DY 66: Poster: Stat. Phys. (Gen., Critical Phen., Biol.)

Time: Thursday 15:30–18:00 Location: Poster A

DY 66.1 Thu 15:30 Poster A

Phase transitions in highly diverse ecosystems — •Mattes Heerwagen and Andreas Engel — Carl-von-Ossietzky Universität Oldenburg, Oldenburg, Deutschland

Ecosystems with many different species and resources are complex systems. Much of our understanding of such ecosystems derives from low-dimensional models with just a few interacting species and a small number of different resources. Nevertheless, most real systems are characterized by a high degree of biodiversity. Recently, Tikhonov and Monasson [1] showed with methods from statistical physics that high dimensional ecosystems may exhibit two phases: a "vulnerable" one with relatively few survivors and, above a critical degree of biodiversity, a "shielded" one in which the competing species cooperate to protect each other from variations in the resource supply and where the number of survivors reaches a maximum. We extend the model of Tikhonov and Monasson to analyse more heterogeneous ecosystems with different types of generalists and specialists. We study the two phases in this more general setting and determine the critical line of the phase transition.

[1] M. Tikhonov and R. Monasson, Collective Phase in Resource Competition in a Highly Diverse Ecosystem, Phys. Rev. Lett. 118, 048103 (2017)

DY 66.2 Thu 15:30 Poster A

The longest increasing subsequence of a sequence problem: A large deviation study — •Jörn Börjes, Hendrik Schawe, and Alexander K. Hartmann — Institut für Physik, Carl von Ossietzky Universität Oldenburg

The longest increasing subsequence (LIS) problem asks for the longest subsequence in which the elements are in sorted order, lowest to highest and part of the given sequence with length n. The elements indices of the sequence do not need to be continuous to become a LIS. There is an exact mapping between a specific polynuclear growth model and the so called LIS problem [1]. This problem is numerically solved by an algorithm with complexity $O(n \log n)$. We study the distribution of the length of the LIS up to the large deviations. We compare our numerical results to the analytically known results. Using specific large-deviation approaches [2], probability distributions can be sampled over a large range of the support, down to probabilities like 10^{-40}.

[1] Satya N. Majumdar and Sergei Nechaev, Phys. Rev. E 69
[2] A.K. Hartmann Phys. Rev. E 65, OSG 202 (2002)

DY 66.3 Thu 15:30 Poster A

Towards a classification of nonequilibrium steady states via invariant manifolds — •Jens Lucht, Prakhar Godara, Marco Giacomo Mazza, and Stephan Herminghaus — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen

Nonequilibrium steady states (NESS) give rise to nontrivial cyclic probability fluxes that breach detailed balance (DB), and thus it is not clear how to define a potential analog to equilibrium case. We argue that there is a formal way to define such a NESS potential for systems describable by a Fokker-Planck equation. DB in NESS can be restored [1] by mapping the phase space into a parameterized family of non-intersecting cycles containing the invariant manifolds of the corresponding deterministic, dynamical system. Transition rates between neighboring cycles are obtained from the microscopic dynamics, i.e., from the drift and diffusive currents. Since fluxes between cycles obey DB, we can integrate over the set of cycles. We present some evidence that this gives us a nonequilibrium potential which reaches minimum solely for NESS.

[1]: Phys. Rev. E., 2012, 85, 041133

DY 66.4 Thu 15:30 Poster A

Non-Flat Histogram Techniques for Spin Glasses — •Fabio Mueller, Stefan Schnabel, and Wolfhard Janke — Institut fuer Theoretische Physik, Universitaet Leipzig, Postfach 100 920, 04009 Leipzig, Germany

We take into consideration the 3D Edwards-Anderson model with bimodal bond distribution. The spin-glass nature of the model implies that finding ground states is an NP-hard problem. The round-trip times, defined as the time one simulation method needs for a specific disorder realization in order to travel from the ground state to the high energy region and back therefore reflects the ability of the method to solve that specific optimization problem.

Employing different simulation techniques the round-trip time distributions are investigated and the performance of the different methods is compared. The methods taken into consideration are among the most established broad-energy ensemble methods including the parallel-tempering method and, in addition, a specially designed non-flat histogram technique which is shown to outperform the currently existing methods.

