DY 22: Poster: Statistical Physics

Time: Wednesday 10:00–12:00 Location: P3

DY 22.1 Wed 10:00 P3

Adaptive Quasi-Monte Carlo Quadrature for Concentrated Distributions in Bayesian Inference — •Jinyi Zhou and Sebastian Matera — Fritz-Haber-Institut der MPG, Berlin

By its probabilistic formulation, Bayesian inference cures many of the problems of the traditional parameter-fitting approach, such as potential ill-posedness and the lack of reliable uncertainty estimates. However, for highly nonlinear and sensitive models, the Bayesian posterior distribution can become complex and is often concentrated in a small fraction of the parameter space. This challenges established sampling approaches, which typically perform well only for smooth distributions. We address this challenge with a novel adaptive Quasi-Monte Carlo (aQMC) quadrature method. This approach combines the highly uniform coverage of Quasi-Monte Carlo with a greedy iterative subdivision algorithm, concentrating the sampling in subdomains where the quadrature error is expected to be largest. In addition to testing on benchmark functions, we demonstrate our approach on a kinetic model from the field of catalysis. In this field, concentrated distributions are expected because, even with the best priors derived from quantum chemical calculations, uncertainties can span several orders of magnitude for the predicted catalytic response, whereas experimental data is highly accurate in comparison.

DY 22.2 Wed 10:00 P3

A novel mathematical model for the coupled binary-fluid surfactant system — •Alexandra Hardy, Steven McDonald, Abdallah Daddi-Moussa-Ider, and Elsen Tjhung — The Open University, Milton Keynes, UK

We propose a new binary-fluid surfactant mathematical model derived from modeling the surfactant molecules as dumbbells. By explicitly taking into account the molecules alignment, we gain new field variable p(r,t); the average orientation of surfactants. Combined with standard phase-field theory for binary fluids gives the system equations, which we both solve numerically and analytically. We employ a hybrid finite difference (FDM) and spectral method for the simulations. Whereas regular perturbation theory is used for the equilibrium solutions, facilitated by assuming weak coupling between surfactant and fluid. Three investigations are presented, firstly we demonstrate excellent agreement between simulation and the analytical solutions for a planar water-oil interface. Second, we prove that our model accurately predicts the decrease in surface tension with increasing surfactant concentration, in line with experiments and related theory. Finally, we show that our model is capable of preventing surfactant-laden droplet coalescence due to the added polarization field p(r,t).

DY 22.3 Wed 10:00 P3

Nonequilibrium mixture dynamics: a model for mobilities and its consequences — •Maryam Akaberian[1], Filipe C Thewes[1,3], Peter Sollich[1,2], and Matthias Krüger[1] — [1]University of Goettingen — [2]King's College London — [3]Max plank institute

extending the famous model b for the time evolution of a liquid mixture, we derive an approximate expression for the mobility matrix that couples the different mixture components. this approach is based on a single component fluid with particles that are artificially grouped into separate species labelled by "colors". The resulting mobility matrix depends on a single dimensionless parameter, which can be determined efficiently from experimental data or numerical simulations, and includes existing standard forms as special cases. we identify two distinct mobility regimes, corresponding to collective motion and interdiffusion, respectively, and show how they emerge from the microscopic properties of the fluid. as a test scenario, we study the dynamics after a thermal quench, providing a number of general relations and analytical insights from a gaussian theory. specifically, for systems with two or three components, analytical results for the time evolution of the equal time correlation function compare well to results of Monte Carlo simulations of a lattice gas. a rich behavior is observed, including the possibility of transient fractionation.

DY 22.4 Wed 10:00 P3

Transport in classical systems with fractionally charged excitations — •Jannis Waldmann, Malte Grunert, Max Grossmann, and Erich Runge — Theoretical Physics I, Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Interacting systems of charged particles can show fractionally charged excitations, as is well known from the Fractional Quantum Hall Effect of electrons in a magnetic field. Fractionally charged excitations in the absence of magnetic fields have also been predicted for certain lattices with geometric frustrations, e.g. for quantum mechanical models of spinless fermions on the criss-crossed checkerboard lattice [1,2]. Here, we present result on transport properties of classical particles with nearest-neighbor repulsion on a Kagome lattice. Using Monte Carlo simulations, we study the transition from classical hopping at high temperatures to transport dominated by half-charged quasi-particles for special filling factors at low temperatures. Furthermore, we provide evidence for a residual entropy at zero temperature and Andreev-like reflection at interfaces to 'normal', i.e. not frustrated systems.

