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ABSTRACTS

of contributions to the

16th International NTZ-Workshop on

New Developments in Computational Physics

CompPhys15

Institut für Theoretische Physik, Universität Leipzig, Germany

26 – 28 November 2015

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

Preface

Welcome to the 16th International NTZ-Workshop *CompPhys15* 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 26 – 27 November 2015 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. Sandy Ehlers who coordinated this difficult task. We also wish to thank the secretaries of the Institute for Theoretical Physics, Ms. Gabriele Menge, Ms. Susan Hussack, and Ms. Lea Voigt, for their invaluable help with all administrative matters.

As in previous years, the Saturday, 28 November 2015, is devoted to various discussion rounds and collaborative meetings which will take place in the Theoretical Physics building. Note that three years ago the Institute for Theoretical Physics has moved from the old location "Vor dem Hospitaltore 1" to the *new* office building in "Brüderstr. 16".

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

Dedicated to the memory of Thomas Neuhaus. His enthusiasm for physics, his cheerfulness and advice will be missed deeply.

Leipzig,
November 2015

Wolfhard Janke

Abstracts

Multicriticality in confined ferromagnets with impurities

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We present a numerical study of the localization-delocalization transition of the interface between magnetic domains of different orientation, in both Ising and Blume-Capel [1] magnets confined between two walls separated by a distance L, where short-range competitive surface magnetic fields act. So, samples are assumed to have a size $L \times M$, L being the width and M the length, respectively. The localization-delocalization transition of the interface becomes a true wetting phase transition when the thermodynamic limit ($L \to \infty, M \to \infty$) is properly taken, as it follows from scaling theory [2]. By considering fixed (quenched) vacancies or nonmagnetic impurities along the centre (i.e., for $x = L/2$) of an Ising sample we found that the wetting transition can be of either of first or second order, depending on the concentration of vacancies. While first-order transitions are precisely located by means of thermodynamic integration methods [3], second-order transitions are accurately determined by using a suitable scaling theory [2]. In this way, at the intersection between second- and first-order lines we found tricritical wetting points. On the other hand, we also considered both standard and modified Blume-Capel models [1] in order to gain insight on the role of mobile impurities. Here, tricritical wetting is also found but for a tiny concentration of impurities. So, our study concludes that a proper density of both quenched and mobile nonmagnetic impurities can effectively cause the pinning-depinning transition of magnetic interfaces. Both cases are fully discussed and the relevance of the results for the design of nano-magnetic storage devices is stressed.

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[3] M. L. Trobo, E. V. Albano, and K. Binder, Phys. Rev. E **90** (2014) 022406.

On the lack of polymorphism in Aβ-peptide aggregates derived from patient brains

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(with Ulrich H.E. Hansmann)

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The amyloid beta (Aβ) oligomers and fibrils that are found in neural tissues of patients suffering from Alzheimer's disease may either cause or contribute to the pathology of the disease. In vitro, these Aβ-aggregates are characterized by structural polymorphism. However, recent solid state NMR data of fibrils acquired post mortem from the brains of two Alzheimer's patients indicate presence of only a single, patient-specific structure. Using enhanced molecular dynamic simulations we investigate the factors that modulate the stability of Aβ-fibrils. We find characteristic differences in molecular flexibility, dynamics of interactions, and structural behavior between the brain-derived Aβ-fibril structure and in vitro models. These differences may help to explain the lack of polymorphism in fibrils collected from patient brains, and have to be taken into account when designing aggregation inhibitors and imaging agents for Alzheimer's disease.

Stabilization of helical structures by bending restraints

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Cooperativity in macromolecular systems, resulting in stable, functional conformations, is achieved by the competition and balance of internal forces. We investigate the influence of bending restraints upon the separation and stabilization of different helical phases and analyze thermal properties of the conformational transitions that accompany helical structure formation processes. These results give evidence that biomolecules can only form stable helical conformations if bending along the chain is effectively confined [1]. Consequently, flexible polymers cannot offer sufficient structural accentuation required for the formation of unique functional biomolecular morphologies, because their propensity to form stable secondary structures is limited.

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Semi-flexible polymers in disordered media (P)

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Presentend are a technique for off-lattice chain growth of semi-flexible polymers in two- and three-dimensional space with underlying disorder of the surrounding medium as well as the corresponding findings concerning the behavior of end-to-end distance and tangent-tangent correlation function. The varying parameters are stiffness of the polymer, density of the disorder and diameter of the obstacles.

