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ABSTRACTS

of contributions to the

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New Developments in Computational Physics

CompPhys21

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Preface

Welcome to the 22nd International NTZ-Workshop *CompPhys21* 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 second time virtually – in a relaxed atmosphere "in Leipzig" at the beginning of Christmas time.

The main part of the Workshop takes place on 25 and 26 November 2021 in the "Zoom Lecture Hall" (talks) and in "Gather Town" (posters and coffee breaks). As in previous years, the Saturday, 27 November 2021, 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 2021

Wolfhard Janke

Abstracts

Corrections to scaling in geometrical clusters of the 2D Ising model (P)

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The geometrical clusters do not capture the critical behaviour of the q-state Potts model: In general, they do not percolate at the critical point, and their critical exponents do not coincide with the thermal ones. In two dimensions and for $0 \leq q \leq 4$, however, they do percolate at the critical temperature, and they are found to encode the tricritical behaviour of a site-diluted Potts model. Here, we study geometrical clusters for the $q = 2$ Potts model (i.e., the Ising model) by means of Monte Carlo simulations. Using finite-size scaling we discuss the appearance of corrections to scaling using different definitions of cluster sets for the average cluster size and percolation strength. For the average cluster size including all percolating clusters, or excluding clusters that percolate in one but not the other direction, leads to smaller corrections to scaling as compared to the other definitions. The percolation strength is less sensitive to the definition used.

Velocity ordering during coarsening in an active matter system

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We perform molecular dynamics simulations to study kinetics of velocity ordering during coarsening in an active matter system with displacement aligning interactions. For this purpose, we calculate the velocity-velocity correlation function. We observed topological defects that annihilate each other as time progresses. The obtained growth picture we compare with ordering in a passive magnetic system.

Spinning particles in quantum Hamilton equations

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Spin in quantum mechanics has no classical description and is described as an intrinsic property that is carried by elementary particles like charge or mass. In the stochastic formalism, however, the spin may be modelled as a rotating charged ball leading to the non-relativistic Pauli-equation. In the recently derived quantum Hamilton equations, the model of a spinning particle is incorporated. This allows to describe the spin as a continuous random variable with the known quantized expectation values in connection with spin which is exemplified by the freely spinning particle and the Stern-Gerlach experiment.

Training normalising flows without action derivative

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Recently an machine learning approach to Monte Carlo simulations called neural Markov chain Monte Carlo is gaining interest. In its most popular form it uses the neural networks to construct normalizing flows which

are then trained to approximate the desired target distribution. As this distribution is usually defined via a Hamiltonian or action the learning algorithm requires calculations of the action gradient with respect to the network weights. In my talk I will present a formulation that avoids this calculation, thus potentially speeding up caclulcations fro model with complex actions.

Spreading processes on vaccinated scale-free networks

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We analyze spreading on scale-free networks, where the distribution of node connectivity k obeys a power-law decay $\sim k^{-\lambda}$. We assume, that only a fraction p of individual nodes can be affected by spreading process, while remaining $1-p$ are immune. We apply the synchronous cellular automaton algorithm and study the stationary states and spatial patterning in SI, SIS and SIR models in a range $2 < \lambda < 3$. Two immunization scenarios, the random immunization and an intentional one, that targets the highest degrees nodes are considered. A distribution of safety patterns is obtained for the case of both scenarios. Estimates for the threshold values of the effective spreading rate β_c as a function of active agents fraction p and parameter λ are obtained and efficiency of both vaccination techniques are analyzed quantitatively. The impact of the underlying network heterogeneous structure is manifest, e.g., in decreasing the β_c values within the random scenario as compared to corresponding values in the case of regular lattice. This result quantitatively confirms the compliency of scale-free networks for disease spreading. On contrary, the vaccination within the targeted scenario makes the complex networks much more resistent to epidemic spreading as compared with regular lattice structures.

