November 25, 2022, 17:24

ABSTRACTS

of contributions to the

23rd International NTZ-Workshop on

New Developments in Computational Physics

CompPhys22

Computational Physics Group,
Institut für Theoretische Physik,
Universität Leipzig, Germany

24–26 November 2022

http://www.physik.uni-leipzig.de/~janke/CompPhys22

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

Preface

Welcome to the 23rd International NTZ-Workshop *CompPhys22* 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 – due to the Covid-19 pandemic for the third time virtually – in a relaxed atmosphere "in Leipzig" at the beginning of Christmas time.

The main part of the Workshop takes place on 24 and 25 November 2022 in the "Zoom Lecture Hall" (talks) and in Leipzig's "Gather Town" (posters and coffee breaks). As in previous years, the Saturday, 26 November 2022, is devoted to various discussion rounds and collaborative meetings which will take place in "Gather Town".

Finally, we and the Centre for Theoretical Sciences (NTZ) gratefully acknowledge financial support of the Workshop from Doctoral College "$\mathbb{L}^4$" of Deutsch-Französische Hochschule (DFH-UFA), DFG Collaborative Research Centre SFB/TRR 102 "Polymers under Multiple Constraints", Research Academy Leipzig (RALeipzig), and Leipzig Graduate School of Natural Sciences "BuildMoNa".

Leipzig,
November 2022

Wolfhard Janke

Abstracts

Metastable states and critical percolation in two-dimensional long-range Ising model

Ramgopal Agrawal
LPTHE - CNRS, Paris, France
ramgopal.sps@gmail.com

In this talk, I will discuss the asymptotic states of two-dimensional long-range Ising model after a quench to zero temperature. I will explain in detail how the abundance of striped metastable states and signature of critical percolation are affected by the long-range interactions.

Geometric clusters in the overlap of the Ising model

Michail Akritidis
Research Centre in Fluid and Complex Systems, Coventry University, United Kingdom
mixaakr@gmail.com

We study the percolation properties of geometrical clusters defined in the overlap space of two statistically independent replicas of a two-dimensional Ising model that are simulated at the same temperature. In particular, we consider two distinct types of clusters in overlap space, which we dub soft and hard constraint clusters, and which are subsets of the regions of constant spin overlap. By means of Monte Carlo simulations and finite-size scaling analyses we estimate the transition temperature, and the set of critical exponents characterising the transitions of these two cluster types. The results suggest that both hard and soft clusters percolate at the transition temperature of the square-lattice Ising model and their critical behaviour is governed by the same correlation length exponent ν as that found by Onsager, but they exhibit non-standard and distinct sets of exponents for the average cluster size and percolation strength.

Numerical study of the critical point of random quantum spin systems in high dimension

Valentin Anfray
Institut Lumière Matière, UMR5306–UCBL–CNRS, France
valentin.anfray@gmail.com

Critical properties of the $2D$ and $3D$ random quantum Potts model with $q = 2, 3, 5, 10, 20$ and 50 states are shown to be governed by an infinite disorder fixed point. We have computed the correlation-length exponent ν, the magnetization exponent d_f and the energy gap exponent ψ. Using finite-size scaling and taking into account finite-size corrections, critical properties of the Potts model are shown to be q-independent. Random quantum Clock models with $q = 2, 3, 5, 8$ and 10 states have been also studied in $2D$ and $3D$. A minimum amount of initial disorder strength is required to flow to an infinite disorder fixed point. Despite large error bars on ψ exponent, our estimates for the critical exponents ν and ψ for all q are compatible with those of the random transverse-field Ising model. Our estimates for the critical exponent d_f are incompatible within error bar but very close. The tricritical point of the random quantum Ashkin-Teller model has been also studied in dimension two and three. We have shown that the correlation-length exponent associated with one of the two unstable directions does not belong to the university class of the random transverse-field Ising model.

