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ABSTRACTS

of contributions to the

14th International NTZ-Workshop on

New Developments in Computational Physics

CompPhys13

Institut für Theoretische Physik,
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28 – 30 November 2013

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

Preface

As in previous years, also the 14th International NTZ-Workshop *CompPhys13* on *New Developments in Computational Physics* covers 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 28 – 29 November 2013 in the Lecture Halls ("Kleiner Hörsaal" and "Theorie 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 place 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, 30 November 2013, is devoted to various discussion rounds and collaborative meetings which will take place in the Theoretical Physics building. Note that last year 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 DFG Graduate School of Excellence "BuildMoNa: Building with Molecules and Nano-objects".

Leipzig, November 2013
Wolfhard Janke

Abstracts

Boundary crossover in non-equilibrium interfaces growth processes

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The growth of stochastic interfaces in the vicinity of a boundary shows a non-trivial crossover between the behaviour deep in the bulk and a more complex boundary behaviour, related to the causal interaction of the interface with the boundary. This calls for a generalization of the usually admitted scaling laws. This is exemplified in the semi-infinite Edwards-Wilkinson model in one dimension, both from its exact solution and numerical simulations, as well as from simulations on the semi-infinite one-dimensional Kardar-Parisi-Zhang model. The scaling of interface heights and widths is analyzed and an universal scaling form for the local height profile is proposed.

Computer simulation of peptide adsorption

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In this talk I shall describe some of our recent work attempting to simulate the statistical mechanical properties of very simple models of polymers and peptides, both in isolation and in the vicinity of surfaces. Some of these methods are well known, and some derived from groundbreaking work in other groups; some aspects, such as the treatment of single-surface adsorption, differ in a few details. I shall summarize the results that we have obtained using lattice models, and set out our preliminary simulations using off-lattice models, setting some of the work in the context of a larger programme of research focusing on the role of peptides on biomineralization.

Transitions in small systems

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Folding and aggregation of molecules, as well as the adsorption of soft organic matter to solid inorganic substrates belong to the most interesting challenges in studies of structure formation and function of complex macromolecules. The substantially grown interest in the understanding of basic physical mechanisms underlying these processes is caused by their impact in a broad field that ranges from the molecular origin of the loss of biological functionality as, for example, in Alzheimer's disease, to the development of nanotechnological applications such as biosensors. Most of these systems are necessarily of finite size, but molecular structure formation exhibits cooperative effects that resemble similar processes in thermodynamic phase transitions. Inspired by the fact that the density of states, and with it the microcanonical entropy, is the natural result of any generalized-ensemble Monte Carlo simulation, we have introduced a method that allows for a systematic and unique identification and Ehrenfest-like classification of structural transitions in small systems by means of microcanonical analysis. This computational approach to phase transitions, which is hardly accessible in theoretical studies, is particularly useful for the analysis of cooperative behavior in folding, aggregation, and adsorption processes of polymers and proteins. In this talk, I am going to discuss thermodynamic properties and statistical analyses of such structural transitions.

MuCa vs WL: A tight race (P)

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We perform a competitive analysis to study the relative performance of the two best-known generalized-ensemble algorithms: the multicanonical Monte Carlo and the Wang-Landau method. To keep things as simple and clear as possible, we take the exactly solvable two-dimensional Ising model as test case and show some preliminary results.

Griffiths phase in a Potts model with correlated disorder

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We discuss the critical behaviour of a q-state Potts model with a long-range correlated disorder. Numerical evidence is given of the existence of a Griffiths phase, where the thermodynamic quantities display an algebraic finite-size scaling, in a finite range of temperatures. The critical exponents are shown to depend on both the temperature and the exponent of the algebraic decay of disorder correlations, but not on the number of states of the Potts model. Hyperscaling relations are violated in the entire Griffiths phase.

Renormalization group for quantum walks

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A renormalization group (RG) treatment of quantum walks holds significant promise for insights into search algorithms for quantum computing and transport phenomena. It extends conventional Fourier analysis to systems that lack translational invariance. The generality of this approach can elucidate systems which at this point are inaccessible and are even difficult to study numerically at any reasonable size. Key questions concern the scaling properties of the (unitary) quantum evolution depending on the geometry. Unlike for random walks, renormalization suggests that quantum walks may exhibit entire spectra of exponents, for instance, for the mean-square displacement, as classical fixed-point analysis gives way to far-more complex RG-flows that pose a severe challenge to existing notions of universality. Effects that are distinctly quantum in their nature, such as interference and localization, can combine in seemingly paradoxical ways as to allow any traveling mode to spread faster than the corresponding random walk while ultimately trapping almost all modes in a finite domain.

