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ABSTRACTS

of contributions to the

18th International NTZ-Workshop on

New Developments in Computational Physics

CompPhys17

Institut für Theoretische Physik, Universität Leipzig, Germany

30 November – 02 December 2017

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Supported by Research Academy Leipzig (RALeipzig), Doctoral College "$\mathbb{L}^4$" of Deutsch-Französische Hochschule (DFH-UFA), EU Marie Curie IRSES Network "DIONICOS: Dynamics of and in Complex Systems", DFG Collaborative Research Centre SFB/TRR 102 "Polymers under Multiple Constraints", Leipzig Graduate School of Natural Sciences "BuildMoNa", and Centre for Theoretical Sciences (NTZ) of Universität Leipzig.

Preface

Welcome to the 18th International NTZ-Workshop *CompPhys17* 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 30 November – 01 December 2017 in the Theory Lecture Hall ("Hörsaal für Theoretische Physik") 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. Antje Heydecke who coordinated this difficult task. We also wish to thank the secretaries of the Institute for Theoretical Physics, Ms. Gabriele Menge and Ms. Susan Moreno, for their invaluable help with all administrative matters.

As in previous years, the Saturday, 02 December 2017, is devoted to various discussion rounds and collaborative meetings which will take place in the Theoretical Physics building. Note that a few 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), Doctoral College "$\mathbb{L}^4$" of Deutsch-Französische Hochschule (DFH-UFA), EU Marie Curie IRSES Network "DIONICOS: Dynamics of and in Complex Systems", DFG Collaborative Research Centre SFB/TRR 102 "Polymers under Multiple Constraints", and Leipzig Graduate School of Natural Sciences "BuildMoNa".

Leipzig,
November 2017

Wolfhard Janke

Abstracts

Reweighting simulations in and out of equilibrium

Marius Bause
Max-Planck-Institut für Polymerforschung, D-55128 Mainz, Germany
mariusbause@gmx.de

Markov State Models (MSM) are a discrete representation of the kinetics of a given system constructed by coarse-graining microtrajectories. While frequently applied to equilibrium systems, a protocol for driven steady state systems has not been developed due to loss of dynamic properties like detailed balance. We propose to apply the principle of Maximum Caliber by Jayne's, postulating that the distribution of paths is given by the maximal path entropy encoding a chosen set of prior information. This reduces the computational effort of constructing an MSM by providing new microscopic relations from macrosopic path-ensemble assumptions. In addition it allows to reweight from equilibrium to non-equilibrium systems and vice versa. Simultaneously the markovian assumption alleviates the combinatorial explosion of microtrajectories. The method is tested on a minimal model under non-conservative forces.

Applications of quantum Hamilton equations of motion

Michael Beyer
Institut für Physik, Martin-Luther Universität Halle, Germany
michael.beyer@student.uni-halle.de

In 1966, E. Nelson established a new interpretation of quantum mechanics, whereby the particles follow some conservative diffusion process, i.e., forward-backward stochastic differential equations (FBSDEs), which are equivalent to the Schrödinger equation [1]. Until now, this equivalence has been applied in such a way that a known solution to the Schrödinger equation is used to integrate the stochastic differential equations numerically and analyze the statistical properties of the sample paths. Compared to the options available to treat classical systems this is limited, both in methods and in scope.

However, in analogy to classical mechanics, we show that finding the Nash equilibrium for a stochastic optimal control problem, which is the quantum equivalent to Hamilton's principle of least action, allows to derive two aspects [2]: i) the Schrödinger equation as the Hamilton-Jacobi-Bellman equation of this optimal control problem and ii) a set of quantum dynamical equations which are the generalization of Hamilton's equations of motion to the quantum world. We derive their general form for the n-dimensional, non-stationary and the stationary case. The resulting forward-backward stochastic differential equations can be solved numerically without using the solution of the Schrödinger equation, which is done for many different systems, e.g., one- and two-dimensional harmonic oscillator, one-dimensional double-well potential or hydrogen atom.

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On the interface tension of the Ising model

Elmar Bittner
Institut für Theoretische Physik, Universität Heidelberg, Germany
e.bittner@thphys.uni-heidelberg.de

We determine the interface tension for the two- and three-dimensional Ising model using multicanonical simulations. We analyse the finite-size scaling behaviour of the interface tension for various temperatures, and compare them to previous results obtained with a combination of the multimagnetic algorithm with the parallel tempering method. We also use exact finite-size scaling functions for the two-dimensional Ising model to validate our results.

