November 19, 2014, 16:50

ABSTRACTS

of contributions to the

15th International NTZ-Workshop on

New Developments in Computational Physics

CompPhys14

Institut für Theoretische Physik,
Universität Leipzig, Germany

27 – 29 November 2014

http://www.physik.uni-leipzig.de/~janke/CompPhys14

Supported by Research Academy Leipzig (RALeipzig), DFG Research Group FOR877, DFG SFB/TRR 102, Alexander von Humboldt Foundation, Deutsch-Französische Hochschule (DFH-UFA), Graduate School "BuildMoNa", and Centre for Theoretical Sciences (NTZ) of Universität Leipzig.

Preface

Welcome to our Jubilee Workshop, the 15th International NTZ-Workshop *CompPhys14* on *New Developments in Computational Physics*. As in previous years, also this year's Workshop will cover a broad spectrum of different fields ranging from general aspects of computational and statistical physics over computer simulation studies in condensed and soft matter physics, including applications to biological systems, and random networks to the intriguing properties of quantum systems and high-energy physics. Following the traditional setup of the Workshop, it is also this year designed to provide a forum for an informal exchange of ideas and to meet in a relaxed atmosphere in Leipzig at the beginning of Christmas time.

The main part of the Workshop takes place from 27 – 28 November 2014 in the Small Lecture Hall ("Kleiner Hörsaal") and the "Aula" of the Experimental Physics building in Linnéstr. 5. We are very grateful to all colleagues who helped moving their regular lecture courses to another location or date, and in particular to Ms. Sandy Ehlers who coordinated this difficult task. We also wish to thank the secretaries of the Institute for Theoretical Physics, Ms. Susan Hussack, Ms. Gabriele Menge, and Ms. Lea Voigt, for their invaluable help with all administrative matters.

As in previous years, the Saturday, 29 November 2014, is devoted to various discussion rounds and collaborative meetings which will take place in the Theoretical Physics building. Note that two years ago the Institute for Theoretical Physics has moved from the old location "Vor dem Hospitaltore 1" to the *new* office building in "Brüderstr. 16".

Finally, we and the Centre for Theoretical Sciences (NTZ) gratefully acknowledge financial support of the Workshop from Research Academy Leipzig (RALeipzig), DFG Research Group FOR877, DFG Collaborative Research Centre SFB/TRR 102, Alexander von Humboldt Foundation, Deutsch-Französische Hochschule (DFH-UFA), and Graduate School "BuildMoNa: Building with Molecules and Nano-objects".

Leipzig, November 2014
Wolfhard Janke

Abstracts

A 20th century physics no-no problem: The reasons of us being

Michael Bachmann

Center for Simulational Physics, Department of Physics & Astronomy, The University of Georgia, Athens, USA

bachmann@smsyslab.org

Biomolecules such as proteins are finite and small – but not microscopic – systems that are of "in-between" sizes, i.e., they exist on mesoscopic length scales. This means, they are too large to allow for a quantum-chemical description of their physical properties and too small for a classical macroscopic approach. They do not even exhibit long-range symmetries, which would be helpful for their theoretical modeling. Nonetheless, processes that lead to functional structures of such molecules in a complex thermal environment surprisingly exhibit features known from thermodynamic phase transitions. Since the thermodynamic limit is out of sight, sophisticated computer simulations are currently the only way for the systematic study of the statistical mechanics of structural transitions in these systems. The striking finite-size effects that influence or even govern processes on mesoscopic scales lead to a couple of fundamental questions such as: What is temperature? In this talk, revised statistical mechanics concepts for finite systems, molecular models, and simulation methods are introduced. Examples of generic molecular structure formation processes such as protein folding, polymer aggregation, and macromolecular adsorption at solid matter will be discussed.

Subtleties of gauge theory in Aharonov-Bohm rings

Bertrand Berche

Groupe de Physique Statistique, Institut Jean Lamour, Université de Lorraine Nancy, France

bertrand.berche@univ-lorraine.fr

The talk will consider several features on gauge transformations in simple one-dimensional mesoscopic rings. The discussion mainly concerns the physics described by multivalued wave functions. The textbook situation of Aharonov-Bohm rings will then be extended to consider more general non-Abelian gauge transformations of spin-orbit interactions.

Modeling many-body van der Waals interactions without electrons

Tristan Bereau

Max-Planck-Institut für Polymerforschung, D-55128 Mainz, Germany

bereau@mpip-mainz.mpg.de

We estimate polarizabilities of atoms in molecules without electron density, using a Voronoi tesselation approach instead of conventional density partitioning schemes. The resulting atomic dispersion coefficients are calculated, as well as many-body dispersion effects on intermolecular potential energies. We also estimate contributions from multipole electrostatics and compare them to dispersion. We assess the performance of the resulting intermolecular interaction model from dispersion and electrostatics for more than 1300 neutral and charged, small organic molecular dimers. Applications to water clusters, the benzene crystal, the anti-cancer drug ellipticine intercalated between two Watson-Crick DNA base pairs, as well as six macro-molecular host-guest complexes highlight the potential of this method and help to identify points of future improvement. The mean absolute error made by the combination of static electrostatics with many-body dispersion reduces at larger distances, while it plateaus for two-body dispersion, in conflict with the common assumption that the simple $1/R^6$ correction will yield proper dissociative tails. Overall, the method achieves an accuracy well within conventional molecular force fields while exhibiting a simple parametrization protocol.