Dimer and monomer statistics using Grassmann analysis (P)

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We present an application of the Grassmann algebra method developed by V.N. Plechko to the problem of dimer and monomer statistics on a regular two-dimensional lattice. The questions of interest are related to the correlation functions between the monomers on such lattice and how they can be computed exactly when the monomers are located on the boundary with a representation in terms of fermionic action.

Self-avoiding walks on critical percolation clusters in 2 to 7 dimensions

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(with Wolfhard Janke)

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Self-avoiding walks (SAWs) on critical percolation clusters are a basic model for polymers in crowded disordered media. The fractal nature of the clusters gives rise to interesting scaling behavior of the SAWs, which is still poorly understood despite considerable efforts in the past. While the analytical results are controversial, those obtained by standard numerical methods are rather imprecise due to very restricted system sizes. We developed an exact enumeration technique [2], which exploits the fractal structure of the critical cluster. The method can handle walks of several thousand steps, amounting to over 10^{1000} conformations. This enabled us to determine the SAW scaling exponents on critical percolation clusters and their backbones with unprecedented accuracy. Varying the lattice dimension beyond the upper critical limit ($D = 6$) allows to check the predictions from field theory and to investigate the influence of the various fractal dimensions of the critical cluster.

Adsorption of a coarse-grained flexible polymer on nanocylinders – A Monte Carlo study

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The thermodynamic behavior of a fully flexible polymer model in the presence of an attractive nanocylinder is subject of this investigation. We are interested in the structural phases of the polymer and how they change with the surface attraction strength of the nanocylinder. The effective monomer-surface attraction strength is associated with the cylinder radius and its material. Previous studies of polymers adsorption on planar surfaces [1, 2, 3] already provide insight in the structures formed by adsorbed polymer chains. Recently also the adsorption on curved surfaces [4, 5, 6] was investigated. We try to connect the results of the adsorption on curved and planar surfaces, since in the limit of an infinite radius of the cylinder, the surface has the same characteristics as a plane. We construct complete pseudo-phase diagrams of a 30-mer interacting with nanocylinders of five different materials as a function of temperature and radius of the cylinders.

[1] A. Milchev and K. Binder, J. Chem. Phys. **114** (2001) 8610.
[2] J. Krawczyk, A.L. Owczarek, T. Prellberg, and A. Rechnitzer, Europhys. Lett. **70** (2005) 726.
[3] M. Möddel, M. Bachmann, and W. Janke, J. Phys. Chem. B **113** (2009) 3314.
[4] A. Milchev and K. Binder, J. Chem. Phys. **117** (2002) 6852.
[5] I. Gurevitch and S. Srebnik, Chem. Phys. Lett. **444** (2007) 96.
[6] T. Vogel and M. Bachmann, Phys. Rev. Lett. **104** (2010) 198302.

Optimising the spatial structure of BLN protein models by means of thermal cycling

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The prediction of the three-dimensional structure of a protein based on its amino acid sequence is a challenging problem. For studying which forces affect the protein folding, highly efficient structure optimisation tools are needed. Here we investigate whether and to what extent the thermal cycling (TC) algorithm [1] is suitable to determine low energy structures of the BLN protein model, designed by J.D. Honeycutt and D. Thirumalai [2]. For this aim, we consider 46-bead, 58-bead, and 69-bead sequences [2, 3] which were constructed to exhibit a

frustrated energy landscape; to the best of our knowledge, the 69-bead sequence is the longest sequence available in the literature. In all these cases, the TC algorithm finds the global minimum within reasonable computing time. In comparison to the multi-start local search and simulated annealing approaches, TC is found to be far more efficient. In the present work, the BLN model for rigid bond lengths is studied in detail for the first time. Comparing the results to the extended model by Berry *et al.* [4], who substitute stiff springs for the rigid bonds, we observe several level crossings when varying the spring constant, even for quite hard springs.