[1] Fulde et al., Ann. Phys. (Leipzig) 11 (2002) 12, 892-900
[2] Pollmann et al., J. Magn. Magn. Mater. 310 (2007), 966-968

DY 22.5 Wed 10:00 P3

Diffusion and order in mixed lattice gas of hard squares — •Piotr Nowakowski[1], Niklas Raake[2], and Ana-Sunčana Smith[2,1] — [1]Institut Ruđer Bošković, Zagreb, Croatia — [2]Friedrich–Alexander–Universität Erlangen–Nürnberg, Erlangen, Germany

We study the diffusion in a crowded environment using a model system of a lattice gas composed of hard square particles of 1×1 and 2×2 size (measured in lattice constant units) undergoing a Brownian motion on a two-dimensional square lattice. For the whole range of concentrations of both types of particles, we numerically test the accuracy and efficiency of an approximation of the motion by a persistent random walk with one or two step memory. A good agreement is observed for very low and very high concentrations of particles.

Additionally, we look at the second order phase transition from a gas phase for low densities of 2×2 particles to a columnar phase. Surprisingly, it seems that the density of large particles at which the transition occurs is not affected by the presence of smaller particles. Moreover, in columnar phase the diffusion constant can be approximated by studying a one-dimensional system.

DY 22.6 Wed 10:00 P3

The bath *remembers*: how many time-scales can we probe through recoil? — •Rupayan Saha[1], Niloyendu Roy[2], Debankur Das[1], Clemens Bechinger[2], and Matthias Krüger[1] — [1]Institute for Theoretical Physics, Georg-August-Universität Göttingen, Göttingen 37073, Germany — [2]Fachbereich Physik, Universität Konstanz, Konstanz 78457, Germany

Recoil experiments, where one studies the transient dynamics of a colloidal particle after driving it externally, are of particular importance to gain insight into the non-Markovian properties prevalent in visoelastic solvents such as micellar suspensions. In an earlier experimental study by Félix Ginot et al. [*New J. Phys. 24.12 (2022): 123013*], the *translational* recoil was found to be governed by a small number of distinct time scales, reproduced by a microscopic model using a small number of so-called bath particles. In this contribution, we investigate *orientational* recoil of such a colloidal probe in a viscoelastic fluid, which, in contrast, appears to exhibit a large number of time scales. In collaboration with experiment, we develop microscopic models to account for such observations, and develop driving protocols to dissect the various time scales involved in this process.

DY 22.7 Wed 10:00 P3

Large-deviation simulation of the coupling time distribution for the CFTP method applied to the heat bath Ising process — •Mathis Groenhagen, Alexander K. Hartmann, and Peter Werner — Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

Coupling from the past (CFTP), introduced by Propp and Wilson [1], is a version of the Markov-chain Monte Carlo method, which is capable of generating exact samples from a finite set with a particular distribution. The performance of the CFTP method for a given application can be characterized by the distribution of the CFTP method's random running time, the *coupling time* τ, for this application.

A large-deviation Monte Carlo algorithm, as described for example

in [2], is used to sample these coupling times for the application of the CFTP method to a single-spin-update heat-bath process for the ferromagnetic two-dimensional square lattice Ising model without an external field. This yields the coupling time distributions over a wide range of coupling times τ down to probability densities of 10^{-80} for different lattice sizes L and temperatures T. These results give additional numerical evidence for the analytical results shown in [3].
[1] J. Propp, D. Willson, Random Struct. Algorithms **9**, 223-252 (1996).
[2] A. K. Hartmann, Phys. Rev. E **65**, 056102 (2002).
[3] A. Collevecchio, E.M. Elçi, T.M. Garoni et al., J Stat Phys **170**, 22-61 (2018).

DY 22.8 Wed 10:00 P3

Large-deviation simulations of non-equilibrium stochastic processes — •Chinmay Chandratre — Heinrichstr. 16, 26131 Oldenburg

For N non-interacting diffusing particles in a harmonic trap where the stiffness is switched randomly between μ_1 and μ_2, the joint distribution of particle positions has been exactly computed [1]. This allowed the computation, in the limit of $N \to \infty$, of the distribution of the position M_k of the k-th rightmost particle. It is governed by a universal scaling function with finite support and tunable shape. However, the behaviour for finite numbers of particles, where the large-deviation corrections become relevant, is analytically not known. Numerically, standard algorithms fail to access the majority of the support, particularly in the tails. Here, special large-deviation algorithms [2] are used to access the tails of the distribution, reaching probabilities as small as 10^{-200} or even smaller. This includes a highly general *black-box* algorithm suitable for studying a wide range of stochastic processes.
[1] Biroli, Marco and Kulkarni, Manas and Majumdar, Satya N. and Schehr, Grégory, Phys. Rev. E **109**, 032106 (2024)
[2] A.K. Hartmann, Phys. Rev. E **89**, 052103 (2014)

