

ABSTRACTS

of contributions to the

24th International NTZ-Workshop on
New Developments in Computational Physics

CompPhys23

Computational Physics Group,
Institut für Theoretische Physik,
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Welcome to the 24th International NTZ-Workshop *CompPhys23* 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 during Christmas time.

The main part of the Workshop will take place on Tuesday/Wednesday, 19 and 20 December 2023, in one of the big lecture halls and the "Aula" of the Experimental Physics building in Linnéstr. 5. As in previous years, the last day, Thursday, 21 December 2023, is devoted to various collaborative meetings and discussion rounds which will take place in the seminar rooms of the Theoretical Physics building in "Brüderstr. 16".

Finally, we and the Centre for Theoretical Sciences (NTZ) gratefully acknowledge financial support of the Workshop from the Doctoral College "L⁴" of Deutsch-Französische Hochschule (DFH-UFA), Research Academy Leipzig (RALeipzig), and Leipzig Graduate School of Natural Sciences "BuildMoNa".

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Wolfhard Janke

Critical dynamics of the $\pm J$ Ising model

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The $\pm J$ Ising model is a simple frustrated spin model, where the exchange couplings independently take the discrete value $-J$ with probability p and $+J$ with probability $1-p$. Here, we investigate the nonequilibrium critical behavior of the bi-dimensional $\pm J$ Ising model, after a quench from different initial conditions to a critical point $T_c(p)$ on the *paramagnetic-ferromagnetic* (PF) transition line, especially, above, below and at the *multicritical Nishimori point* (NP). The *dynamical* critical exponent z_c seems to exhibit non-universal behavior for quenches above and below the NP, which is identified as a pre-asymptotic feature due to the *repulsive* fixed point at the NP. Whereas, for a quench directly to the NP, the dynamics reaches the asymptotic regime with $z_c \simeq 6.02(6)$. We also consider the geometrical spin clusters (of like spin signs) during the critical dynamics. Each universality class on the PF line is uniquely characterized by the stochastic Loewner evolution (SLE) with corresponding parameter κ .

Ralph Kenna's scaling relations in critical phenomena

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In this short talk, we want to revisit and propose an alternative derivation of some of the scaling relations among “hatted critical exponents” which were first derived by Ralph Kenna, Des Johnston and Wolhard Janke. For the scaling relation involving the behavior of the correlation function we will propose an alternative form since we believe the expression is incomplete in the work of Ralph and his collaborators.

CTMRG study of interacting dimers

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The 2D dimer model does not display any phase transition, even upon the introduction of a fixed density of monomers. However, numerical simulations revealed the existence of a phase transition when an interaction favors the parallel alignment of dimers within the same plaquette. The critical behavior has been investigated by means of transfer matrix calculations and Monte Carlo simulations. I will review the recent efforts to apply Tensor Networks techniques to this model and present preliminary results from a study conducted using the Corner Transfer Matrix Renormalization Group (CTMRG).

Self-tuning Hamiltonian Monte Carlo

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The performance of Hamiltonian Monte Carlo simulations crucially depends on its parameters, in particular the integration timestep and the number of integration steps. We present an adaptive general-purpose framework

to automatically tune both parameters based on a local loss function which promotes the fast exploration of phase-space. We show that a good correspondence between loss and autocorrelation time can be established, allowing for gradient-based optimization using a fully-differentiable set-up. The loss is constructed in such a way that it also allows for gradient-driven learning of a distribution over the number of integration steps. Our approach is demonstrated for the one-dimensional harmonic oscillator and alanine dipeptide, a small protein common as a test case for simulation methods. Through the application to the harmonic oscillator, we highlight the importance of not using a fixed timestep to avoid a rugged loss surface with many local minima, otherwise trapping the optimization. In the case of alanine dipeptide, by tuning the only free parameter of our loss definition, we find a good correspondence between it and the autocorrelation times, resulting in a > 100 fold speed up in optimization of simulation parameters compared to a grid-search. For this system, we also extend the integrator to allow for atom-dependent timesteps, providing a further reduction of 25% in autocorrelation times.