Random walks in power-law correlated disordered environment

Viktoria Blavatska[1]
(with Niklas Fricke[2], Martin Marenz[2], Johannes Zierenberg[2], and Wolfhard Janke[2])

[1] Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Lviv, Ukraine
[2] Institut für Theoretische Physik, Universität Leipzig, Germany
viktoria@icmp.lviv.ua

We study the statistical properties of random walks in a disordered environment with quenched defects that obey power-law correlations $\sim r^{-a}$ for large separations r. This type of disorder describes the impurities organized in complex fractal structures, characterized by fractal dimension $d_f = d - a$ in d-dimensional space. Applying both the Pruned-Enriched Rosenbluth Method (PERM) and an exact enumeration technique, we numerically estimate the universal size and shape characteristics such as the scaling exponent ν governing the effective size of a random walk trajectory and averaged asphericity A_d of typical random walk configuration in $d = 2$ at various values of the correlation parameter a.

Semi-flexible polymers in disordered media (P)

Johannes Bock
(with Wolfhard Janke)

Institut für Theoretische Physik, Universität Leipzig, Germany
jbock@itp.uni-leipzig.de

We report computational studies of the behavior of semi-flexible polymers in disordered media. An off-lattice chain growth algorithm based on the Monte Carlo method is used to examine configurational properties of the polymers such as the end-to-end distance and tangent-tangent correlation. Particular attention is paid to the effects of the disordered environment on the properties of the polymers. These studies are validated by comparison with previous work done in our group in two dimensions, which is now expanded into the third dimension.

On the mixing of the single-bond dynamics for the random-cluster model

Eren Metin Elçi
(with Martin Weigel)

Applied Mathematics Research Centre, Coventry University, United Kingdom
eren.metin.elci@gmail.com

The Markov Chain Monte Carlo method is a ubiquitous tool in Statistical Physics. It is standard lore that close to a point of a second-order phase transition a phenomenon called "critical slowing down" hampers efficient sampling. A major breakthrough in reducing this slowing down for the random-cluster model has been the invention of the Swendsen-Wang-Chayes-Machta algorithm. Recently, however, it has been shown, both rigorously and numerically, that local chains can be as or even more efficient than non-local chains. Examples are the Worm algorithm for the Ising model and the single-bond dynamics for the random-cluster model. Here we present results of a numerical study of the coupling time of the single-bond chain dynamics for the random-cluster model. A careful analysis allows us to obtain high-precision (upper) bounds for auto-correlation, relaxation and mixing times for both critical and off-critical temperatures on square and simple-cubic lattices. The numerical results give strong evidence in favor of the rapid-mixing property of the single-bond dynamics for the random-cluster model, both at a second-order phase transition and off criticality. In particular for the square lattice we show that super- and sub-critical efficiencies are, due to duality, tied together. Furthermore we also present, to our knowledge, a novel heuristic method for detecting a first-order phase transition in the coupling-time distribution. This work has been done in collaboration with Timothy Garoni and Andrea Collevecchio, School of Mathematical Sciences, Monash University, Melbourne, Australia.

Rare-event simulations for score statistics of multiple sequence alignments

Pascal Fieth
Institute for Physics, University of Oldenburg, Germany
pascal.fieth@uni-oldenburg.de

Assessing the significance of alignment scores of optimally aligned DNA or amino acid sequences requires knowledge of the score distribution in the biologically relevant high-scoring region. For gapless local alignments of infinitely long sequences this distribution is known to follow a Gumbel distribution analytically. Distributions for gapped local alignments and global alignments can only be obtained numerically. The rare-event region of the distribution has to be known to determine the significance of alignments with biological relevance. To cover this region, previous studies utilised parallel tempering for the analysis of pairwise local alignments with gaps [1]. They showed that, contrary to results from previous simple sampling studies, a Gaussian correction to the Gumbel distribution is necessary in case of finite sequence lengths. Here, this study is expanded to global alignments and to sum-of-pair scores of multiple sequence alignments, i.e. the alignments of more than two sequences, with gaps. The results for score distributions of local and global multiple sequence alignments will be shown, where regions with probabilities smaller than 10^{-100} could be obtained.

[1] S. Wolfsheimer, B. Burghardt, and A.K. Hartmann, *Local sequence alignment statistics: Deviations from Gumbel statistics in the rare-event tail*, Algorithms for Molecular Biology **2** (2007) 9.

True asymptotics of self-avoiding walks on 3D percolation clusters

Niklas Fricke
(with Wolfhard Janke)
Institut für Theoretische Physik, Universität Leipzig, Germany
niklas.fricke@itp.uni-leipzig.de

We study self-avoiding walks on three-dimensional critical percolation clusters using a new exact enumeration method. It overcomes the exponential increase in computation time by exploiting the clusters' fractal nature. We enumerate walks of over 10^4 steps, far more than has ever been possible. The scaling exponent ν for the end-to-end distance turns out to be smaller than previously thought and appears to be the same on the backbones as on full clusters. We find strong evidence against the widely assumed scaling law for the number of conformations and propose an alternative, which perfectly fits our data.