DY 66.5 Thu 15:30 Poster A

Self-learning Monte Carlo simulations of classical and quantum many-body systems — •Kai Meinerz and Simon Trebst — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

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. Such a self-learning approach employs reinforcement learning techniques to learn the distribution of accepted updates and is 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 66.6 Thu 15:30 Poster A

study ab Initio of the effect of a-Site substitution on the fe1.12te system — •Mir Ali — Computational Physics Laboratory of Materials, Liabes Djillali University of Sidi Bel-Abbes, Algeria

Abstract: In the present work, our aim is to verify the structural, electronic and magnetic properties of both systems Fe1.12Te and *RTX*(R = Fe, X = Te and T = Ni, Co) in the P4/nmm structure. For this task, we use the density functional theory (DFT) as a theoretical tool integrated into wien2k code (Blaha 2001). The solid Fe1 xMxTe (M =Ni, Co) have been synthesized by Kazakov et al.(Chem.Met. Alloys 3, 155*160 2010). They have observed a systematic shift of the lattice parameters for both systems for M = Ni and Co till x = 0.1, then a second phase with the NiAs-type structure appeared when x passes 0.15. Fe1-xNixTe retains its structure in a concentration between x = 0.1 and 0.15, and Fe1-xCoxTe retains its structure when x is between 0.05 and 0.1 (Blaha 2001)[1]. [1].Blaha, P., Schwarz, K., Madsen, G.K.H., Kvasnicka, D., Luitz,J.: WIEN2K,An Augmented Plane Wave plus Local Orbitals Program for Calculating Crystal Properties. Vienna University of Technology, Austria (2001).

DY 66.7 Thu 15:30 Poster A

Wave localization in locally centrosymmetric disordered lattices — •Christian Morfonios[1], Malte Röntgen[1], and Peter Schmelcher[1,2] — [1]Zentrum für Optische Quantentechnologien, Universität Hamburg — [2]Center for Ultrafast Imaging, Universität Hamburg

Since the work of Anderson, disorder in a medium is known to generically induce wave localization due to multiple destructive interference, in turn suppressing the transport through a sample. This may be altered by different forms of correlations between the constituents of the disordered medium which typically lead to the delocalization of wave excitations on configuration average, as indicated by various measures. On the other hand, the presence of global centrosymmetry (spatial inversion symmetry) in an otherwise disordered system has recently been argued to enhance the transport efficiency between given sites via delocalized parity eigenstates. Seeing local centrosymmetry - restricted to different subparts of the system - as a particular type of correlation, we address the question of its impact on wave localization and transport properties in one-dimensional tight-binding lattices.

DY 66.8 Thu 15:30 Poster A

Irreversible Markov chains in spin models: Topological excitations — •Ze Lei[1] and Werner Krauth[1,2] — [1]Ecole Normale Superieure, Paris, France — [2]The University of Tokyo, Tokyo, Japan

We analyze the convergence of the irreversible event-chain Monte Carlo algorithm for continuous spin models in the presence of topological excitations.

In the two-dimensional XY model, we show that the local nature of the Markov-chain dynamics leads to slow decay of vortex–antivortex correlations in comparision with the fast decorrelation of spin waves.

We propose an assignment algorithm for pairing vortices and antivortices, and show that the maximum vortex–antivortex distance follows a Fréchet description. The contributions of topological excitations to the equilibrium correlations vary from a dynamical critical exponent $z \sim 2$ at the critical temperature to $z \sim 0$ in the limit of zero temperature.

In the harmonic approximation of spin waves for dimensions higher than 2, we confirm the event-chain algorithm's fast relaxation (corresponding to $z = 0$). Its mixing times however remain much larger than equilibrium correlation times at low temperatures.

We also describe the respective influence of topological monopole–antimonopole excitations and of spin waves on the event-chain dynamics in the three-dimensional Heisenberg model.

We expect that the fast relaxation of phonon modes explains the success of the event-chain algorithm at high densities for particle systems.

DY 66.9 Thu 15:30 Poster A

Occupation time statistics for single molecule dynamics — •Alessio Lapolla and Aljaz Godec — Mathematical Biophysics Group, Max-Planck-Institute for Biophysical Chemistry (Göttingen)

State-of-the art experimental methods nowadays routinely probe dynamical properties of individual molecules, and thereby provide unprecedented insight into biophysical phenomena at low-copy numbers. Yet, despite the consensus about its relevance, a general theory of single molecule dynamics remains elusive.