XY model on a SAW

Evgeni Burovski
HSE University, Moscow, Russia
evgeny.burovskiy@gmail.com

tba

Bond order parameters in crystallization of short polymer chains in thin films: SAMC simulation (P)

Evgeniia Filimonova
Institut für Physik, Martin-Luther Universität Halle, Germany
evgeniia.filimonova@physik.uni-halle.de

Our research is devoted to crystallization in polymer melts in the presence of hard walls. An interface to a solid material can initiate crystallization in polymer liquids by either heterogeneous nucleation or prefreezing. Our goal is to reveal physical factors which are responsible for one of these two scenarios of surface-induced polymer crystallization. We use coarse-grained model and perform stochastic approximation Monte Carlo (SAMC) simulation. We have developed an approach that allows us to identify the translational and orientational local ordering by means of comparing our system configurations with reference crystalline structures of different symmetries. In addition to calculating the usual order parameters (Steinhardt parameters, common neighbours analysis, nematic order parameter, etc.), we suggested new order parameters based on scalar products of bonds between nearest neighbours. We observe a coexistence of an isotopic structure in the center of the film with ordered structures at the walls at intermediate values of energies (in microcanonical analysis). A change in the crystal structure accompanying a change in density at different energies is also shown. We are able to localise the transition points between different pseudo-phases quite precisely.

Financial support of the International Graduate School AGRIPOLY supported by the European Social Fund (ESF) and the Federal State Saxony-Anhalt is acknowledged.

Superdiffusion-like behavior in zero-temperature coarsening of the $d = 3$ Ising model

Denis Gessert
(with Henrik Christiansen and Wolfhard Janke)
Institut für Theoretische Physik, Universität Leipzig, Germany
denis.gessert@itp.uni-leipzig.de

For coarsening to a temperature below the critical temperature of the non-conserved Ising model in three dimensions a power-law growth of domains of like spins with exponent $\alpha = 1/2$ is predicted. Including recent work, it was not possible to clearly observe this growth law when the quench temperature was set to zero. In an attempt to verify the prediction we run large-scale Monte Carlo simulations of lattice sizes up to $L = 2048$ and make a surprising discovery. At late times domains show superdiffusive growth, i.e., $\alpha > 1/2$, which we show may be caused by sponge-like structures emerging at early times.

Replica symmetry breaking for Ulam's problem

Alexander Hartmann
Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany
a.hartmann@uni-oldenburg.de

The description of complex system by the concept of Replica Symmetry Breaking (RSB), which was introduced by Giorgio Parisi in the 1980s, was honored by the Nobel price in 2021. RSB has been used to analyze and describe the behavior of many systems, such as spin glasses, neural networks, optimization problems, or data

analysis using machine learning. From the numerical side, for a thorough analysis of almost all RSB-exhibiting problems only algorithms are available with exponentially growing running times, which has restricted the system sizes considerably.

We study increasing subsequences (IS) for an ensemble of sequences given by permutation of numbers $\{1, 2, ..., n\}$. We consider a Boltzmann ensemble at temperature T. Thus each IS appears with the corresponding Boltzmann probability where the energy is the negative length $-l$ of the IS. For $T \to 0$, only ground states, i.e., longest IS (LIS) contribute, also called Ulam's problem. We introduce an algorithm which allows us to directly sample IS in perfect equilibrium in polynomial time, for any given sequence and any temperature. Thus, we can study very large sizes. We obtain averages for the first and second moments of number of IS as function of n and confirm analytical predictions. Furthermore, we analyze for low temperature T the sampled ISs by computing the distribution of overlaps and performing hierarchical cluster analyses. In the thermodynamic limit the distribution of overlaps stays broad and the configuration landscape remains complex. Thus, Ulam's problem exhibits RSB. This means it constitutes a model with complex behavior which can be studied numerically exactly in a highly efficient way.

The cubic fixed point for $N = 3$ and 4 in three dimensions: Monte Carlo simulations of the ϕ^4 model on the lattice

Martin Hasenbusch

Institut für Theoretische Physik, Universität Heidelberg, Germany
hasenbusch@thphys.uni-heidelberg.de

We study the cubic fixed point for $N = 3$ and 4 by using finite size scaling applied to data obtained from Monte Carlo simulations of the ϕ^4 model on the simple-cubic lattice. We generalize the idea of improved models to a two-parameter family of models. The two-parameter space is scanned for the point, where the two leading corrections to scaling vanish. Here we like to present the basic concepts and central numerical results.

From 2d Ising to 0d electron transport

Fred Hucht

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

The two-dimensional Ising model is one of the most extensively studied models in statistical physics. It is used to describe, e.g., magnetism, liquids, epidemics, neural nets, just to name a few. In its simplest form, the model consists of spins $s_i = \pm 1$ on a square lattice. Neighboring spins have energy $E = -Js_is_j$ and favor parallel orientation if $J > 0$. The 2d Ising model is one of the few exactly solvable models that show a nontrivial continuous phase transition from a para- to a ferromagnet at a finite temperature $T_c > 0$. Near this phase transition, long-range correlations emerge that lead to interesting nontrivial effects such as strong fluctuations or critical Casimir forces, just to name a few. From a recent exact solution of the 2d Ising model with arbitrary exchange couplings J_{ij} we were able to analyse systems with quenched surface disorder, where the couplings $J_{ij} = \pm 1$ are random at one system boundary [1]. The talk will give an overview over the recent developments as well as an unexpected relation to path integrals in the framework of interacting electron transport through a quantum dot [2].