[1] A. Möbius, A. Neklioudov, A. Díaz-Sánchez, K.H. Hoffmann, A. Fachat, and M. Schreiber, Phys. Rev. Lett. **79** (1997) 4297.
[2] J.D. Honeycutt and D. Thirumalai, Biopolymers **32** (1992) 695.
[3] M.T. Oakley, D.J. Wales, and R.L. Johnston, J. Phys. Chem. B **115** (2011) 11525.
[4] R.S. Berry, N. Elmaci, J.P. Rose, and B. Vekhter, Proc. Natl. Acad. Sci. USA **94** (1997) 9520.

The Kosterlitz-Thouless transition in thin films: A Monte Carlo study of three-dimensional lattice models

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We study the phase transition of thin films in the three-dimensional XY universality class. To this end, we perform a Monte Carlo study of the improved two-component ϕ^4 model, the improved dynamically diluted XY model and the standard XY model on the simple cubic lattice. We study films of a thickness up to $L_0 = 32$ lattice spacings. In the short direction of the lattice, free boundary conditions are employed. Using a finite-size scaling (FSS) method, proposed recently, we determine the transition temperature with high accuracy. The effectively two-dimensional finite-size scaling behaviour of the Binder cumulant U_4, the second-moment correlation length over the lattice size $\xi_{2\mathrm{nd}}/L$, the ratio of the partition functions with anti-periodic and periodic boundary conditions Z_a/Z_p and the helicity modulus Υ clearly confirm the Kosterlitz-Thouless nature of the transition. We analyse the scaling of the transition temperature with the thickness L_0 of the film. We compute the universal ratio of the thickness of the film L_0 and the transverse correlation length ξ_T in the three-dimensional thermodynamic limit at the Kosterlitz-Thouless transition temperature of a film of thickness L_0: $[L_{0,\mathrm{KT}}/\xi_T]^* = 1.595(7)$. This result can be compared with experimental results on thin films of ^{4}He near the λ-transition.

Statistical mechanics of the coagulation-diffusion process with a stochastic reset

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The effects of a stochastic reset, to its initial configuration, is studied in the exactly solvable one-dimensional coagulation-diffusion process. A finite resetting rate leads to a modified non-equilibrium stationary state. If in addition the input of particles at a fixed given rate is admitted, a competition between the resetting and the input rates leads to a non-trivial behaviour of the particle-density in the stationary state. From the exact inter-particle probability distribution, a simple physical picture emerges: the reset mainly changes the behaviour at larger distance scales, while at smaller length scales, the non-trivial correlation of the model without a reset dominates.

Confined semiflexible chains in a good solvent: A Monte Carlo test of scaling concepts

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Single semiflexible polymer chains under good solvent conditions are described by self-avoiding walks (SAWs) on the square and simple cubic lattices with an additional bending energy penalty ε_b at each 90^o kink along the chains. Varying the bending energy ε_b allows to vary the effective persistence lengths ℓ_p of polymer chains in the bulk covering the range up to 52 lattice spacings and 120 lattice spacings in $d = 3$ [1] and $d = 2$ [2], respectively. Employing the pruned-enriched Rosenbluth method (PERM), chain lengths of polymers confined between two hard walls that are apart from each other at a distance D are up to $\mathcal{O}(10^5)$ [3, 4]. With our large-scale Monte Carlo simulations of confined semiflexible chains, the scaling laws predicted in Flory, Daoud-de Gennes, and Odijk regimes are checked. While under weak confinement ($D \gg l_p$) the model (for very long chains) still is compatible with the Daoud-de Gennes scaling theory, for strong confinement ($D \leq l_p$) strong deviations from the predictions based on the Kratky-Porod model are found. However, Odijk's deflection length plays no role for semiflexible chains with discrete bond angles. We also estimate the critical fugacity, the force of compression exerted by the walls, and the monomer density profiles, and compare those results to theoretical predictions.

[1] H.-P. Hsu, W. Paul, and K. Binder, Europhys. Lett. **92** (2010) 28003.
[2] H.-P. Hsu, W. Paul, and K. Binder, Europhys. Lett. **95** (2011) 68004.
[3] H.-P. Hsu and K. Binder, Soft Matter **9** (2013) 10512.
[4] H.-P. Hsu and K. Binder, Macromolecules **46** (2013) 8017.

