DY 17: Statistical Physics (General) I

Time: Tuesday 10:00–12:45 Location: H19

DY 17.1 Tue 10:00 H19

Fluctuations and correlation functions of occupation measures in single-file diffusion — •Alessio Lapolla and Aljaz Godec — Mathematical Biophysics Group, Max Planck Institute for Biophysical Chemistry, Goettingen, Germany

Dynamical processes in statistical physics are predominantly Markovian, at least within a sufficiently high-dimensional setting. However, single-particle experiments in fact probe functionals of lower-dimensional projected dynamics, which typically turns out to be non-Markovian. While the statistical behavior of functionals of trajectories of Markov processes is meanwhile rather well understood, much less is known about the respective behavior in non-Markovian systems. We will present rigorous results for fluctuations and two-tag correlations of bounded additive functionals of ergodic Markov processes having a diagonalizable propagator. Our results relate the statistics of functionals on arbitrary time-scales to the relaxation eigenspectrum. As an application, we will present exact results for one- and two-tag local times in single-file diffusion (SFD), which is central to several phenomena, i.e. the transport in biological channels. In SFD individual particles diffuse in a narrow, effectively one-dimensional channel, which prevents their crossing. Tagging the trajectory of a particular particle corresponds to a projection to a one-dimensional system and introduces a persistent memory. Our analytical results unveil the intricate meaning of such a projection-induced memory on a trajectory level and allow for a detailed analysis of related experiments.

[1] Alessio Lapolla and Aljaž Godec *New J. Phys.* **20** 113021, 2018

DY 17.2 Tue 10:15 H19

Universal Finite-Size Scaling for Kinetics of Phase Separation in Multicomponent Mixtures — Suman Majumder[1], •Subir K. Das[2], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany — [2]Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur P.O., Bangalore 560064, India

From Kawasaki-exchange Monte Carlo simulations of the q-state Potts model, we present results for the kinetics of phase separation in multicomponent mixtures, for $q \leq 10$, in space dimension $d = 2$. A particular focus has been on the quantification of finite-size scaling functions for various values of q and quench depths. For a range of final quench temperatures, our analyses, via finite-size scaling and other state-of-the-art methods, show that the growth follows the Lifshitz-Slyozov behavior, expected for a diffusive mechanism, irrespective of the number of components. We show that the growth for different q values and quench temperatures, in finite systems, can be described by a universal scaling function with a nonuniversal metric factor, originating from the differences in the amplitudes. We also demonstrate the morphological and kinetic equivalence between a q-component equal proportion mixture and an off-critical binary mixture, in the framework of the Ising model, with relative concentration of the minority component in the latter being $x_c = 1/q$.

DY 17.3 Tue 10:30 H19

Effective temperatures in equilibrium: ring statistics in 2D-silica — Projesh Kumar Roy and •Andreas Heuer — Institut f. Phys. Chemie, WWU Münster

The thermodynamic properties of subsystems in strong interaction with the neighborhood can largely differ from the standard behavior. For example the energy distribution of a harmonic dumbbell in a solvent can be described as if it would experience a broad distribution of temperatures, albeit with the correct average temperature [1]. Here we analyse for the case of 2D-silica [2] the energy distribution for rings of a given size via computer simulations [3]. It turns out that the observed energy distribution of also displays non-standard behavior. However, the observed energy distribution is related to a single strongly reduced temperature as compared to the temperature of the heat bath. This effective temperature approaches the temperature of the heat bath for larger ring sizes. From a systematic analysis of the 1D Ising model and an analytically solvable model we suggest that these observations reflect the presence of strong local energy correlations [4].

[1] P.D. Dixit, Phys. Chem. Chem. Phys.17, 13000 (2015).

[2] L. Lichtenstein, M. Heyde, and H.-J. Freund, J. Phys. Chem. C 116, 20426 (2012).

[3] P. K. Roy, M. Heyde, and A. Heuer, Phys. Chem. Chem. Phys. 20, 14725 (2018).