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Random-bond antiferromagnetic Ising model in a field

Ferenc Iglói

Wigner Research Centre for Physics, Budapest, Hungary
igloi@szfki.hu

Using combinatorial optimization techniques we study the critical properties of the two- and three-dimensional Ising models with uniformly distributed random antiferromagnetic couplings ($1 \leq J_i \leq 2$) in the presence of a homogeneous longitudinal field, h, at zero temperature. In finite systems of linear size, L, we measure the

average correlation function, $C_L(\ell, h)$, when the sites are either on the same sublattice, or they belong to different sublattices. The phase transition, which is of first order in the pure system, turns to mixed order in two dimensions with critical exponents $1/\nu \approx 0.5$ and $\eta \approx 0.7$. In three dimensions we obtain $1/\nu \approx 0.7$, which is compatible with the value of the random-field Ising model, but we cannot discriminate between second-order and mixed-order transitions.

The importance of mutual information for simulation based inference (P)

Giulio Isacchini

Institut für Theoretische Physik, Universität Leipzig, Germany
giulio.isacchini@uni-leipzig.de

Simulation-based inference enables learning the parameters of a model even when its likelihood cannot be computed in practice. One class of methods uses data simulated with different parameters to infer models of the likelihood-to-evidence ratio, or equivalently the posterior function. Here we frame the inference task as an estimation of an energy function parametrized with an artificial neural network. We present an intuitive approach, named MINIMALIST, in which the optimal model of the likelihood-to-evidence ratio is found by maximizing the likelihood of simulated data. Within this framework, the connection between the task of simulation-based inference and mutual information maximization is clear, and we show how several known methods of posterior estimation relate to alternative lower bounds to mutual information. These distinct objective functions aim at the same optimal energy form and therefore can be directly benchmarked. We compare their accuracy in the inference of model parameters, focusing on four dynamical systems that encompass common challenges in time series analysis: Dynamics driven by multiplicative noise, nonlinear interactions, chaotic behavior, and high-dimensional parameter space.

Adsorption of dopamine on the b-AsP surface based on first principles

Pinar Kaya

(with Okay Tercan, Cagil Kaderoglu, Ethem Aktürk, and Handan Olgar)

Ankara University, Department of Physics Engineering, 06100, Ankara, Turkey
pinar.kaya.fizmuh@gmail.com

In recent years, 2D nanomaterials have become a very interesting subject with the discovery of the unique properties of 2D graphene [1]. As the size of the materials decreases, the surface area increases and a very small effect on it has big consequences. Especially the changes in the physical, chemical, mechanical and magnetic properties of the material also affect the usage area in technology. The electronic and optical properties of 2-dimensional biocompatible materials, which have started to be used with organic molecules, can be adjusted. These 2D hybrid structures have application areas in biotechnology, especially as biosensors and drug carriers. Dopamine (DA) is a naturally produced hormone in the body and is a neurotransmitter. Depending on the secretion of DA more or less, it causes many serious diseases such as Schizophrenia [2], Parkinson [3], depression [4]. Therefore, it is vital to design a biosensor that can accurately detect the DA level in the body. In addition, DA is a highly researched biomolecule in many interface material designs with its adhesion, biocompatibility and other properties [5]. On the other hand, b-AsP has a semiconductor monolayer structure with indirect bandgap [6]. In this study, hybrid structure formed by combining b-AsP monolayer with DA molecule was investigated using Density Functional Theory based on first principles. The structural and electronic properties of each obtained combination were studied with different adsorption configurations on clean and defective b-AsP monolayers of the DA molecule. As a result, all the obtained calculations were compared to discuss whether this substrate has good biosensor and drug transporter properties for the DA molecule.

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Three-dimensional Potts model in a random field

Manoj Kumar

Chemnitz University of Technology, Germany
manojkmr8788@gmail.com

The Potts model is a generalization of an Ising model for q arbitrary states of spins. Like an Ising model, the random field in a Potts model has also a significant effect on magnetic ordering. In this talk, I will be presenting my recent work on the three-dimensional random-field Potts model for $q = 3$ and 4. I will show how the various quantities like magnetization, energy, specific heat, and susceptibility, behave with respect to the strength of the random field and discuss different critical exponents resulting from their finite-size scaling.