Collapse dynamics of the helix-coil transition in polyaniline (P)

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The collapse transition of polymers can provide important insights into the folding of proteins. In this work the influence of the formation of α -helices on the nonequilibrium pathways of the collapse of polyaniline was investigated. To this end, the full-time evolution of the helix-coil transition in polyaniline was simulated using molecular dynamics (MD) simulations with the Andersen, the Langevin and the Nosé-Hoover thermostat. The pathway of the collapse in general seems to follow the pearl-necklace picture, with an initial formation of small globular clusters that eventually merge into one bigger cluster. This cluster then loses its globular shape, as the formation of helices dominates and a helical structure forms. The dynamics of this transition can be described by a critical exponent z for which we find a value of $z \approx 5/4$ in the simulations with both the Langevin and Andersen thermostat. In contrast to this the Nosé-Hoover thermostat shows significantly faster dynamics with an exponent of $z \approx 3/5$. While the first one agrees with the usually obtained values of $z = 1 - 2$ for nonbiological polymers, the second value is more in agreement with the exponent of $z \approx 0.5$ which was recently observed in the collapse of polyglycine [1].

[1] S. Majumder, U. H. E. Hansmann, and W. Janke, *Macromolecules* **52** (2019) 5491.

Phases and topological defects in passive and active systems in two dimensions

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Long-range translational order is forbidden in low-dimensional systems with short-range interactions: Solid phases can only have quasi long-range translational order while they keep long-range orientational order. The standard picture is that the melting transition occurs in two steps: An intermediate phase with quasi long-range orientational order is reached by the unbinding of dislocations while the transition to the liquid is triggered by the unbinding of disclinations. In this talk I will revisit all these issues and I will extend their analysis to systems of self-propelled particles, the constituents of active matter, a new kind of soft matter relevant to describe numerous biological problems. The dynamics across various phase transitions will also be discussed. A new scenario emerges from extensive molecular simulations studies.

Analytical and numerical investigation of star polymers in confined geometries

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The analysis of the impact of the star polymer topology on the depletion interaction potentials, the depletion forces and the monomer density profiles was carried out analytically and by molecular dynamic simulations. The following calculations were made: the dimensionless depletion interaction potentials, the dimensionless depletion forces and the layer monomer density profiles for a dilute solution of ideal star polymers with number $f = 3, 4, 5$ of legs in a Θ -solvent confined in a slit geometry of two parallel walls with repulsive surfaces and for the case of one repulsive and the other one inert surface. Furthermore, the dimensionless layer monomer density profiles for ideal star polymers with different number $f = 3, 4, 5$ of legs immersed in a dilute solution of big colloidal particles with different adsorbing or repelling properties in respect to polymers were calculated, bearing in mind the Derjaguin approximation. Taking into account the small sphere expansion made it possible to get the monomer density profiles for a dilute solution of ideal star polymers with different number $f = 3, 4, 5$ of legs immersed in a solution of small spherical particles, or nano-particles of finite size, which are much smaller than the polymer size and the other characteristic mesoscopic length of the system. Besides, we performed molecular dynamics simulations of a dilute solution of star-shaped polymers with $N = 901$ ($3 \times 300 + 1$ -star polymer with three legs), 1201 ($4 \times 300 + 1$ -star polymer with four legs) and 1501 ($5 \times 300 + 1$ -star polymer with five legs) beads accordingly. The analytical and numerical results for star polymers that we obtained are compared with the results for linear polymers in confined geometries. The acquired results show that a dilute solution of star polymer chains can be applied for the production of new functional materials because the behavior of these solutions is strictly correlated with the topology of polymers, and also with the nature and geometry of confined surfaces. The above mentioned properties can find extensive practical application in nano-technology, as well as in bio-technology and medicine for drug and gene transmission.