Ground states of Edwards-Anderson spin glasses

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Extensive computations of ground-state energies of the Edwards-Anderson spin glass on bond-diluted, hypercubic lattices are conducted in dimensions $d = 3, \ldots, 7$. Results are presented for bond densities exactly at the percolation threshold, $p = p_c$, and deep within the glassy regime, $p > p_c$, where finding ground states becomes a hard combinatorial problem. We measure the exponents for the stiffness exponent and for finite-size corrections, which allow us to test scaling relations and test mean-field predictions for $d > 6$.

Interfacial adsorption in Potts models on the square lattice

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We study the effect of interfacial phenomena in two-dimensional perfect and random q-state Potts models with continuous phase transitions, using Monte Carlo techniques. In particular, for the total interfacial adsorption, the critical behavior, including corrections to scaling, are analyzed. The role of randomness is scrutinized. Results are discussed applying scaling arguments and invoking findings for bulk critical properties. In all studied cases, i.e., $q = 3$, 4, and $q = 8$, the spread of the interfacial adsorption profiles is observed to increase linearly with the lattice size at the bulk transition point.

Multi-objective solver for inverse parametric problems

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We propose a multi-objective strategy for solving challenging inverse parametric problems. We perform optimization with objectives being misfits of different physical descriptions of a considered phenomenon. The resulting Pareto set constitutes various alternatives of minimizing individual misfits. The set of alternatives is narrowed to the ones that are sufficiently coherent. The proposed strategy is illustrated by solving benchmark problems and a real-world engineering problem of recognizing natural resources under the Earth's surface with magnetotelluric measurement.

Comparing atomistic and coarse-grained simulations of P3HT

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(with Monchil Ivanov and Wolfhard Janke)

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Poly(3-hexylthiophene) (P3HT) is a key material used in organic photovoltaics (OPVs). In this study we assess the validity of two coarse-grained models of P3HT. We compare coarse-grained Monte Carlo simulations to fully atomistic molecular dynamics simulations. Structural properties of single polymer chains of short to medium lengths are compared between the three representations.

Distribution of convex hulls for single and multiple random walks

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We study the convex hull of the set of points visited by one or several two-dimensional random walkers of T discrete time steps. Two natural observables that characterize the convex hull in two dimensions are its perimeter L and area A. While the mean perimeter $\langle L \rangle$ and the mean area $\langle A \rangle$ have been studied before, analytically and numerically, and exact results are known for large T (Brownian motion limit), little is known about the full distributions $P(A)$ and $P(L)$. We provide numerical results for these distributions. We use a sophisticated large-deviation approach that allows us to study the distributions over a larger range of the support, where the probabilities $P(A)$ and $P(L)$ are as small as 10^{-300}. We analyze (open) single and multiple random walks as well as (closed) Brownian bridges on the two-dimensional discrete grid as well as in the two-dimensional plane. The resulting distributions exhibit, for large T, a universal scaling behavior (independent of the details of the jump distributions) as a function of A/T and $L/\sqrt{T}$, respectively. We also study the behavior as a function of the number n of walkers. We are also able to obtain the rate function, describing rare events at the tails of these distributions, via a numerical extrapolation scheme and find for a single walker a linear and square dependence as a function of the rescaled perimeter and the rescaled area, respectively. For multiple walkers, a second power-law regime appears to emerge.

Exact results on the kinetics of growing interfaces

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Exactly solvable models provide useful insight to guide further numerical studies. Recent exact reuslts on the dynamical behaviour of growing interfaces on either spatially infinite or half-infinite systems will be presented. The exactly solvable Edwards-Wilkinson and Arcetri universality classes will be used for illustration. The validity of dynamical scaling will be analysed. Results will be compared to simulations in the Kardar-Parisi-Zhang universality class, whenever possible.

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[2] M. Henkel and X. Durang, J. Stat. Mech. P05022 (2015) [arxiv:1501.07745]; and work in progress.