Molecular dynamics simulations of the monomer density profiles of knotted ring polymer chains confined in a slit of two parallel walls with one attractive and another repulsive surface (P)

Piotr Kuterba

(with Zoriana Danel, Henrik Christiansen, and Wolfhard Janke)

Institute of Physics, Jagiellonian University, Cracow, Poland
zussini@gmail.com

Molecular dynamics simulations have been performed to obtain the monomer density profiles for linear and ring polymer chains of 360 monomer length in a slit geometry of two parallel walls with one attractive and another repulsive surface. The ring structures have different knots: 3_1, 6_1, 9_1, 10_{124}, $3_1 3_1 5_1$ and there are also twisted knots with $n = 10$ and $n = 20$. The monomer pairs were simulated with Lennard-Jones 12-6 potential, bonds were simulated with Finitely Extensible Nonlinear Elastic (FENE) potential, lastly the monomer-wall interaction used the Lennard-Jones 9-3 potential. It has been shown that polymers with complicated structure have lower monomer density profiles near the attractive wall, but it becomes opposite at some distance in the direction of the repulsive wall. The twisted knots with $n = 10$ and $n = 20$ twists present additional local maxima in their monomer density profiles for narrow slits with limiting value, which is not the case for the wide slits.

Diffusion in presence of topological defects

Andy Manapany

Université de Lorraine, Nancy, France
andy.manapany@univ-lorraine.fr

We study the diffusion processes of a real scalar field in the presence of the distortion field induced by a chiral topological defect. The defect modifies the usual Euclidean background geometry into a non-diagonal Riemann-Cartan geometry characterized by a singular torsion field. The new form of the diffusion equation is established and the scalar field distribution in the vicinity of the defect is investigated numerically. Results show a high sensitivity to the boundary conditions. In the transient regime, we find that the defect vorticity generates an angular momentum associated with the diffusion flow and we discuss its main properties.

Phase separation in the long-range Ising model

Fabio Müller
(with Henrik Christiansen and Wolfhard Janke)

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

We study the phase separation of the long-range Ising by means of a newly developed algorithm which allowed for the first time to verify a long-standing theoretical prediction for the growth of the characteristic length scale $\ell(t)$.

Percolation properties of the two-dimensional Ising spin glass

Lambert Münster
(with Martin Weigel)

Institut für Physik, Technische Universität Chemnitz
lambert.muenster@physik.tu-chemnitz.de

Suitable cluster definitions have allowed researchers to describe many ordering transitions in spin systems as geometric phenomena related to percolation. For spin glasses and some other systems with quenched disorder, however, such a connection is missing to date. The Fortuin-Kasteleyn–Coniglio-Klein clusters originally defined for the ferromagnetic problem cannot be directly linked to the spin-glass transition since they percolate already in the high-temperature paramagnetic phase [1, 2]. More relevant for spin glasses are clusters defined on the basis of the overlap of several replicas. In the present work we hence study a two-replica cluster representation [3] of the two-dimensional Ising spin glass by performing Monte Carlo simulations at low temperatures. We show that clusters within this representation have percolation thresholds that shift to lower temperature by increasing the system size, in agreement with the zero-temperature spin-glass transition in two dimensions. The overlap is proportional to the difference in density of the two largest clusters, thus supporting a picture where the spin-glass transition corresponds to an emergent density difference of the two largest clusters inside the percolating phase [3].

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Activity mediated globule to coil transition of a flexible polymer in poor solvent

Subhajit Paul
(with Suman Majumder and Wolfhard Janke)

ICTS-TIFR, Bangalore, India
subhajit.paul@icts.res.in

tba

Dimensional crossover on multileg attractive-U Hubbard ladders

Ian Pilé

HSE University, Moscow, Russia
pileyan@gmail.com

We study the ground state properties of a polarized two-component Fermi gas on multileg attractive-U Hubbard ladders. Using exact diagonalization and density matrix renormalization group method simulations, we

construct grand canonical phase diagrams for ladder widths of up to $W = 5$ and varying perpendicular geometries, characterizing the quasi-one-dimensional regime of the dimensional crossover. We compare our findings with mean-field studies which bring artifacts in the quasi-one-dimensional regime.

A simple algorithm for uniform sampling on the surface of a hypersphere

Stefan Schnabel

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

We propose a simple method for uniform sampling of points on the surface of a hypersphere in arbitrarily many dimensions. By avoiding the evaluation of computationally expensive functions like logarithms, sines, cosines, or higher-order roots the new method is faster than alternative techniques.

