DY 51: Poster: Stat. Phys., Comp. Meth

Time: Thursday 15:00–18:00 Location: Poster B2

DY 51.1 Thu 15:00 Poster B2

Random Field Ising Model with spatially disorder strength gradient — •Christoph Polle and Alexander K. Hartmann — Institut für Physik, University of Oldenburg, Germany

We study numerically [1] a three-dimensional Random Field Ising Model (RFIM) in which a spatially disorder strength gradient $h(x)$ is introduced. The gradient was chosen so that $h(x)$ is equal to the critical value $h_c = 2.28$ [2] at the half of the lattice in x-direction. The actual magnetic field acting on a spin i is defined as $h_i = h(x) * n_i$, where n_i is a (0,1) quenched Gaussian number.

To investigate the system efficiently the RFIM was transformed to a network, then the maximum flow problem was solved to determine the ground state [3]. This is done for different system sizes and realizations. From the ground state the magnetization, a specific-heat like quantity and the susceptibility where calculated as a function of x. Also the system was analyzed in the spirit of gradient percolation problems[4].

[1] A.K. Hartmann, Big Practical Guide to Computer Simulations, World Scientific Publishing, Singapore 2015.
[2] A.K. Hartmann and A.P. Young, Physical Rewiew B **64**, 214419 (2001).
[3] J.-C. Picard and H.D. Ratliff, Networks **5**, 357 (1975).
[4] B. Sapoval, M. Rosso, J.-F. Gouyet, Journal de Physique Lettres **46** (4), pp.149-156 (1985).

DY 51.2 Thu 15:00 Poster B2

Semi-automatic construction of Lattice Boltzmann models — •Dominic Spiller[1] and Burkhard Duenweg[1,2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Department of Chemical Engineering, Monash University, Melbourne, Australia

A crucial step in constructing a Lattice Boltzmann model is the definition of a suitable set of lattice velocities, and the correct assignment of the associated weights. The poster outlines the functioning of a publicly available Python script which has been written to assist researchers in that task. The speed of sound c_s is considered as a parameter, which can, within limits, be chosen at will. Under this premise, the Maxwell–Boltzmann constraint equations are a system of linear equations to determine the weights, and hence amenable to numerical solution by standard linear algebra library routines. By suitable contractions, the tensor equations are mapped to a set of equivalent scalar equations, which simplifies the treatment significantly. Using a singular-value decomposition, the software is able to distinguish between (i) no solution, (ii) one unique solution, and (iii) infinitely many solutions. Case (ii) is analyzed in detail, and the range of permitted c_s values is calculated. The script can treat arbitrary spatial dimensions, and an arbitrarily large degree of isotropy, measured in terms of tensorial velocity moments of the weights. New models that have been found in two and three dimensions are isotropic up to tenth order.

DY 51.3 Thu 15:00 Poster B2

Self-learning Monte Carlo Methods — •Kai Meinerz and Simon Trebst — ITP, University of Cologne

The application of machine learning approaches has seen a dramatic surge across a diverse range of fields that aim to benefit from their unmatched core abilities of dimensional reduction and feature extraction. In the field of computational many-body physics machine learning approaches bear the potential to further improve one of the stalwarts in the field * Monte Carlo sampling techniques. Here we explore the capability of *self-learning* Monte Carlo approaches to dramatically improve the update quality in Markov chain Monte Carlo simulations. We implement such a self-learning approach using restricted Boltzmann machines which are trained to learn the probability distribution of the configuration space and are then used to suggest updates that are almost always accepted, thereby dramatically reducing autocorrelation effects. It can, in principle, be applied to all existing Monte Carlo flavors and is tested here for both classical and quantum Monte Carlo techniques applied to a variety of many-body problems.