Crystallization in melts of semiflexible polymer chains: How to distinguish noisy crystal structures

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We study conformational properties of short polymer chains in melts between two hard walls. Our final goal is to reveal physical factors which are responsible for a particular scenario of surface-induced polymer crystallization (e.g., the nucleation and growth or the first-order prefreezing [1]). We use a coarse-grained model and perform flat-histogram Monte Carlo (MC) simulations based on the stochastic approximation Monte Carlo (SAMC) algorithm [2]. We suggest a new way of calculating bond order parameters (Steinhardt parameters [3]) to distinguish between different crystal structures and observe coexistence of several symmetries. We also analyse different order parameters: Nematic orientational order parameter, bond order parameters, hexagonal order parameter (which shows a quasi-two-dimensional stacking of chain cross sections in a plane perpendicular to the director).

[1] A.-K. Flieger, M. Schulz, and T. Thurn-Albrecht, *Macromolecules* **51** (2018) 189–194.

[2] T. Shakirov and W. Paul, *Phys. Rev. E* **97** (2018) 042501.

[3] P. J. Steinhardt, D. R. Nelson, and M. Ronchetti, *Phys. Rev. E* **28** (1983) 784–805.

Self-learning population simulations for a frustrated Ising model (P)

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Population annealing (PA) is a Monte Carlo method well suited for problems with a rough free energy landscape such as glassy systems. PA is similar to repeated simulated annealing, with the addition of a resampling step at each temperature. To achieve best performance, the PA parameters have to be chosen carefully. Both the

set of temperatures, as well as the number of sweeps carried out at each temperature, form a several hundred-dimensional parameter space. In practice, these are often chosen a priori following very simple patterns, e.g. a temperature set given by linearly increasing inverse temperature with a constant number of updates at each temperature. While it is now common to choose the temperatures adaptively, the number of updates still is usually either constant or piece-wise constant. We propose a fully adaptive variant of the PA algorithm in which both the temperature step and the number of updates are chosen adaptively. Besides few hyper parameters, this method requires no previous knowledge on the underlying model and works in an online self-learning manner. To test our method we study the Ising model with competing ferromagnetic ($J_1 > 0$) nearest and antiferromagnetic ($J_2 < 0$) next-to-nearest neighbor interactions on the honeycomb lattice.

First-passage area distribution and optimal fluctuations of fractional Brownian motion

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(with Baruch Meerson, Jerusalem, Israel)

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We study the probability distribution $P(A)$ of the area $A = \int_0^T x(t)dt$ swept under fractional Brownian motion (fBm) $x(t)$ until its first passage time T to the origin. The process starts at $t = 0$ from a specified point $x = L$. We show that $P(A)$ obeys exact scaling relation

$$P(A) = \frac{D^{\frac{1}{2H}}}{L^{1+\frac{1}{H}}} \Phi_H \left(\frac{D^{\frac{1}{2H}} A}{L^{1+\frac{1}{H}}} \right),$$

where $0 < H < 1$ is the Hurst exponent characterizing the fBm, D is the coefficient of fractional diffusion, and $\Phi_H(z)$ is a scaling function. The small- A tail of $P(A)$ has been recently predicted by Meerson and Oshanin [Phys. Rev. E **105**, 064137 (2022)], who showed that it has an essential singularity at $A = 0$, the character of which depends on H . Here we determine the large- A tail of $P(A)$. It is a fat tail, in particular such that the average value of the first-passage area A diverges for all H . We also verify the predictions for both tails by performing simple-sampling as well as large-deviation Monte Carlo simulations. The verification includes measurements of $P(A)$ up to probability densities as small as 10^{-190} . We also perform direct observations of paths conditioned on the area A . For the steep small- A tail of $P(A)$ the “optimal paths”, *i.e.*, the most probable trajectories of the fBm, dominate the statistics. Finally, we discuss extensions of theory to a more general first-passage functional of the fBm.

Understanding neural network models for phase recognition (P)

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Neural Networks have been used successfully to detect the different phases of various spin systems. We investigate and compare the performances of a few different models and use the smallest networks to visualise the loss landscape which can be used to understand the training of the network.