Structure of poly-glutamines studied by Monte Carlo simulation (P)

Arne Böker
Institut für Physik, Martin-Luther Universität Halle, Germany
arne.boeker@physik.uni-halle.de

Much effort has recently been put into understanding amyloid formation in polypeptides. The amyloid state is a structure in which polypeptides aggregate as a stack of β-sheets, which is usually not the native state, leading to loss of function. Amyloids can cause a variety of diseases (amyloidoses) such as Huntington's chorea, which is linked to an amyloidic state of expanded poly-glutamine sequences. The relation between conformations of a polypeptide is governed by local minima in the free energy function. Coarse-grained models tend to simplify the free energy in such a way that these local minima are ignored. To circumvent this problem, the level of coarse-graining needs to be chosen appropriately. PRIME20 [1] provides reasonable detail by mapping each amino acid to four beads, but keeps parameter space simple with the set of interactions reduced to 19 energy parameters. We perform thermodynamic simulations of single PRIME20 chains using the SAMC [2] variation of Wang-Landau Monte Carlo sampling. The structure formation of single poly-glutamines is investigated, configurations of which may also serve as templates in amyloid formation.

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Efficient method of simulating with long-range interactions: The case of coarsening in the Ising model

Henrik Christiansen
(with Suman Majumder and Wolfhard Janke)
Institut für Theoretische Physik, Universität Leipzig, Germany
henrik.christiansen@itp.uni-leipzig.de

Simulations of systems with long-range interactions are computationally more challenging than its short-range counterpart, e.g., in the long-range Ising model all spins have to be considered in the calculation of the local energy change. For several models, this problem has been overcome by the introduction of cluster algorithms for equilibrium simulations. As those cluster methods do not capture the dynamics, one cannot rely on them for simulating kinetics of phase transitions. Here, we present a novel and efficient approach of tackling such problems, concerning nonequilibrium dynamics via Monte Carlo simulations by storing a local "pseudo heatbath" for the energy calculation. As an illustration, we present results for coarsening of the long-range Ising model in $d = 2$ dimensions. In contradiction to all available simulation results in this context (using an cut-off to make the simulation feasible), our results establish agreement with the theoretical predictions.

Efficient implementation of connectivity changing moves for dense polymers

Nathan Clisby
Dept. of Mathematics, Swinburne University of Technology, Hawthorn, Victoria, Australia
nclisby@swin.edu.au

I will describe how to efficiently implement connectivity changing moves which allow for rapid Monte Carlo sampling of dense polymer configurations, such as Hamiltonian paths. This involves the development of a novel binary tree data structure which allows moves to be performed in CPU time $O(\log N)$ for a polymer with N monomers. I will discuss differences that have been observed between two- and three-dimensional systems, and sketch a framework for describing a family of connectivity changing moves. This is work in progress, and the focus of the talk will be on algorithmic aspects rather than physical applications.

On critical speeding-up in an irreversible worm dynamics for high-dimensional Ising models

Eren Metin Elçi

(with Jens Grimm, Lijie Ding, Abrahim Nasrawi, Timothy M. Garoni and Youjin Deng)

School of Mathematical Sciences, Monash University, Clayton, Victoria, Australia
elci@posteo.de

We present a study of an irreversible worm algorithm for the zero-field ferromagnetic Ising model by using the lifting technique. We study the dynamic critical behaviour of an energy estimator on both the complete graph and toroidal grids, and compare our findings with reversible algorithms such as the Prokof'ev-Svistunov worm algorithm. Our results show that the lifted worm algorithm improves the dynamic exponent of the energy estimator on the complete graph, and leads to a significant constant improvement (up to two orders of magnitude) on toroidal grids.

On the effect of disorder on first-order phase transitions: The case of the 2D random-bond Blume-Capel mode

Nikolaos Fytas

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

We present new results on the effect of quenched disorder on first-order phase transitions, using as a platform the Blume-Capel model in two-dimensions. By means of Monte Carlo simulations and a finite-size scaling analysis based on the correlation length we show that the low-temperature randomness-induced (ex-first-order) continuous transition of the random-bond Blume-Capel model belongs to the universality class of the pure Ising ferromagnet. These results settle down previous claims of violation of universality obscured by strong scaling orrections, as monitored in our analysis. An overview of results at the originally second-order regime of the model is also given together with a most recent reproduction of the phase diagram of the pure model and its well-known scaling behavior.

Crumpling transition and low-temperatures properties of crystalline membranes with perforation patterns

Antonio Gordillo-Guerrero

Department of Electric Engineering, Electronics and Automatics, Universidad de Extremadura, Badajoz, Spain
anto@unex.es

We present a Monte Carlo study of two-dimensional triangular lattices with fixed connectivity, living in a 3D space. We define two interactions between points: an elastic term (like springs) and a curvature one (tending to parallel all plaquettes in the same plane). The strength of the latter is defined by a coupling constant called κ. For κ large, we expect an almost plane membrane, while for κ small we except a crumpled surface. It is believed that this model belongs to the same universality class as graphene sheets. We define several sizes and densities of perforations, using different periodic patterns on the lattice and free boundary conditions. We estimate numerically the critical values of the coupling for each pattern, performing a finite-size scaling (FSS) study of the specific heat and gyration ratio behaviors computing the associated critical exponents [1]. We compare with very recent results obtained using Molecular Dynamics simulations [2] obtaining good agreement. Finally, we have performed a detailed study of the low-temperature phase (flat phase) computing some elasticity constants such as the Poisson Ratio and the Young Modulus [1].