Universality in the three-dimensional random-field Ising model

Nikolaos Fytas
Applied Mathematics Research Centre, Coventry University, United Kingdom
ab5298@coventry.ac.uk

By performing a high-statistics simulation of the $D = 3$ random-field Ising model at zero temperature for different shapes of the random-field distribution, we show that the model is ruled by a single universality class. We compute the complete set of critical exponents for this class, including the correction-to-scaling exponent, and we show, to high numerical accuracy, that scaling is described by two independent exponents. Discrepancies with previous works are explained in terms of strong scaling corrections.

Poly(3-hexylthiophene) adsorption on Au(001)

Jonathan Gross[1]
(with Stefan Förster[2], Erik Kohl[2], Momchil Ivanov[1], Wolf Widdra[2], and Wolfhard Janke[1])

[1] Institut für Theoretische Physik, Universität Leipzig, Germany
[2] Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany
gross@itp.uni-leipzig.de

We employ Monte Carlo algorithms to simulate coarse-grained poly(3-hexylthiophene) (P3HT) chains of different lengths adsorbed on a Au(001) surface. The polymer–surface interaction is represented by a 10–4 Lennard-Jones layered potential, with a height modulation of the top layer to incorporate the stripe-like pattern induced by the surface reconstruction at the vacuum interface. We compare the findings of our simulations to scanning tunneling microscopy (STM) images. To quantify the agreement of experiment and simulations we measure end-to-end distances and radii of gyration [1].

[1] S. Förster, E. Kohl, M. Ivanov, J. Gross, W. Widdra, and W. Janke, J. Chem. Phys. **141** (2014) 164701.

Large deviations for work distributions

Alexander Hartmann
Institute for Physics, University of Oldenburg, Germany
a.hartmann@uni-oldenburg.de

Here, we study rare events in non-equilibrium processes using numerical simulations. We develop a very general black-box method, based on sampling vectors of random numbers within an artificial finite-temperature (Boltzmann) ensemble to access rare events and large deviation for almost arbitrary equilibrium and non-equilibrium processes. In this way, we obtain probabilities as small as 10^{-180}, hence rare events and large-deviation properties can be easily obtained. We study the distribution of work performed for a critical two-dimensional Ising system of size $L \times L = 128 \times 128$ upon rapidly changing the external magnetic field. To obtain, e.g., free-energy differences from the work distributions (using the Jarzynski theorem), they must be studied in ranges where the probabilities are as small as 10^{-240}. The present approach allows one to obtain the free energy with a very high relative precision of 10^{-4}. This works well also for non-zero field, i.e., for a case where standard umbrella-sampling methods are not efficient to calculate free energies. Furthermore, for the present case it is verified that the resulting distributions of work for forward and backward processes fulfill Crooks theorem with high precision.

Phase transition of films in the Ising universality class

Martin Hasenbusch
Institut für Physik, Humboldt-Universität zu Berlin, Germany
martin.hasenbusch@physik.hu-berlin.de

We study the transition of films with free and periodic boundary conditions. We determine accurately the transition temperature and the scaling of this temperature with the thickness of the film. We confirm that the transition belongs to the universality class of the two-dimensional Ising model.

Ring polymers in disordered environment: Conformational properties (P)

Khrystyna Haydukivska
(with Viktoria Blavatska)

Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Lviv, Ukraine
wja4eslawa@icmp.lviv.ua

We analyze the universal size characteristics of flexible ring polymers in solutions in presence of structural obstacles (impurities) in d dimensions. One encounters such situations when considering polymers in gels, colloidal solutions, intra- and extracellular environments. Applying the direct polymer renormalization scheme, we evaluate the estimates for averaged gyration radius R_g and spanning radius $R_{1/2}$ of typical ring polymer conformation. Our results quantitatively reveal an extent of the effective size and anisotropy of closed ring macromolecules in disordered environment.

Spherical models of interface growth

Malte Henkel

Groupe de Physique Statistique, Institut Jean Lamour, Université de Lorraine Nancy, France
malte.henkel@ijl.nancy-universite.fr

In magnetic phase transitions, the spherical model of Berlin & Kac is a well-known device which replaces non-linear interactions by the so-called "spherical constraint". In this way, one obtains a new universality class with an exactly solvable member; and with non-trivial properties near their critical point. Here, we shall discuss to what extent the Kardar-Parisi-Zhang equation of interface growth can be represented by a conveniently chosen "spherical variant". The Arcetri models so obtained will be carefully defined and their stationary and non-stationary scaling behaviour will be analysed.

Simulating three-body Casimir interactions in colloidal suspensions (P)

Hendrik Hobrecht
(with Fred Hucht)

Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany
hendrik@thp.uni-due.de

We study the fluctuation-induced (Casimir) interactions in colloidal suspensions, especially between colloids immersed in a binary liquid close to its critical demixing point for two-dimensional systems. To simulate those systems, we present a Monte Carlo cluster algorithm based on geometric symmetries of the Hamiltonian. Utilizing the principle of universality, the suspension is represented by an Ising system while the colloids are areas of spins with fixed orientation. Our results for the Casimir interaction potential between two particles agree quantitatively with the theoretical predictions [1], where we find that the behavior depends strongly on whether the order parameter is hold fixed or is allowed to fluctuate. Finally we present our results for the three-body interaction Casimir potential.

[1] T.W. Burkhardt and E. Eisenriegler, Phys. Rev. Lett. **74** (1995) 3189.