[4] P. K. Roy, A. Heuer, arXiv:1808.03869; Phys. Rev. Lett. (accepted)

DY 17.4 Tue 10:45 H19

Strong Coupling and non-Markovian Effects in the Statistical Notion of Temperature — •Camilo Alfonso Moreno and Juan Diego Urbina — Institut für Theoretische Physik, Universität Regensburg, Germany

We investigate the emergence of temperature T in the system-plus-reservoir paradigm starting from the fundamental microcanonical scenario at total fixed energy E. As shown by Schwinger [1] for the regime of weak coupling γ between system and environment, $T(E)$ emerges from the saddle-point analysis that leads to the usual ensemble equivalence in the thermodynamic limit [2]. By extending these ideas for finite γ, in [3] we provide a consistent generalization of temperature $T(E, \gamma)$ in strongly coupled systems and we illustrate its main features for the specific model of Quantum Brownian Motion where it leads to consistent microcanonical thermodynamics. Interestingly, we show that while this $T(E, \gamma)$ is a monotonically increasing function of the total energy E, its dependence with γ is a purely quantum effect drastically different for Markovian and non-Markovian regimes. We also derive a generalization of the idea of equivalence of ensembles for systems with finite coupling and discuss possible issues when the observables are not smooth and must be taking into account in the saddle-point analysis.

[1] P. C. Martin, J. Schwinger, *Phys. Rev* **6**, 115 (1959).
[2] N. J. Morgenstern, *Quantum Statistical Field Theory* (2017)
[3] C. A. Moreno, J. D. Urbina, *arXiv:1811.12110*, (2018).

DY 17.5 Tue 11:00 H19

Isotropic-anisotropic phase transition in a three-dimensional lattice model of sticky rods — •Paul Quiring, Miriam Klopotek, and Martin Oettel — Institute for applied Physics, Theoretical and Computational Soft Matter/Nano-Science and Experimental Colloidal Physics, Tübingen, Germany

We investigate the isotropic-anisotropic phase transition in a three-dimensional lattice model of 1x1xL-sized hard rods with nearest-neighbor attractions using grand-canonical Monte Carlo simulations. We find that the topology of the phase diagram strongly depends on the rod length L.

For higher temperatures and L>4, we generally find a very weak first order isotropic-nematic transition as in the corresponding system with no attractions [1]. There is no appreciable widening for increasing attractions. For L=8 and decreasing temperature, this transition line ends in a quasi-tricritical point, below which there is a first-order transition between an isotropic vapor and a nematic liquid.

For L=5, the critical point for the liquid-vapor transition between isotropic states is not affected. The nematic order is of "layered-disordered" type, i.e. one of the three directions is suppressed. The line of isotropic-nematic transitions presumably ends in a critical endpoint on the liquid side of the binodal.

[1] A. Gschwind, M. Klopotek, Y. Ai und M. Oettel, "Isotropic-nematic transition for hard rods on a three-dimensional cubic lattice", Physical Review E, Bd. 96, Nr. 1, S. 012 104, 2017.

15 min. break

DY 17.6 Tue 11:30 H19

The Ising model on finite projective geometries — •Kai Klede and Klaus Mecke — Institut für Theoretische Physik 1, FAU Erlangen-Nürnberg

Various attempts to reconcile quantum field theories with general relativity have not yet led to a breakthrough in the construction of a unified theory of quantum gravitation. We investigate a fundamentally new approach to quantum spacetime, using finite projective geometries, that inherently incorporate finite features in the model of spacetime. In order to understand this geometry better, the Ising Model is studied on two dimensional finite projective spaces, over finite fields of prime order. I will discuss in particular numerical results for the critical be-

havior, suggesting a notion of system size, proportional to the square root of the field order.

DY 17.7 Tue 11:45 H19

The phases of a 2D lattice system of hard rods 'through the eyes' of unsupervised and generative machine-learning algorithms — •Miriam Klopotek, Shang-Chun Lin, Cristoph Mony, Paul Quiring, and Martin Oettel — Institute for Applied Physics, University of Tübingen, Germany

There has been a recent burst of effort from the statistical physics community to apply machine learning algorithms to workhorse lattice spin models, e.g. often the Ising, XY, but also other variants [1,2]. We examine how unsupervised and generative machine learning algorithms 'interpret' raw configurational data in a different model that is very simple in construction, yet nontrivial with respect to its spatial structure and phases. It entails global and local orientational ordering, anisotropies, both continuous transitions and phase coexistence, and is non-fully-packed [3]. The neural-network architectures we test are convolutional autoencoders, variational autoencoders, as well as generative adversarial networks. We pay special attention to the internally-learned, 'boiled-down' representation of the data – the *latent space* variables – which correlate with the order parameters [2].