Namely, most available experimental techniques are limited by short, typically subergodic observation times. As a result, their interpretation cannot rely neither on ensemble statistical mechanics nor ergodic theory. This poses the need for a statistical mechanics of time-averaged observables, explicitly taking into account the fluctuations between different realizations.

In our work we focused on the statistics of occupation time: the fraction of time a random process spends in any given region of configuration space. We obtained rigorous general results for the lower order moments of the occupation time in Markovian dynamics, which go beyond large-deviation theory. To illustrate the predictive power of the theory we provide exact results for a selection of simple diffusive models of single-molecule dynamics.

DY 66.10 Thu 15:30 Poster A

Accounting for the context-dependent effects in the modelling of synthetic genetic circuits — •Johannes Falk[1], Maleen Hanst[2], Heinz Koeppl[2], and Barbara Drossel[1] — [1]Technische Universität Darmstadt, Institut für Festkörperphysik, Germany — [2]Technische Universität Darmstadt, Bioinspired Communication Systems, Germany

Synthetic biology aims at designing modular genetic circuits that can be assembled according to the desired function. When embedded in a cell, a circuit module becomes a small subnetwork within a larger environmental network, and its dynamics is therefore affected by interactions with the environment. The environment not only causes extrinsic noise but also memory effects, which means that the dynamics of the subnetwork is affected by its past states via a memory function that is characteristic of the cellular environment. Using a modification of the Mori-Zwanzig projection formalism, we show how the modifications of the subnetwork dynamics due to the environment can be calculated for stochastic models. In particular, we derive analytical expressions of memory kernels for specific classes of environments that are derived from linear reaction networks. Furthermore, we present computer simulation results showing how the environment can destroy the periodic oscillations displayed by the isolated subnetwork.

DY 66.11 Thu 15:30 Poster A

Effects of a flexible pinning on the statics and dynamics of a thermalized thin sheet — •Josip Augustin Janeš[1,2], Daniel Schmidt[2], Udo Seifert[3], and Ana-Sunčana Smith[1,2] — [1]Institute Ruđer Bošković, Zagreb, Croatia — [2]PULS Group, Department of Physics and Cluster of Excellence: EAM, FAU Erlangen-Nürnberg, Erlangen, Germany — [3]II. Institut für Theoretische Physik, Universität Stuttgart, Stuttgart, Germany

Mechanical characteristics of freely suspended 2D membranes are commonly determined from their fluctuation spectrum. However, this task is significantly more challenging for the case of membranes attached by proteins to underlying scaffolds. Actually, a complete theoretical description of the effect of a pinning on the dynamic correlations in a membrane is still missing. Here we rectify this situation by modelling the spatial and dynamic correlations by several complimentary analytical methods. We construct a complete theoretical framework for the problem in question and validate our approach by obtaining excellent agreement with the explicit Langevin simulations.

DY 66.12 Thu 15:30 Poster A

Superposition of survival curves as a tool for epistasis analysis of longevity interventions — Stefan Nowak[1,2], Johannes Neidhart[1,2,3], •Jonas Rzezonka[1,2], Ivan G. Szendro[1,2], Rahul Marathe[1,2,4], and Joachim Krug[1,2] — [1]Sybacol, Universität zu Köln, Köln, Germany — [2]ITP, Universität zu Köln, Köln, Germany — [3]MBR Optical Systems, Wuppertal, Germany — [4]Department of Physics, IIT Delhi, New Delhi, India

A problem in ageing research is to understand how different factors contributing to longevity should be expected to act in combination under the assumption that they are independent. Standard epistasis analysis compares the extension of mean lifespan achieved by a combination of interventions to the prediction under an additive or multiplicative null model, but neither model is fundamentally justified. Moreover, the target of longevity interventions is not mean life span but the entire survival curve. We formulated superposition principles that predict the survival curve resulting from a combination of two interventions based on the survival curves of the individual treatments, and quantify epistasis as the deviation from this prediction [1]. We test the method on a published data set comprising survival curves for all combinations of 4 different longevity interventions in *Caenorhabditis elegans* [2]. We find that epistasis is generally weak even when the standard analysis indicates otherwise.