DY 22.9 Wed 10:00 P3

Residual entropy of ice: A study based on transfer matrices — •De-Zhang Li[1], Yu-Jie Cen[2], Xin Wang[3], and Xiao-Bao Yang[4] — [1]Quantum Science Center of Guangdong-Hong Kong-Macao Greater Bay Area — [2]Institute of Materials Chemistry, Vienna University of Technology — [3]Department of Physics, City University of Hong Kong — [4]Department of Physics, South China University of Technology

The residual entropy of ice systems has long been a significant and intriguing issue in condensed-matter physics and statistical mechanics. This study focuses on two typical realistic ice systems: hexagonal ice (ice Ih) and cubic ice (ice Ic). We present a transfer-matrix description of the number of ice-ruled configurations for these systems. A transfer matrix M is constructed for ice Ic, where each element represents the number of ice-ruled configurations of a hexagonal monolayer under certain conditions. The product of M and M^T corresponds to a bilayer unit in the ice Ih lattice, thus forming an exact transfer matrix for ice Ih. Utilizing this, we show that the residual entropy of ice Ih is not less than that of ice Ic in the thermodynamic limit, first proved by Onsager in the 1960s. Additionally, we introduce an alternative transfer matrix M' for ice Ih based on a monolayer periodic unit. Various interesting properties of M, MM^T and M' are analyzed, including the sum of all elements, the element in the first row and first column, and the trace. Each property corresponds to the residual entropy of a certain 2-d ice model. This work provides an effective description, based on transfer matrices, for the residual entropies of various 2-d ice models.

DY 22.10 Wed 10:00 P3

Beyond mean-field kinetic theory of nematic self-propelled particles — •Benjamin Kohler, Horst-Holger Boltz, and Thomas Ihle — Institute for Physics, University of Greifswald, 17489 Greifswald, Germany

We present Landau kinetic theory and direct simulation results for systems of self-propelled particles with alignment interactions of higher-order symmetry with a particular focus on nematic couplings. Systematically expanding the BBGKY-hierarchy approximation beyond the mean-field contributions, we employ the one-sided molecular chaos assumption and an diagrammatic approach to account for higher order correlations. Our calculations yield predictions with no free parameters that are in quantitative agreement with direct agent-based simulations without being restricted to low densities.

DY 22.11 Wed 10:00 P3

Barrier crossing and rare fluctuations of active Brownian particles — •Rafael Diaz Hernandez Rojas[1], Karthik Cheruvary[1,2], and Peter Sollich[1] — [1]University of Göttingen — [2]IISER Pune

Understanding noise-induced transitions is crucial for modelling complex systems where random fluctuations can affect both the local stability and the global behaviour of a system. Noise-activated escape processes are a key instance, and were solved by Kramers long ago for barrier crossing driven by thermal noise. A natural question is how different noise sources might change the picture, in particular those postulated in active matter models. Here we study the escape problem for the paradigmatic case of an Active Brownian Particle, where the direction of the self-propulsion velocity rotates randomly on a timescale known as persistence time. Using a path integral formalism in the weak thermal noise limit. We map the problem of finding the most likely escape trajectory to the minimisation of an appropriate action. We show that optimal trajectories always consist of an initial relaxation in a tilted potential, beyond which the escape becomes genuinely activated. We apply our approach to convex potentials (to study barrier climbing by rare fluctuations) as well as potentials with multiple minima (to analyse barrier crossing). We highlight the effects of directionality induced by the self-propulsion and its non-trivial interplay with the shape of the potential. A key result is that, for potentials with a symmetry axis along the line between two minima, activity can generate optimal escape paths that break this symmetry.

