DY 56: Poster - Statistical Physics

Statistical Physics (general); Statistical Physics far from Thermal Equilibrium; Statistical Physics in Biological Systems; critical phenomena

Time: Thursday 16:00–18:00 Location: Poster A

DY 56.1 Thu 16:00 Poster A

From classical to quantum and back: Hamiltonian coupling of classical and Path Integral models of atoms — Karsten Kreis[1,2], Davide Donadio[1], Kurt Kremer[1], and •Raffaello Potestio[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Graduate School Materials Science in Mainz, Mainz, Germany

Quantum delocalization of atomic nuclei affects the physical properties not only of low temperature systems, such as superfluid helium, but also of room temperature molecules containing light atoms. An accurate modeling of these effects can be achieved making use of the Path Integral formulation of Quantum Mechanics, which is however computationally very demanding. By restricting this numerically expensive description to a small region of space, while modeling the remaining atoms as classical particles, the amount of computational resources required for a simulation can be significantly reduced. In the present work we derive a Hamiltonian formulation for a bottom-up, theoretically solid coupling between a classical model and a Path Integral description of the same system. The validity of this approach is demonstrated by means of simulations of low temperature parahydrogen.

DY 56.2 Thu 16:00 Poster A

The symmetric Anderson impurity model in a continuum limit of the Hubbard model — •Yahya Öz and Andreas Klümper — Bergische Universität Wuppertal

Starting from a generalizaton of the Hubbard model by use of Shastry's R-matrix with two independent spectral parameters an integrable lattice model can be constructed, which yields the symmetric Anderson impurity model in the continuum with all interaction parameters. We use the continuum limit for the deriviation of the thermodynamic equations of the symmetric Anderson impurity model from those of the Hubbard model. We consider two alternative formulations and obtain the infinite set of TBA equations, but also a finite set of nonlinear integral equations which allows a much more efficient numerical treatment.

DY 56.3 Thu 16:00 Poster A

Large deviations in Taylor diffusion — •Marcel Kahlen and Andreas Engel — Institut für Physik, Universität Oldenburg, Deutschland

Diffusion of particles in streaming liquids is ubiquitous. Taylor diffusion addresses the dispersion of particles in shear flow.

Using a large-deviation principle, we approximate the time dependent particle distribution for large times in a Taylor diffusion setting with N layers. The stochastic transitions of the particles between the layers is modelled as a Markovian jump process. Applying the contraction principle to the rate function for the empirical density of this process as given by Donsker and Varadhan, we obtain a set of non-linear equations for the lateral particle distribution at large times. For the simplest case of $N = 2$ layers the contraction can be performed analytically and reproduces known results. In the general case a linearisation yields an approximate solution which we compare with simulation results.

DY 56.4 Thu 16:00 Poster A

Transverse correlation functions in the Ising antiferromagnet on the anisotropic kagome lattice — •Walter Apel[1] and Hans-Ulrich Everts[2] — [1]PTB Braunschweig, PSt4, 38116 Braunschweig — [2]LUH, Inst. f. Theoret.Physik, 30167 Hannover

We study the anisotropic kagome Ising antiferromagnet, i.e. a model in which the coupling along one of the three directions differs from the couplings along the other two directions.

In previous work [J of Statistical Mechanics: Theory and Experiment 2011], we calculated rigorously the correlation function parallel to the chains. Now, we devise a method to calculate rigorously the correlation functions transverse to the chains. The phase diagram and first results for the correlation functions are given.

DY 56.5 Thu 16:00 Poster A

Poly(3-hexylthiophene) (P3HT) Molecules Interacting with Au(001) Substrates — •Momchil Ivanov, Jonathan Gross, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig

One of the main objectives of this project is to gain, with the help of computer simulations, a better understanding of adsorption properties and recognition of surface patterns of macromolecules such as polymers and proteins when interacting with material surfaces and nanoparticles (external constraints), and of the interplay of these phenomena with polymer collapse, crystallization, aggregation and folding (internal constraints). This study reports on an approach to combine the experimental observation of polymer chain conformations adsorbed on a metal surface with coarse-grained Monte Carlo simulations. P3HT chains with a maximum length of 60 monomers were simulated in contact with an Au(001) surface and the end-to-end distance as well as the radius of gyration of the molecules were determined.