Multicriteria optimization of molecular force field models

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To reach the quantitative precision required in engineering applications, molecular force field models of fluids need to be adjusted to experimental data for diverse physical properties. This implies the presence of multiple conflicting objectives in the optimization task, making it difficult to achieve an optimal agreement for the different properties with a single model parameterization. In the present work, this problem is solved by computing the Pareto set, i.e. the set of all rational compromises between objectives, from which a user can choose the one which fits best to a particular application scenario. As an example, the following optimization task is studied: For ten different pure fluids, the two-centre Lennard-Jones plus point quadrupole (2CLJQ) model is applied to simultaneously describe the vapour pressure, the liquid density, and the vapour-liquid surface tension. The surface tension is computed by MD simulation of systems containing a vapour-liquid interface, with a novel, numerically efficient correction scheme for long-range interactions, which remains valid even for short cutoff radii. Literature models, which were adjusted to bulk properties, but not to interfacial properties, are validated against the surface tension of real fluids. The literature models are consistently found to overestimate the surface tension (by 20% on average). It is discussed how the agreement with the surface tension can be improved, based on experimental data and a correlation of the thermodynamic properties of the 2CLJQ model fluid. Multicriteria optimization provides a versatile framework to realize this in practice. The Pareto sets are determined, yielding an overview and a rational basis for assessing the capabilities of the molecular model for reproducing and predicting different thermodynamic properties. However, it is computationally expensive to determine the Pareto set. Brute force methods usually cannot be applied even for moderate dimensionalities of the objective and parameter spaces, whereas Monte Carlo methods often yield poor results. For the present study, two algorithms are combined: Sandwiching and hyperboxing. This is computationally efficient and facilitates a specification of the numerical error. In the studied case, it is found that any pair of two out of the three properties can be described by a 2CLJQ model with an accuracy close to the accumulated error from experiment and simulation, whereas it is impossible to reconcile all three properties to that level of accuracy. The outcome is visualized by a novel technique, employing self-organizing patch plots. Furthermore, an interactive modelling tool is provided by which users can develop fine-tuned molecular models within a few minutes, illustrating that multicriteria optimization provides a versatile framework within computational physics and engineering.

Static and dynamic properties of large polymer melts in equilibrium

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We present a detailed study of the static and dynamic behavior of semiflexible polymer chains with the Flory characteristic ratio, $C_\infty \sim 2.86$, in a melt. Starting from the previously obtained fully equilibrated high molecular weight polymer melts by Zhang *et al.* [ACS Macro Lett. **3** (2014) 198] we carefully investigate the scaling behavior

for polymer melts predicted by theory. We find that for semiflexible chains in a melt, results of the internal mean square end-to-end distance, the probability distributions of the end-to-end distance, and the chain structure factor are all described very well by the theoretical predictions for ideal chains. We also examine the motion of monomers in polymer melts by molecular dynamic simulations using the ESPResSo++ package. The scaling predictions of the mean square displacement of innermost monomers, center of mass, and the relative behavior between them based on the Rouse model, and the reptation theory are verified, and the related characteristic relaxation time scales are determined. Finally, we check the topological structures of polymer chains through the primitive path analysis (PPA), and give the evidence that the entanglement length N_e from the standard expression of the plateau modules $G_N^0 = \frac{4}{5}(\rho k_B T/N_e)$ with N_e determined through PPA is consistent with the value obtained from stresses.

Boltzmann inversion of harmonic oscillators (P)

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We apply the Boltzmann inversion method analytically to obtain a coarse-grained model from a simple system and compute statistical quantities of interest of the original and the coarse-grained system. We compare these observables to gain an understanding of the differences between both systems. The energy distributions as well as the expected values of the energy in the original and the coarse-grained systems differ. However, the method produces equal distance distributions in both systems.

Monolayer growth in a hard-rod lattice model

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The adsorption process of anisotropically-shaped particles at surfaces or interfaces (thin film growth) demonstrates structure formation away from equilibrium, and is the basis for modern materials like organic semiconductors. Whereas in the 3D bulk rod-like particles exhibit numerous phases such as the liquid, nematic, etc., they also exhibit transitions in ordering when near to or "stuck" onto a substrate. It seems worthwhile to study the interplay between such equilibrium phases and the dynamics of the thin films growing via deposition. We model rods on a discrete, cubic lattice which have simple, classical interactions. At first, we limit ourselves to steric exclusions and we treat the formation of the first monolayer of these rods on a substrate. We later include "sticky" interactions between rods and/or attractions with the substrate. Kinetic Monte Carlo is utilized to simulate the (time-dependent) growth of such a monolayer, whereby the rods find themselves in both near- and far-from-equilibrium assemblages. Our simulations are compared with descriptions of these lattice-monolayers using classical density functional theory (DFT), both static and dynamic.