Lattice Monte Carlo simulations of polymer melts

Hsiao-Ping Hsu
Max-Planck-Institut für Polymerforschung, D-55128 Mainz, Germany
hsu@mpip-mainz.mpg.de

Polymer melts consisting of fully flexible and moderately stiff chains are studied by Monte Carlo simulations, using the bond fluctuation model at a volume fraction 0.5. A pre-packing process for the preparation of the initial configuration of the polymer melts, which reduces the local density fluctuations, is tested before the excluded volume interaction is switched on completely. This process leads to a significantly faster decrease of the number of overlapping monomers on the lattice. It is useful for simulating very large systems, where the statistical properties of the model with a marginally incomplete elimination of excluded volume violations are the same as those of the model with strictly excluded volume. We find that the internal mean square end-to-end distance for moderately stiff chains in a melt can be very well described by a freely rotating chain model with a precise estimate of the bond-bond orientational correlation between two successive bond vectors in equilibrium. The plot of the probability distributions of the reduced end-to-end distance of chains of different stiffness also shows that the data collapse is excellent and described very well by the Gaussian distribution for ideal chains. However, while our results confirm the systematic deviations between Gaussian statistics for the chain structure factor $S_c(q)$ (minimum in the Kratky plot) found by Wittmer *et al.* [EPL 77 (2007) 56003] for fully flexible chains in a melt, we show that for the available chain length these deviations are no longer visible, when the chain stiffness is included. The mean square bond length and the compressibility estimated from collective structure factors depend slightly on the stiffness of the chains.

Casimir force scaling functions in 2d Ising systems with open boundaries: The importance of corner contributions

Fred Hucht
(with Felix M. Schmidt)
Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany
fred@thp.uni-due.de

We consider the two-dimensional square lattice Ising model with free boundary conditions, aiming at universal critical Casimir force scaling functions. Surprisingly, no closed form solution exists for finite $L_\parallel \times L_\perp$ lattices due to the lack of translational invariance in both directions. However, the exact partition function polynomial can be efficiently calculated from the determinant of a $(4L_\parallel L_\perp)$-dimensional sparse matrix using arbitrary integer arithmetics. For infinite systems, we derive exact expressions for the bulk, surface and corner free energies at arbitrary temperatures using q-products [1]. Combining these results, we derive universal finite-size-scaling functions of the Casimir force and the residual free energy for different values of the aspect ratio $\rho = L_\perp/L_\parallel$. We find a unusual logarithmic divergence of the residual free energy scaling function at $x = tL_\perp \to 0$, which is directly related to the logarithmic L-dependence of the free energy at criticality predicted by Cardy and Peschel [2]. Furthermore, we find a crossover from attractive to repulsive Casimir forces, similar to the simpler periodic case [3].

[1] E. Vernier and J. L. Jacobsen, J. Phys. A: Math. Theor. **45** (2012) 045003.
[2] J.Cardy and I. Peschel, Nucl. Phys. B **300** (1988) 377.
[3] A. Hucht, D. Grüneberg, and F. M. Schmidt, Phys. Rev. E**83** (2011) 051101.

Random transverse-field Ising chain with long-range interactions

Ferenc Iglói
Wigner Research Centre, Budapest, Hungary
igloi@szfki.hu

We study the low-energy properties of the long-range random transverse-field Ising chain with ferromagnetic interactions decaying as a power α of the distance. Using variants of the strong-disorder renormalization group method, the critical behavior is found to be controlled by a strong-disorder fixed point with a *finite* dynamical exponent $z_c = \alpha$. At the critical point, the correlation length diverges exponentially, the magnetization shows

an α-independent logarithmic finite-size scaling and the entanglement entropy satisfies the area law. These observations are argued to hold for other systems with long-range interactions, even in higher dimensions.

P3HT molecules interacting with Au(001) substrates (P)

Momchil Ivanov[1]
(with Stefan Förster[2]**, Erik Kohl**[2]**, Jonathan Groß**[1]**, Wolf Widdra**[2]**, and Wolfhard Janke**[1]**)**
[1] Institut für Theoretische Physik, Universität Leipzig, Germany
[2] Institute of Physics, Martin-Luther-Universitt Halle-Wittenberg, Halle, Germany
momchil@itp.uni-leipzig.de

One of the main objectives of this project is to gain, with the help of computer simulations, a better understanding of adsorption properties and recognition of surface patterns of macromolecules such as polymers and proteins when interacting with material surfaces and nanoparticles (external constraints), and of the interplay of these phenomena with polymer collapse, crystallization, aggregation and folding (internal constraints). This study reports on an approach to combine the experimental observation of polymer chain conformations adsorbed on a metal surface with coarse-grained Monte Carlo simulations. P3HT chains with a maximum length of 60 monomers were simulated in contact with an Au(001) surface and the end-to-end distance as well as the radius of gyration of the molecules were determined.

Corner contribution to free energy for 2D dimer model

Nikolay Izmailyan
Applied Mathematics Research Centre, Coventry University, United Kingdom
ab5223@coventry.ac.uk

According to conformal field theory for models on the finite $L \times L$ plane there is a corner contribution to the free energy proportional to $\log L$. However for the dimer model on the rectangular lattice with free boundary conditions there is no such contribution to the free energy, while for the dimer model on the plane with one monomer on the boundary of the lattice and for the dimer model on the cylinder with one monomer on the perimeter of the cylinder there is the term proportional to $\log L$. We have explained such unusual behavior of the dimer model in terms of $c = -2$ conformal field theory by using bijection between dimer and spanning tree models.