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Monte Carlo studies of P3HT aggregation (P)

Jonathan Groß
(with Mochil Ivanov, David Nicolai Oberthür and Wolfhard Janke)

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

Poly(3-hexylthiophene) (P3HT) is a semiconducting polymer that has applications in organic photovoltaics. It is widely used as a semiconducting layer in organic thin film field effect transistors (FETs) and solar cells. We found that a recently developed coarse-grained model [1] of P3HT, is suitable and able to reproduce not only fully atomistic simulations, but also experimental results [2, 3, 4]. On the basis of those single-chain studies, we now take the next step and look at aggregation of a few polymers, to gain an understanding of the fundamental processes that happen during the crystallization of P3HT. With replica-exchange (parallel tempering) simulations we investigate a system of four P3HT polymer chains with 10 repeat units each in the presence of a Au(001) surface and without a substrate. In addition to that, we aim to apply the parallel multicanonical (PMUCA) sampling method [5] to our system. A recent implementation of PMUCA on graphics processing units [6], promises vast increase in efficiency of the multicanonical weight recursion and production run. An early implementation for polymer aggregation using this novel approach is presented here.

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Enhanced sampling simulations of folding and aggregation

Ulrich H. E. Hansmann

Dept. of Chemistry and Biochemistry, University of Oklahoma, Norman, OK, USA
uhansmann@ou.edu

Folding, association and aggregation of proteins are key processes in the biochemistry of cells but often difficult to probe in experiments or computer simulations. The later suffer from the problem that these processes happen on time scales that in general are not accessible in atomistic simulations, and the required computational resources even increase exponentially with size of the molecules. In this talk, I will describe variants of replica exchange sampling designed to overcome this sampling-problem in studies of fold-switching proteins and amyloid-forming peptides.

High-precision simulation of height distribution for directed polymers in random media

Alexander Hartmann

Institute for Physics, Carl von Ossietzky University of Oldenburg, Germany
a.hartmann@uni-oldenburg.de

The distribution of relative free energies H of directed polymers in disordered media is studied, which is in the KPZ universality class. We study the distribution at large and medium small temperatures, corresponding to short and medium long times in KPZ. Using a statistical mechanics-based large-deviation approach, the distribution can be obtained over a large range of the support, down to a probability density as small as 10^{-1000}. We compare with analytical predictions for short and long times, respectively. For short times a very good agreement is found for $H < 0$ and a convergence is visible for $H > 0$. For large times, an asymptotic convergence in the tails is visible.

Interface tension and the cluster exchange algorithm

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

We study interfaces with periodic boundary conditions in the low temperature phase of the improved Blume-Capel model on the simple-cubic lattice. The interface free energy is defined by the difference of the free energy of a system with anti-periodic boundary conditions in one of the directions and that of a system with periodic boundary conditions in all directions. It is obtained by integration of differences of the corresponding internal energies over the inverse temperature. These differences can be computed efficiently by using a variance reduced estimator that is based on the exchange cluster algorithm.

Shape characteristics of partially directed polymers in anisotropic environment (P)

Khristine Haydukivska
Institute for Condenced Matter Physics, National Academy of Sciences of Ukraine, Lviv, Ukraine
wja4eslawa@gmail.com

We consider a lattice model of a partially directed self-avoiding walk on a cubic lattice with an anisotropic disorder. The obstacles are considered to be in the form of unpenetrable lines that are oriented in one direction and randomly distributed in the perpendicular plane. We analyze two cases, when polymers are considered to be oriented in direction perpendicular as well as at the 45 degree angle to the direction of the columnar defects. We apply the Pruned-Enriched Rosenbluth Method (PERM) in order to analyze conformational properties of polymers, which include both scaling exponents and shape characteristics. For the case of perpendicular orientation of the stretching field and columnar defects, we observe a reorientation transition of polymers, while in the other case this transition is absent.