Driven DNA: Does a dynamic transition exist in the thermodynamic limit? (P)

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(with Sanjay Kumar[3] **and Wolfhard Janke**[1]**)**

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We propose a generic model of driven DNA under the influence of an oscillatory force of amplitude F and frequency ν and show the existence of a dynamical transition for a chain of finite length. We find that the area of the hysteresis loop, $A_{\rm loop}$, scales with the same exponents as observed in a recent study based on a much more

detailed model. However, towards the true thermodynamic limit, the high-frequency scaling regime extends to lower frequencies for larger chain length L, and the system has only one scaling ($A_{\mathrm{loop}} \approx \nu^{-1}F^{2}$). Expansion of an analytical expression for A_{loop} obtained for the model system in the low-force regime revealed that there is a new scaling exponent associated with force, ($A_{\mathrm{loop}} \approx \nu^{-1}F^{2.5}$), which has been validated by high-precision numerical calculation. By a combination of analytical and numerical arguments, we also deduce that for large but finite L, exponents are robust and independent of temperature and friction coefficient.

Aging and dynamical scaling during collapse of a polymer

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We investigate a newly framed two-time property for the nonequilibrium evolution dynamics during the collapse of a homopolymer via Monte Carlo simulations of a model polymer. Our results show evidence of aging effects, as observed in the slow dynamics of structural and spin glasses, along with the presence of a dynamic scaling of the autocorrelation functions $\sim x^{-\lambda_c}$ (x being the ratio of the cluster sizes at two different times). We estimate the value of λ_c unambiguously by applying a finite-size scaling analysis to the numerical data. The value thus obtained obeys a bound which we predict via general theoretical arguments. The results presented should be of general validity and may trigger direct experimental verification in single-polymer dynamics.

Knots as topological order parameter for semiflexible polymers

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We used a combination of the multicanonical Monte Carlo algorithm and the replica-exchange method to investigate the phase diagram of a semiflexible polymer in dependence of the polymer stiffness. We found a novel phase in the phase diagram which is best described by the knot type of the polymer conformation. Almost all conformations in these phases have the same knot type after applying a procedure which connects the termini of the polymer. Therefore, they are thermodynamically stable and considerable different from the knots found in the swollen and globular phase of flexible polymers. We also showed that a derivative of the Alexander polynomial is a well suited order parameter to distinguish the "knotted" phases. Moreover, the transitions into the knotted conformations exhibit a phase coexistence, but happen at an almost constant mean total energy, hence we observed no latent heat.

A strange surprise in teaching basic numerics: The question matters

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Finding a root of a nonlinear function of one continuous variable is a basic task. Various methods are available for solving such problems, in particular bisection, false position (regula falsi) and secant methods, as well as the Newton approach. To ensure that a code works simultaneously stable and fast, they can be combined appropriately. Thus, for almost half a century, the van Wijngaarden-Dekker-Brent algorithm, a combination of inverse quadratic interpolation and bisection, has been considered as method of choice.

The talk demonstrates how thinking on the aim of the elementary steps leads to a new hybrid algorithm, which seems to be roughly as efficient as the van Wijngaarden-Dekker-Brent algorithm in the immediate vicinity of the root, but considerably more stable far away from it.

Planar ("fuki-nuke") ordering and finite-size effects for a model with four-spin interactions (P)

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We analyse a model with local four spin interaction of Ising spins, which appears as a special, plaquette-only case of the so-called gonihedric Ising model, a discrete variant when describing interacting surfaces. In three dimensions, it shows a strong first-order phase transition from a disordered high-temperature phase to a phase with exponentially degenerate low-temperature states and this degeneracy gives rise to a nonstandard finite-size scaling of the transition temperature. Our multicanonical simulations that confirmed this unusual finite-size scaling in the first place also provide a way of measuring planar order parameters. These come from considering an exactly solvable anisotropic limit of the model and can distinguish the low- and high-temperature phases in both the anisotropic and isotropic cases. In two dimensions, the model may serve as a pedagogical example on calculating how different finite-size corrections appear from different boundary conditions.

