches Kolloquium, Universität Duisburg-Essen, 11. November 2009

M. Möddel: *Polymer Adsorption Transitions at Attractive Substrates Analysed from a Canonical and a Microcanonical Perspective*, Spring Meeting of the German Physical Society, TU Dresden, 23.–27. March 2009

M. Möddel: *The Adsorption Transition of a Single Coarse-Grained Polymer in the Microcanonical Ensemble*, Workshop and Tutorial *Modeling and Simulating Macromolecules*, ITP, Universität Leipzig, 09.–10. July 2009

M. Möddel: *Systematic Microcanonical Analyses of Polymer Adsorption Transitions*, 2nd *BuildMoNa* Workshop for Doctoral Candidates, Neukirchen/Pleiße, 08.–09. October 2009

M. Möddel: *Systematic Microcanonical Analyses of Polymer Adsorption Transitions*, 10th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys09*, Universität Leipzig, 26.–29. November 2009

S. Schnabel: *Solid-Solid Transitions of Flexible Polymers*, Saxonian Theory Seminar, Chemistry Department, Universität Leipzig, 26.–27. February 2009

S. Schnabel: *Solid-Solid Transitions of Flexible Polymers*, Spring Meeting of the German Physical Society, TU Dresden, 23.–27. March 2009

S. Schnabel: *Tieftemperaturverhalten minimalistischer Polymermodelle*, PhD Defense talk, ITP, Universität Leipzig, 28. Oktober 2009

S. Schöbl: *Semiflexible Polymers in Random Disorder*, Seminar talk, DFH-UFA guest stay, Nancy Université, France, 14. September 2009

S. Schöbl: *Effect of Disorder on Equilibrium Conformations of Semiflexible Polymers*, 2nd *BuildMoNa* Workshop for Doctoral Candidates, Neukirchen/Pleiße, 08.–09. October 2009

T. Vogel: *Secondary Structure Formation of Tubelike Polymers*, Saxonian Theory Seminar, Chemistry Department, Universität Leipzig, 26.–27. February 2009

T. Vogel: *Thickness-Dependent Secondary Structure Formation of Tubelike Polymers*, Spring Meeting of the German Physical Society, TU Dresden, 23.–27. March 2009

T. Vogel: *Secondary Structure Formation of Tubelike Polymers*, Seminar talk, Universidad Complutense de Madrid, Spain, 15. April 2009

T. Vogel: *Structural Behavior of Polymers from Monte Carlo Studies of Coarse-Grained Models*, invited talk, Symposium *Simulation of Molecules and Nanotubes*, Technion, Haifa, Israel, 13. October 2009

T. Vogel: *Structural Behavior of Polymers from Monte Carlo Studies of Coarse-Grained Models*, PhD Defense talk, ITP, Universität Leipzig, 13. November 2009

B. Wacław: *Condensation in Mass Transport Models with Factorized Steady States*, Seminar talk, Universität Freiburg, 04. March 2009

B. Wacław: *Condensation in 1D Systems with Pair-Factorized Steady States*, Spring Meeting of the German Physical Society, TU Dresden, 23.–27. March 2009

B. Wacław: *Localization in Maximal-Entropy Random Walk*, TKM Seminar, ITP, Universität Leipzig, 29. April 2009

B. Wacław: *Localization in Maximal-Entropy Random Walk*, Seminar talk, Physics Department, Humboldt Universität zu Berlin, 06. May 2009

B. Wacław: *Condensation in Pair-Factorized Steady States*, Conference *ENRAGEing Perspectives – Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*, MPI PKS, Dresden, 18.–22. May 2009

S. Wenzel: *Quantum Phase Transitions in Systems of Coupled Spin Dimers*, Spring Meeting of the German Physical Society, TU Dresden, 23.–27. March 2009

S. Wenzel: *Evidence for an Unconventional Universality Class From a Two-Dimensional Dimerized Quantum Heisenberg Model*, 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34*, Universität Leipzig, 29. March – 01. April 2009

S. Wenzel: *Monte Carlo Investigations of Low-Dimensional Classical and Quantum Spin Systems: Unconventional Criticality and Orbital Ordering*, PhD Defense talk, ITP, Universität Leipzig, 22. April 2009

S. Wenzel: *The Compass Model with Screw-Periodic Boundary Conditions*, Seminar talk, Ecole Polytechnique Fédéral de Lausanne (EPFL), Switzerland, 09. December 2009