Disassembling Casimir scaling functions at finite aspect ratios

Hendrik Hobrecht
(with Fred Hucht)
Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany
hendrik@thp.uni-due.de

The finite-size scaling functions for the free energy of the two-dimensional Ising universality class are known exactly only either for finite aspect ratios at criticality due to conformal field theory (CFT), or for thin films at arbitrary temperatures. Beyond the thin films and CFT there are but a few results, namely for the torus, the open cylinder, and approaches for topologically more exotic forms like the open Möbius strip and the Klein bottle. Despite their role as potential for the critical Casimir force, even less is known in the presence of surface fields. We present a systematic calculation of the interlink between those limiting cases, implementing both symmetric (++) and asymmetric (+-) symmetry-breaking boundary conditions (BCs) on the cylinder with finite aspect ratio, as well as the often discussed Brascamp-Kunz BC. We show that the scaling limit of the latter one is indeed equal to open boundaries, as both are believed to represent Dirichlet BCs. Therefore we start with Kasteleyn's dimer representation of the Ising model, follow McCoy and Wu to introduce boundary fields, and implement an anisotropic scaling theory together with a hyperbolic parametrisation of the Onsager dispersion. An impressive feature of these scaling functions is the possibility to disassemble them not only into recurring bulk, surface, and finite-size contributions, but even beyond. We can distinguish different building blocks for the surfaces and surface fields, as well as for the breaking of the Z_2-symmetry and the surface tension due to imposed domain walls.

MD simulations on martensitic transformations in iron-palladium

Alexander Holm

Leibniz-Institute for Surface Modification (IOM) and Division of Surface Physics, University of Leipzig, Germany
alexander.holm@iom-leipzig.de

We report about molecular dynamics (MD) simulation studies on martensitic transitions in iron-palladium (Fe_7Pd_3) shape memory alloys, mentioning custom-designed embedded atom method (EAM) potentials based on density functional theory (DFT) calculations. Upon application of an uniaxial compressive strain to the simulation cell it was found that the transformation from a face-centered cubic crystal-lattice-configuration to a body-centered tetragonal configuration occurs, exhibiting orientation variants which can be connected to the structural phenomenon of twinning, which is a prerequisite for the shape memory effect in Fe_7Pd_3. The focus of this presentation will lie on the structural properties of the martensitic phase transition, regarding transformation paths and the introduction of a new method to determine structural changing incidents from a series of radial distribution functions, the RDF-Separation-Function.

Non-linear viscoelasticity of highly strained polymer melts: Primitive path analysis

Hsiao-Ping Hsu
(with Kurt Kremer)

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

Polymer melt dynamics is strongly affected by entanglement effects due to topological constraints between chains both in the linear and non-linear viscoelastic regime. Starting from fully equilibrated and highly entangled bead-spring chains in a melt [1, 2, 3], the entanglement structure and force distribution within the system are investigated after the system is strongly deformed by isochoric elongation with fixed strain rate. We relate the stress relaxation in both linear and non-linear viscoelastic regimes to changes in the primitive paths of chains extracted from the primitive path analysis (PPA) [4]. We have also shown that the tension forces both along the original paths and along primitive paths in the stretching direction follow the same pattern. Finally, we find that there exists a long lived clustering of topological constraints along the chains in the strongly deformed state [5].

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Analytic finite-size scaling functions in the anisotropic Ising rectangle

Fred Hucht

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

The partition function of the square lattice Ising model on the rectangle, with open boundary conditions in both directions, is calculated exactly for arbitrary system size $L \times M$ and temperature. We start with the dimer method of Kasteleyn, McCoy & Wu, construct a highly symmetric block transfer matrix and derive a factorization of the involved determinant, effectively decomposing the free energy of the system into two parts, $F(L,M) = F_{\text{strip}}(L,M) + F^{\text{res}}_{\text{strip}}(L,M)$, where the residual part $F^{\text{res}}_{\text{strip}}(L,M)$ contains the nontrivial finite-L contributions for fixed M [1]. It is given by the determinant of a $M/2 \times M/2$ matrix and can be mapped onto an effective spin model with M Ising spins and long-range interactions. While $F^{\text{res}}_{\text{strip}}(L,M)$ becomes exponentially small for large L/M or off-critical temperatures, it leads to important finite-size effects such as the critical Casimir force near criticality. In the finite-size scaling limit $L, M \to \infty$, $T \to T_c$, with fixed temperature scaling variable $x \propto (T/T_c - 1)M$ and fixed aspect ratio $\rho \propto L/M$, we derive exponentially fast converging series for the related universal Casimir potential and Casimir force scaling functions [2]. At the critical point $T = T_c$ we confirm

predictions from conformal field theory. The presence of corners and the related corner free energy has dramatic impact on the Casimir scaling functions and leads to a logarithmic divergence of the Casimir potential scaling function at criticality.

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Contact process in inhomogeneous environment

Ferenc Iglói

Wigner Research Centre for Physics, Budapest, Hungary
igloi.ferenc@wigner.mta.hu

We consider the contact process near an extended surface defect, where the local control parameter deviates from the bulk one by an amount of $\lambda(l) - \lambda(\infty) = Al^{-s}$, l being the distance from the surface [1]. We concentrate on the marginal situation, $s = 1/\nu_\perp$, where $\nu_\perp$ is the critical exponent of the spatial correlation length, and study the local critical properties of the one-dimensional model by Monte Carlo simulations. The system exhibits a rich surface critical behavior. For weaker local activation rates, $A < A_c$, the phase transition is continuous, having an order-parameter critical exponent, which varies continuously with A. For stronger local activation rates, $A > A_c$, the phase transition is of mixed order: the surface order parameter is discontinuous, at the same time the temporal correlation length diverges algebraically as the critical point is approached, but with different exponents on the two sides of the transition. The mixed-order transition regime is analogous to that observed recently at a multiple junction [2] and can be explained by the same type of scaling theory.