(Z2) lattice gerbe theory

Desmond A. Johnston
Department of Mathematics, School of Mathematical and Computer Sciences, Heriot-Watt University, Edinburgh, United Kingdom
D.A.Johnston@hw.ac.uk

2-form abelian and non-abelian gauge fields on d-dimensional hypercubic lattices have been discussed in the past by various authors and most recently by Lipstein and Reid-Edwards. In this note we recall that the Hamiltonian of a Z2 variant of such theories is one of the family of generalized Ising models originally considered by Wegner. For such "Z2 lattice gerbe theories" general arguments can be used to show that a phase transition for Wilson surfaces will occur for $d > 3$ between volume and area scaling behaviour.

Boundary driven open quantum XXZ chain

Dragi Karevski

Groupe de Physique Statistique, Institut Jean Lamour, Université de Lorraine Nancy, France
dragi.karevski@univ-lorraine.fr

We consider an open Heisenberg quantum spin chain, coupled at the ends to boundary reservoirs polarized in different directions, which sets up a twisting gradient across the chain. We demonstrate that the exact nonequilibrium steady state of the chain driven by boundary Lindblad operators can be constructed explicitly with a matrix product ansatz where the matrices satisfy the quantum algebra $U_q[SU(2)]$. Using this matrix product ansatz in the isotropic case, we calculate explicitly the magnetization profiles and magnetization currents.

Effects of the bond elasticity on the structural transitions of a flexible polymer

Tomas Koci
(with Michael Bachmann)

Center for Simulational Physics, Department of Physics & Astronomy, The University of Georgia, Athens, USA
koci24@uga.edu

Utilizing advanced parallel Monte Carlo methods we examine the structural transitions of coarse-grained flexible polymers as a function of the elasticity of the FENE bond. In the course of the study we encounter the notoriously difficult sampling of the entropically suppressed conformations in the region of very strong first order transitions. Improved sampling of the region is obtained by generalized ensemble methods. Pseudophase diagrams are constructed using energy dependent canonical quantities to demonstrate the effects of the changes in the elasticity of the FENE bond to the liquid and solid structural phases. With increasing elasticity of the FENE bond we observe the disappearance of the liquid phase and the fusion of the theta and the freezing transitions.

Lee-Yang-Fisher zeros for the Ising model on complex network

Mariana Krasnytska[1,2]
(with Bertrand Berche[2] **and Yurij Holovatch**[1]**)**

[1] Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Lviv, Ukraine
[2] Groupe de Physique Statistique, Institut Jean Lamour, Université de Lorraine Nancy, France
kras_mariana@icmp.lviv.ua

We analyze the partition function of the Ising model on graphs of two different types: a complete graph, when all graph nodes are mutually linked and an annealed scale-free (SF) network with the node-degree distribution decaying for high node degrees as $P(k) \sim k^{-\lambda}$. We are interested in zeros of the partition function Z in the case of complex temperature t or external field h (Fisher and Lee-Yang zeros correspondingly) [1, 2]. The study of partition function zeros gives quantitative information about phase transitions occurring in the system. In particular, for the second-order phase transition, location and motion of the zeros allows to calculate the critical temperature, critical exponents α, β, δ and the critical amplitude ratio A_+/A_-. By the present study, we accomplish the Lee-Yang [3] and Fisher [4] zeros analysis for the Ising model on a complete graph. For the model on an annealed scale-free network, we find an appropriate integral representation for the partition function. For a SF network with $\lambda > 5$ we reproduce behavior of zeros for the Ising model on a complete graph. For $3 \leq \lambda < 5$ the angle φ appears to be λ-dependent. In turn, this gives access to the (λ-dependent) values of the critical exponents and critical amplitudes ratios of the Ising model on the scale-free network.

[1] M.E. Fisher, Phys. Rev. Lett. **40** (1978) 1610.
[2] C.N. Yang and T.D. Lee, Phys. Rev. **87** (1952) 404; *ibid.* **87** (1952) 410.
[3] Z. Glumac and K. Uzelac, Phys. Rev. E **66** (2013) 022140.
[4] M.L. Glasser, V. Privman, and L.S. Schulman, J. Stat. Phys. **66** (1986) 451.

Anistropic spin-glass models

Anastasios Malakis
Department of Physics, University of Athens, Greece
amalakis@phys.uoa.gr

We study two versions of the anisotropic $\pm J$ three-dimensional Ising model. In the first case (ani_z), $\pm J$ random exchange is applied only in the xy planes with the z interactions ferromagnetic, while in the second one (ani_{xy}), only z interactions are random with x and y ferromagnetic. Using parallel tempering and finite-size analysis, we determine their phase diagrams and compare them to the isotropic model. In particular, at their symmetry points, we report a striking coincidence of the transition temperatures of the isotropic and the ani_z case, while the ani_{xy} case yields a significantly higher critical temperature. For the ferromagnetic–spin-glass transition line we find forward behavior for the ani_{xy} case, in contrast to the reentrant behavior of the isotropic and the ani_z models. We estimate the critical behavior along the transition lines, and conclude that all three models share the same universality class, indicating the irrelevance of the introduced spatial anisotropy for the critical exponents.