Aggregation and ordering in small alkane systems

Timur Shakirov

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

Ordering of small alkanes differs drastically from the bulk one. The difference is not only quantitative but also qualitative: short-chain single alkanes fold at low temperatures into non-trivial structures [1] in contrast to fully-stretched-chain lamellae in bulk. For the few chain systems we demonstrate the leading role of torsional stiffness in the ordered structure formation and investigate the corresponding conformations, which vary from spirals to tilted lamellae. For the fully stretched chain lamellae we find a two-step ordering, the indications of which remain at least up to 16 chain aggregates. In contrast to the low-temperature ordering, the aggregation or liquid-vapor transition leads to similarly disordered structures for all system sizes, which allows correction of size effects and extrapolation of the estimated aggregation temperatures to the thermodynamic limit. Our calculations of aggregation/boiling temperatures at normal pressure are in good agreement with experimental data. The presented equilibrium results are based on Wang-Landau-type Monte Carlo simulations [2, 3] of a chemically realistic united atom model [4].

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Finite-size analysis of the variance of machine learning output function

Lev Shchur

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

We explore the possibilities of using neural networks to study phase transitions. The main question is the level of accuracy which can be accessed in the estimation of the critical point and critical exponents of the statistical physics models. We generate data for two spin models in two dimensions for which analytical solutions exist, the Ising model and Baxter-Wu model. We applied six neural networks with three different architectures to the data and estimated critical temperature and correlation length exponent. We found that accuracy of estimation does depend on the neural network. The critical exponent of Baxter-Wu model is estimated by the deep machine learning technique for the first time.

Molecular dynamics study on elastic properties and intrinsic vibrations of fullerenes (P)

Jacek Siódmiak
Institute of Mathematics and Physics, UTP University of Science and Technology, Bydgoszcz, Poland
siedem@pbs.edu.pl

The best-known form of fullerenes one of the allotropic forms of carbon is C60. This fullerene is made of sixty carbon atoms arranged in a pattern of alternating 20 hexagons and 12 pentagons, just like in a soccer ball. Carbon atoms are joined by 90 covalent bonds: 60 are single bonds and 30 are double bonds. From a mechanical point of view, these bonds can be considered as springs. The adequate term describing the interactions of bonded atoms is found in every force field in molecular dynamics simulations. Here, the results of simulations of intrinsic vibrations of various forms of fullerenes in a vacuum and in water will be presented. We distinguished different vibrational modes, as well as a shift and change in the intensity of the natural frequency of vibrations in water compared to oscillations in a vacuum. We confirmed that the fundamental frequencies are closely related to the size of the fullerene. In addition, results of simulations in which fullerene, initially compressed, expands, and tends to a state of equilibrium are shown.

Universality in the two-dimensional dilute Baxter-Wu model

Alexandros Vasilopoulos
Research Centre in Fluid and Complex Systems, Coventry University, United Kingdom
vasilopa@uni.coventry.ac.uk

We study the question of universality in the two-dimensional spin-1 Baxter-Wu model in the presence of a crystal field Δ. We employ extensive numerical simulations of two types, providing us with complementary results: Wang-Landau sampling at fixed values of Δ and a parallelized variant of the multicanonical approach performed at constant temperature T. A detailed finite-size scaling analysis in the regime of second-order phase transitions in the (Δ, T) phase diagram indicates that the transition belongs to the universality class of the 4-state Potts model. Previous controversies with respect to the nature of the transition are discussed and possibly attributed to the presence of strong finite-size effects, especially as one approaches the pentacritical point of the model.

News from population annealing: From weighted averages to quantum Monte Carlo

Martin Weigel
Institut für Physik, Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Germany
martin.weigel@physik.tu-chemnitz.de

Population annealing is a generalized-ensemble Monte Carlo simulation algorithm that proves useful for the simulation of systems with complex free-energy landscapes and that offers superior parallelizability properties. As a meta-algorithm, population annealing can be combined with a wide range of simulation methods, including Monte Carlo and molecular dynamics. In the past, we have analyzed the approach regarding the scaling of statistical and systematic errors, proposed improvements and implemented the method on highly-efficient graphics processing units. In the present talk I will discuss recent developments regarding the optimal choice of the resampling protocol and the combination of several population annealing simulations using weighted averages. Finally, I will discuss a combination of population annealing with quantum Monte Carlo simulations.