Random quantum magnets in $d > 2$ dimensions: Critical behavior and entanglement entropy

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Using the strong disorder renormalization group method, we study numerically the quantum critical behavior (i.e. at $T = 0$) of the random transverse-field Ising model in $d = 2, 3$ and 4 dimensions. In all cases the critical behavior is controlled by an infinite disorder fixed point and the critical exponents in the bulk, as well as at a free surface, corner and edge are disorder independent. The entanglement entropy satisfies the area law to which there are universal logarithmic corrections at the critical point due to corners.

[1] I.A. Kovács and F. Iglói, Phys. Rev. B **83** (2011) 174207; J. Phys.: Condens. Matter **23** (2011) 404204; Europhys. Lett. **97** (2012) 67009; Phys. Rev. B **87** (2013) 024204.

Polymer adsorption onto a stripe-patterned surface (P)

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In recent years, polymer systems have received a great deal of attention from both, the experimental and the theoretical perspectives. However, a complete description of the properties of these materials does not currently exist. Therefore, further research is needed. This particular study is part of an ongoing effort to try to understand these systems and is focused on the adsorption of single polymer chains. Previous theoretical studies have provided phase diagrams that lay the foundations for a better understanding of the basic mechanisms of polymer adsorption.

This particular study focuses on a single polymer chain in a confined volume and its adsorption onto a stripe-patterned surface. A minimalistic simple-cubic lattice model was used where the chain is represented by an interacting self-avoiding walk (ISAW) and was confined between an attractive patterned wall and a steric wall with no interaction whatsoever. The pattern consisted of parallel stripes of defined width and separation. Besides the pattern parameters, three energy scales determine the phase diagram of the system: chain-surface attraction, chain-pattern attraction and chain self-attraction. Chains of lengths up to $N = 19$ monomers were studied using the method of exact enumeration. The influence of the energy scales and pattern parameters on the system was analysed with the help of temperature vs. chain-pattern attraction phase diagrams. These diagrams were constructed by means of both canonical and microcanonical analysis of the enumeration data.

Potts models with invisible states

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The number of so-called invisible states which need to be added to the q-state Potts model to transmute its phase transition from continuous to first order has attracted recent attention. In the $q = 2$ case, a Bragg-Williams, mean-field approach necessitates four such invisible states while a 3-regular, random-graph formalism requires seventeen. In both of these cases, the changeover from second- to first-order behaviour induced by the invisible states is identified through the tricritical point of an equivalent Blume-Emery-Griffiths model. Here we investigate the generalised Potts model with invisible states on both a Bethe lattice with z neighbours and random regular graphs.

On the uniform sampling of ground states in the 2D $\pm J$ Ising spin-glass model

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It is well known that the Edwards-Anderson Ising spin glass with discrete coupling distribution results in an extensive ground-state degeneracy. As the number of ground states hence grows exponentially with system size L, an exact enumeration is not practical, except for very small systems. This even applies to the otherwise well tractable model in two dimensions. There, exact ground states can be generated in polynomial time using one of several known mappings to minimum-weight perfect matching problems. While the resulting algorithm can be modified to generate random ground states in the presence of degeneracies, these are not in general produced with uniform probabilities. Here, we introduce an approach that achieves approximate uniform sampling. The algorithm is based on a cluster analysis of connected domains of free spins resulting from inputs generated by the matching approach which are then used as state space for a suitably adapted Markov chain sampling.

Effect of bending stiffness on a homopolymer inside a spherical cage

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We study the change of the pseudo phase transition of a simple homopolymer inside a spherical confinement. Of particular interest is the shift of the collapse and freezing transitions with shrinking radius of the sphere and how it changes with varying stiffness of the polymer. Therefore we use a modified bead-stick model, with an additional cosine potential to introduce a bending stiffness. We used the multicanonical Monte Carlo method to get an overview of the complete phase space of this model. To characterize the pseudo phase transition we analyse fluctuations of energetic and conformational observables. We observed a clear dependence of the shift of

the collapse transition with the stiffness of the polymer. For very flexible polymers the transition temperature goes to lower temperatures with shrinking sphere radius. This effect turns around with increasing stiffness of the polymer.