Effects of stiffness in a generic polymer model and where knots come into play (P)

Martin Marenz
(with Wolfhard Janke)
Institut für Theoretische Physik, Universität Leipzig, Germany
martin.marenz@itp.uni-leipzig.de

In this work we give an overview of the influence of bending stiffness on the conformational phases of a generic bead-stick polymer model. Although this is a simplistic model, we have observed a rich variety of conformational phases which are comparable to conformations observed for real polymers and proteins. Just by changing the internal bending stiffness, the polymer model features different pseudo-phases like bended, knot-like, hairpin or toroidal phases. To identify these phases we have calculated, besides standard observables, the knot type of the polymer via the Alexander polynomial.

The stability of foam films: Remarks on the concept of disjoining pressure

Harald Morgner
Wilhelm-Ostwald Institute for Physical and Theoretical Chemistry, Fakultät für Chemie und Mineralogie, University of Leipzig, Germany
hmorgner@rz.uni-leipzig.de

Liquid soap films have a long history of attracting the attention of renowned scientists like Hooke, Newton, Plateau, Gibbs and Marangoni [1]. Today, the accepted theory for describing thin liquid films is the DLVO theory named after their founders Derjaguin, Landau [2] and Verwey, Overbeek [3]. The key quantity when investigating foam films is the pressure difference between the vapor phase outside the liquid film and the pressure inside the liquid phase connected to the liquid film. This pressure difference is named disjoining pressure $P_{\text{disjoining}} = P_{\text{vap}} - P_{\text{liq}}$. The vapor pressure P_{vap} exceeds the pressure in the liquid phase P_{liq}. Thus the question arises why the film is not destroyed by the outside pressure. The explanation relies on the repulsive interaction between the two interfaces [4] which acts perpendicular to the film surfaces and is understood to consist of electrostatic, van der Waals and steric forces. The distance between the interfaces should have influence upon the distribution of charges in the interfaces and, indeed, this could recently be explicitly investigated by the surface spectroscopy NICISS (= Neutral Impact Collision Ion Scattering Spectroscopy) [5]. In spite of the experimental data that can successfully be fitted by the available theory, the concept of the disjoining pressure deserves some attention. It is based on the understanding that the repulsive interaction between the interfaces causes a pressure which keeps the interfaces apart and, thus, stabilizes the film. In experiment the separation between the interfaces (or film thickness) is varied by varying the outside pressure exerted by a gas, e.g. air. It is difficult to vary the thickness of the foam film at constant gas pressure experimetally, at least it has not been done so far. However, in a simulation one can vary the thickness of the film while keeping all other parameters constant. This leads to the surprising result

that the disjoining pressure is not affected by the film thickness down to the point where the films ruptures. This is incompatible with the notion that the disjoining pressure depends on the interaction between the interfaces. It will be discussed why this seemingly surprising result follows from simple thermodynamic considerations.

[1] V. Bergeron, *Forces and structures in thin liquid soap films*, J. Phys.: Condens. Matter **11** (1999) R215–R238.
[2] B. Derjaguin and L. Landau, *Theory of the stability of strongly charged lyophobic sols and of the adhesion of strongly charged particles in solutions of electrolytes*, in: Acta Physico Chemica URSS **14** (1941) p. 633.
[3] E.J.W. Verwey and J.Th.G. Overbeek, *Theory of the Stability of Lyophobic Colloids* (Elsevier, Amsterdam, 1948).
[4] C. Stubenrauch, J. Schlarmann, and R. Strey, *A disjoining pressure study of n-dodecyl-D-maltose foam films*, Phys. Chem. Chem. Phys. **4** (2002) 4504–4513.
[5] C. Ridings and G. Andersson, *Deconvolution of NICISS profiles involving elements of similar masses*, NIMB Proceedings 2014, published online ahead of print.

Macroscopic degeneracy influences the finite-size scaling at first-order phase transitions

Marco Mueller[1]
(with Desmond A. Johnston[2] and Wolfhard Janke[1])

[1] Institut für Theoretische Physik, Universität Leipzig, Germany
[2] Department of Mathematics, School of Mathematical and Computer Sciences, Heriot-Watt University, Edinburgh, United Kingdom
marco.mueller@itp.uni-leipzig.de

We explore how a macroscopic low-temperature phase degeneracy influences the leading finite-size corrections of systems with periodic boundaries at a first-order phase transition and provide an example of a four-spin interaction, plaquette Hamiltonian that displays such a degeneracy, growing exponentially with linear system size in 3d. We confirm the modified scaling of different quantities with high-precision multicanonical data, back it up by canonical data and discuss potential candidate order parameters.

Open boundary conditions in stochastic transport processes with pair-factorized steady states (P)

Hannes Nagel[1]
(with Darka Labavić[2], Hildegard Meyer-Ortmanns[2], and Wolfhard Janke[1])

[1] Institut für Theoretische Physik, Universität Leipzig, Germany
[2] School of Engineering and Science, Jacobs University Bremen, Germany
hannes.nagel@itp.uni-leipzig.de

Using numerical methods we discuss the effects of open boundary conditions on condensation phenomena in the zero-range process (ZRP) and transport processes with pair-factorized steady states (PFSS), an extended model of the ZRP with nearest-neighbor interaction. For the zero-range process we compare to analytical results in the literature with respect to criticality and condensation. For the extended model we find a similar phase structure, but observe supercritical phases with droplet formation for strong boundary drives.