[1] Nowak S, Neidhart J, Rzezonka J, Szendro IG, Marathe R and Krug J (2017) bioRxiv https://doi.org/10.1101/147173.
[2] Yen K, Mobbs CV (2010). AGE 32:39-49

DY 66.13 Thu 15:30 Poster A

Reweighting Simulation in and out of Equilibrium — Marius Bause, Tristan Bereau, and •Kurt Kremer — Max Planck Institute for Polymer Research, Mainz, Germany

Markov State Models(MSM) are a discrete representation of the kinetics of a given system constructed by course-graining microtrajectories. While frequently applied to equilibrium systems, a protocol for driven steady state systems has not been developed due to loss of dynamic properties like detailed balance. We propose to apply the principle of Maximum Caliber by Jayne's, postulating that the distribution of paths is given by the maximal path entropy encoding a chosen set of prior information. This reduces the computational effort of constructing an MSM by providing new microscopic relations from macrosopic path-ensemble assumptions. Simultaneously the markovian assumption alleviates the combinatorial explosion of microtrajetories. The method is tested on a minimal model under non-conservative forces.

DY 66.14 Thu 15:30 Poster A

Conformational dynamics of growing polymers under non-stationary conditions — •Jörn H. Appeldorn, Ali Malek, and Reiner Kree — Inst. f. Theoret. Physik, Univ. Göttingen, Friedrich-Hund. Pl. 1, 37077 Göttingen

The time scales of conformational evolution of a poylmer chain and of ongoing polymerization reactions may become comparable for living polymers and for biopolymer reactions. In particular this happens under non-stationary conditions, if the polymerization velocity decreases, for example due to depletion of monomers or activators. We extend both the Rouse model and the dynamical model of a semi-flexible chain in the approximation of constant average line tension to include instationary growth with velocities decreasing as $t^{-\gamma}$. We demonstrate and discuss the appearance of well-defined dynamical transitions in a dragged chain and in a chain in homogeneous shear flow, which are signalled by sudden, qualitative changes in conformational or rheological properties as functions of γ.

DY 66.15 Thu 15:30 Poster A

Synaptic Miniature Transmitter Release:Random in Nature or Partly Deterministic? — •Daungruthai Jarukanont — University of Kassel, Kassel

The mechanism of how synaptic terminals release neurotransmitters by spontaneous vesicle fusion is still unclear. *Since the early work of Fatt and Katz (1952), the spontaneous release of neurotransmitters is assumed to be a purely stochastic process that occurs randomly and can be described by Poisson processes. In this work, we investigate the statistical behavior of the miniature excitatory postsynaptic currents (mEPSCs) in mouse Hippocampal neurons, and of the miniature excitatory junctional potentials(mEJPs) in the neuromuscular junctions (NMJ) of Drosophila larvae. We find that, in contrast to the previous assumptions, neither mEPSCs nor mEJPs could be described the Poisson process. Instead, the inter-event interval histograms of the mEPSCs from mouse Hippocampal neurons are well described by inverse-Gaussian distributions, while the inter-event interval histograms of mEJPs in the neuromuscular junctions of Drosophila larvae are well fitted by gamma distributions. Further study and analysis is still needed to understand the mechanism of the spontaneous release of neurotransmitter. However, it is clear from our analysis that the spontaneous release process is partly-deterministic and not random like as is currently assumed.

DY 66.16 Thu 15:30 Poster A

Two Perspectives on the Condensation-Evaporation Transition — •Franz Paul Spitzner[1], Johannes Zierenberg[1,2], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig Postfach 100 920, 04009 Leipzig, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Göttingen, Germany

The particle condensation-evaporation transition is a standard example of a first-order phase transition. In equilibrium, the consideration may be reduced to the coexistence of a homogeneous gas phase and an inhomogeneous phase consisting of a single macroscopic droplet with surrounding vapour. The transition can either be driven by density or temperature – keeping the respective "orthogonal" quantity constant. While this problem can be rigorously treated only at fixed temperature and in two dimensions, a heuristic derivation of the leading-order finite-size scaling behaviour exists that holds for the transition at fixed temperature and at fixed density.