Fluid adsorption in mesopores: Critical remarks on the validity of thermodynamics for confined systems

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Adsorption of fluids in mesopores is often accompanied by the phenomenon of hysteresis. One observes that the states realized in experiment do not comply with thermodynamics in that one set of boundary conditions may lead to more than one response of the system, and that the actual response depends on the systems' history. This is well known to be in disagreement with the rules of thermodynamics. It is common practice to bridge the discrepancy between thermodynamics and experiment by postulating the existence of metastable states the lifetime of which is conceived to exceed the typical duration of experiments. The concept of metastability cannot be separated from the notion that a ground state must exist into which a metastable state will decay with a characteristic lifetime. Thus, postulating metastable states calls for a theoretical description that is suited to handle the time dependence of the system. Let us assume that the characteristic relaxation time of the system has the value τ_0. Then it would be of interest to compare with the time scale of the experiment that is used for studying the system. In principal one can distinguish three cases: 1. time independent theory in Ref. [1], via the concept of COS, 2. time dependent theory, to be established, 3. basic assumption for the time independent theory of thermodynamics. For a typical adsorption system it has been found that the life time is orders of magnitude larger than the age of the universe [2]. In this case one would seek a time independent theory, corresponding to case 1. Obviously, the appropriate theory cannot be thermodynamics, as it is based on case 3. We will discuss possible strategies towards a time dependent theory that is generally valid for confined systems and why schemes that are found in the literature are inappropriate for the purpose.

[1] H. Morgner, *Fluids in mesopores V: A new theory and applications*, J. Chem. Chem. Eng. **5** (2011) 456–472.
[2] H. Morgner, *Time dependent aspects of adsorption: Pressure jumps and fluctuations*, J. Chem. Chem. Eng. **7** (2013) 260–274.

Multicanonical analysis of the gonihedric Ising model (P)

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The gonihedric Ising model originates from catching basic properties of fluctuating random surfaces in a bosonic string theory. Formulated as a lattice model of interacting classical spins it has been investigated by means of multicanonical Monte Carlo computer simulations to resolve open questions on its first-order phase transition. The transition temperature has been determined consistently for the original plaquette model and its dual representation. Also the interface tension has been obtained for both models for the first time.

Application of a steady states transport model to condensation of water droplets on a substrate (P)

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Condensation of water droplets on a substrate proves as a good test ground for condensation phenomena in basic stochastic transport processes. The modeled physical situation consists of a substrate at constant temperature exposed to a constant influx of microscopic water droplets from surrounding vapor. We consider a simple one-dimensional stochastic transport process with constant particle influx. This process can be parameterized so that particles condense to droplets. The employed transport model consists of a periodic lattice and a gas of indistinguishable particles, so that each site i is occupied by zero or m_i particles. At every time step a random site i is chosen and a particle may leave to an adjacent site with probability proportional to a hopping rate $u(m_i|m_{i1}, m_{i+1})$. The hopping rate is chosen so that particles tend to condensate by incorporating a zero-range repulsive interaction and surface tension like short-range interaction [1]. The envelope shape of condensates can be tuned to have the same scaling of volume to droplet width as real droplets [2]. Particle influx from environmental vapor is mimicked by adding at random sites randomly with a constant influx rate. We compare our observations with a recent study of water droplet size distributions obtained in experiment and simulation by Blaschke et al. [3]. In the experiment water vapor condenses on a glass substrate. The simulation mimicks experiment by adding a new constant inital volume droplet at some point to the substrate and subsequently merging any overlapping droplets at every time step. In contrast to the previous simulations [3] our model intrinsically includes diffusion of particles and droplet merging occurs due to movement as well as particle placement in the influx step.

[1] M.R. Evans, T. Hanney, and S.N. Majumdar, Phys. Rev. Lett. **97** (2006) 010602.
[2] B. Wacław, J. Sopik, W. Janke, and H. Meyer-Ortmanns, Phys. Rev. Lett. **103** (2009) 080602.
[3] J. Blaschke, T. Lapp, B. Hof, and J. Vollmer, Phys. Rev. Lett. **109** (2012) 068701.

