DY 44: Poster Session: Statistical Physics and Critical Phenomena

Time: Thursday 15:00–18:00 Location: P2

DY 44.1 Thu 15:00 P2

How to distinguish between indistinguishable particles — •Michael te Vrugt — Institut für Theoretische Physik, Center for Soft Nanoscience, Philosophisches Seminar, 48149 Münster, Germany

Does exchanging two indistinguishable particles lead to a new physical state? While the answer appears to be clear in quantum mechanics (no), the situation in *classical* statistical mechanics is up to considerable debate. In this work [1], we show that order-preserving dynamics, a recently developed formalism that allows for an accurate treatment of single-file diffusion within dynamical density functional theory, provides a strong argument for haecceitism (the view that such an exchange does make a difference) since it requires treating observationally indistinguishable particle configurations as being different. This result turns out to have interesting consequences for the concept of thermodynamic equilibrium.

[1] M. te Vrugt, Br. J. Phil. Sci. (forthcoming), doi: 10.1086/718495

DY 44.2 Thu 15:00 P2

Operationally Accessible Uncertainty Relations for Thermodynamically Consistent Semi-Markov Processes — •Benjamin Ertel, Jann van der Meer, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Semi-Markov processes generalize Markov processes by adding temporal memory effects as expressed by a semi-Markov kernel. We recall the path weight for a semi-Markov trajectory and the fact that thermodynamic consistency in equilibrium imposes a crucial condition called direction-time independence for which we present an alternative derivation. We prove a thermodynamic uncertainty relation that formally resembles the one for a discrete-time Markov process. The result relates the entropy production of the semi-Markov process to mean and variance of steady-state currents. We prove a further thermodynamic uncertainty relation valid for semi-Markov descriptions of coarse-grained Markov processes that emerge by grouping states together. A violation of this inequality can be used as an inference tool to conclude that a given semi-Markov process cannot result from coarse-graining an underlying Markov one. We illustrate these results with representative examples [1].

[1] Benjamin Ertel, Jann van der Meer and Udo Seifert, Phys. Rev. E 105, 044113 (2022)

DY 44.3 Thu 15:00 P2

Lane formation of gravitationally driven model colloids in two-dimensional linear channels — •Marc Isele, Kay Hofmann, and Peter Nielaba — Physics Department, University of Konstanz, Konstanz, Germany

We conducted Brownian dynamics simulations to investigate the segregation phenomena of driven model colloids in two-dimensional linear channels. Two kinds of spherical particles of different sizes were driven in the same direction by a gravitational force. The difference in driving force acting on these particles creates a segregation similar to the lane formation of oppositely driven colloids. We had a closer look at parameter values facilitating lane formation and the resulting lanes were examined more closely. This approach creates a system which is easier to reproduce in experiments than the conventional oppositely driven setups by tilting a linear channel with two particle kinds of different size.

DY 44.4 Thu 15:00 P2

Geometric Brownian Information Engine : Essentials of optimal work and performance. — •Rafna Rafeek, Syed Yunus Ali, and Debasish Mondal — Department of Chemistry and Center for Molecular and Optical Sciences & Technologies, Indian Institute of Technology Tirupati, Yerpedu 517619, Andhra Pradesh, India

We investigate a Geometric Brownian Information Engine (GBIE) in the presence of an error-free feedback controller that transforms the information gathered on the state of particles entrapped in mono-lobal geometric detention into extractable work. We determine the benchmarks for utilizing the available information in an output work and the optimum operating requisites for best performance. Apart from a reference measurement distance xm and feedback site xf , upshots of the information engine also depend on the transverse constant bias force(G). G tunes the entropic contribution in the effective potential and the standard deviation (σ) of the equilibrium marginal probability distribution.

We find that the upper bound of the achievable work shows a crossover from (5/3-2ln2)kBT to 1/2kBT when the system changes from entropy to an energy-dominated one.The higher loss of information during the relaxation process, accredits the lower value of work in entropic instances of GBIE. We recognize that the work extraction reaches a global maximum when xf=2xm with xm=0.6σ, irrespective of the extent of the entropic limitation. Also we explore the effect of entropic control on the unidirectional passage of the particle and efficacy of the GBIE.