DY 22.12 Wed 10:00 P3

Rarefied gas transport in a narrow channel induced by an asymmetric wall geometry — •Constantin Rein[1], Klaus Kroy[1], and Viktor Holubec[2] — [1]Brüderstr. 16, D-04103 Leipzig — [2]V Holešovičkách 747/2, Praha 8, Czech Republic

Since the work of Knudsen on gas transport in a narrow channel, it is known that gases in the dilute limit, where the mean free path is larger than the characteristic length scale, behave different as compared to the well known finite density regime[1]. So-called Knudsen pumps use temperature differences along channel walls to induce gas particle transport along the channel[2]. Inspired by the working principle of our recently introduced active Brownian ratchet[3], we investigate numerically and analytically the gas transport phenomenon appearing in a narrow channel with specular walls, except for a diffusively reflecting triangle that protrudes into the channel from one of the walls. Despite the absence of a variation in the wall temperature, a flow emerges. It arises solely from an asymmetry of the incoming and outgoing orientational distribution. The magnitude, direction and flow pattern of the induced transport is discussed.

[1] Knudsen, M. Eine revision der Gleichgewichtsbedingung der Gase, Thermische Molekularströmung. Ann. Phys. 336,205*229 (1909). [2] Wang, X., Su, T., Zhang, W., Zhang, Z. & Zhang, S. Knudsen pumps: a review. Microsyst Nanoeng 6, 26 (2020). [3] Rein, C., Kolář, M., Kroy, K. & Holubec, V. Force-free and autonomous active Brownian ratchets(a). EPL 142, 31001 (2023).

DY 22.13 Wed 10:00 P3

Dielectric response and fluctuation-dissipation-theorem for moving bodies — •Daniele Gamba, Philip Rauch, and Matthias Krüger — Georg-August University, Göttingen

Casimir forces operate at microscopic scales and are integral to phenomena such as gecko adhesion and functionality of nano-devices. Recent research has unveiled new effects, arising from thermal and mechanical non-equilibrium, such as levitation or propulsive forces capable to driving heat engines, or novel effects tied to optically non-reciprocal materials [1,2]. In this contribution we formulate scattering theory for objects in respective motion. Specifically, we find the dielectric response and the fluctuation-dissipation theorem for arbitrary moving bodies. The dielectric response of a moving body is found to be nonlocal in space, optically non-reciprocal, and can also appear as being active. Conversely, it is possible to design an active medium that appears optically passive when in motion. Finally, we derive closed expressions for Casimir forces and heat transfer between moving bodies using scattering theory.
1. Krüger et al., Physical Review B, 2012.
2. Gelbwaser-Klimovsky et al., Physical Review Letters, 2021.

DY 22.14 Wed 10:00 P3

Criticality in non-reciprocal spin modells — •Max Hässler and Martin Weigel — TU Chemnitz, Chemnitz, Deutschland

Equilibrium statistical physics is based on symmetric, Hamiltonian interactions fulfilling Newton*s Third Law. On the other hand, active matter like bacteria or other self-propelled particles such as bird flocks violates time-reversal symmetry and is often characterized by non-reciprocal interactions. Simple models are of interest for exploring fundamental features of such systems. We examine classical spin systems including the Ising model with non-reciprocal interactions, using Monte Carlo simulations to study criticality in such models. For several systems we determine critical exponents and compare the observed universality classes to those of the corresponding reciprocal, equilibrium models.

DY 22.15 Wed 10:00 P3

Harnessing finite-size effects to gauge aging in the $2D$ Ising model — •Dustin Warkotsch[1,2], Malte Henkel[2,3], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany — [2]Laboratoire de Physique et Chimie Théoriques (CNRS UMR 7019), Université de Lorraine, Nancy, France — [3]Centro de Física Teórica e Computacional, Universidade de Lisboa, Lisbon, Portugal

The finite-size effects in a $2D$ Ising model with nearest-neighbor interactions are investigated at low temperature with respect to the two-time autocorrelation function $C(t,s)$, where t is the observation and s the waiting time. Using a finite-size scaling ansatz established for the spherical model linking the resulting plateaus in $C(t,s)$ to waiting time s and lattice size L, a precise and reproducible estimation for the autocorrelation exponent λ and dynamical exponent z is developed.

DY 22.16 Wed 10:00 P3

Theoretical and Experimental Advances in Non-Equilibrium Statistical Physics — •Anton Zizenko — Bolshaya Semenovskaya 38

Research helps to understand how complex systems behave when they are far from equilibrium, such as in cases of anomalous transport or phase transitions. Main achievements: Relaxation and fluctuations: Describing the behavior of systems after external influence. Critical phenomena: Studying changes in systems out of equilibrium. Entropy production: Connection with energy loss processes and irreversibility. Applications: Development of materials with new properties, improvement of thermal conductivity, and optimization of processes in chemistry and biology.