Critical and geometric properties of magnetic polymers across the globule-coil transition

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We study a lattice model of a single magnetic polymer chain, where Ising spins are located on the sites of a lattice self-avoiding walk in $d = 2$. We consider the regime where both conformations and magnetic degrees of freedom are dynamic, thus the Ising model is defined on a dynamic lattice and conformations generate an annealed disorder. Using Monte Carlo simulations, we characterize the globule-coil and ferromaget-to-paramagnet transitions, which occur simultaneously at a critical value of the spin-spin coupling. We argue that the transition is continuous — in contrast to $d = 3$ where it is first-order. Our results suggest that at the transition the metric exponent takes the theta-polymer value $\nu = 4/7$ but the crossover exponent $\phi \approx 0.7$, which differs from the expected value for a θ-polymer.

A multivariate approach to relate shape fluctuations and dynamics of

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In entangled linear polymer melt, at intermediate time scales, motion of a typical chain is constrained in a tube-like region. Whereas, the equilibrium dynamics is governed by "reptation", whereby kinks or structural defects propagate along the contour of the tube. We employ a multidimensional approach for a high-resolution view of the shape fluctuations, and to relate these conformational changes with the dynamics. To this end, configurational internal coordinates (invariant under global translation or rotation) are used to form the higher-dimensional feature space. We obtain the data from molecular dynamics simulations of long semiflexible linear polymer chains in a melt. Principal component analysis (PCA) shows that the shape changes can be captured with relatively small number of observables or principal components (PC). Dynamics of PCs reveal that small wavelength fluctuations are important for subdiffusive reptation dynamics. Further we determine dynamic cross correlation among the chains and relate it to entanglement.

Yet another Quantum Monte Carlo algorithm for strongly correlated systems

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We propose a new numerical approach for the Fermi-Hubbard model, combining Quantum Monte Carlo (QMC) simulation with a Linked-Cluster Expansion performed stochastically. The method is not a QMC algorithm per se: Any QMC algorithm can be used to estimate the partition function of the small clusters that are considered. Using the simplest Determinantal QMC, we show that the sign problem is alleviated, even without any resummation of the tadpoles by a shift of the action, and that the efficiency is brought much closer to that of the CDET algorithm.

Critical behavior of curvature dependent interfacial tension

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We study liquid-liquid phase coexistence in symmetric binary mixtures. Via the application of a successive umbrella sampling Monte Carlo simulation technique we obtain results on curvature dependence of interfacial tension. From the analysis of these results, obtained at different temperatures, we verify an expression for the universal critical behavior of this quantity. Our primary result is, however, related to an nonuniversal aspect. We show, via studies of different models, how the above mentioned critical behavior is influenced by the variation in the critical temperature.

Mpemba Effect: How common is it?

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Should a hotter body of water freeze quicker than a colder one when placed inside a refrigerator? An answer in affirmative is counter-intuitive and is now known as the Mpemba effect (ME). While the existence of ME is still debated, despite finding mentions from the times of Aristotle, there are efforts to discover ME-like effect in other systems. The general question being asked: Should a hotter body of a material equilibrate faster than a colder one when quenched to the same final low temperature? In this talk I will discuss results showing evidence of the effect in some simple model systems.

Crystallization of short polymer chains between two hard walls: Flat histogram Monte Carlo simulation (P)

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Our work is devoted to the study of the crystallization process in the melt of short polymer chains between two walls. To reveal the polymer structure and crystallization mechanism (1st order prefreezing or nucleation and growth), we analyse order parameters such as nematic orientational order parameter, bond orientation order parameters (Steinhardt parameters), hexagonal order parameter (which shows a quasi-two-dimensional stacking of chain cross sections in a plane perpendicular to the director). Research of these parameters in layers parallel to walls allows to plot corresponding profiles along the normal to the walls. We implement a Stochastic Approximation Monte Carlo (SAMC) using coarse-grained model. During microcanonical analysis, we can distinguish between isotropic regions in the center of the cell and crystallized structures near the walls.