DY 44.5 Thu 15:00 P2

Shear flow induced instability of a trapped colloidal particle in a complex medium — •Lea Fernandez and Sabine H.L. Klapp — Institute for Theoretical Physics, TU Berlin

The motion of a colloidal particle in a complex medium, bound by an optical trap and subjected to a shear flow can be modelled by the Lanvegin equations for an over-damped harmonic oscillator in n dimensions. Here we treat n_{obs} observed, physical variables, with $n = n_{obs} + n_{int}$, and n_{int} internal, auxiliary variables modelling a complex medium. Analytical and numerical results are presented for $n_{obs} = 2$ and $n_{int} = 1$, where the coupling between the observed variables is given by a plane Couette flow. We analyse the dynamics of averages, probability densities, and trajectories using Brownian dynamics and the Smoluchowski equation. Of special interest is the effect of the coupling with the auxiliary variable. The focus is on coupling parameters where the steady shear flow causes a transition from a stationary state to an in-stationary state, corresponding to a delocalisation of the particle, when the shear rate exceeded a critical value.

DY 44.6 Thu 15:00 P2

Quantifying the potential energy landscape within nanoconfinements by MD simulations — •Simon Hefner, Robin Horstmann, and Michael Vogel — TU Darmstadt, Institut für Physik kondensierter Materie, Hochschulstr. 6, 64289, Darmstadt, Germany

Nanoconfinements find applications in various fields from catalysis to electronics, [1] although the properties of confined systems are still not fully understood. For instance, the effects of different kinds of confinements on the dynamical and structural properties of confined liquids are still elusive. To obtain a better understanding of those effects MD simulations are well suited [2]. Here, we performed simulations for TIP4P/2005 water. Neutral pores of water were prepared. From the time-averaged static density profile in the pore the potential energy landscape was reconstructed and the energy barrier against water motion at the wall and in bulk were calculated and compared. We calculated the temperature and radial dependence of the energy barrier. The translational dynamics of water can be derived form the obtained energy landscape using the Arrhenius law. We further applied these methods to other kinds of pore systems and liquids and compared the results.

[1] Clancy,Adam J. et al. Chem. Rev., **2018**, *118* (16), 7363-7408
[2] Horstmann, R. et al, Langmuir, https://doi.org/10.1021/acs.langmuir.2c005

DY 44.7 Thu 15:00 P2

Fluctuations of work and heat in a driven entropic potential — •Syed Yunus Ali, Prashanta Bauri, and Debasish Mondal — Department of Chemistry and Center for Molecular and Optical Sciences & Technologies, Indian Institute of Technology Tirupati, Yerpedu 517619, Andhra Pradesh, India

We consider the motion of an over-damped Brownian particle in two-dimensional bilobal confinement driven by a periodic field in the presence of a transverse bias force. The confinement results in an entropic bistable potential in a reduced dimension. We calculate the work done and absorbed heat over a period and their mean and relative variance fluctuations in entropy and energy-dominated regimes. The average work done and absorbed heat over a period show turnover behavior as a function of noise strength and frequency input. Therefore, these observables can be considered potential quantifiers of the entropic stochastic resonance phenomena. We find that the heat fluctuations

over a single period are always greater than the work fluctuations. We also discuss the applicability of steady-state fluctuation theorems in this system.

DY 44.8 Thu 15:00 P2

Exploiting Brownian motion and correlations for computing — •Alessandro Pignedoli[1] and Karin Everschor-Sitte[2] — [1]Twist Group, Faculty of Physics, University of Duisburg-Essen — [2]Twist Group, Faculty of Physics, University of Duisburg-Essen

Brownian motion is a natural phenomenon that can be exploited for computing [1]. Particle swarm optimization [2] based on the ideas of swarm intelligence is an example of this sort of computation. While the random motion of particles allows the exploration of the entire phase space of the system, interactions and driving forces break ergodicity. This allows for an efficient solution to an optimization problem, which can be identified by looking at the system's correlations and statistical observables. To accomplish Brownian computation, we employ a Langevin model to describe magnetic skyrmions [3], which are topologically stable magnetic whirls that have been shown to behave like interacting Brownian particles [4].

[1] C.H. Bennett, Int. J. Theor. Phys. 21, 905 (1982). [2] J. Kennedy and R. Eberhart, Proc. of ICNN'95 * Int. Conf. on Neural Networks, 4, 1942 (1995) [3] K. Everschor-Sitte, J. Masell, R. M. Reeve and M. Kläui, J. Appl. Phys. 124, 240901 (2018) [4] J. Zázvorka, et al. Nat. Nanotechnol. 14, 658 (2019)

DY 44.9 Thu 15:00 P2

Overload wave-memory induces amnesia of a self-propelled particle — •Maxime Hubert[1], Stéphane Perrard[2], Nicolas Vandewalle[3], and Matthieu Labousse[4] — [1]PULS group, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]PMMH, ESPCI Paris and PSL University, Paris, France — [3]GRASP, University of Liège, Liège, Belgium — [4]Guliver, ESPCI Paris and PSL University, Paris, France