DY 56.6 Thu 16:00 Poster A

Computer Simulations of Semiflexible Polymers in Disordered Environments — •Johannes Bock and Wolfhard Janke — ITP Leipzig

We report computational studies of the behavior of semi-flexible polymers in disordered media. An off-lattice chain growth algorithm based on the Monte Carlo method is used to examine configura- tional properties of the polymers such as the end-to-end distance and tangent-tangent correlation. Particular attention is paid to the comparison of the occuring phenomena in two and three dimensions.

DY 56.7 Thu 16:00 Poster A

Comparability of microcanonical data sampled by Molecular Dynamics and Monte Carlo simulations — •Philipp Schierz, Johannes Zierenberg, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

In this work we performed microcanonical simulations with statistical Monte Carlo (MC) sampling [1,2,3] and dynamical Molecular dynamics (MD) integrations. Our aim was to get both methods into agreement which needed a careful consideration of the conservation laws we encountered in MD simulations [4,5]. We applied a time series reweighting technique to transform the MD sampling to the full NVE ensemble without conservation laws. For a higher number of degrees of freedom the differences between the simulation techniques diminished as expected. We adapted the known multi histogram reweighting technique WHAM to use it for microcanonical MD simulation data. Therefore we got an estimate of the density of states from MD simulations. For this procedure we needed an accurate knowledge of the sampled ensembles.

[1] J. R. Ray, Phys. Rev. A 44 (1991) 4061.

[2] B.A. Berg and T. Neuhaus, Phys. Lett. B 267 (1991) 249; Phys. Rev. Lett. 68 (1992) 9;

[3] W. Janke, Int. J. Mod. Phys. C 03 (1992) 1137; Physica A 254 (1998) 164.

[4] R. Lustig, J. Chem. Phys 100 (1994) 3048.

[5] F. Calvo, J.P. Neirotti, D.L. Freeman, and J.D. Doll, J. Chem. Phys 112 (2000) 10350.

DY 56.8 Thu 16:00 Poster A

crumpling of plastic wires in spherical cavities — ali farnudi[1], javad najafi[2], m reza shaebani[3], and •mehdi habibi[1,4] — [1]Department of Physics, Institute for Advanced Studies in Basic Sciences, Zanjan, Iran — [2]Department of Experimental Physics, Saarland University, Saarbrucken, Germany — [3]Department of Theoretical Physics, Saarland University, Saarbrucken, Germany — [4]Van der Waals-Zeeman Institute, University of Amsterdam, Amsterdam, The Netherlands

We study the morphology of crumpled plastic wires irreversibly packed into spherical cavities. The total length of the injected wire follows a power-law dependence on the relative system size, that is the ratio of sphere and wire radii. The exponent (or, equivalently, the mass-size fractal dimension) depends on the friction coefficient between the

wire and the cavity walls, reflecting friction-dependent structural differences. While ordered coil formation is partially observed at low frictions, highly disordered structures emerge at large friction limit, where the number of folds exhibits a power-law scaling in the relative system size. The probability distribution of the fold-size broadens and becomes more asymmetric for relatively larger spheres. We present a self-avoiding random walk model for the injection of the plastic wire at high friction regime, which provides a new insight into the underlying mechanism and remarkably reproduces the experimental results.