M. Wiedenmann: *Evaporation/Condensation Transition of 3D Ising Droplets*, 2nd *BuildMoNa* Workshop for Doctoral Candidates, Neukirchen/Pleiße, 08.–09. October 2009

Posters

M. Aust, E. Bittner, W. Janke: *Free Energy Inherent Structures in Spin Glass Models*, Spring Meeting of the German Physical Society, TU Dresden, 23.–27. March 2009

M. Aust, E. Bittner, W. Janke: *Free Energy Inherent Structures in Spin Glass Models*, 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34*, Universität Leipzig, 29. March – 01. April 2009

R. Bischof, W. Janke: *Plateau Formation in the Twist Parameter of the Bond Alternating Antiferromagnetic S=1/2 Heisenberg Spin Chain*, Spring Meeting of the German Physical Society, TU Dresden, 23.–27. March 2009

R. Bischof, W. Janke: *Formation of a Plateau in the Twist Parameter of the Bond Alternating Antiferromagnetic S=1/2 Heisenberg Spin Chain*, 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34*, Universität Leipzig, 29. March – 01. April 2009

R. Bischof, W. Janke: *Phase Diagram of a Mixed Quantum Spin Chain with Bond Alternation and Exchange-Anisotropy*, 10th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys09*, Universität Leipzig, 26.–29. November 2009

E. Bittner, A. Nußbaumer, W. Janke: *Anisotropy of the Interface Tensions of the Three-Dimensional Ising Model*, Spring Meeting of the German Physical Society, TU Dresden, 23.–27. March 2009

E. Bittner, A. Nußbaumer, W. Janke: *Anisotropy of the Interface Tensions of the Three-Dimensional Ising Model*, 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34*, Universität Leipzig, 29. March – 01. April 2009

E. Bittner, A. Nußbaumer, W. Janke, M. Weigel: *Fußballfieber*, Wissenschaftsmesse *Studieren in Mitteldeutschland*, Neue Messe Leipzig, 05. September 2009

E. Bittner, A. Nußbaumer, W. Janke: *Anisotropy of the Interface Tensions of the Three-Dimensional Ising Model*, 10th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys09*, Universität Leipzig, 26.–29. November 2009

W. Janke, E. Bittner: *Replica-Exchange Cluster Algorithm*, *The XXVII International Symposium on Lattice Field Theory – Lattice 2009*, Peking University, Beijing, China, 26.–31. July 2009

M. Weigel, W. Janke: *Cross Correlations in Scaling Analyses of Phase Transitions*, 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34*, Universität Leipzig, 29. March – 01. April 2009

S. Karalus, W. Janke, M. Bachmann: *Cutting the Energy Range in Multicanonical Monte Carlo Simulations*, 10th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys09*, Universität Leipzig, 26.–29. November 2009

M. Möddel, M. Bachmann, W. Janke: *Conformational Mechanics of Polymer Adsorption Transitions at Attractive Substrates*, Workshop *BioStruct09*, Florence, Italy, 16.–18. February 2009

M. Möddel, M. Bachmann, W. Janke: *Conformational Mechanics of Polymer Adsorption Transitions at Attractive Substrates*, SimBioMa Workshop *Challenges in Modelling the Interface Between Biomolecules and Inorganic Surfaces*, Schloss Waldthausen, Mainz, 18.–20. March 2009

M. Möddel, M. Bachmann, W. Janke: *Conformational Mechanics of Polymer Adsorption Transitions at Attractive Substrates*, 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34*, Universität Leipzig, 29. March – 01. April 2009

M. Möddel, M. Bachmann, W. Janke: *Conformational Mechanics of Polymer Adsorption Transitions at Attractive Substrates*, 2nd Scientific Symposium of the Graduate School *BuildMoNa*, Universität Leipzig, 02.–03. April 2009

M. Möddel, M. Bachmann, W. Janke: *Conformational Mechanics of Polymer Adsorption Transitions at Attractive Substrates*, Workshop *Statistical Physics and Low Dimensional Systems 2009*, Nancy, France, 13.–14. May 2009

M. Möddel, M. Bachmann, W. Janke: *Conformational Mechanics of Polymer Adsorption Transitions at Attractive Substrates*, Workshop *ProSurf – Protein Surface Interaction*, Sestri Levante, Italy, 04.–06. July 2009