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Spin chain SUSY

Desmond A. Johnston

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

Supersymmetry (SUSY), a symmetry between bosons and fermions, has been conspicuous by its absence in particle physics where it was originally formulated. However, an *exact* lattice supersymmetry does exist in various 1D spin chains where it relates chains of different lengths. We discuss its formulation for the XXZ spin chain with various boundary conditions.

Site-diluted Ising model in two dimensions – Towards long-range correlated defects (P)

Stanislav Kazmin
(with Wolfhard Janke)

Max Planck Institute for Mathematics in the Sciences (MPI-MIS) and Institut für Theoretische Physik, Universität Leipzig, Germany
kazmin@mis.mpg.de

We investigate the critical behavior of a long-range correlated site-diluted Ising model in two dimensions. In this model the spatial correlation function between two sites ϵ_i and ϵ_j decays according to a power-law $C(d) = \langle \epsilon_i \epsilon_j \rangle \propto d^{-a}$. The Harris criterion states that in the region where the correlation between the defects is important one expects a new universality class with continuous critical exponents and $\nu = 2/a$. Our aim is to find the critical a_c at which the system falls into another universality class and find the critical exponents and critical temperatures below and above this value. To this end, we first analyze the two-dimensional uncorrelated site-diluted Ising model and the pure Ising model as the edge cases of the long-range correlated site-diluted Ising

model. At present state we obtained the critical temperature as a function of dilution concentration as well as critical exponents of the pure system and are about to extract critical exponents for the diluted system.

Applications of quantum Hamilton equations of motion (P)

Jeanette Köppe
Institut für Physik, Martin-Luther Universität Halle, Germany
jeanette.koeppe@physik.uni-halle.de

See abstract of Michael Beyer's talk.

Complexity and optimization: Physical science meets biological science via computer simulations

David P. Landau
Center for Simulational Physics, The University of Georgia, Athens, GA, USA
dlandau@hal.physast.uga.edu

Complexity is everywhere in nature, and it often manifests itself in the existence of a rough free energy landscape that is extraordinarily difficult to investigate. Other problems have no free energy but can be mapped onto complex free energy landscapes. Ground state searches correspond to optimization problems, but often knowledge of the thermodynamic behavior at different temperatures is also desired. Computer simulations have become the method of choice for studying a wide variety of systems, but traditional algorithms fail when the free energy has multiple minima and maxima that are widely separated in phase space. We will introduce a generic, parallel Replica Exchange Wang-Landau (REWL) Monte Carlo sampling method [1] that is naturally suited for implementation on massively parallel, petaflop supercomputers. The approach introduces a replica-exchange framework involving densities of states that are determined iteratively for overlapping windows in energy space, each via traditional Wang-Landau sampling. The framework is valid for models of soft and hard condensed matter, including systems of biological interest. The significant scalability, performance advantages, and general applicability of the method are demonstrated using thousands of computing cores for several quite different models of interacting particles. Systems studied may have discrete or continuous degrees of freedom, and include those with both complex free energy landscapes and topological constraints.

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Thermodynamics of single polyethylene and polybutylene glycols with hydrogen-bonding ends

Eunsang Lee
Institut für Physik, Martin-Luther Universität Halle, Germany
eunsang.lee@physik.uni-halle.de

A variety of linear polymer precursors with hydrogen bonding motif at both ends enable to design supramolecular polymer systems with tailored macroscopic properties including self-healing. In this study, we investigate thermodynamic properties of single polyethylene and polybutylene glycols with hydrogen bonding motifs. In this context, we first build a coarse-grained model of building blocks of the supramolecular polymer system based on all-atom molecular structures. The density of states of the single precursor is obtained using the Stochastic Approximation Monte Carlo (SAMC) method. Constructing canonical partition functions from the density of states, we find the transition from looped to open conformations at transition temperatures which are non-monotonously changing with increasing degree of polymerization N due to the competition between chain stiffness and loop-forming entropy penalty. In the complete range of N under investigation, the transition is shown to be first-order-like according to clear two peaks in a two-dimensional energy distribution, even if the latent heat for long chains is buried in other energy contributions. Polyethylene and polybutylene glycols show similar behavior in all the thermodynamic properties but the transition temperature of the more flexible polybutylene glycol is shown to be gradually changing.