Open boundary conditions in stochastic transport processes with with short-range interactions

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

Line contribution to the critical Casimir force between a homogeneous and a chemically stepped surface

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Recent experimental realizations of the critical Casimir effect have been implemented by monitoring colloidal particles immersed in a binary liquid mixture near demixing and exposed to a chemically structured substrate. In particular, critical Casimir forces have been measured for surfaces consisting of stripes with periodically alternating adsorption preferences, forming chemical steps between them. Motivated by these experiments, we analyze the contribution of such chemical steps to the critical Casimir force for the film geometry and within the Ising universality class. By means of Monte Carlo simulations, mean-field theory and finite-size scaling analysis we determine the universal scaling function associated with the contribution to the critical Casimir force due to individual, isolated chemical steps facing a surface with homogeneous adsorption preference or with Dirichlet boundary condition. In line with previous findings, these results allow one to compute the critical Casimir force for the film geometry and in the presence of arbitrarily shaped, but wide stripes. In this latter limit the force decomposes into a sum of the contributions due to the two homogeneous parts of the surface and due to the chemical steps between the stripes. We assess this decomposition by comparing the resulting sum with actual simulation data for the critical Casimir force in the presence of a chemically striped substrate.

Simulating emergent phenomena (with GPU-based molecular dynamics)

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Emergent phenomena are especially fascinating because they are not obvious consequences of the design of the systems in which they appear, a characteristic equally relevant when attempting to simulate them. Several systems that exhibit surprisingly rich emergent behavior will be described, each studied by MD (molecular dynamics) simulation. (a) In the case of fluids studied at the atomistic level, not only can complex hydrodynamic phenomena in convecting and rotating fluids – the Rayleigh-Benard and Taylor-Couette instabilities – be reproduced within the limited length and time scales accessible to MD, but there is even quantitative agreement. (b) Modeling self-assembly processes associated with virus capsid growth reveals the ability to achieve complete, error-free shells, where paradoxically, high yields are due to reversible bond formation. (c) Studies of granular mixtures show behavior that, in the case of a rotating drum, reproduces known but counterintuitive axial and radial segregation, and in the case of a vertically vibrated layer, predicts a novel form of horizontal segregation. These simulations tend to be comparatively large and lengthy, and in some cases multiple runs are needed because the outcomes are unpredictable, so the use of GPU-based parallel computing is beneficial; the methodology involved will be outlined. While MD is subject to limitations, both conceptual and computational, the results offer exciting indications of what can be accomplished.

Kolmogorov-Anosov C-systems and MIXMAX random number generator

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We are developing further our earlier suggestion to use hyperbolic Anosov C-systems for the Monte Carlo simulations in high-energy particle physics. The hyperbolic dynamical systems have homogeneous instability of all trajectories and as such they have mixing of all orders, countable Lebesgue spectrum and positive Kolmogorov entropy. These extraordinary ergodic properties follow from the C-condition introduced by Anosov. The C-condition defines a rich class of dynamical systems which span an open set in the space of all dynamical systems. The important property of C-systems is that they have a countable set of everywhere dense periodic trajectories and that their density exponentially increases with entropy. Of special interest are C-systems that are defined on a high-dimensional torus. The C-systems on a torus are perfect candidates to be used for Monte Carlo simulations. Recently an efficient algorithm MIXMAX was found, which allows very fast generation of long trajectories of the C-systems. These trajectories have high quality statistical properties and we are suggesting to use them for Monte Carlo simulations. The MIXMAX generator is currently the default generator in the ROOT software package at CERN.

Theoretical studies on embedded chromophores (P)

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Cyanobacteriochromes (CBCR) are photosensory proteins that can be found in cyanobacteria. They exist in two electronic ground states; a so-called dark stable state and a photoproduct state. By reversibly photochemical switching between those two states, CBCRs mediate various biochemical reactions. Interestingly, the absorption spectrum of various CBCRs covers the full range of the visible spectrum, from the blue to the far-red region. AnPixJ, for instance, possesses a red absorbing dark stable state, denoted as Pr and a green photoproduct state called Pg. Due to the ability of CBCRs to perform a reversible photocycle, numerous fields of application can be imagined, from fluorescence microscopy to optogenetics. This requires a fundamental understanding of the factors underlying the absorption properties of CBCRs, hence the interplay of the supramolecular and the electronic