Simulated quantum annealing for general Ising models

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We perform high precision Quantum Monte Carlo annealing simulations within a class of general Ising models on lattice manifolds that can be easily embedded into the connectivity graph of an existing annealing board: The D-Wave quantum computer. We predict correlations in-between classical and quantum annealing algorithms, which in a later step may be confronted to actual experiments on the physical chip. We review aspects of our current knowledge on the usefulness of the D-wave quantum computer.

Critical Casimir forces between homogeneous and chemically striped surfaces

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Recent experiments have measured the critical Casimir force acting on a colloid immersed in a binary liquid mixture near its continuous demixing phase transition and exposed to a chemically structured substrate. Motivated by these experiments, we study the critical behavior of a system, which belongs to the Ising universality class, for the film geometry with one planar wall chemically striped, such that there is a laterally alternating adsorption preference for the two species of the binary liquid mixture, which is implemented by surface fields. For the opposite wall we employ alternatively a homogeneous adsorption preference or homogeneous Dirichlet boundary conditions, which within a lattice model are realized by open boundary conditions. By means of mean-field

theory, Monte Carlo simulations, and finite-size scaling analysis we determine the critical Casimir force acting on the two parallel walls and its corresponding universal scaling function. We show that in the limit of stripe widths small compared with the film thickness, on the striped surface the system effectively realizes Dirichlet boundary conditions, which generically do not hold for actual fluids. Moreover, the critical Casimir force is found to be attractive or repulsive, depending on the width of the stripes of the chemically patterned surface and on the boundary condition applied to the opposing surface.

The Janus family: A special purpose computer generation devoted to spin glasses

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The Special Purpose Computer Janus [1, 2], based on a FPGA-architecture, was designed and developed as a multipurpose reprogramable supercomputer some years ago. During its childhood (it is now around 5 years old), Janus has been focused on the study and simulation of spin glasses, paradigm of complex systems. Indeed it has revealed as a very fruitful scientific computer for studying these disordered systems, reaching simulation times up to 0.1 seconds of an experiment for very large lattices and low temperatures, or finding evidences for a finite phase transition in the Edwards-Anderson model in a magnetic field. In addition, Janus is now open to other researchers not belonging to the Janus Collaboration. Any application which can be fitted in a FPGA-architecture, will be very welcome. Encouraged by the good results reported by Janus, the "Janus Collaboration" decided to go a step further developing and designing Janus II [3], born just around three months ago.

[1] Janus Collaboration: F. Belletti *et al.*, Comput. Phys. Commun. **178** (2008) 208–216.
[2] Janus Collaboration: F. Belletti *et al.*, Computing in Science & Engineering **11-1** (2009) 48–58.
[3] Janus Collaboration: M. Baity-Jesi *et al.*, preprint arXiv:1310.1032.

Magnetic catalysis in 2 color QCD at finite temperature

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A lattice calculation on the phase diagram of two color QCD at finite temperature and magnetic field. A discussion of the results in view of claims of magnetic catalysis vs inverse magnetic catalysis.

Analysis of localization-delocalisation transitions in corner-sharing tetrahedral lattices (P)

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The corner-sharing tetrahedral lattice appears as a sublattice in different materials, e.g. spinels and pyrochlore. We consider the transport of non-interacting electrons and analyse the localisation-delocalisation (LD) transition induced by random on-site potentials. Three different methods (multifractal analysis, Green resolvent method, energy-level statistics) are used to explore the phase diagram, which is then compared to the results of a recent study [1]. Furthermore these methods yield detailed insight into the critical behaviour at the LD transition, i.e. the divergence of the correlation length, which is characterized by the value of the universal critical exponent.

[1] F. Fazileh, X. Chen, R. J. Gooding, and K. Tabunshchyk, Phys. Rev. B **73** (2006) 035124.