DY 22.17 Wed 10:00 P3

Frustrated Self-Assembly — •Andrey Zelenskiy and Martin Lenz — Université Paris-Saclay, CNRS, LPTMS, 91405, Orsay, France

Biomolecular self-assembly lies at the very heart of the function of living cells, where it organizes individual components into functional biological machines. The macromolecular sub-units typically correspond to proteins, whose shapes have been optimized over millions of years of evolution to ensure a proper functionality of the self-assembled structures. However, in pathological cases, proteins fail to achieve the optimal folding, which often leads to complex ill-fitting shapes. This produces geometrical incompatibility, which leads to frustrated interactions between the sub-units. Surprisingly, despite a huge variability in protein structure, such misfolded units tend to robustly self-assemble into aggregates with well-defined morphologies. Interestingly, these structures display a clear preference for slimmer topologies, such as fiber aggregates. This emergent principle of dimensionality reduction suggests that the aggregation of irregular components derives from the generic physical principles, rather than the microscopic details of the interactions.

Inspired by this idea, we model the frustrated self-assembly of ill-shaped proteins as coarse-grained anisotropic particles, whose interactions depend on their relative orientations and positions in space. This simple model successfully reproduces a hierarchy of aggregate morphologies and gives pointers to the origins of dimensionality reduction.

DY 22.18 Wed 10:00 P3

Topological and thermodynamic inference in Markov networks with observed and hidden transitions — •Alexander M. Maier[1], Udo Seifert[1], and Jann van der Meer[2] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Kyoto University, Graduate School of Science, Division of Physics and Astronomy, Oiwakecho 145-10, Kyoto 606-8224, Japan

The number of observable degrees of freedom is typically limited in experiments. Here, we consider discrete Markov networks in which an observer has access to a few visible transitions. We present what information, locally and globally, of such a Markov network can be inferred from the observed data. In particular, we shed light on operationally accessible information about the topology of shortest paths between visible transitions in the underlying graph and show a rule that allows us to identify potential clusters of states or exclude their existence. Moreover, we show how to estimate entropy production along an observable, coarse-grained path. Combining this with further inferable information, we propose two strategies to reconstruct a graph that is compatible with the observations and part of the original graph underlying the Markov network. This approach highlights how much information waiting-time distributions contain while also paving the way to infer thermodynamically consistent models of observed partially accessible systems.

DY 22.19 Wed 10:00 P3

Stroboscopic measurements in Markov networks: Thermodynamic inference vs. exact generator reconstruction — •Malena Thea Bauer[1], Udo Seifert[1], and Jann van der Meer[2] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Kyoto University, Graduate School of Science, Division of Physics and Astronomy, Oiwakecho 145-10, Kyoto 606-8224, Japan

A major goal of stochastic thermodynamics is to estimate the inevitable dissipation that accompanies particular observable phenomena in an otherwise not fully accessible system. Quantitative results are often formulated as lower bounds on the total entropy production, which capture a part of the total dissipation that can be determined based on the available data alone. In this work, we discuss the case of a continuous-time dynamics on a Markov network that is observed stroboscopically, i.e., at discrete points in time in regular intervals. We compare the standard approach of deriving a lower bound on the entropy production rate in the steady state to the less common method of reconstructing the generator from the observed propagators by taking the matrix logarithm. Provided that the timescale of the stroboscopic measurements is smaller than a critical value that can be determined from the available data, this latter method is able to recover all thermodynamic quantities like entropy production or cycle affinities and is therefore superior to the usual approach of deriving lower bounds. We conclude the comparison of both methods with numerical illustrations and a discussion of the requirements and limitations of both methods.

DY 22.20 Wed 10:00 P3

Brownian particles for unconventional computing — •Alessandro Pignedoli, Atreya Majumdar, and Karin Everschor-Sitte — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen

Brownian particles naturally explore a system's configuration space offering an energy efficient approach to optimisation problems [1]. We demonstrate that interacting Brownian particles can solve optimisation problems [2,3] more efficiently than individual particles acting alone. This collective efficiency arises from their local interactions, which mimic the principles of swarm intelligence, where the whole systems emergent behaviour outperforms the sum of its individual components [4].

[1] C. H. Bennett, Int. J. Theor. Phys. 21, 905 (1982); [2] German Patent Application DE 10 2023 131 171, K. Everschor-Sitte, A. Pignedoli, B. Dörschel (2023); [3] German Patent Application DE 10 2023 131 706, K. Everschor-Sitte, A. Pignedoli, B. Dörschel (2023); [4] Bonabeau, et al, Oxford University Press (1999).