structure has to be investigated. To date, the mechanism behind the color-tuning is poorly understood. This work addresses a detailed description of the structure and dynamics of the Pr state of the second GAF domain of AnPixJ on the molecular level using classical molecular dynamics. Special regard is given to the influence of the amino acid tryptophane-90 (Trp90) that is located in the chromophore binding pocket and which is assumed to play a crucial role in stabilizing the Pr-state. Our results indicate the existence of two stable structural substates of AnPixJ in its Pr state in solution, from which only one was observed by X-ray crystallography. These structural substates differ mainly regarding the conformation adopted by the chromophore and also regarding the relative orientation of Trp90, which in turn influences the mobility of the chromophore. Furthermore the two substates exhibit different patterns of hydrogen bond interactions between the chromophore and the adjacent amino acids. These structural and dynamical differences can potentially lead to significant alterations in the electronic and spectral properties of the chromophore and should be considered in future theoretical efforts to investigate the color-tuning mechanism in CBCRs.

First-order phase transitions in the advantageous full microcanonical ensemble

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Most statistical physics textbooks start from the full microcanonical ensemble. Here momentum and configuration space is considered in the partition function. Nonetheless it is possible to define a simple Metropolis sampling in this ensemble [1] since the momentum part of the phase space can be treated analytically. Martin-Mayor already discovered an advantageous sampling behaviour of the full microcanonical ensemble for lattice spin systems [2] which is now tested for a continuum Lennard-Jones gas. The sampling behaviour will be explained and compared to other simulation techniques for first-order phase transitions.

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Greedy Monte Carlo for spin glass gound-state search

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When spin glasses are investigated standard Monte Carlo methods are severly hampered by the system's rough energy landscape which is dominated by local energy minima separated by barriers. We show how the greedy algorithm can be used to be combined with traditional Monte Carlo methods and that the resulting algorithm is very effective in finding ground states of the three-dimensional Edwards-Anderson model.

Multifractal analysis of electronic states on random Voronoi-Delaunay lattices (P)

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The random Voronoi-Delaunay lattice (VDL) is a simple model for amorphous solids and foams. It is defined as a set of bonds between randomly positioned sites. The bonds connect neighboring Voronoi cells and are obtained by the Delaunay triangulation. The resulting topologically disordered lattice features strong anticorrelations between the coordination numbers of neighboring sites. The disorder fluctuations therefore decay qualitatively

faster with increasing length scale than those of generic random systems. A recent study showed that this modifies the Harris and Imry-Ma criteria and leads to qualitatively changes of the scaling behavior at magnetic phase transitions [1].

We consider the transport of non-interacting electrons on two- and three dimensional random VDLs and study the electronic wave functions by multifractal analysis. We observe localized states for all energies in the two-dimensional system. In three dimensions, we find two phase transitions towards extended states very close to the band edges. The scaling analysis shows that the scaling exponent of the localization length is 1.6, in accordance with the usual orthogonal universality class. An additional generic energetic randomness by on-site potentials does not lead to qualitative changes. We obtain a phase diagram by varying the disorder strength of these potentials.

In conclusion, the unusual coordination number anticorrelations of random VDLs do not lead to qualitatively different behavior compared to the well-known Anderson model of localization on regular lattices.

[1] H. Barghathi and T. Vojta, Phys. Rev. Lett. **113** (2014) 120602.

Wang-Landau simulation of short single polyethylene chain's crystallization

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The phase behaviour of polyethylene has been under wide investigation during the last six decades. But investigation of single-chain crystallization is a technically difficult problem. In the case of molecular dynamics simulations, it is not so easy to distinguish kinetic and thermodynamic effects on chain folding. We present results of a Wang-Landau type Monte Carlo study at thermodynamical equilibrium of folding of a single polymer chain. Our simulations are based on a chemically realistic united atom model [1].

[1] W. Paul, D. Y. Yoon, and G. D. Smith, J. Chem. Phys. **103** (1995) 1702–1709.

Current state-of-the-art in kinetic Monte Carlo simulations

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We review recent developments in the parallel techniques developed for kinetic Monte Carlo simulations.