DY 56.9 Thu 16:00 Poster A

Infinitesimal Monte Carlo Algorithms — •Manon Michel[1], Sebastian C. Kapfer[2], and Werner Krauth[1] — [1]Laboratoire de Physique Statistique, 24 rue Lhomond 75005 Paris France — [2]Institut für Theoretische Physik 1 Staudtstr. 7 91058 Erlangen Germany

Monte Carlo methods, most notably the Metropolis algorithm, are a powerful tool in statistical physics. But local random walks induce a high rate of rejections, making any simulations around a phase transition point too expensive. To address this problem, we reformulate the Metropolis algorithm at the most fundamental level, upgrading the diffusive dynamics to a convective one. We therefore construct a new framework for Monte Carlo algorithms, based on a new factorization of the Metropolis acceptance probability. It leads to a class of rejection-free Markov chain Monte Carlo algorithms for sampling general multidimensional probability distributions, without introducing discretizations in time or in space [1]. These algorithm break detailed balance yet satisfy global balance. They generalize the recent and successful hard-sphere event-chain Monte Carlo method and were recently used in bidimensional melting with soft interactions. Finally, this new framework allows direct access to quantities as pressure and stress in multiparticle systems. Generally, it leads also to new insights on elastic constants derivation from first principles, yielding a precise determination of existence of hexatic phase[2].

[1] M. Michel, S. C. Kapfer, W. Krauth, Journal of Chemical Physics 140 54116 (2014)

[2] M. Michel, S. K. Kapfer, W. Krauth, manuscript in preparation

DY 56.10 Thu 16:00 Poster A

Deriving elasticity theory for non-ideal crystals: application to cluster crystals — •Johannes Häring, Matthias Fuchs, and Christof Walz — Universität Konstanz, 78457 Konstanz

For non-ideal crystals density fluctuations can be expressed by deformations of the underlying lattice structure plus changes in the occupancy of the single lattice sites. In our approach these density variations from a equilibrium density play the role of the displacement from the equilibrium position in normal elasticity theory.

Through classical density functional theory it is possible to obtain the hydrodynamic equations of motion, a wave equation , expressions for the constants of elasticity and the isothermal compressibility.

A well-known model for cluster crystals, the so called generalized exponential model is used to demonstrate the capability of the theory because its big differences in occupancy of each lattice site (e.g. fluctuations from 12 to 15 particles per lattice site) lead to a significant deviation from the ideal crystal.

DY 56.11 Thu 16:00 Poster A

Stiff Directed Lines in Random Media — •Horst-Holger Boltz and Jan Kierfeld — TU Dortmund, Dortmund, Germany

We investigate the behaviour of stiff directed lines with bending energy in a random medium. We show that a stiff directed line in 1+d dimensions undergoes a localization transition with increasing disorder for d>2/3. We demonstrate that this transition is accessible by numerical transfer matrix calculations in 1+1 dimensions and analyze the properties of the disorder-dominated phase. On the basis of the two-replica problem, we propose a relation between the localization of stiff directed lines in 1+d dimensions and of directed lines under tension in 1+3d dimensions, which is strongly supported by identical free energy distributions. This shows that pair interactions in the replicated Hamiltonian determine the nature of directed line localization transitions with consequences for the critical behavior of the Kardar-Parisi-Zhang (KPZ) equation. Furthermore, we quantify how the persistence length of the stiff directed line is reduced by disorder. Additionally, we study the depinning of stiff directed lines. Their equation of motion is the (quenched) Herring-Mullins equation, which also describes surface growth governed by surface diffusion. We employ analytical arguments and numerical simulations to determine the critical exponents and compare our findings with previous works and functional renormalization group results, which we extend to the different line elasticity. We see evidence for two distinct correlation length exponents.

DY 56.12 Thu 16:00 Poster A

Second law-like inequality for periodic, feedback-driven quantum engines — •Michael Bauer, Kay Brandner, Michael Schmid, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

A genuine feature of projective quantum measurements is that they inevitably alter the mean energy of the observed system if the measured quantity does not commute with the Hamiltonian of the observed system. Compared to the classical case, Jacobs proved that this additional energetic cost leads to a stronger bound on the work extractable after a single measurement from a system initially in thermal equilibrium [Phys. Rev. A 80, 012322 (2009)]. Here, we show that the same bound holds for a large class of feedback-driven quantum engines operating periodically and in finite time. The bound thus implies a natural definition for the efficiency of information to work conversion in such devices.