Current-current correlations in lattice QCD: Continuum study of quark diffusion (P)

Thomas Neuhaus

JSC, Forschungszentrum Jülich, Germany
t.neuhaus@fz-juelich.de

We present continuum results for quark diffusion constants in the quark-gluon plasma.

Fermionic quantum criticality in honeycomb and π-flux Hubbard lattice models

Francesco Parisen Toldin

Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany
francesco.parisentoldin@physik.uni-wuerzburg.de

We numerically investigate the critical behavior of the Hubbard model on the honeycomb and the π-flux lattice, which both exhibit a direct transition from Dirac fermions to an antiferromagnetic Mott phase. We use projective auxiliary-field quantum Monte Carlo simulations and a careful finite-size scaling analysis that exploits improved renormalization-group invariant observables. This approach, which is successfully verified for the 3D XY transition of the Kane-Mele-Hubbard model, allows us to extract estimates for the critical couplings and the critical exponents. The results confirm that the critical behavior for the semimetal to Mott insulator transition in the Hubbard model belongs to the Gross-Neveu-Heisenberg universality class on both lattices.

Comparison of microcanonical MD and MC simulations for liquid-gas like phase transitions

Philipp Schierz

(with Johannes Zierenberg and Wolfhard Janke)

Institut für Theoretische Physik, Universität Leipzig, Germany
schierz@itp.uni-leipzig.de

In this work we do a quantitative comparability study of Molecular Dynamics (MD) and Monte Carlo (MC) simulations in the microcanonical ensemble. The microcanonical MC simulations are done with a Metropolis like scheme [1] and additionally with MUCA [2]. We look at three application examples: Single polymer collapse, 4-particle Lennard-Jones gas condensation and aggregation for a 8×13 polymer system. For the 4-particle Lennard-Jones gas condensation and polymer aggregation we encounter two different ensembles in the MD simulation due to conservation laws. While the angular momentum is conserved in MD for a condensate or aggregate (NVEPJ ensemble) it is not conserved any longer for gas-like states (NVEP ensemble). We apply a WHAM like reweighting scheme for the estimation of the density of states from MD data. For this application it was necessary to differentiate between the two ensemble regions in MD.

[1] J.R. Ray, Phys. Rev. A **44** (1991) 4061.
[2] B.A. Berg and T. Neuhaus, Phys. Lett. B **267** (1991) 249; Phys. Rev. Lett. **68** (1992) 9; W. Janke, Int. J. Mod. Phys. C **03** (1992) 1137; Physica A **254** (1998) 164.

Wang-Landau type Monte Carlo study of crystallization in melts of short semi-flexible polymers

Timur Shakirov

Institut für Physik, Martin-Luther Universität Halle, Germany
timur.shakirov@physik.uni-halle.de

Wang-Landau type Monte Carlo simulations are employed to obtain the complete thermodynamic equilibrium information for a melt of short, semi-flexible polymer chains. We show that our model system undergoes a first-order crystallization transition into a rotator-like phase upon increasing the chain stiffness at fixed density. The intermolecular interaction is purely repulsive so that the transition is of lyotropic type, driven by maximization of the system entropy.

On the accuracy of the Wang-Landau algorithm

Lev Shchur

Landau Institute for Theoretical Physics and Science Center, Chernogolovka, Moscow region, Russia
lev@itp.ac.ru

We check for the 2D Ising model the relaxation of the density of states function to the exact value using the Wang-Landau algorithm. We found that the accuracy saturates to some finite value which weakly depends on the algorithm parameters and variations. We discuss possible modifications of the algorithm which may improve the accuracy.

Adsorption of semiflexible polymers (P)

Semjon Stepanow

Institut für Physik, Martin-Luther Universität Halle, Germany
semjon.stepanow@physik.uni-halle.de

To describe the adsorption of a worm-like chain in a potential well we consider the solution of the distribution function of one polymer end in a piecewise constant potential by using the representation of the distribution function $\langle l, m, E, k, \mathbf{r}|P\rangle$ in terms of quantum numbers l, m of the orbital momentum. The truncations of the infinite order system of equations occurs with respect to the eigenvalue of the square of the orbital momentum l, which is related to the number of the exact moments of the end-to-end distance of the free chain. We present explicit results for $l_{\max} = 1$ and $l_{\max} = 2$.

Fourier Monte Carlo renormalization group approach to crystalline membranes

Andreas Tröster

Institute for Theoretical Physics, Vienna University of Technology, A-1040 Wien, Austria
andreas.troester@tuwien.ac.at

The computation of the critical exponent η characterizing the universal elastic behavior of crystalline membranes in the flat phase continues to represent challenges to theorists as well as computer simulators that manifest themselves in a considerable spread of numerical results for η published in the literature. We present new insight to this problem that results from combining Wilson's momentum shell renormalization group method with the power of modern computer simulations based on the Fourier Monte Carlo algorithm. After discussing the ideas and difficulties underlying this combined scheme, we present a calculation of the renormalization group flow of the effective 2d Young modulus for momentum shells of different thickness. Extrapolation to infinite shell thickness allows us to produce results in reasonable agreement with those obtained by functional renormalization group or by Fourier Monte Carlo simulations in combination with finite-size scaling. Moreover, our new method allows one for the first time to obtain a decent estimate for the value of the Wegner exponent ω that determines the leading correction to scaling.