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Ising universality in the two-dimensional Blume-Capel model with quenched random crystal field

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Using high-precision Monte Carlo simulations based on a parallel version of the Wang-Landau algorithm and finite-size scaling techniques, we study the effect of quenched disorder in the crystal-field coupling of the Blume-Capel model on a square lattice. We mainly focus on the part of the phase diagram where the pure model undergoes a continuous transition, known to fall into the universality class of a pure Ising ferromagnet. A dedicated scaling analysis reveals concrete evidence in favor of the strong universality hypothesis with the presence of additional logarithmic corrections in the scaling of the specific heat. Our results are in agreement with an early real-space renormalization-group study of the model as well as a very recent numerical work where quenched randomness was introduced in the energy exchange coupling. Finally, by properly fine tuning the control parameters of the randomness distribution we also qualitatively investigate the part of the phase diagram where the pure model undergoes a first-order phase transition. For this region, preliminary evidence indicate a smoothing of the transition to second-order with the presence of strong scaling corrections.

Population annealing Monte Carlo using the rejection-free n-fold way update applied to a frustrated Ising model on the honeycomb lattice

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Population annealing (PA) is a MC method well suited for the study of systems with a rough free energy landscape, e.g. glassy systems. PA is similar to an equilibrium version of parallel simulated annealing runs with the addition of a resampling step at each temperature. While a large population may improve imperfect equilibration, it is evident PA will fail when almost no spins are flipped in the equilibration routine. This is the case in systems with a low-temperature phase transition where high Metropolis rejection rates make sampling phase space near infeasible. To overcome this slowdown we propose a combination of the PA framework with the rejection-free "n-fold way" update and achieve an exponential speed-up at low temperatures compared to Metropolis. To test our method we study the Ising model with competing ferromagnetic nearest and antiferromagnetic next-to-nearest neighbor interactions of strengths $J_1 > 0$ and $J_2 < 0$, resp., on the honeycomb lattice. As T_c becomes arbitrarily small, when approaching the special point $J_2 = -J_1/4$ with $T_c = 0$, we consider this a good choice to test the efficacy of our method.

The dynamic critical exponent z of the three-dimensional Ising universality class: Monte Carlo simulations of the improved Blume-Capel model

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We study purely dissipative relaxational dynamics in the three-dimensional Ising universality class. To this end, we simulate the improved Blume-Capel model on the simple-cubic lattice by using local algorithms. We perform a finite-size scaling analysis of the integrated autocorrelation time of the magnetic susceptibility in equilibrium at the critical point. We obtain $z = 2.0245(15)$ for the dynamic critical exponent. As a complement, fully magnetized configurations are suddenly quenched to the critical temperature, giving consistent results for

the dynamic critical exponent. Furthermore, our estimate of z is fully consistent with recent field theoretic results.

On the swelling properties of pom-pom polymers indilute solutions

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We consider the simplest representative of the class of multiply branched polymer macromolecules, known as a pom-pom structure. The molecule consists of a backbone linear chain terminated by two branching points that may have different functionalities. The molecule is considered in the dilute solution regime where it is the easiest to study the influence of topology on size characteristics. In this work we study the pom-pom polymers using both analytical and numerical approaches. To describe the influence of branching on the size of the macromolecule a number of size characteristics were considered. The main attention in this talk is directed to the influence of the asymmetric branching on the size of the pom-pom polymers.

Quantum Langevin dynamics of the spherical model

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The collective and purely relaxational dynamics of quantum many-body systems, quenched to temperature $T = 0$ from a disordered initial state, is studied through the exact solution of the quantum Langevin equation of the quantum spherical model. The stationary state of the quantum dynamics is shown to be a non-equilibrium state. The long-time behaviour of single-time and two-time correlation and response functions and the resulting quantum ageing behaviour is analysed. A detailed comparison with classical ageing as well as with an effective markovian dynamics is presented.