For a simple model consisting of a laser-driven two level system, we maximize the efficiency with respect to the observable whose measurement is used to control the feedback protocol. We find that the optimal observable typically does not commute with the Hamiltonian and hence would not be available in a classical two level system. This result reveals that periodic feedback engines operating in the quantum realm can exploit quantum coherences to reach high efficiency.

DY 56.13 Thu 16:00 Poster A

Brownian motion with external force: investigation of validity of the Jarzynski equality — •Nina Megier and Walter T. Strunz — Institut für Theoretische Physik, TU Dresden

We examine a harmonic oscillator coupled linearly to a harmonic bath. Initially our system of interest is in equilibrium, at later times it is driven far away from equilibrium by a time dependent force. We investigate both, the classical and the quantum case for the validity of the Jarzynski equality, also in strong coupling limit. Our analysis is based on the Gaussian statistics of the stochastic force acting on the harmonic oscillator in the Langevin picture.

DY 56.14 Thu 16:00 Poster A

Fluctuating efficiency for a microscopic Carnot engine — •Johannes Hoppenau — Carl-von-Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

Recently the probability density function of the efficiency of microscopic heat engines gained particular interest. In [1,2] G. Verley et al. analyze the distribution of efficiencies by using large deviation techniques. We propose a simple model of a microscopic Carnot engine to illustrate their results. In addition, we analyze the efficiency distribution in the limiting case of slow driving. Even in this case we find strong fluctuations of work and heat not compatible with a normal distribution of these quantities.

[1] G. Verley, M. Esposito, T. Willaert, and C. Van den Broeck, Nat. Commun. 5, 4721 (2014).

[2] G. Verley, T. Willaert, C. Van den Broeck, and M. Esposito, Phys. Rev. E 90, 052145 (2014).

DY 56.15 Thu 16:00 Poster A

A minimalistic but realistic evolutionary food web model — •Tobias Rogge, Barbara Drossel, and Korinna T. Allhoff — TU Darmstadt, Germany

We present an evolutionary food web model that includes no population dynamics but is nevertheless able to generate a large variety of complex, multi-trophic networks with an ongoing turnover of species. The nodes represent species, which are characterized by three traits, namely body mass, feeding center and feeding range. These traits also define the links to other species in the network representing feeding and competition interactions.

The evolutionary algorithm starts with a simple initial network. At each iteration step, a new species is added to the system as a modification of a randomly chosen parent species. This "mutant" changes the environment for those species that now have a new predator, prey or competitor species. Some species are therefore removed from the system, if they no longer fulfill a survival criterion that depends on the interactions of the species. Subsequently, the next "mutant" is introduced. In contrast to many other evolutionary food web models,

population dynamics is not explicitely taken into account. However, its effects are captured in the survival criterion. Thus, realistic network structures emerge and evolve with little computational effort. The model is therefore a valuable tool to evaluate statistical properties over long timescales, over a large parameter space, and for larger communities of coupled networks. We present selected results obtained from our simulations of the model.

DY 56.16 Thu 16:00 Poster A

Markov state modeling of polymers in shear flow — •Fabian Knoch and Thomas Speck — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany

The dynamical properties of polymers driven by shear flow have been investigated intensively. In shear flows, polymers show a coil to globular transition. This switch-like dynamics is not only relevant in the context of biology (proteins flowing through blood vessels are also exposed to shear flows) but also from the point of non-equilibrium statistical dynamics. We study numerically a generic polymer model [1]. Instead of performing constant shear rate simulations, we investigate the dynamics subjected to constant interparticle stress σ_{const}. Similar to the constant shear rate case, the constant stress simulations also show a switch-like dynamics depending on σ_{const}. Using stochastical thermodynamics, we develop a new method to construct dynamical Markov state models [2] for polymers in shear flow.