"Walking droplets" constitute a model system to investigate active transport dynamics driven by complex memory kernels. The droplet stores positional information in a wavefield at an oil interface that in return serves as a propulsive mechanism. The complexity of the wavefield and the amount of positional information are remotely controlled through a single scalar value, the memory of the system, which corresponds to the persistence time of the waves. In this study, we investigate the high-memory limit of both the droplet and the wavefield dynamics. We show that an overload of memory brings the droplet to a diffusive dynamics which cannot be distinguished from a active markovian dynamics. The wavefield however contains all the correlations of the dynamics and exhibits an energy-minimization principle and equipartition of energy in the eigenmodes of the wavefield.

DY 44.10 Thu 15:00 P2

Coarse-graining of systems with discrete Markovian dynamics — Stefan Klumpp and •Miguel Rodríguez Martín — Institute for the Dynamics of Complex Systems, University of Göttingen, Göttingen.

There exists a wide range of physical systems that can be described by discrete Markovian dynamics. In many cases it is desirable to reduce the number of states in order to lower the computational cost or obtain an effective description that captures the most relevant effects at a given scale. A steady state-conserving method of coarse graining based on merging adjacent states and obtaining new transition rates from the optimization of the Kullback-Leibler divergence is generalized by minimizing the Rényi divergence instead. The resulting transition rates depend on the quotients between the steady state probabilities of the merged states in the original system, so a method is developed to compute these transition rates without the need of finding the steady state probabilities. Making use of the similarities between the master equation and Schrödinger's equation, a formulation for classical discrete Markov processes analogous to quantum mechanics is developed, both in the frame of Schrödinger's formulation and second quantization. These are used to study coarse graining under the constraint that the steady state must be conserved.

DY 44.11 Thu 15:00 P2

Molecular dynamics simulations of binary mixtures in nanostructured pores — Niels Müller, Michael Vogel, and •Markus Haneke — TU Darmstadt, Institut für Physik kondensierter Materie, Hochschulstr. 6, 64289, Darmstadt, Germany

Water and its mixtures are fairly common in nature and technology.

Here, we seek to understand the influence of solid surfaces with nanostructured porous confinements on binary aqueous mixtures. For this purpose, we exploit that MDS allow us to determine structural and dynamical properties in a spatially resolved manner. The inner surfaces and the aqueous mixtures of the simulated systems are made of differently polarized molecules. The composition and temperature are varied, approaching the regime of spinodal decomposition.

We find that the nanostructured surfaces impose a corresponding nanoscopic phase separation onto the confined mixtures. Explicitly, the concentration of the mixture components varies along the pore axis in phase with the surface patterning, where the effect is stronger near the pore walls. Moreover, the particle mobility differs between the components and depends on the position within the porous confinement. In particular, the imposed concentration fluctuations cause diffusion barriers.

DY 44.12 Thu 15:00 P2

Microcanonical analysis of model polymers interacting via many-body dispersion — •Benedikt Ames, Mario Galante, Matteo Gori, and Alexandre Tkatchenko — Department of Physics and Materials Science, Université du Luxembourg

Non-covalent interactions play a crucial role in the energetics and structure formation of many systems of interest for physics, chemistry and biology.

Among computational methods which include van der Waals (vdW) interactions, the many-body dispersion framework (MBD) attains an excellent accuracy by accounting for all orders of the coupling. Its application has shown the importance of going beyond the pairwise (PW) approximation, for example to obtain the correct energy ordering of molecular crystals and for the adhesion of 2D structures. Nevertheless, the phenomena of MBD-driven dynamics remain largely unexplored.

Here, as a means to probe these dynamics, we study the phase transitions of a simplified model polymer via microcanonical inflection point analysis [1], a recent generalization of the notion of phase transitions from the thermodynamic limit to finite-size systems. By contrasting simulations using MBD and PW methods, we explore whether the different characteristics of each vdW model manifest themselves in distinct properties of the polymer's clustering transition.

[1] Koci, Qi and Bachmann, J. Phys.: Conf. Ser. 759, 012013 (2016).