Growth of entanglement entropy under local projective measurements

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Non-equilibrium dynamics of many-body quantum systems under the effect of measurement protocols is attracting an increasing amount of attention. It has been recently revealed that measurements may induce an abrupt change in the scaling-law of the bipartite entanglement entropy, thus suggesting the existence of

different non-equilibrium regimes. However, our understanding of how these regimes appear and whether they survive in the thermodynamic limit is much less established. Here we investigate these questions on a one-dimensional quadratic fermionic model: this allows us to reach system sizes relevant in the thermodynamic sense. We show that local projective measurements induce a qualitative modification of the time-growth of the entanglement entropy which changes from linear to logarithmic. However, in the stationary regime, the logarithmic behavior of the entanglement entropy does not survive in the thermodynamic limit and, for any finite value of the measurement rate, we numerically show the existence of a single area-law phase for the entanglement entropy. Finally, exploiting the quasi-particle picture, we further support our results by analysing the fluctuations of the stationary entanglement entropy and its scaling behavior.

Entropic force in a dilute solution of real ring polymer chains with different topological structures in a slit of two parallel walls with mixed boundary conditions (P)

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We have performed molecular dynamics simulations to examine the radius of gyration in real ring polymer chains composed of 360 monomers with diverse topological structures. Our focus was on the entropic force exerted by a dilute solution of these polymers, considering their different topologies and the excluded volume interaction (EVI) in a good solvent, on the confining parallel walls within a slit geometry. We employed mixed boundary conditions, comprising one repulsive wall and another at the adsorption threshold. The results, especially for wider slit regions, show qualitative agreement with prior analytical findings for ideal ring polymers.

Critical and tricritical singularities from small-scale Monte Carlo simulations: The Blume-Capel model in two dimensions

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We show that the study of critical properties of the Blume-Capel model at two dimensions can be deduced from Monte Carlo simulations with good accuracy even for small system sizes when one analyses the behaviour of the zeros of the partition function. The phase diagram of the model displays a line of second-order phase transitions ending at a tricritical point, then a line of first-order transitions. We concentrate on critical and tricritical properties and compare the accuracy achieved via standard finite-size scaling of thermodynamic quantities with that from the zeros analysis. This latter analysis showcases spectacular precision, even for systems as small as 64 spins! We also show that the zeros are very sensitive to subtle crossover effects.

Fast, hierarchical, and adaptive algorithm for Metropolis Monte Carlo simulations of long-range interacting systems

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We present a fast, hierarchical, and adaptive algorithm for Metropolis Monte Carlo simulations of systems with long-range interactions that reproduces the dynamics of a standard implementation exactly, i.e., the generated configurations and consequently all measured observables are identical, allowing in particular for nonequilibrium studies [1]. The method is demonstrated for the power-law interacting long-range Ising and XY spin models with nonconserved order parameter and a Lennard-Jones particle system, all in two dimensions. The measured

run times support an average complexity $O(N \log N)$, where N is the number of spins or particles. Importantly, prefactors of this scaling behavior are small, which in practice manifests in speedup factors larger than 10^4 . The method is general and will allow the treatment of large systems that were out of reach before, likely enabling a more detailed understanding of physical phenomena rooted in long-range interactions.

[1] F. Müller, H. Christiansen, S. Schnabel, and W. Janke, Phys. Rev. X **13** (2023) 031006.

The Griffiths phase and beyond: A large-deviations study

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The Griffiths phase is a temperature range in systems with quenched disorder that reaches from the critical temperature of the pure system to the corresponding critical temperature in the presence of disorder. In this phase, the possibility of large fluctuations in the disorder degrees of freedom leads to broad distributions in response functions. For example, inside the Griffiths phase of the two-dimensional bond-diluted Ising model the distribution of the magnetic susceptibility is expected to have an exponential tail [1]. A large-deviation Monte Carlo algorithm is used to sample this distribution, and the exponential tail is extracted over a wide range of the support, down to probabilities of the order of 10^{-300} [2, 3]. A connection between the local fraction of ferromagnetic bonds and the size of the magnetic susceptibility is demonstrated numerically. Furthermore the distribution of the magnetic susceptibility is also investigated at the ferromagnetic phase transition, inside the ferromagnetic phase and at zero temperature, revealing interesting differences and similarities between the cases.