[1] Alexander-Katz, A. and Schneider, M. F. and Schneider, S. W. and Wixforth, A. and Netz, R. R., PRL 97(13), 2006
[2] Noé, F. and Horenko, I. and Schütte, C. and Smith, J. C., J. Chem. Phys. 126(15), 2007

DY 56.17 Thu 16:00 Poster A

Markov State Model with reweighting: application to small molecules with perturbed potential — Luca Donati and •Bettina Keller — Freie Universität Berlin, Berlin, Germany

We have studied the effect of small perturbations in the potential energy surface of molecular systems by performing numerical simulations and constructing Markov State Model of the trajectories. The Markov State Models are a valid tool to analyze the large amounts of data generated by Molecular Dynamics simulations and to extract information on the timescales. In general, it is necessary to perform a new simulation after having changed the potential to construct the Markov State Model of the perturbed molecule. However, if we consider small perturbations of the system, we can use reweighting methods [1] to construct a Markov State Model that does not need a new simulation, but that uses the trajectory of the initial not-perturbed molecule. Our method is based on the Girsanov theorem [2], that has been already tested successfully for diffusive processes (e.g. a double well potential perturbed by an external force). We applied it on small molecules subjected to alchemical transformations. We studied the effect of varying the charges and the van der Waals radii on the conformational dynamics. The approach is relevant to force-field optimization, but it could eventually also be used to study mutations in proteins.
[1] Jan-Hendrik Prinz et.al., The Journal of Chemical Physics, **134**, 2011
[2] Schütte Christof et.al., Molecular Physics, **00**, 2014

DY 56.18 Thu 16:00 Poster A

Vortex arrays and mesoscale turbulence of self-propelled particles — •Robert Großmann[1], Pawel Romanczuk[2], Markus Bär[1], and Lutz Schimansky-Geier[3] — [1]Physikalisch-Technische Bundesanstalt, Abbestraße 2-12, 10587 Berlin, Germany — [2]Princeton University, Princeton, New Jersey 08543, USA — [3]Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany

We present a self-propelled particle model with Turing-like interactions: short-range alignment and anti-alignment at larger distances. The model is able to produce polarly ordered states, periodic vortex patterns and mesoscale turbulence, which resembles observations in dense suspensions of swimming bacteria. The model allows a systematic derivation and analysis of a kinetic theory as well as hydrodynamic equations for density and momentum fields. A phase diagram with regions of pattern formation as well as orientational order is obtained from a linear stability analysis of these continuum equations. Microscopic Langevin simulations of self-propelled particles are in agreement with these findings.

DY 56.19 Thu 16:00 Poster A

Emergent large-scale structures of Boolean networks optimized for criticality — Marco Möller[1] and •Tiago P. Peixoto[2] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt — [2]Institut für Theoretische Physik, Universität Bremen

We construct statistical ensembles of modular Boolean networks which are constrained to lie at the critical line between frozen and chaotic dynamic regimes. The ensembles are maximally random given the imposed constraints, and thus represent null models of critical networks. The structures of the ensembles undergo several phase transitions from a fully random structure to several ordered ones, including a prominent core-periphery structure, and an "attenuated" two-group structure, where the network is divided in two groups of nodes, and one of them has Boolean functions with very low sensitivity. This shows that such simple large-scale structures are the most likely to occur when optimizing for criticality, in the absence of any other constraint or competing optimization criteria.

DY 56.20 Thu 16:00 Poster A

Characterization of K-Complexes and Slow Wave Activity in a Neural Mass Model — Arne Weigenand[1], •Michael Schellenberger Costa[1], Hong-Viet Victor Ngo[1,2], Jens Christian Claussen[3,1], and Thomas Martinetz[1] — [1]Institut für Neuro- und Bioinformatik, Univ. Lübeck — [2]Institut for Medical Psychology and Behavioral Neurobiology, Univ. Tübingen — [3]Computational Systems Biology Lab, Jacobs Univ. Bremen