We present how the well known multicanonical method can be adopted to the grand canonical ensemble, allowing us to investigate the condensation-evaporation transition of a 2D Lennard-Jones gas in both regimes. The careful adjustment of simulation parameters and subtle implementation choices will be discussed, in order to provide insight into the method and consistent results that support the existing prediction of the scaling behaviour.

DY 66.17 Thu 15:30 Poster A

Integer quantum Hall transitions on tight-binding lattices — •Martin Puschmann[1,2], Philipp Cain[1], Michael Schreiber[1], and Thomas Vojta[2] — [1]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Department of Physics, Missouri University of Science and Technology, Rolla, MO, United States

We investigate the integer quantum Hall transition in the lowest Landau band of two-dimensional tight-binding lattices for non-interacting electrons affected by a perpendicular magnetic field. Specifically, we consider both simple square lattices, where Landau levels are broadened by random potentials, and random Voronoi-Delaunay lattices in which (topological) disorder is introduced by bonds between randomly positioned sites. Based on a recursive Green function approach, we calculate the smallest positive Lyapunov exponent describing the long-range behavior of the wave function intensities along a quasi-one-dimensional lattice stripe. In both systems, we observe that the critical exponent of the localization length takes a value of $\nu \approx 2.60$. Our critical estimates, thus, coincide with those based on the semi-classical Chalker-Coddington (CC) network model, see e.g. [1]. They do not agree with the reduced critical exponent, $\nu \approx 2.37$, found by Gruzberg et al. in a recently proposed geometrically disordered CC model [2].

[1] K. Slevin and T. Ohtsuki, Phys. Rev. B 80, 041304 (2009)
[2] I. A. Gruzberg et al., Phys. Rev. B 95, 125414 (2017)

DY 66.18 Thu 15:30 Poster A

Full Counting Statistics of the non-equilibrium Dicke model — •Christopher W. Wächtler and Gernot Schaller — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We consider the single-mode Dicke-Hamiltonian coupled to two Markovian bosonic baths at different temperatures. In the thermodynamic limit the closed system untergoes a second order quantum phase transition from a normal phase to a superradiant phase as the atom-field coupling is increased. In this work, we microscopically derive a generalized master equation with counting fields. We use it to describe the non-equilibrium steady state with constant energy or heat flow through the system. By the use of full counting statistics [1] we investigate for finite system size the energy current as well as its higher moments for evidence of the underlying quantum phase transition. Additionally we consider the thermodynamic limit of the system and disspators by means of a Holstein-Primakoff transformation and displaced bosonic modes [2].

[1] M. Esposito *et al.*, Rev. Mod. Phys. 81, 1665 (2009).
[2] C. Emary, T. Brandes, PRE 67, 66203 (2003).

DY 66.19 Thu 15:30 Poster A

Directed negative-weight percolation — •Christoph Norrenbrock, Mitchell Mkrtchian, and Alexander K. Hartmann — Carl-von-Ossietzky Universität Oldenburg, Oldenburg (Germany)

We consider a directed variant of the negative-weight percolation model [1] in a two-dimensional, periodic, square lattice. The problem exhibits edge weights which are taken from a distribution that allows for both positive and negative values. Additionally, in this model variant all edges are directed. For a given realization of the disorder, a minimally weighted loop/path configuration is determined by performing a non-trivial transformation of the original lattice and solving a minimum weight perfect matching problem. For this problem, fast polynomial-time algorithms are available, thus we could study large systems with high accuracy. Depending on the fraction of negatively and positively weighted edges in the lattice, a continuous phase transition can be identified, whose characterizing critical exponents we have estimated by a finite-size scaling analysis of the numerically obtained data. We observe a strong change of the universality class with respect to standard directed percolation, as well as with respect to undirected negative-weight percolation.

[1] Melchert, O. and Hartmann, A. K., New J. Phys. **10** 043039 (2008)

DY 66.20 Thu 15:30 Poster A

Critical exponents from a Landau-like approach — •Sören Sanders — Carl von Ossietzky Universität, Oldenburg, Deutschland

Landau's approach to continuous phase transitions provides an effective theory for the description around the critical point but falls short in correctly establishing non-trivial critical exponents. Using the example of the Mott-insulator to superfluid transition of the Bose-Hubbard model, we derive from the microscopic properties a Landau-like description not restricted by this limitation and correctly reproduce the best known value for the critical exponent β of the XY-universality class.