Determinant representation for integrable spin-boson models

Hugo Tschirhart

Groupe de Physique Statistique, Institut Jean Lamour, Université de Lorraine Nancy, France
hugo.tschirhart@laposte.net

In this work, we construct an alternative formulation to the traditional Algebraic Bethe ansatz for quantum integrable models derived from a generalised rational Gaudin algebra realised in terms of a collection of spins 1/2 coupled to a single bosonic mode. The ensemble of resulting models which we call Dicke-Jaynes-Cummings-Gaudin models are particularly relevant for the description of light-matter interaction in the context of quantum optics. Having two distinct ways to write any eigenstate of these models we then combine them in order to write overlaps and form factors of local operators in terms of partition functions with domain wall boundary conditions.

We also demonstrate that they can all be written in terms of determinants of matrices whose entries only depend on the eigenvalues of the conserved charges. Since these eigenvalues obey a much simpler set of quadratic Bethe equations, the resulting expressions could then offer important simplifications for the numerical treatment of these models.

Anisotropic extension of the quantum spherical model (P)

Sascha Sebastian Wald

Groupe de Physique Statistique, Institut Jean Lamour, Université de Lorraine Nancy, France
sascha-sebastian.wald@univ-lorraine.fr

We study a modified version of the quantum spherical model by introducing a tunable pair creation and annihilation. Through a Bogoliubov-like transformation we diagonalise the quantum Hamiltonian and study the dependence of thermodynamic properties at zero temperature in dependence of the tuning parameter λ. Particularly we treat the case without pair creation and annihilation and the non-standard regime, namely $\lambda \neq 1$. Thermodynamic observables like correlation length, specific heat, magnetisation and correlation functions are derived explicitly and studied near the quantum phase transition of the system. Finally, we studied the universality class of the 1D quantum chain by quantum field theory. We derive explicitly the central charge and proof it to be $c = 1$.

Fragmentation of fractal random structures

Martin Weigel

Applied Mathematics Research Centre, Coventry University, United Kingdom
martin.weigel@coventry.ac.uk

We analyze the fragmentation behavior of random clusters in a lattice geometry under a process where bonds between neighboring sites are successively broken. Modeling such structures by configurations of a generalized Potts or random-cluster model allows us to discuss a wide range of systems with fractal properties including trees as well as dense clusters. We present exact results for the densities of fragmenting edges and the distribution of fragment sizes for critical clusters in two dimensions and discuss generalizations to the problem of vertex fragmentation. Dynamical fragmentation protocols lead to broad distributions of fragments, following power laws. Analytical results are complemented by extensive numerical simulations.

Specific interactions in a hard sphere model (P)

Benno Werlich

Institut für Physik, Martin-Luther Universität Halle, Germany
benno.werlich@physik.uni-halle.de

For studying structure formation of homopolymers chains we use an off-lattice hard-sphere coarse grained model with square-well interactions. We start with a phase diagram for chain length $N = 40$ that shows a variety of stable structures depending on the chain stiffness for different temperatures. Afterwards an extra square-well (SW) potential is introduced as specific interaction. Therewith the density of states (DOS) shows new interesting features which also result in canonical and microcanonical analysis. Thus, chains with enabled or disabled extra SW potentials will be checked against each other. In practice number of monomers and the stiffness approaches the modelling of protein-like structures and the new potential could be understood as hydrogen bonds. For the generation of the DOS we use the Stochastic Approximation Monte Carlo Method (SAMC). There we fine tuned the simulation parameters to converge the DOS in a reasonable time.

Structural transitions in helical polymers

Matthew Williams
(with Michael Bachmann)

Center for Simulational Physics, Department of Physics & Astronomy, The University of Georgia, Athens, USA
mjw532@uga.edu

Helical structures, as well as more complex tertiary structures, made up of helixes are relevant in biological systems. We perform generalized-ensemble Monte Carlo simulations to examine homopolymer models which include a torsional potential energy associated with each bond. With the inclusion of a torsional potential, helical structures emerge and can contort to form a variety of tertiary structural phases. We explore the two-dimensional space, parametrized by temperature and torsional energy scale, to map helical structures and to locate structural transitions. We see transitions occur between helical and non-helical secondary structures and also between various tertiary structures.

Aggregation of semiflexible polymers under constraints

Johannes Zierenberg
(with Marco Mueller, Philipp Schierz, Martin Marenz, and Wolfhard Janke)

Institut für Theoretische Physik, Universität Leipzig, Germany
zierenberg@itp.uni-leipzig.de

Applying parallel multicanonical simulations [1], we study the aggregation transition of finite semiflexible polymers in dependence on the stiffness and density. The polymer length is here fixed as a chemical property. Considering a spherical confinement, we show that the competition between single-polymer collapse and many-polymer aggregation yields a lower temperature bound for the isolated chain approximation [2]. For dilute flexible polymers, we present entropic and energetic arguments that allow to relate the inverse aggregation to the density of the monodisperse systems [2]. In a systematic approach for a small number of polymers, we construct generic temperature-stiffness structural phase diagrams [3]. This highlights the key role of stiffness in polymer aggregation, responsible for a wide range of structural motifs from amorphous aggregates to polymer bundles.

[1] J. Zierenberg, M. Marenz, and W. Janke, Comput. Phys. Comm. **184** (2013) 1155.
[2] J. Zierenberg, M. Mueller, P. Schierz, M. Marenz, and W. Janke, J. Chem. Phys. **141** (2014) 114908.
[3] J. Zierenberg and W. Janke, submitted (2014).