M. Möddel, W. Janke, M. Bachmann: *Systematic Microcanonical Analyses of Polymer Adsorption Transitions*, Jülich Soft Matter Days 2009, Bonn, 10.–13. November 2009

H. Nagel, P. Białas, B. Wacław, W. Janke: *Monte Carlo Generation of Equilibrated Graphs*, Spring Meeting of the German Physical Society, TU Dresden, 23.–27. March 2009

H. Nagel, P. Białas, B. Wacław, W. Janke: *Monte Carlo Generation of Equilibrated Graphs*, 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34*, Universität Leipzig, 29. March – 01. April 2009

A. Nußbaumer, E. Bittner, W. Janke: *A Nearly Local Observable for a Global Quantity*, 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34*, Universität Leipzig, 29. March – 01. April 2009

A. Nußbaumer, E. Bittner, W. Janke: *A Nearly Local Observable for a Global Quantity*, Conference *ENRAGEing Perspectives – Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*, MPI PKS Dresden, 18.–22. May 2009

S. Schnabel, M. Bachmann, W. Janke: *Solid-Solid Transitions of Flexible Polymers*, 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34*, Universität Leipzig, 29. March – 01. April 2009

S. Schnabel, M. Bachmann, W. Janke: *Solid-Solid Transitions of a Flexible Elastic Off-Lattice Polymer Model*, 2nd Scientific Symposium of the Graduate School *BuildMoNa*, Universität Leipzig, 02.–03. April 2009

S. Schöbl, K. Kroy, W. Janke: *Effect of Disorder on Equilibrium Conformations of Semiflexible Polymers*, Spring Meeting of the German Physical Society, TU Dresden, 23.–27. March 2009

S. Schöbl, K. Kroy, W. Janke: *Effect of Disorder on Equilibrium Conformations of Semiflexible Polymers*, 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34*, Universität Leipzig, 29. March – 01. April 2009

S. Schöbl, K. Kroy, W. Janke: *Effect of Disorder on Equilibrium Conformations of Semiflexible Polymers*, 2nd Scientific Symposium of the Graduate School *BuildMoNa*, Universität Leipzig, 02.–03. April 2009

T. Vogel, T. Neuhaus, M. Bachmann, W. Janke: *Thickness-Dependent Secondary Structure Formation of Tubelike Polymers*, 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34*, Universität Leipzig, 29. March – 01. April 2009

T. Vogel, T. Neuhaus, M. Bachmann, W. Janke: *Thermodynamics of Tubelike Flexible Polymers*, Jülich Soft Matter Days 2009, Bonn, 10.–13. November 2009

S. Wenzel, W. Janke: *Monte Carlo Simulations on the 2D Compass Model*, School on *Modern Theories of Correlated Electron Systems*, Les Houches, France, 11.–29. May 2009

M. Wiedenmann, A. Nußbaumer, E. Bittner, W. Janke: *Monte Carlo Study of the Evaporation/Condensation Transition of Ising Droplets*, 34th Conference of the Middle European Cooperation in Statistical Physics *MECO34*, Universität Leipzig, 29. March – 01. April 2009

M. Wiedenmann, A. Nußbaumer, E. Bittner, W. Janke: *Monte Carlo Study of the Evaporation/Condensation Transition of Ising Droplets*, 2nd Scientific Symposium of the Graduate School *BuildMoNa*, Universität Leipzig, 02.–03. April 2009

M. Wiedenmann, A. Nußbaumer, E. Bittner, W. Janke: *Monte Carlo Study of the Evaporation/Condensation Transition of Ising Droplets*, 10th International NTZ-Workshop on *New Developments in Computational Physics – CompPhys09*, Universität Leipzig, 26.–29. November 2009

11.22 Graduations

Doctorate

- Sandro Wenzel
  Monte Carlo Investigations of Low-Dimensional Classical and Quantum Spin Systems: Unconventional Criticality and Orbital Ordering
  22. April 2009
- Stefan Schnabel
  Tieftemperaturverhalten minimalistischer Polymermodelle
  28. Oktober 2009
- Thomas Vogel
  Structural Behaviour of Polymers from Monte Carlo Studies of Coarse-Grained Models
  13. November 2009