Diagrams of states for single flexible-semiflexible multiblock copolymer chains in different selective solvents: Computer simulations by means of stochastic approximation Monte Carlo (P)

Daria Maltseva

Faculty of Physics, Moscow State University, Russia, and Institut für Physik, Martin-Luther Universität, Halle, Germany

dv.maljtceva@physics.msu.ru

Diagrams of states for single flexible-semiflexible multiblock copolymer chains in different selective solvents have been calculated by means of computer simulations using the Stochastic Approximation Monte Carlo (SAMC) method. We study conformational properties of a single multi-block copolymer chain consisting of flexible (F) and semi-flexible (S) blocks with equal composition of F- and S-units and with different affinity to a solvent. We perform Monte Carlo (MC) simulations based on the Stochastic Approximation algorithm [1, 2] which is one of the most recent realizations of flat-histogram-type MC algorithms [3]. SAMC algorithm is based on the idea of equally frequent sampling of all energy states of the system and accumulating the density of states function. We use the two-dimensional density of states function, which depends on the energy of intramolecular stiffness and on the energy of non-valence interactions. We present data on different non-trivial globular morphologies, including several structures with high orientational ordering of bonds, which we have obtained in our model for different values of the chain length, the block length and the stiffness parameter. Preliminary diagrams of states in variables temperature vs. stiffness parameter are also presented for different values of the block length. We compare our results with those obtained previously for a single SF-copolymer chain in a non-selective solvent [4, 5] and discuss the observed differences.

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Simulated annealing, effective but inefficient? A case study for the 3D136 instance of the HP model of protein folding

Arnulf Möbius[1]

(with Florian Guenther[2]**)**

[1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW), Dresden, Germany
[2]TU Dresden, Germany

a.moebius@ifw-dresden.de

Because of its clarity, the simulated annealing algorithm (SA) is very popular and is taught in most courses on computational physics or applied numerics. However, its efficiency seems to be rather weak. Thus, for the last decades, various new heuristic optimisation approaches have been demonstrated to be advantageous over SA. To keep such a comparison for a difficult protein folding task as fair as possible, we pushed SA to its limits for the 3D136 instance of the HP model. Studying the dependence of the mean energy of the resulting state on the number of move trials over five orders of magnitude, we were surprised to which enormous extent SA can be accelerated by very simple means. The following four modifications enable to speed up this low-energy state search by up to a factor of 3000 in total. (1) We focus on the best state hit within the SA run rather than on the final one; this is advantageous due to the non-equilibrium nature of the SA process. (2) Generalising this idea, we stop the cooling process and restart it from the respective best-so-far state (without temperature change) an optimised number of times. (3) We determine the most appropriate initial and final temperatures of the exponential schedule used. (4) By means of OpenMP parallelisation, we simultaneously perform a number of only weakly interacting SA runs. Although these ideas are rather obvious and, in part, have been used in various studies before, they seem to be not as widely used as they deserve to be. Therefore, we suggest to study the corresponding efficiency gain for further challenging optimisation problems. At least, the acceleration approach (1), which can be very easily implemented and which does not exhibit any adjustable parameter, should always be included in teaching and application of SA.

Non-flat histogram methods for spin glasses (P)

Fabio Mueller
(with Stefan Schnabel and Wolfhard Janke)
Institut für Theoretische Physik, Universität Leipzig, Germany
fabio.mueller@itp.uni-leipzig.de, flabons@posteo.de

We take into consideration the 3D Edwards-Anderson model with bimodal bond distribution. Since the model is characterized by spin-glass behavior, finding ground states is an NP-hard problem. Employing different simulation techniques the round trip time distribution is investigated and the performance of the different methods is compared. The methods taken into consideration are the most established broad energy ensemble methods including the parallel tempering method and, in addition, a specially designed non-flat histogram technique which is shown to outperform the currently existing methods.

Finite-size effects in canonical and grand-canonical quantum Monte Carlo simulations for fermions

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

We introduce a quantum Monte Carlo method at finite temperature for interacting fermionic models in the canonical ensemble, where the conservation of the particle number is enforced. Although general thermodynamic arguments ensure the equivalence of the canonical and the grand-canonical ensembles in the thermodynamic limit, their approach to the infinite-volume limit is distinctively different. Observables computed in the canonical ensemble generically display a finite-size correction proportional to the inverse volume, whereas in the grand-canonical ensemble the approach is exponential in the ratio of the linear size over the correlation length. We verify these predictions by quantum Monte Carlo simulations of the Hubbard model in one and two dimensions in the grand-canonical and the canonical ensemble. We prove an exact formula for the finite-size part of the free energy density, energy density and other observables in the canonical ensemble and relate this correction to a susceptibility computed in the corresponding grand-canonical ensemble. This result is confirmed by an exact computation of the one-dimensional classical Ising model in the canonical ensemble, which for classical models corresponds to the so-called fixed-magnetization ensemble. Our method is useful for simulating finite systems which are not coupled to a particle bath, such as in nuclear or cold atom physics.