From the critical Casimir effect to the Ising model on the rectangle

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The critical Casimir effect describes an emergent interaction between particles embedded in a fluctuating medium, as well as between its surfaces. It is caused by the nontrivial dependency of the medium free energy F on its boundary conditions and geometry, determined by the particles position and shape: If $F \mapsto F + \delta F$ changes under a particle displacement $r \mapsto r + \delta r$, a Casimir force $F_\mathrm{C} = -\delta F/\delta r$ on the particle emerges. The range of this fluctuation-induced force is determined by the correlation length $\xi(T)$ of the medium fluctuations, and it becomes long-ranged near a critical point T_c, where $\xi(T \to T_\mathrm{c})$ diverges. The critical Casimir effect is a universal finite-size effect, and it has been investigated both theoretically and experimentally in various universality classes and geometries. The talk will give an overview over recent developments.

In the case of the exactly solvable square-lattice Ising model, the Casimir potential and force can be calculated exactly for many geometries and boundary conditions, including the finite rectangle, for which an exact solution in terms of a Toeplitz determinant could be found recently. Finally, first results for the critical Casimir effect in the presence of quenched surface disorder are discussed.

Statistics of percolating clusters in a model of photosynthetic bacteria

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In photosynthetic organisms, the energy of light during illumination is absorbed by the antenna complexes, which is transmitted by excitons and is either absorbed by the reaction centers (RCs), which have been closed in this way, or emitted by fluorescence. The basic components of the dynamics of light absorption have been integrated into a simple model of exciton migration, which contains two parameters: The exciton hopping probability and the exciton lifetime. During continuous radiation with light the fraction of closed RCs, x, continuously increases and at a critical threshold, x_c, a percolation transition takes place. Performing extensive Monte Carlo simulations we study the properties of the transition in this correlated percolation model. We measure the spanning probability in the vicinity of x_c, as well as the fractal properties of the critical percolating cluster, both in the bulk and at the surface.

Cabana: An exascale particle simulation toolkit (P)

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Cabana is a performance portable library for particle-based simulations, developed as part of the Co-Design Center for Particle Applications (CoPA) within the Exascale Computing Project (ECP) under the U.S. Department of Energy. Applications include but are not limited to Molecular Dynamics (MD) with either short- and/or long-range interactions and various flavors of Particle-in-Cell (PIC) methods, including applications to fluid and solid mechanics and plasma physics. Cabana provides particle data structures, algorithms, and utilities to enable simulations on a variety of platforms including many-core architectures and GPUs (LA-UR-21-31489).

Effects of measures on phase transitions in two cooperative Susceptible-Infectious-Recovered (SIR) dynamics

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In recent studies, it has been shown that a cooperative interaction in a co-infection spread can lead to a discontinuous transition at a decreased threshold. Here, we investigate effects of immunization with a rate proportional to the extent of the infection on phase transitions of a cooperative co-infection. We use mean-field approximation to illustrate how measures that remove a portion of the susceptible compartment, like vaccination, with high enough rates can change discontinuous transitions in two coupled SIR dynamics into continuous ones while increasing the threshold of transitions. First, we introduce vaccination with a fixed rate into a symmetric spread on two diseases and investigate the numerical results. Second, we set the rate of measures proportional to the size of the infectious compartment and scrutinized the dynamics. We solve the equations numerically and analytically and probe the transitions for a wide range of parameters. We also determine transition points from the analytical solutions. Third, we adopt a heterogeneous mean-field approach to include heterogeneity and asymmetry in the dynamics and see if the results corresponding to homogeneous symmetric case stand.

Efficient algorithms for computing ground states of the 2D random-field Ising model (P)

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We investigate the application of graph-cut methods for the study of the critical behaviour of the two-dimensional random-field Ising model. We focus on exact ground-state calculations, crossing the phase boundary of the model at zero temperature and varying the disorder strength. For this purpose we employ two different minimum-cut–maximum-flow algorithms, one of augmenting-path and another of push-relabel style. We implement these approaches for the square and triangular lattice problems and compare their computational efficiency.