11.23 Guests

- Prof. Dr. Günter Ahlers
  University of California at Santa Barbara, USA
  Stochastically Driven Large-Scale Circulation in Turbulent Rayleigh-Benard Convection
  29. March – 02. April 2009
- Prof. Dr. Hagen Kleinert
  Institut für Theoretische Physik, FU Berlin
  Multivalued Fields
  29. March – 02. April 2009
- Prof. Dr. David P. Landau
  University of Georgia, Athens, USA
  Monte Carlo Simulations of Systems with Complex Energy Landscapes
  29. March – 05. April 2009

- Prof. Dr. Hartmut Löwen
  Institut für Theoretische Physik II, Universität Düsseldorf
  Colloidal Suspensions Subjected to External Fields
  29. March – 02. April 2009
- Prof. Dr. Georg Maret
  Dept. of Physics, Universität Konstanz
  Melting and Glass Transition of a 2D Colloidal Model System
  29. March – 02. April 2009
- Prof. Dr. Sidney Redner
  Dept. of Physics, Boston University, USA
  Dynamical Approach for Solving Complex Networks
  29. March – 02. April 2009
- Prof. Dr. Matthias Troyer
  Theoretische Physik, ETH Zürich, Switzerland
  Continuous Time QMC Solvers for Quantum Impurity Problems
  29. March – 02. April 2009
- Prof. Dr. Royce K. P. Zia
  Virginia Tech, Blacksburg, USA
  Non-Equilibrium Statistical Mechanics: A Growing Frontier of "Pure and Applied" Theoretical Physics
  29. March – 02. April 2009
- Prof. Dr. Bertrand Berche
  Statistical Physics Group, IJL, Nancy Université, France
  Gauge Field Theory Approach to Spin Transport in 2D Electron Gas
  29. March – 02. April 2009
- Prof. Dr. Thomas Nattermann
  Institut für Theoretische Physik, Universität zu Köln
  Localized States and Interaction Induced Delocalization in Bose Gases with Quenched Disorder
  29. March – 02. April 2009
- Prof. Dr. Handan Arkin (Olgar)
  Physics Engineering, Ankara University, Turkey
  Study of the Conformational Changes of Hydrophobic-Polar Polymer Chain near a Hydrophobic Chain
  29. March – 02. April 2009
- Prof. Dr. Malte Henkel
  Nancy Université, France
  Non-Equilibrium Kinetics and Ageing in Non-Glauberian Ising Models
  29. March – 02. April 2009
- Prof. Dr. Ferenc Iglói
  Institute of Theoretical Physics, Research Institute for Solid State Physics and Optics, Budapest, Hungary
  Entanglement Entropy of Quantum Spin Chains
  29. March – 02. April 2009

- Prof. Dr. Bernd A. Berg
  Florida State University, Tallahassee, USA
  Research Prize Winner of the Alexander von Humboldt Foundation
  01. May – 31. July 2009
- Dr. Viktoria Blavatska
  Institute for Condensed Matter Physics, Lviv, Ukraine
  Humboldt Fellow/FOR877 guest
  01. May – 31. July 2009
- Marcin Zagorski
  Jagellonian University, Krakow, Poland
  22.–31. May 2009
- Prof. Dr. Stefan Boettcher
  Emory University, Atlanta, USA
  Heuristische Bestimmung und die Auswertung von Ising Spin-Glas-Grundzuständen
  5.–6. November 2009
- Prof. Dr. Nobuyasu Ito
  Department of Applied Physics, Graduate School of Engineering, The University of Tokyo, Japan
  Simulation Study on Nonequilibrium Transport Phenomena
  26.–30. November 2009
- Jean-Charles Walter
  Université Henri Poincaré, Nancy, France
  Numerical Investigation of the Aging of the Fully-Frustrated XY Model
  25.–29. November 2009
- Prof. Dr. Victor Martín-Mayor
  Departamento de Fisica Teorica I, Universidad Complutense de Madrid, Spain
  Large-Scale Equilibrium Simulation of the 3D Edwards-Anderson Model
  25.–29. November 2009
- PD Dr. Stefan Wessel
  Institut für Theoretische Physik III, Universität Stuttgart
  Optimized Broad-Histogram Ensembles for the Simulation of Quantum Systems
  25.–29. November 2009
- Dr. Viktoria Blavatska
  Institute for Condensed Matter Physics, Lviv, Ukraine
  Polymers in Crowded Environment Under Stretching Force: Globule-Coil Transitions
  25. November – 02. December 2009