Numerical construction of the Aizenman-Wehr metastate

Juan J. Ruiz-Lorenzo
Department of Physics, Universidad de Extremadura, Badajoz, Spain
ruiz@unex.es

Chaotic size dependence makes it extremely difficult to take the thermodynamic limit in disordered systems. Instead, the metastate, which is a distribution over thermodynamic states, might have a smooth limit. So far, studies of the metastate have been mostly mathematical. We present a numerical construction of the metastate for the $d = 3$ Ising spin glass. We work in equilibrium, below the critical temperature. Leveraging recent rigorous results, our numerical analysis gives evidence for a "dispersed" metastate, supported on many thermodynamic states.

Linear programming and cutting planes for ground states and excited states of the traveling salesperson problem

Hendrik Schawe
Institute for Physics, Carl von Ossietzky University of Oldenburg, Germany
hendrik.schawe@uni-oldenburg.de

The Traveling Salesperson problem asks for the shortest cyclic tour visiting a set of cities given their pairwise distances and belongs to the NP-hard complexity class, which means that typical realizations are not solvable in polynomial time (if P $\neq$ NP holds). Nevertheless, there are subsets of the problem which are typically easy to solve. To examine a transition from an easy to a hard phase, we study an ensemble of random configurations of cities in a Euclidean plane, characterized by a parameter σ, which governs the strength of the randomness. The realizations are treated using a linear programming approach with selected cutting planes. We observe several phase transitions from easy to hard phases, depending on the types of cutting planes used. These transitions are related to physical properties of the shortest tours and analyzed using finite-size scaling techniques. Further, we look at excited states to explore the energy landscape in detail. The linear programming approach offers capable tools to find excited states fulfilling very specific requirements. This allows us, e.g., to find the second shortest tour, the shortest tour not using half the edges of the optimal tour or the tour most different to the optimal tour within some allowed excitation ϵ, e.g., 1% longer than the optimum. We are especially interested whether the energy landscape is complex and how to determine the level of complexity.

Coarse-graining the state space of a spin glass

Stefan Schnabel
(with Wolfhard Janke)

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

The Edwards-Anderson model is the standard model for two- and three-dimensional spin glasses and due to its rugged energy landscape the investigation by means of Monte Carlo techniques is exceptionally difficult. Based on our previous work [1] we have developed a novel algorithm that exclusively samples the metastable states, i.e., the local minima. This means that every valley or basin of attraction in the energy landscape of the standard model is reduced to the respective local minimum. The associated ensemble, the energy landscape and the state space can thus be considered coarse-grained versions of their counterparts. We present measurements of the distribution of local minima as well as overlap distributions and correlation length.

[1] S. Schnabel and W. Janke, Comput. Phys. Commun. **220** (2017) 74.

Convergence estimation of flat-histogram algorithms based on simulation results

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

The present work considers the question of convergence of Wang-Landau, multi-canonical and stochastic approximation Monte Carlo algorithms, which was previously investigated on very different level. In the case of the multi-canonical algorithms, a convergence behavior similar to either the original Wang-Landau or the stochastic approximation Monte Carlo algorithms is shown, depending on details of the algorithm. I suggest a method for error estimation based only on the results of simulations, not involving an information about the exact density of states, which is unknown for most practically interesting problems.

Control of accuracy in the Wang-Landau algorithm

Lev Shchur

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

The Wang-Landau (WL) algorithm has been widely used for simulations in many areas of physics. Our analysis of the WL algorithm explains its properties and shows that the difference of the largest eigenvalue of the transition matrix in the energy space from unity can be used to control the accuracy of estimating the density of states. Analytic expressions for the matrix elements are given in the case of the one-dimensional Ising model. The proposed method is further confirmed by numerical results for the one-dimensional and two-dimensional Ising models and also the two-dimensional Potts model.

Two perspectives on the condensation-evaporation transition (P)

Franz Paul Spitzner

(with Johannes Zierenberg and Wolfhard Janke)

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

The particle condensation-evaporation transition is a standard example of a first-order phase transition. In equilibrium, the consideration may be reduced to the coexistence of a homogeneous gas phase and an inhomogeneous phase consisting of a single macroscopic droplet with surrounding vapour. The transition can either be driven by density or temperature – keeping the respective "orthogonal" quantity constant. While this problem can be rigorously treated only at fixed temperature and in two dimensions [1], a heuristic derivation of the leading-order finite-size scaling behaviour exists that holds for the transition at fixed temperature and at fixed density [2].

We present how the well known multicanonical method can be adopted to the grandcanonical ensemble, allowing us to investigate the condensation-evaporation transition of a 2D Lennard-Jones gas in both regimes. The careful adjustment of simulation parameters and subtle implementation choices will be discussed, in order to provide insight into the method and consistent results. Not only does our data support the existing prediction of the scaling behaviour, but it is also for the first time that the theory by Biskup et al. [1] is confirmed to hold for continuous, off-lattice systems.