DY 44.13 Thu 15:00 P2

Arcsine laws in non-equilibrium regime — •Avijit Kundu[1,2], Raunak Dey[2], Biswajit Das[2], and Ayan Banerjee[2] — [1]University of Bayreuth, Universitystrasse 30, 95447, Bayreuth, Germany — [2]Indian Institute of Science Education and Research Kolkata, Mohanpur, Kalyani, 741246, India

Most of the processes in the mesoscopic world especially inside living cell are far from thermal equilibrium. The time evolution of such processes is important to study to characterize the processes. Remarkably, Paul Lévy defined arcsine laws for three variables related to the stochastic Wiener process. Here we have studied stochastically driven colloidal particle in a viscous fluid and observed the entropic current, work done on the system or dissipated by it, follow the Lévy arcsine laws in the large time limit. The significant lead of this work is to show the convergence of cumulative distribution to the arcsine law is faster for the case of near equilibrium system where the entropy production rate is smaller. We also have tested the convergence rates of cumulative distributions for different non-equilibrium systems by driving the optically trapped colloidal probe with external noise parameters and changing the flow field by introducing a microbubble in its vicinity.

DY 44.14 Thu 15:00 P2

Phase transition in clustering algorithms — •Julian Zitterich and Alexander K. Hartmann — Institute of Physics, University of Oldenburg, Germany

A well known problem in data analysis and machine learning is the clustering problem. It consists of grouping a set of data vectors into subsets, such that *similar* vectors end up in the same subset. How to define similarity and how to find these subgroups depend much on the investigated problem, thus many algorithms and metrics exists. Also it may that an algorithm is not able to successfully detect structure in the given data. Thus, we study here ensembles of artificially generated data controlled by parameters such that for some parameter values the clustering is *easy* or at least *possible* while for other values it is *hard* or *impossible*. Thus, from a statistical physics viewpoint we are interested in phase transitions of the clustering problem between such phases. Previously, the existence of such phase transitions was

observed for a single ensemble in high-dimensional space by using the AMP algorithm [1]. Here, we investigate numerically [2] four different state-of-the-art cluster algorithms and analyse their behaviour for increasingly complex ensembles. Low complexity ensembles are realized by direct sampling of data vectors, while high complexity ensembles are implemented by short simulations of simple models of interacting particles.

[1] T. Lesieur et al., 54th Annual Allerton Conference on Communication, Control, and Computing (Allerton), arXiv:1610.02918 (2016)
[2] A.K. Hartmann, *Big Practical Guide to Computer Simulations*, World Scientific (2015)

DY 44.15 Thu 15:00 P2

Chemfiles: reading and writing atomistic modeling files — •Guillaume Fraux — Institute of Materials, EPFL, Lausanne, Switzerland

Running atomistic simulations produces enormous amounts of data, which has to be post-processed in order to extract scientifically relevant information. Unfortunately, this task is made much harder by the vast menagerie of existing file formats, all containing similar data in a different formatting.

Chemfiles is a software library providing a unified interface to these formats, allowing researchers to spend their time analyzing their data instead of writing file parsers over and over. Chemfiles is implemented in C++, and provides programming interfaces to most of the scientific languages: Python, Fortran, C, Rust and Julia. 21 different formats are currently supported, including both text and binary (i.e. XTC, TNG, DCD, ...) formats. All text formats can be read and written with multiple compression standards (gzip, xz, bzip2). Chemfiles also offers a comprehensive atom selection language, including the unique feature of simultaneous selection of multiple atoms (e.g. `pairs: name(#1) == H and name(#2) == O and distance(#1, #2) < 3.0`).

Overall, chemfiles one of the fastest libraries for reading files used in atomistic simulation, being between 20% and 10 times faster than other commonly used libraries; while offering a simpler and easy to use programming interface; freeing up time for scientists working with these file formats.

DY 44.16 Thu 15:00 P2

Phase transitions for two-stage stochastic minimum spanning tree optimisation problem — •Robert Strassen and Alexander K. Hartmann — Institute of Physics, University of Oldenburg

Phase transitions in classical optimization problems have been studied extensively in statistical physics [1]. Here, we consider two-stage stochastic optimization problems, where the optimization is performed in two different stages, such that in the first stage not all information is available. In particular, we consider the two-stage stochastic minimum spanning tree (MST) problem for undirected graphs with given initial edge costs. In the second stage, one of a set of random scenarios is realized, involving different edge costs. In each stage, edges can be selected such that a spanning tree is finally formed, aiming at a minimum expected total costs. Unlike the conventional MST problem, the two-stage version is generally worts-case "hard" to solve, even though there are problem instances that are "easy". We investigate numerically [2] the problem by the calculation of bounds and applying several approximation algorithms, including one of Dhamdere et al. [3] on various random ensembles of graphs. Our aim is to find out whether there are phase transitions between typical easy and hard problem phases.