DY 51.4 Thu 15:00 Poster B2

Finite temperature structure of Hybrid Perovskites from ab-initio and classical MD — •Jonathan Lahnsteiner[1], Georg Kresse[1], Jurn Heinen[2], and Menno Bokdam[1] — [1]University of Vienna — [2]University of Amsterdam

Determining the finite temperature structure of the hybrid perovskite MAPbI3 is a challenge for both experimental and theoretical methods. A very powerful computational method that can resolve the atomic structure is molecular dynamics (MD). The resulting structure depends on the density functional approximation (DFA) in the case of ab-initio MD and the force field in classical MD. We compare the structure between 250 K and 400 K obtained with different DFAs and force fields in one consistent manner. In a previous study, we observed a low level of a dynamic correlation between MA molecules in large scale PBEsol MD calculations. Therefore the relative ordering of the neighboring organic molecules as well as the symmetry of the PbI3 framework is analyzed. The distribution function of the molecules is used to map out an effective energy surface for the rotation of a single molecule. This surface is accurately modeled by a pair of cubic harmonics. Available experimental data in literature are compared to the structure obtained with the different methods. The spread in these data is still too large to uniquely determine the method that *best* describes the perovskite, however promising candidates and outliers have been identified. In agreement with our previous benchmarking study based on RPA perturbation theory calculations , we find the SCAN functional is the most likely choice for the MD calculations of the hybrid perovskite.

DY 51.5 Thu 15:00 Poster B2

Entropy Production in Non Equilibrium Steady State Systems — •Timon Wittenstein, Marius Bause, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

Entropy production is believed to contain structural information of non-equilibrium steady states. For further insight, the entropy production is calculated along an ensemble of stochastic off-equilibrium trajectories. By fixing start and end point, a localized entropy production for a transition between two states in conformational space is introduced. The trajectory based entropy production is compared to statistics based Markov State Model and a theory based value on a minimal two dimensional model. This quantity is a special case of the detailed fluctuation theorem by Crooks and extends detailed balance towards non-equilibrium steady states. Trajectory based calculation of local entropy production can be used for improved sampling in simulation or as a physics based constrained for Markov Sate Modeling.

DY 51.6 Thu 15:00 Poster B2

Phase transition for parameter learning of Hidden Markov Models — •Nikita Rau[1], Jörg Lücke[2], and Alexander K. Hartmann[1] — [1]Institut of Physics, University of Oldenburg — [2]Department of Medical Physics, University of Oldenburg

We study by computer simulations [1] the learning process during which the parameters of Hidden Markov Models (HMMs) [2] are estimated from a sequence of observed data which is generated artificially. Using the Baum-Welch algorithm [3], an Expectation-Maximization algorithm from the field of Machine Learning, we are capable of observing the learning process of different sized HMMs. By changing the amount of accessible learning data and its noise level, we observe a phase-transition-like change in the performance of the learning algorithm. For bigger HMMs and more learning data, the learning behaviour improves tremendously by reaching a certain threshold in the noise strength. Before reaching the threshold, the parameter-learning is prone to errors, after exceeding it, the learning process becomes nearly perfect. This observation is strongly dependant of the amount of learning data.

[1] A. K. Hartmann, Big Practical Guide to Computer Simulations, World-Scientific, Singapore 2015)
[2] R. Durbin, S. Eddy, A. Krogh, and G. Mitchison, Biological Sequence Analysis (Cambridge University Press 2001)
[3] L. E. Baum, Ann. Math. Statist., vol. 41, 164–171, 1970

DY 51.7 Thu 15:00 Poster B2

Critical Exponent ν of the Ising Model in Three Dimensions with Long-range Correlated Disorder — •Stanislav Kazmin[1,2] and Wolfhard Janke[1] — [1]University of Leipzig — [2]Max Planck Institute for Mathematics in the Sciences

We analyze the critical behavior of the site-diluted Ising model in three dimensions using Monte-Carlo simulation techniques. The case of uncorrelated defects is compared to the long-range correlated case where the space correlation function between the defects obeys a power-law decay. We discuss different methods of critical exponent ν extraction and compare our results to theoretical predictions.