Structure of polymer-grafted nanoparticle melts

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The structure of neat melts of polymer-grafted nanoparticles (GNPs) is studied via coarse-grained molecular dynamics simulations. We systematically vary the degree of polymerization and grafting density at fixed nanoparticle (NP)radius and study in detail the shape and size of the GNP coronas. For sufficiently high grafting density, chain sections close to the NP core are extended and form a dry layer. Further away from the NP, there is an interpenetration layer, where the polymer coronas of neighboring GNPs overlap and the chain sections have almost unperturbed conformations. To better understand this partitioning, we develop a two-layer model, representing the grafted polymer around an NP by spherical dry and interpenetration layers. This model quantitatively predicts that the thicknesses of the two layers depend on one universal parameter, x, the degree of overcrowding of grafted chains relative to chains in the melt. Both simulations and theory show that the chain extension free energy is nonmonotonic with increasing chain length at a fixed grafting density, with a well-defined maximum. This maximum is indicative of the crossover from the dry layer-dominated to interpenetration layer-dominated regime, and it could have profound consequences on our understanding of a variety of anomalous transport properties of these GNPs. Our theoretical approach therefore provides a facile means for understanding and designing solvent-free GNP-based materials

Time series analysis of data sets provided on the COVID-19 dashboard of the RKI: What was the influence of telephone sick certificates in 2020?

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For evaluating the effects of non-pharmacological measures against the spreading of the Covid-19 pandemic, characteristic changes of the time series of the number of infected persons have to be identified. To ensure a high resolut ion of such relations, a data preparation was performed as follows: (i) Focus on those patients for whom the disease dates (first occurrence of symptoms) are known, (ii) determination of a specific 7-day sliding average of the number of daily new cases, (iii) ascribing this average value to the respective mean day of the interval under consideration, and (iv) graphical presentation in a simple logarithmic diagram, as is motivated by the mathematics of spreading mechanisms. The obtained simple logarithmic charts of the averaged time series exhibit several longer, almost straight-line segments. In these time intervals, the dispersion conditions seem to vary only slightly. Remarkably, the transitions between two successive straight-line segments occur mostly within a few days, usually with in about a week. These changes indicate significant, abrupt modifications of the pandemic's spread conditions. With regard to such transitions, two precise temporal coincidences are particularly noteworthy: Both in March 2020 and in October 2020, the phases of rapidly growing numbers of cases ended within approximately one week immediately after the introduction of the possibility of telephone sick certificates.

On the other hand, neither for the contact restrictions imple mented at 22.03.2020 nor for the start of the wave breaker lockdown at 02.11.2020, associated effects are detectable in the obtained diagrams.

Percolation properties of the two-dimensional Ising spin glass (P)

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In the Ising model there exists a direct connection between percolation of Fortuin-Kasteleyn clusters and the ferromagnetic phase transition. In contrast, due to frustration percolation of Fortuin-Kasteleyn clusters in spin glasses occurs at a higher temperature than the spin-glass transition [1, 2].

In this work we focus on percolation of clusters defined from the overlap of two replicas. This approach is beneficial since the overlap is the order parameter of the spin-glass transition. To be more concrete, we study the CMR representation of Chayes, Machta and Redner [3] as well as the two-replica Fortuin-Kasteleyn representation of Newman and Stein [4] in the two-dimensional Ising spin glass with Gaussian disorder by performing Monte Carlo simulations. Our data suggest the existence of a zero-temperature percolation transition in agreement with the zero-temperature spin-glass transition in two dimensions.