[1] A.K. Hartmann and M. Weigt, *Phase Transitions in Optimization Problems*, Wiley-VCH, Berlin 2005
[2] A.K. Hartmann, *Big Practical Guide to Computer Simulations*, World-Scientific, Singapore, 2015
[3] K. Dhamdhere, R. Ravi, M. Singh, IPCO 2005, LNCS **3509**, pp. 321-334, (2005)

DY 44.17 Thu 15:00 P2

Critical Casimir effect in the square-lattice Ising model with quenched surface disorder — •Luca Cervellera and Alfred Hucht — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

For the square-lattice Ising model, the critical Casimir amplitude and force can be calculated exactly for many geometries and boundary conditions. From a recent exact solution for the cylinder with length L, circumference M, and with arbitrary random boundary conditions at one boundary, we determine the full density of thermodynamic states $\omega(\delta F, m_B)$, with residual free energy δF and boundary magnetization m_B at criticality. From this quantity we can derive the disorder averaged Casimir potential for different aspect ratios and disorder ensembles.

DY 44.18 Thu 15:00 P2

Anomalous collective dynamics of auto-chemotactic populations — Jasper van der Kolk[1], Florian Rasshofer[1], •Richard Swiderski[1], Astik Haldar[2], Abhik Basu[2], and Erwin Frey[1,3] — [1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Munich, Germany — [2]Theory Division, Saha Institute of Nuclear Physics, HBNI, 1/AF Bidhannagar, Calcutta 700 064, West Bengal, India — [3]Max Planck School Matter to Life, Hofgartenstraße 8, 80539 Munich, Germany

While the role of local interactions in nonequilibrium phase transitions is well studied, a fun- damental understanding of the effects of long-range interactions is lacking. We study the critical dynamics of reproducing agents subject to auto-chemotactic interactions and limited resources. A renormalization group analysis reveals distinct scaling regimes for fast (attractive or repulsive) interactions; for slow signal transduction the dynamics is dominated by a diffusive fixed point. Further, we present a novel nonlinear mechanism that stabilizes the continuous transition against the emergence of a characteristic length scale due to a chemotactic collapse.

DY 44.19 Thu 15:00 P2

Multifractality at the integer quantum Hall transition — •Martin Puschmann[1], Daniel Hernangómez-Pérez[2], Bruno Lang[3], Soumya Bera[4], and Ferdinand Evers[1] — [1]Institute of Theoretical Physics, University of Regensburg, D-93053 Regensburg, Germany — [2]Department of Molecular Chemistry and Material Science, Weizmann Institute of Science, Rehovot 7610001, Israel — [3]IMACM and Institute of Applied Computer Science, Bergische Universität Wuppertal, D-42119 Wuppertal, Germany — [4]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India

The quantum Hall transitions are still one of the bigger mysteries of condensed matter theory. In the past twenty years several conjectures have been made as to what the field theory of the critical fixed point of the integer (class A) quantum Hall transition could be. The multifractal spectrum provides a characteristic fingerprint of the phase transition. Here, recent analytical work predicts a parabolic dependency of the anomalous dimension $\Delta_q = q(1-q)/4$, where the exponents $\tau_q = 2(q-1) + \Delta_q$ describe the system-size scaling of wavefunction moments $|\Psi|^{2q}$ [1]. In great analogy to our previous analysis on the spin (class C) quantum Hall transition [2], we investigate the multifractal spectrum of the class A transition and similarly demonstrate the presence of quartic terms in Δ_q. Our findings are thus clearly inconsistent with the strict parabolicity predicted for "traditional" conformal field theories. [1] M. R. Zirnbauer, Nucl. Phys. B 941, 458 (2019) [2] M. Puschmann et al., Phys. Rev. B 103, 235167 (2021)

DY 44.20 Thu 15:00 P2

Detection of defects in soft quasicrystals with neural networks — •Ali Doener and Michael Schmiedeberg — Theoretische Physik I, Erlangen, DE

The aim of this work is to construct and employ a neural network for the detection of topological defects in dodecagonal quasicystalline patterns. Even though quasircrystals are aperiodic, they exhibit a longe-range order. Furthermore, in principle any discrete rotational symmetry can occur.

In this work, dodecagonal quasicrystalline patterns in two-dimensions with a built-in dislocation are generated and employed as input images of the neural network. The network then should figure out not only the position but also the type of the Burgers vector of the defect.

Our trained neural network is able to recognize the type of the Burgers vector very good. The position of the dislocation is recognized up to a mean deviation from the real position that is much smaller that the small length scale in the quasicrystals. In future, we want to train the network with patterns that contain multiple dislocations as well as phasonic excitations.