DY 51.8 Thu 15:00 Poster B2

A Theoretical Investigation of Hydrocarbon Decomposition at High Temperature and High Pressure — •Nehzat Safaei, Kurt Kremer, and Omar Valsson — Max Planck Institute for Polymer Research, Ackerman- nweg 10, 55128, Mainz, German

We have studied reaction kinetics of hydrocarbon decomposition at high pressures and temperatures using variationally enhanced sampling method. Investigation of hydrocarbons decomposition witch provides valuable information about the rate of radical creation and subsequent reactions, specially at extreme conditions where there is a serious lack of both thermodynamic and kinetic data, can reveals new insights to the synthesis of most interesting carbon-based compounds such as graphene and nanodiamond which are the promising materials for a variety of applications. In order to calculate the decomposition rate of hydrocarbons in different thermodynamics conditions, we have performed molecular dynamics simulation to explore the phase space of different systems of hydrocarbons with different chain lengths. Variationally enhanced sampling method along with metadynamics is employed to calculate the rate of decomposition reactions. In this approach, an effective bias potential is constructed and implemented as a fixed bias which speeds up the molecular dynamics time by facilitating escape over dissociation barrier. We employed metadynamics with an infrequent deposition stride to ensure that the trajectory does not stuck in any regions. We have measured the validity of the rare event assumption by the p-value test of cumulative distribution function of the data fitted to the Poisson expression.

DY 51.9 Thu 15:00 Poster B2

Non-flat histogram techniques in application to complex free energy landscapes — •Fabio Mueller, Stefan Schnabel, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

Simulation of systems with rugged free-energy landscapes such as spin glasses and polymers are intrinsically difficult and algorithmic improvements for such systems are still needed to enlighten the nature of their low-temperature phase. We developed Monte Carlo non-flat histogram methods, which base on parametric optimization of well-known flat histogram techniques in generalized ensembles, tailored explicitly for systems with complex free-energy landscapes.

DY 51.10 Thu 15:00 Poster B2

Critical properties of long-range ferromagnetic quantum Ising chains — •Stephan Humeniuk — Institut für Theoretische Physik III, Universität Stuttgart — Current address: Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

The ferromagnetic Ising chain is of great historical value, being one of the first models for which a Kosterlitz- Thouless (KT) transition was found and due to its important role in the creation of renormalization group theory [1,2]. In this work some gaps are filled in in the understanding of this well-studied model in the presence of a transverse field, notably the role of a diverging kink size for observing the KT transition in finite-size simulations. The quantum critical point of the inverse-square ferromagnet is highly anisotropic in real space and imaginary time, with a dynamical critical exponent z=1/2.

[1] Anderson et al., PRB 1, 4464 (1970); Kosterlitz, PRL 37, 1577 (1976). [2] Bhattacharjee et al., PRB 24, 3862 (1981).

DY 51.11 Thu 15:00 Poster B2

Serially-Connected Domain Model for Phase Transitions in Disordered Porous Solids — •Henry R.N.B. Enninful, Adrianna Wójciak, Dirk Enke, and Rustem Valiullin — Leipzig University, Leipzig, Germany

Detailed elucidation of the pore structure of (nano-)porous solids is important for their optimization for various applications such as energy storage, separations and catalysis. While existing characterization approaches work well for ordered, single-pore mesoporous solids, the complex morphological structure of pore network and accompanying them cooperativity effects in phase transitions render the currently used approaches inapplicable for disordered materials.

In this work, we demonstrate the potentials of a recently developed connected domain model (CDM), which intrinsically contains both the structural complexity and cooperativity effects [1]. It is essentially based on a statistical average over linear chains of pores connected to each other and takes account of the change of the transition mechanisms depending on the phases state in adjacent pores. The model is validated by comparing its predictions to the results of GCMS simulations and is further used to rationalize the freezing and melting transitions in a family of porous glasses with different pore sizes.

[1] D. Schneider; D. Kondrashova; R. Valiullin, *Phase transitions in disordered mesoporous solids*, Scientific Reports, 2017, 7, 7216.