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Boundary criticality of the 3d O(N) model: From normal to extraordinary

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It was recently realized that the three-dimensional O(N) model possesses an extraordinary boundary universality class for a finite range of $N \geq 2$. For a given N, the existence and universal properties of this class are predicted to be controlled by certain amplitudes of the normal universality class, where one applies an explicit symmetry breaking field to the boundary. In this paper, we study the normal universality class for $N = 2, 3$ using Monte Carlo simulations on an improved lattice model and extract these universal amplitudes. Our results are in good agreement with direct Monte Carlo studies of the extraordinary universality class serving as a non-trivial quantitative check of the connection between the normal and extraordinary classes.

Kinetics of coil-globule transition of an active polymer with Vicsek-like alignment

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Dynamics of various biological filaments can be understood within the framework of active polymer models. Here we consider a bead-spring model for a flexible polymer chain in which the active interaction among the beads is introduced via an alignment rule adapted from the Vicsek model. Following a quench from the high-temperature coil phase to a low-temperature state point, we study the coarsening kinetics via molecular dynamics (MD) simulations using the Langevin thermostat. For the passive polymer case the low-temperature equilibrium state is a compact globule. Results from our MD simulations reveal that though the globular state is also the typical final state in the active case, the nonequilibrium pathways to arrive at such a state differ from the passive

picture due to the alignment interaction among the beads. We notice that deviations from the intermediate "pearl-necklace"-like arrangement, that is observed in the passive case, and the formation of more elongated dumbbell-like structures increase with increasing activity. Furthermore, it appears that while a small active force on the beads certainly makes the coarsening process much faster, there exists nonmonotonic dependence of the collapse time on the strength of active interaction. We quantify these observations by comparing the scaling laws for the collapse time and growth of pearls with the passive case.

1D-to-3D crossover on multileg attractive-U Hubbard ladders (P)

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We study ground state properties of a polarized two-component Fermi gas on multileg attractive-U Hubbard ladders. Using DMRG simulations, we construct grand canonical phase diagrams for varying perpendicular geometries and ratios of hopping amplitudes, and charactrize the 1D-to-3D crossover. We compare our findings with recent experiemental and theoretical studies of quasi-one-dimensional polarized Fermi gases.

Randomised mixed labyrinth fractals

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Fractals, introduced by Benoit Mandelbrot in the early 1980s, allow the analysis of physical properties of natural geometries and structures in non-integer dimensions. It has been shown recently, that utilizing fractals structures, for instance for gas sensors made of carbon nanotubes increase their efficiency or give new insights to complex quantum phenomena. Here, we are interested how the effect of randomness, as observed in real materials, alter the topology and thus dynamics of the resulting fractal structures in comparison to the pure cases. We focus on a special class of Sierpinski carpets, i.e., the labyrinth fractals [1], that can be used for dendritic networks or porous materials. Therefore, we mix to fractal patterns, with different properties, i.e., shortest path and random walk dimension, randomly together at different mixing ratios. Surprisingly we found that even in cases where the initial patterns exhibit the same non-integer dimensions the resulting randomised fractals give a different property [2].

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Electron phonon entanglement

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In this talk we overview the results about entanglement between electrons and phonons in coupled systems, including the case of H2+ molecules, approximate results in exciton systems, and analytical results in Luttinger liquids (this is our contribution). These results show, that at phase transitions there might be a maximum of the entanglement entropy, there is a temperature limit in the Luttinger system, above this limit there is zero entanglement.

Scaling and entropy of the hard-sphere polymer

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We investigate hard-sphere polymers in two to five dimensions. Using a recently developed simulation technique [1, 2] we are able to treat very long chains and can test the predicted scaling behavior. To ensure homogeneity along the chain we introduce periodic boundary conditions. We find that theory describes the observations very well, however, a discontinuity emerges when the sphere diameter δ is varied. Measurements of the system's entropy suggest that this is likely related to the excluded volume's dependency on δ.