[1] Carrasquilla and Melko, *Nat. Phys.* **13**, 431 (2017). Hu, Singh and Scalettar, *PRE* **95**, 062122 (2017). Ch'ng, Vazquez, and Khatami, *PRE* **97**, 013306 (2018)., *etc.*
[2] S. Wetzel., *PRE* **96**, 022140 (2017).
[3] Longone, Linares, and Ramirez-Pastor, *JCP* **132**, 184701 (2010). Mortazavifar and Oettel, *PRE* **96**, 032608 (2017).

DY 17.8 Tue 12:00 H19

Discovering physical concepts with neural networks — •Raban Iten, Tony Metger, Henrik Wilming, Lidia del Rio, and Renato Renner — Institute for Theoretical Physics, ETH Zürich, 8093 Zürich, Switzerland

We introduce a neural network architecture that models the physical reasoning process and that can be used to extract simple physical concepts from experimental data without being provided with additional prior knowledge. We apply the neural network to a variety of simple physical examples in classical and quantum mechanics, like damped pendulums, two-particle collisions, and qubits. The network finds the physically relevant parameters, exploits conservation laws to make predictions, and can be used to gain conceptual insights. For example, given a time series of the positions of the Sun and Mars as observed from Earth, the network discovers the heliocentric model of the solar system - that is, it encodes the data into the angles of the two planets as seen from the Sun. Our work provides a first step towards answering the question whether the traditional ways by which physicists model nature naturally arise from the experimental data without any mathematical and physical pre-knowledge, or if there are alternative elegant formalisms, which may solve some of the fundamental conceptual problems in modern physics, such as the measurement problem in quantum mechanics.

DY 17.9 Tue 12:15 H19

Low-energy physics of the bilinear-biquadratic spin-1 chain — •Moritz Binder and Thomas Barthel — Department of Physics, Duke University, Durham, North Carolina 27708, USA

The bilinear-biquadratic spin-1 chain features various interesting quantum phases, including the Haldane phase, a dimerized phase, and an extended critical phase. Here, we apply an efficient density matrix renormalization group (DMRG) algorithm utilizing infinite boundary conditions [1] to compute precise dynamic spin structure factors for a comprehensive set of points in the phase diagram. Analyzing both dynamic spin and quadrupolar correlations, we gain detailed insights into the nature of low-lying excitations of the model. We compare our results to Bethe ansatz solutions at the SU(3)-symmetric ULS point and the TB point as well as at the pure biquadratic point, which can be mapped to an anisotropic spin-1/2 XXZ chain in the gapped Néel phase. In the Haldane phase, we relate our results to the approximate description in terms of the non-linear sigma model.

[1] M. Binder and T. Barthel, Phys. Rev. B **98**, 235114 (2018).

DY 17.10 Tue 12:30 H19

Multiscale model for heterogeneous catalysis in open-cell metal foam structures — •Sebastian Mühlbauer, Severin Strobl, and Thorsten Pöschel — Institute for Multiscale Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg

Heterogeneous catalysis in metallic or ceramic foam structures represents a very promising alternative to catalysis in packed beds or monoliths. Due to high porosity, specific surface and tortuosity, these structures provide excellent mass transport properties at moderate pressure drops. To investigate the reaction rate in such open-cell foam structures in the mass transfer limited regime, we develop a particle based simulation software. We combine an isotropic, lattice-free variant of Stochastic Rotation Dynamics with specialized boundary condition capable of modeling inlet and outlet for reactive flow. The foam structure itself is modeled as an inverse sphere packing, which is described via constructive solid geometry.

Using the developed simulation tool, we first investigate the flow through single unit cells for a wide range of parameters. The gathered results are then condensed to relations for pressure drop and reaction rate, which can be validated based on experimental data. Exploiting the derived relations, we follow a multiscale approach enabling us to investigate reactive flow through complex porous metal foam structures on macroscopic scale. We apply this multiscale model to find optimum foam structures which, for example, minimize flow resistance, while maximizing the reaction rate in a macroscopic catalytic converter.