Autocorrelation study for a coarse-grained polymer model

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By means of Metropolis Monte Carlo simulations of a coarse-grained model for flexible polymers, we investigate how the integrated autocorrelation times of different energetic and structural quantities depend on the temperature. We show that, due to critical slowing down, an extremal autocorrelation time can also be considered as an indicator for the collapse transition that helps to locate the transition point. This is particularly useful for finite systems, where response quantities do not necessarily exhibit clear indications for pronounced thermal activity

Microcanonical molecular dynamics meets (multi)canonical Monte Carlo (P)

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Since the beginning of computational physics, both Molecular Dynamics and Monte Carlo simulations have been applied to the study of thermodynamic systems. The principle algorithm for Molecular Dynamics (MD) remained unchained, except for integrators and thermostats. On the other hand, there exists an increasing variety of different algorithms for Monte Carlo simulations like Metropolis, Parallel Tempering, Wang-Landau and the multicanonical method (MUCA). While MD and Parallel Tempering can be parallelized intuitively, MUCA and Wang-Landau have only recently been parallelized (see, e.g., [1]).

In this case study, we considered microcanonical MD simulations (NVE), avoiding the use of thermostats. The MD simulation was parallelized on GPUs and we compared the results to parallel multicanonical simulations. For each simulation approach, we performed both a microcanonical and a canonical analysis.

[1] J. Zierenberg, M. Marenz, and W. Janke, Comput. Phys. Comm. **184** (2013) 1155.

Liquid-glass transition in equilibrium

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We have studied the equilibrium phase diagram of a system of two coupled replicas of a binary mixture of hard spheres. Thanks to the "tethered Monte Carlo" method, we have been able to compute numerically the so-called "replica potential", characteristic of analytical mean-field computations. This potential has let as to confirm the validity of some mean-field predictions in realistic systems. In particular, this system undergoes a random first-order phase transition at a lower density than the unreplicated system, a precursor of the standard ideal glass transition. In the presence of a coupling field the glass transition point becomes a coexistence line that finishes in a critical point. We have also studied this second-order point, checking that its critical properties are compatible with those of an Ising system, as mean-field calculations suggested. The talk will be based on the recent work at http://arxiv.org/abs/1311.1465.

Wang-Landau simulation of polymer melts phase behaviour (P)

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Phase transitions in polymer melts have been under intensive investigation during the last years using both theoretical and experimental methods. But Wang-Landau simulations of polymer melts weren't successive and concerned mainly single chains and dilute systems or lattice models. We present results of off-lattice Wang-Landau simulations of melts of linear semi-flexible chains with stiffness bond potential. The simulated phase behavior of such system corresponds qualitatively to known results and can be estimated for model systems with maximal to minimal number of state ratio of over a few thousand orders of magnitude.

Polymer dynamics in confinement: MD simulations of 1,4-polybutadiene at a graphite interface (P)

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Polymer dynamics in confinement is both of fundamental interest concerning our understanding of the glass transition, as well as of high technological importance for the performance of composite materials. The results here presented are concerned with atomistic MD simulations of a chemically realistic model of a 1,4-polybutadiene melt (55% trans and 45% cis content) confined between two walls of graphite. The focus of our study is to investigate the effects of confinement on the chain dynamics in the melt and to reveal to what extent the walls are influencing structure and dynamics of the melt. As an example, it is well known and of interest to look at the conformation that a chain adopts at an interface by forming trains, loops and tails. It is evident that the chain dynamics of an adsorbed chain may be strongly constrained in comparison to a chain which is not adsorbed at an interface.

Partition function zeros and finite-size scaling for polymer adsorption

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The zeros of the canonical partition functions for a flexible polymer chain tethered to an attractive flat surface are computed for chains up to length $N = 1024$. We use a bond-fluctuation model for the polymer and obtain the density of states for the tethered chain by Wang-Landau sampling. The partition function zeros in the complex $\exp(1/T)$-plane are symmetric about the real axis and densest in a boundary region that has the shape of a nearly closed circle, centered at the origin, terminated by two flaring tails. This structure defines two root-free zones about the positive real axis. With increasing chain length, the circular boundary pinches down towards the positive real axis, dividing the axis into two sections, in accord with Yang-Lee theory. We apply finite-size scaling theory for partition function zeros to locate the adsorption transition in the thermodynamic limit and obtain values for the polymer crossover, order parameter, and specific heat exponents. These values allow us to construct universal scaling functions for the average number of surface contacts and the specific heat from our data.