[1] A. J. Bray, Phys. Rev. Lett. **59** (1987) 586.

[2] A. K. Hartmann, Phys. Rev. E **65** (2002) 056102.

[3] K. Hukushima and Y. Iba, J. Phys.: Conf. Ser. **95** (2008) 012005.

Universal finite-size scaling in the extraordinary-log phase

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Recent advancements in boundary critical phenomena have led to the discovery of a new surface universality class in the three-dimensional $O(N)$ model. The newly found “extraordinary-log” phase can be realized on a two-dimensional surface for $N < N_c$, with $N_c > 3$, and on a plane defect embedded into a three-dimensional system, for any N . One of the key features of the extraordinary-log phase is the presence of logarithmic violations of standard Finite-Size Scaling, whose amplitude is determined by a universal parameter $\alpha(N)$. In this work we study Finite-Size Scaling in the extraordinary-log universality class by means of MC simulations of an improved lattice model, where leading scaling corrections are suppressed. We simulate the model with open boundary conditions, realizing the extraordinary-log phase on the surface for $N = 2, 3$, as well as for fully periodic boundary conditions and in the presence of a plane-defect for $N = 2, 3, 4$. In line with field-theory predictions, renormalization-group invariant observables studied here exhibit a logarithmic dependence on the size of the system.

Dynamics and correlations of a tracer in a linear chain of run-and-tumble particles

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We consider a linear chain of run-and-tumble particles (RTP) interacting harmonically with nearest neighbors. For tagged particles in bulk, we obtain a closed-form expression for the mean-squared displacement (MSD). Different scaling forms were extracted to show the cross-over from ballistic to diffusive to sub-diffusive behavior,

and finite-size effects were also studied. The activity in this system is characterized by the persistence time, defined as the inverse of the tumbling rate α of a particle, the passive limit corresponds to $\alpha \rightarrow \infty$. We also compute the full distribution of tagged particle displacement and find that it evolves from highly non-Gaussian forms (bimodal, heavy-tailed, etc.) at early times ($t < \alpha^{-1}$) to a Gaussian one at large times when interaction with other particles are dominant. Finally we computed static and dynamic correlations in the steady state for the “stretch” variables, defined as relative displacements between nearest neighbors, and pointed out interesting differences between the active and passive systems. For example, we show that the dynamical correlation shows very different scaling in the active case (small α) compared to the diffusive scaling for the passive case. Our results easily extend to other active particle models such as active Brownian particles and active Ornstein-Uhlenbeck particles.

Population annealing in the real microcanonical ensemble (P)

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A simulation method is introduced to study systems with a first-order phase transition. It uses the population annealing algorithm in the real microcanonical ensemble where the total energy consisting of a potential and a kinetic energy contribution is set to be constant. The method is tested on the two-dimensional q -state Potts model which exhibits a first-order phase transition for $q > 4$. This work is part of my master’s thesis.

Sampling states of spin models using generative neural networks

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A neural network based sampling approach for discrete models such as the Ising model is presented, which yields uncorrelated states and is therefore not subject to slowing down effects. Here, we use so called Variational Autoregressive Networks (VANs) for this purpose, for which the exact sampling probability can be calculated. This feature allows for the asymptotically unbiased estimation of thermodynamic properties such as the average energy and specific heat. Training VANs can be realized either by a supervised learning scheme, that requires a database of training states, or by a reinforcement learning approach, that minimizes variational free energy. As detailed studies reveal, the latter approach leads to difficulties in overcoming large free energy barriers and thus to mode collapse. Finally, we discuss how VANs can be conditioned on certain input parameters such as temperature or energy