Spin representation without fixed quantization axis

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Spin models are very common in studying electronic, magnetic and ferroelectric properties. Due to the non-commuting spin operators the quantization axis is usually fixed, for instance in z-direction. As result one can examine the case that the continuous rotational symmetry is broken by the ground state which is not invariant under the same symmetry group as the underlying Hamiltonian. Here we propose a representation of spin operators where the quantization axis is not fixed. Such a representation can be also assigned to classical spin variables. The consequences are discussed for the isotropic Heisenberg model or alternatively for the non-linear sigma model. There appear additional terms breaking the rotational symmetry. As a consequence the elementary excitation of the spin waves becomes massive. Another example discussed is the occurrence of helical structures.

Stochastic Thermodynamics: Nonequilibrium Response (tentative)

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tba

Regular packings on periodic lattices

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We investigate the problem of packing identical hard objects on regular lattices in d dimensions. Restricting configuration space to parallel alignment of the objects, we study the densest packing at a given aspect ratio X. For rectangles and ellipses on the square lattice as well as for biaxial ellipsoids on a simple cubic lattice, we calculate the maximum packing fraction $\varphi_d(X)$. It is proved to be continuous with an infinite number of singular points $X_\nu^{\min}$, $X_\nu^{\max}$ $\nu = 0, \pm1, \pm2, \ldots$. In two dimensions, all maxima have the same height, whereas there is a unique global maximum for the case of ellipsoids. The form of $\varphi_d(X)$ is discussed in the context of geometrical frustration effects, transitions in the contact numbers and number theoretical properties. Implications and generalizations for more general packing problems are outlined.

Stiffness of homopolymer chains (P)

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For studying structure formation of homopolymer chains we use an off-lattice hard-sphere coarse grained model with square-well interactions. The indication of first and second order like pseudophase-transitions has been done with the help of microcanonical and canonical analysis. Therefore, a stiffness dependent state-diagram is shown for 40-mers. An example of various chain lengths for fixed stiffness shows an evolution of pseudophase-transitions. Beside nonspecific square-well interactions we introduced additional specific square-well interactions and study its effects. The simulations have been performed with the help of the Stochastic Approximation Monte Carlo Method (SAMC).

Evolutionary accessibility of fitness landscapes with multiple alleles

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The question of accessibility of the global fitness maximum has a long history. Dating back to works of Wright and Fisher, there are two competing pictures about how increasing dimensionality of fitness landscape affects its accessibility. On the one hand, increasing size of fitness landscape results in higher number of local fitness peaks that act as evolutionary dead-ends rendering the global peak inaccessible. On the other hand, with increasing dimensionality of fitness landscape local peaks become saddle points keeping the global peak accessible. For the fitness landscape with two alleles (genes being ON or OFF) the former picture dominates. However, it remains unclear how considering multiple alleles instead of only two will affect the accessibility. To address this, we

performed exhaustive enumeration of all accessible pathways for fitness landscapes with up to 16 alleles and 2^{28} genotypes. We also run a Moran type simulation of population evolution to independently verify our conclusions. The resulting estimates of asymptotic accessibility give 12%, 50%, 69%, 81% for fitness landscapes with 2, 4, 8 and 16 alleles, respectively. The evolutionary pathways on fitness landscapes with multiple alleles are typically much longer (a few times) and have more backward mutations than on landscapes with two alleles.

Exploring different regimes in finite-size scaling of the droplet condensation-evaporation transition

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We present a finite-size scaling analysis of the droplet condensation-evaporation transition of a lattice gas (in two and three dimensions) and a Lennard-Jones gas (in three dimensions) at fixed density [1]. Parallel multicanonical simulations allow sampling of the required system sizes with precise equilibrium estimates. In the limit of large systems, we verify the theoretical leading-order scaling prediction for both the transition temperature and the finite-size rounding. In addition, we present an emerging intermediate scaling regime, consistent in all considered cases and with similar recent observations for polymer aggregation. While the intermediate regime locally may show a different effective scaling, we show that it is a gradual crossover to the large-system scaling behavior by including empirical higher-order corrections. This implies that care has to be taken when considering scaling ranges, possibly leading to completely wrong predictions for the thermodynamic limit. In this study, we consider a crossing of the phase boundary orthogonal to the usual fixed temperature studies. We show that this is an equivalent approach and, under certain conditions, may show smaller finite-size corrections.

[1] J. Zierenberg and W. Janke, Phys. Rev. E **92** (2015) 012134-1–11.