Fourier MC simulation of criticality in solid and hexatic membranes

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Hexatic membranes are extremely difficult to study both in theory as well as in simulations based on conventional real space algorithms. We present new results for the flat phase of hexatic membranes using a unique

simulation approach based on an recently developed optimization [1] of our Fourier Monte Carlo algorithm [2, 3]. In our present treatment, the case of hexatic membranes is found to closely resemble that of solid membranes for which our algorithm has already proven to be quite successful. This success is based on tuning the Monte Carlo acceptance rates separately for each wavevector, which enables us to drastically reduce critical slowing down and thus observe critical behavior with excellent statistical accuracy. The resulting simulation scheme provides a new tailor-made approach to study critical behavior of systems with long-range interactions. In detail, we calculate correlation function $\langle |f(q)| \rangle^2 = G(q)$ and the related mean squared displacement $\langle (\Delta f)^2 \rangle$ of the membrane's out-of-plane deformations in the Monge parametrization and give a detailed finite-size scaling analysis of these data. For hexatic membranes, our simulations yield evidence for a logarithmic singularity of the critical exponent $\eta = 0_{\log}$. For the solid case, our numerical estimate for η is markedly smaller than that derived from other recent simulations, and we find clear evidence against "intrinsic ripples", whose existence has recently been claimed in the graphene-related literature.

[1] A. Tröster, Phys. Rev. B **87** (2013) 104112.
[2] A. Tröster, Phys. Rev. B **76** (2007) 012402.
[3] A. Tröster, Phys. Rev. Lett. **100** (2008) 140602.

Environmental impact on DNA denaturation

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We reconsider simple models for DNA denaturation focussing in particular on the impact of the environment in which the process occurs. We show how solvent quality, temperature and correlations of the environment may influence the denaturation process.

Corner contribution to cluster numbers in the Potts model

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For the two-dimensional Q-state Potts model at criticality, we study the average number of clusters N_Γ that intersect a given contour Γ. This quantity, which in the percolation limit $Q \to 1$ is related to the entanglement entropy of the random-field Ising model, is determined by the length of the curve Γ. Additionally, however, there occur logarithmic contributions related to the corners of Γ. These are found to be universal and their size can be calculated exactly employing techniques from conformal field theory. For the Fortuin-Kasteleyn clusters relevant to the thermal phase transition we find agreement with these predictions from large-scale numerical simulations. For the spin clusters, on the other hand, the cluster numbers are not found to be consistent with the tricritical branch of the Potts model as conventionally assumed.

Disentanglement of two qubits coupled to an Ising chain: Sudden quench dynamics

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We study the disentanglement of two qubits coupled at different sites of an Ising chain. At the initial time, the transverse field of the chain is suddenly quenched from an initial value up to a final value, leading to a non-equilibrium dynamics. The dependence of the decoherence on the quench parameters and the distance between

the qubits is evaluated exactly through the so called Loschmidt Echo. A special focus is set on the influence of the critical point on the disentanglement properties.

Specific interactions in a coarse-grained hard-sphere model (P)

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Synthetic- and biopolymers are topics for various areas of scientific interest. This wide range stretches from convenience products like television screens to biological questions like Alzheimer's disease. Although both polymer types are related by their structural background, e.g., monomeric units, their structure formation shows non-trivial differences. For a better understanding of these differences by molecular simulations it is a good starting point to use simple coarse-grained models. To understand the structure formation of biopolymers we started with a coarse-grained hard-sphere model which is also a common starting point for synthetic polymer modeling. By varying parameters and introducing specific interactions the attention can be shifted to biopolymers for investigating, e.g., peptide aggregation which can cause neurodegenerative diseases like the before mentioned Alzheimer's disease. For simulations with our coarse-grained hard-sphere model we started with Wang-Landau Monte Carlo and switched to Stochastic Approximation Monte Carlo. This brought an improved performance.

Numerical study of the branching tree of states in spin glasses

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We present a numerical method to generate explicit realisations of the ultrametric tree of states in mean-field spin glasses. We can thus obtain detailed information on the structure of the spin-glass phase. In particular, a cavity computation allows us to evaluate sophisticated observables, such as correlation functions. Our approach sheds light on the physical meaning of the full-RSB solution and has the potential to extend this solution to systems where replica computations are not available (such as the Bethe lattice). We show a sample application to peak counting and finite-size effects in the single-sample probability distributions of the spin overlap, a problem that has generated some debate recently.