Density of states from microcanonical averages

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When Monte Carlo simulations are employed to investigate equilibrium properties of some system of interest, one intermediate aim is often to determine the density of states. Once obtained, it allows for the calculation of quantities like the partition function, the mean energy, or the specific heat. These, in turn, reveal aspects of the system’s thermodynamic behavior like temperature or order of phase transitions. While the methods predominantly used utilize one or more histograms which once reweighted provide an estimator for the density of states, histograms are prone to relatively large statistical errors which can impede further analysis of the data. However, as an alternative technique, the derivative of the logarithmic density of states can be calculated from microcanonical averages of spatial derivatives of the Hamiltonian like gradient, Laplacian, and Hessian. I will review the established method [1, 2] and discuss a recently introduced formula [3] that avoids the use of the computationally demanding Hessian.

- [1] G. Gilat, *Calculation of derivatives of spectral functions in solids*, Solid State Commun. **14** (1974) 263.
- [2] H. H. Rugh, *Dynamical approach to temperature*, Phys. Rev. Lett. **78** (1997) 772.

[3] S. Schnabel and W. Janke, *Surveying an energy landscape*, *Front. Phys.* **11** (2023) 1218107.

Flat-histogram simulation: Optimal convergence and extended sampling

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Recent developments in Monte Carlo sampling methods, particularly in flat-histogram algorithms, have expanded our understanding of complex physical systems. Despite a long history and established mathematical convergence, optimal parameter choice and the relationship between different techniques remain less explored in computational physics. This study aims to address this gap by estimating general rules for optimal parameter choice in Stochastic Approximation Monte Carlo (SAMC) and comparing its convergence with Multicanonical sampling (MUCA). We also explore the integration of importance sampling with SAMC to reduce the sensitivity of convergence to parameter variations. This integration not only stabilizes the convergence process but also enhances the robustness of the simulations. Furthermore, this combined approach allows extension of flat-histogram sampling. It enables a broader exploration of model parameters, such as examining the relative contributions of different energy components or pressure estimation in isochoric Monte Carlo simulations without the need for direct force or virial calculations.

Finite-size analysis of second-order phase transitions in classical spin models using machine learning

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We analyze the Ising model and the Baxter-Wu model in two dimensions using deep learning networks trained to classify paramagnetic (PM) and ferromagnetic (FM) phases using supervised machine learning [1]. Snapshots of spin configurations used as training data are labeled as belonging to the PM state or FM state using analytically known phase transition temperatures depending on a given set of parameters. We use the variation $V(T)$ of the output function $P(T)$ to estimate the critical temperature and correlation length exponent [2]. The approach was tested with two models of two universality classes using six neural networks. Supervised learning was carried out for the isotropic Ising model on a square lattice. There are two testing models. First, it is Onsager case with different horizontal M and vertical N couplings on a square lattice [3]. Second, it is Houtappel case of Ising model with ferromagnetic couplings on the square lattice bonds equipped with couplings J_d in one of the diagonal directions. The critical temperature is known for both cases [3, 4]. It is well known that anisotropy changes the value of the Binder cumulant [5] and thereby determines the limitations of universality [6]. Accordingly, we demonstrate the limitations of knowledge transfer in machine learning due to anisotropy. In the case of Onsager model, the deviation of critical temperature looks like the ratio of the correlation length amplitudes [7]. In both cases, the estimate of critical correlation exponent is reliable.

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- [1] J. Carrasquilla and R. G. Melko, *Nature Phys.* **13** (2017) 431.
- [2] V. Chertentkov, E. Burovski, and L. Shchur, *Phys. Rev. E* **108** (2023) L032102.
- [3] L. Onsager, *Phys. Rev.* **65** (1944) 117.
- [4] R. M. F. Houtappel, *Physica* **16** (1950) 425.
- [5] V. Dohm, *Phys. Rev. E* **77** (2008) 061128.
- [6] W. Selke and L. N. Shchur, *Phys. Rev. E* **80** (2009) 042104.
- [7] T. T. Wu, B. M. McCoy, C. A. Tracy, and E. Barouch, *Phys. Rev. B* **13** (1976) 316.