NREM sleep is characterized by two hallmarks, namely K-complexes (KCs) during sleep stage N2 and cortical slow oscillations (SOs) during sleep stage N3. While the underlying dynamics on the neuronal level is well known and can be easily measured, the resulting behavior on the macroscopic population level remains unclear. On the basis of an extended neural mass model of the cortex, we suggest a new interpretation of the mechanisms responsible for the generation of KCs and SOs [1]. As the cortex transitions from wake to deep sleep, in our model it approaches an oscillatory regime via a Hopf bifurcation. Importantly, there is a canard phenomenon arising from a homoclinic bifurcation, whose orbit determines the shape of large amplitude SOs. A KC corresponds to a single excursion along the homoclinic orbit, while SOs are noise-driven oscillations around a stable focus. The model generates both time series and spectra that strikingly resemble real electroencephalogram data and points out possible differences between the different stages of natural sleep.
[1] A. Weigenand, M. Schellenberger Costa, H-VV Ngo, JC Claussen, T. Martinetz, PLoS Comput Biol 10, e1003923 (2014)

DY 56.21 Thu 16:00 Poster A

Wilson-Cowan oscillators as minimal bifurcation models of Non-REM sleep — •Annika Reinke[1], Arne Weigenand[1], and Jens Christian Claussen[2,1] — [1]Institut für Neuro- und Bioinformatik, Univ. Lübeck — [2]Computational Systems Biology Lab, Jacobs Univ. Bremen

When sleep deepens to sleep stages N2 and N3, specific oscillations emerge, namely speep spindles in N2, and slow oscillations and K complexes in N3. While several models, after sufficient fit of parameters, can be made to reproduce experimental data, often several parameter sets or even slightly different models yield similar match with data. This calls for a simplification of the models. Here we adopt standard models of neural oscillators that are generic for a normal form of the same bifurcation phenomenology, and compare them to EEG time series. We conclude that a simple Wilson-Cowan oscillator can be adapted to exhibit the essential bifurcations when transiting to N2 and N3, including the canard phenomenon associated with the onset of the anharmonic sleep oscillations.

DY 56.22 Thu 16:00 Poster A

On the effect of the drive on self-organized criticality — Marco Winkler[1], •Johannes Falk[2], and Wolfgang Kinzel[1] — [1]Institute of Theoretical Physics, University of Würzburg, 97074 Würzburg, Germany — [2]Institute for Condensed Matter Physics, Technical University of Darmstadt, 64289 Darmstadt, Germany

The well known Sandpile model of self-organized criticality generates avalanches of all length and time scales, without tuning any parameters. In the original models the external drive selects sites randomly. We analyse a drive which depends on the present state of the system, namely the effect of favouring sites with a certain height in the deposition process. We investigate, that the system stays in a critical state, if sites of height three are favoured. Our numerical results indicate the

same universality class as the original model with random deposition, although the stationary state is approached very differently. In contrast, when favouring sites of height two, only avalanches which cover the entire system occur. Furthermore, we study the distributions of sites with a certain height, as well as the transient processes of the different variants of the external drive.

DY 56.23 Thu 16:00 Poster A

Multifractal analysis of states in Voronoi-Delaunay lattices — •Martin Puschmann, Philipp Cain, and Michael Schreiber — Institute of Physics, Technische Universität Chemnitz, Chemnitz

The Voronoi-Delaunay lattice (VDL) is a set of nearest-neighbor connections between randomly positioned sites. It is a simple model for amorphous solids and foams. We consider the transport of non-interacting electrons in this lattice and assume that all connections have the same strength. Consequently, the VDL is topologically disordered by connectivity only. Whether this form of disorder is sufficient to obtain localized states in two- and three-dimensional lattices was studied by the multifractal analysis of electronic wave functions and the finite-size scaling approach. We observe localized states in both dimensionalities with energies very close to the band edges. A localization-delocalization transition was found only in the three-dimensional lattice, in accordance with the localization theory. The corresponding critical exponent of localization is equal to the exponent of the orthogonal Wigner-Dyson class. Furthermore, we analyzed the case of additional random on-site potentials in the three-dimensional lattice. We obtain a phase diagram by varying the disorder strength of these potentials. The mixing of these different disorders does not affect the critical exponent.