[1] M. Biskup, L. Chayes, and R. Kotecký, Europhys. Lett. **60** (2002) 21.
[2] J. Zierenberg and W. Janke, Phys. Rev. E **92** (2015) 012134.

Dynamically order-disorder transition in triangular lattice driven by a time dependent magnetic field (P)

Erol Vatansever

Department of Physics, Dokuz Eylul University, Izmir, Turkey
erol.vatansever@deu.edu.tr

We have elucidated the dynamic phase transition features and finite-size scaling analysis of the triangular lattice system under the presence of a square-wave magnetic field. It has been found that as the value of half-period of the external field reaches its critical value, whose location is estimated by means of Binder cumulant, the system presents a dynamic phase transition between dynamically ordered and disordered phases. Moreover, at the dynamic phase transition point, finite-size scaling of the Monte Carlo results for the dynamic order parameter and susceptibility give the critical exponents $\beta/\nu = 0.143 \pm 0.004$ and $\gamma/\nu = 1.766 \pm 0.036$, respectively. The obtained critical exponents show that present magnetic system belongs to same universality class as the two-dimensional equilibrium Ising model.

Monte Carlo study of hysteresis features of a cylindrical nanowire under quenched disorder (P)

Zeynep Demir Vatansever
Department of Physics, Dokuz Eylul University, Izmir, Turkey
zeynep.demir@deu.edu.tr

Hysteresis properties of a quenched disordered binary alloy cylindrical nanowire of the type A_p $B_{(1-p)}$ have been studied by Monte Carlo simulation technique. The nanowire system consists of two types of magnetic components, A with spin-1/2 and B with spin-1, which are randomly located on the sites of the nanowire. We have investigated the effects of the active concentration of type-A magnetic components, p, and the strength of the spin-spin coupling between type-A and -B components on the remanence magnetization and coercivity field in a wide range of temperature. It has been shown that it is possible to modify the magnetic properties (coercivity, remanence as well as hysteresis loops) of the nanowire by varying the concentration of the magnetic components and the exchange coupling strength between unlike magnetic components. Moreover, a qualitative agreement has been found between our simulations results and recent experimental studies.

Critical behavior of the quantum Potts chain with aperiodic perturbation

Dimitris Voliotis[1]
(with Christophe Chatelain[2]**)**

[1]São Carlos Institute of Physics, University of São Paulo, Brazil
[2] Groupe de Physique Statistique, Institut Jean Lamour, Université de Lorraine Nancy, France
dimvoliotis@gmail.com

The quantum q-state Potts chain with various aperiodic perturbations is studied under the Strong-Disorder Renormalization Group (SDRG) approach. The magnetic scaling dimension is extracted and found to be independent of q for aperiodic sequences with a vanishing wandering exponent. On the other side, the dynamical exponent found to increase with q and to remain finite for all the aperiodic sequences. Finally, for the Rudin-Shapiro sequence, the results are compatible with an Infinite-Disorder Fixed Point (IDFP).

Stiff homopolymer chains and specific interactions (P)

Benno Werlich
(with Timur Shakirov, Mark P. Taylor and Wolfgang Paul)

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

We studied the stiffness of a hard-sphere homopolymer model with attractive interactions by variation of the bond length. Therefore, a state diagram for a chain length of 40 monomers is presented. For very short bond lengths the high-temperature line of the state diagram changes from a collapse to a knot transition, which appears below a biologically meaningful bond length. The shrinked configuration space of very stiff chains leads to an intuitive access to the knot-folding process. Regarding biological systems we introduced specific interactions as additional short-range potential and show some consequences of its strength with respect to the non-specific interactions. The simulations were performed off-lattice with Stochastic-Approximation Monte Carlo (SAMC) to gain the microcanonical entropy.

Diversity of dynamic states in neural networks induced by homeostatic plasticity

Johannes Zierenberg

Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany
johannes.zierenberg@ds.mpg.de

Dynamics of spiking neural networks exhibit clear differences, depending whether recorded in living organisms and artificial cultures. In living organisms, the neural activity shows continuous, fluctuating dynamics, whereas cultured networks develop strong bursts separated by periods of silence. We propose that this is a result of an interplay between (1) network input, which is much stronger in the intact brain than in isolated cultures, and (2) homeostatic plasticity, a slow negative feedback mechanism adapting the neural spike rate. Based on our theoretical work, we predict that homeostasis can be harnessed to tune the dynamic state of a network by altering its input strength. Most importantly, this could allow to abolish the bursts in cultured neurons and render the dynamics brain-like instead – a key prerequisite to study neurological and psychiatric disorders on the network level under laboratory conditions.