Phase separation of a magnetic fluid: Asymptotic states and non-equilibrium kinetics

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We study self-assembly in a colloidal suspension of magnetic particles by performing comprehensive molecular dynamics simulations of the Stockmayer model (SM) which comprises spherical particles decorated by a magnetic moment. The SM potential incorporates dipole-dipole interactions along with the usual Lennard-Jones interaction, and exhibits a gas-liquid phase coexistence observed experimentally in magnetic fluids. When this system is quenched from the high-temperature homogeneous phase to the coexistence region, the non-equilibrium evolution to the condensed phase proceeds with the development of spatial as well as magnetic order. We observe density-dependent coarsening mechanisms – a diffusive growth law $\ell(t) \sim t^{1/3}$ in the nucleation regime, and hydrodynamics-driven inertial growth law $\ell(t) \sim t^{2/3}$ in the spinodal regimes. [$\ell(t)$ is the average size of the condensate at time t after the quench.] While the spatial growth is governed by the expected conserved order parameter dynamics, the growth of magnetic order in the spinodal regime exhibits unexpected non-conserved dynamics. The asymptotic morphologies have density dependent shapes which typically include the isotropic sphere and spherical bubble morphologies in the nucleation region, and the anisotropic cylinder, planar slab, cylindrical bubble morphologies in the spinodal region. The structures are robust and non-volatile, and exhibit characteristic magnetic properties. For example, the oppositely magnetized hemispheres in the spherical morphology impart the characteristics of a Janus particle to it. The observed structures have versatile applications in catalysis, drug delivery systems, memory devices and magnetic photonic crystals, to name a few.

Dynamical scaling of the two-dimensional pure and dilute Baxter-Wu model

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We investigate the relaxation dynamics of the dilute (spin-1) Baxter-Wu model in the presence of a crystal-field Δ at the regime of continuous transitions. We employ a set of Monte Carlo simulation schemes, particularly the heat-bath single spin-flip algorithm and a hybrid approach that combines a cluster with the heat-bath update. A finite-size scaling analysis of the integrated autocorrelation time for the order parameter at equilibrium provides estimates of the dynamical critical exponent z . Our results indicate that, while for $\Delta \leq 0$ the effective values of z seem to converge to a universal value, for $\Delta > 0$, z appears to increase with Δ , rendering the hybrid update almost as efficient as a single spin-flip update near the multicritical point. Some additional reference results are also presented for the pure Baxter-Wu model.

Simulation of non-equilibrium dynamics: Harnessing finite-size effects to measure ageing in the 2D Ising model (P)

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The finite-size effects in a 2D Ising model with nearest-neighbour interactions are investigated at $T = 0.1T_c$ with respect to the two-time autocorrelation function $C(t, s)$ where t is the observation and s the waiting time. Using an ansatz established for the spherical model linking the resulting plateaus in $C(t, s)$ to waiting time s and lattice size L , a precise and reproducible estimation for the autocorrelation exponent λ and dynamical exponent z is developed.

Universal fragility of spin-glass ground-states under single bond changes

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We consider the effect of perturbing a single bond on ground states of nearest-neighbor Ising spin glasses, with a Gaussian distribution of the coupling constants, across various two and three-dimensional lattices and regular random graphs. Our results reveal that the ground-states are strikingly susceptible to such changes. Altering the strength of only a single bond beyond a critical threshold value leads to a new ground state that differs from the original one by a droplet of flipped spins whose boundary and volume diverge with the system size – an effect that is reminiscent of the more familiar phenomenon of disorder chaos. These elementary fractal-boundary zero-energy droplets and their composites feature robust characteristics and provide the lowest-energy macroscopic spin-glass excitations. Remarkably, within numerical accuracy, the size of such droplets conforms to a nearly universal power-law distribution with exponents dependent on the spatial dimension of the system. Furthermore, the critical coupling strengths adhere to a stretched Gaussian distribution that is predominantly determined by the local coordination number.