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On the collective excitations of the drop crystals moving in liquid

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We simulate solid particles flowing in the two-dimensional channel pumped with the Poiseuille velocity profile using the Immersed Boundary and Lattice Boltzmann methods. We found the collective excitations of the particle emerge with the increasing number of particles in the chain. We measure the spectrum of the chain oscillations varying the width of the channel. We found that the spectrum of oscillations is sensitive to the channel's width and argue that the collective oscillation spectrum is formed by the interaction of the solid particles with the waves reflected from channel boundaries. We compare our results with the experiments of the drop movement in the quasi-two-dimensional channel and with the simulations of other groups. Supported by Russian Science Foundation, grant 19-21-00286.

Functionalization of Boron-Carbide monolayer for the adsorption of organic molecules (P)

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Because of their specific structure, graphene and graphene like nano materials have attracted great attention in biomedical applications such as biosensor and drug delivery studies. In this study, as a biosensor, the adsorption of dopamine and 5-fluoroacil (5-Fu) biomolecules have been investigated by means of first principles calculations. Geometric optimizations of the systems formed with different configurations on the monolayer surface of biomolecules have been made and the effect on the structural differences on the electronic properties have been examined.

Influence of roughening transition on nonequilibrium dynamics of the three-dimensional Ising model

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Via Monte Carlo simulations of the Glauber Ising model we investigate the dependence of nonequilibrium

dynamics on temperature in the case of an ordering ferromagnetic system in space dimension d = 3. In this dimension there exists a non-zero roughening transition temperature, which is related to the roughness of interface between different ordering phases. Here we present results on structure, growth and aging, for the above-mentioned system, over a wide range of temperature, and show that the unexpected slow dynamics, that was earlier reported for the zero temperature quenches, occurs at all temperatures below the roughening transition. This demonstrates an important structure-dynamics connection in phase-ordering dynamics.

Universality aspects of the two-dimensional spin-1 Baxter-Wu model in a crystal field (P)

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We investigate the universality aspects of the two-dimensional spin-1 Baxter-Wu model in the presence of a crystal-field coupling Δ. We employ extensive numerical simulations of two types which provide us with complementary results: Wang-Landau entropic sampling simulations at fixed values of Δ and a parallelized variant of the multicanonical approach at constant temperatures T. A detailed finite-size scaling analysis at the regime of second-order phase transitions of the $\Delta - T$ 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 phase transition are resolved and attributed to the presence of strong finite-size effects, especially as one approaches the pentacritical point of the model.

Monte Carlo study of the two-dimensional kinetic Blume-Capel model in a quenched random crystal field

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We investigate by means of Monte Carlo simulations the dynamic phase transition of the two-dimensional kinetic Blume-Capel model under a periodically oscillating magnetic field in the presence of a quenched random crystal-field coupling. We analyze the universality principles of this dynamic transition for various values of the crystal-field coupling at the originally second-order regime of the corresponding equilibrium phase diagram of the model. A detailed finite-size scaling analysis indicates that the observed nonequilibrium phase transition belongs to the universality class of the equilibrium Ising ferromagnet with additional logarithmic corrections in the scaling behavior of the heat capacity. Our results are in agreement with earlier works on kinetic Ising models.

Autocorrelations in homeostatic spiking neural networks as a result of emergent bistable activity

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Using a neuromorphic processor, we emulate networks of excitatory and inhibitory leaky integrate and fire neurons with spiking rates regulated by homeostatic plasticity. The latter incorporates stochastic updates that give rise to heterogeneous weight distributions. As predicted by theory, the network becomes more recurrent for decreasing input strength, which manifests in an increase of the autocorrelation time. Surprisingly, this rise can be attributed to emergent bistable population activity that (i) can be well approximated by a hidden Markov model, (ii) does not appear to vanish for increasing system sizes, and (iii) is likely stabilized by the heterogeneous weight distribution. In addition, we show that networks with bistable population activity allow for a more precise, yet slower representation of additional input that may still be read out once the input is removed.