DY 22.21 Wed 10:00 P3

Investigating hydrogen isotopologues at cryogenic temperature in the gas, liquid, and solid phase with the T2ApIR experiment — •Alexander Marsteller, Dominic Batzler, Beate Bornschein, Lutz Bornschein, Tobias Falke, Florian Hanss, Joshua Kohpeiss, Bennet Krasch, Simone Wadle, and Robin Grössle — Karlsruher Institut für Technologie, Karlsruhe, Deutschland

Cryogenic hydrogen is of interest for a wide range of research topics such as fundamental phyiscs of liquids, astrophysics or energy storage. Tritium, the radioactive isotope of hydrogen, is of particular use as an electron source for neutrino mass measurement, and also the most promising contender for fuel in nuclear fusion for power generation. In spite of this, literature on the material properties of tritium is sparse. To improve upon this, the Tritium Absorption InfraRed Spectroscopy

2 (T2ApIR) Experiment has been designed and built at the Tritium Laboratory Karlsruhe (TLK), and is currently in its scientific commissioning phase. The main focus of this experiment is to enable the investigation of the properties of all six hydrogen isotopologues and their mixtures in the gaseous, liquid, and solid phase. This is achieved using infrared absorption spectroscopy, a polariscope setup, Raman spectroscopy, as well as a temperature and pressure measurement. On this poster I will present the T2ApIR setup as well as some of the first measurements performed with it.

DY 22.22 Wed 10:00 P3

GEANT4 based design to measure the solubility of tritiated molecules in dual phase xenon — •J.R. Braun[1], V. Aures[2], D. Forck[1], R. Grössle[1], and M. Röllig[1] — [1]Tritium Laboratory Karlsruhe, Eggenstein-Leopoldshafen, Germany — [2]Technische Universität München, Garching bei München, Germany

Detection of trace amounts of tritium is a challenging task that can be tackled using scintillation. Liquid xenon is an excellent scintillator for this purpose. A fundamental property in designing analytical systems for tritium detection is the solubility of tritiated molecules. Trace detection of tritium is critical for experiments aimed at the detection of rare physical interactions, such as the direct detection of dark matter, where naturally occurring tritium background is a challenge to overcome. Consequently, systems for both detection and removal of tritium are required. The aim of the "Tritium in Xenon" (TriXe) experiment is to determine the Henry solubility and the diffusion constant of tritiated hydrogen, water and methanes in dual-phase xenon in thermal equilibrium. TriXe employs a dual-phase chamber in which the xenon is present at operating conditions of DARWIN. By detecting VUV scintillation light with photomultipliers, the concentration of the tritiated molecules in each phase can be determined, as the concentration is proportional to the counting rate. Together with the second diffusion law, the diffusion constant can be deduced from the change in the count rate over time. The results of TriXe can be used to make qualitative and quantitative suggestions for changes in background reduction and direct tritium monitoring by cryogenic distillation.

DY 22.23 Wed 10:00 P3

Precise Estimation of the Liquid-Gas Critical Point of Water — •Mayank Sharma and Peter Virnau — Institute of Physics, Johannes Gutenberg University Mainz

We perform Molecular Dynamics simulations to investigate the liquid-gas critical point for the TIP4P water model. In the canonical (NVT) ensemble, density fluctuations are quantified and analyzed using a recently developed method [1] based on cumulant crossings. Complementary simulations in the isothermal-isobaric (NPT) ensemble yield density and energy distributions, which are mapped onto the universal 3D Ising master curve via histogram reweighting. The critical points determined by the two approaches exhibit very good agreement, highlighting the robustness of this methodology. This work establishes a reliable framework for accurately locating the critical point which is applied to test the influence of ionic conditions on the latter.

[1] J.T. Siebert et al., Phys. Rev. E (R) 98, 030601 (2018).

DY 22.24 Wed 10:00 P3

Linking Local and Macroscopic Transport Properties in Confined Electrolyte Systems: Molecular Dynamics Simulations of Water Swollen Hectorite — •Bastian Füsser, Aqsa Nisar, and Michael Vogel — Technische Universität Darmstadt, Darmstadt, Germany

In this work, we study the structural and dynamic properties of water and ions in hectoriete slit confinements using molecular dynamics simulations. Our goal is to develop a detailed understanding of the relationship between local interactions and macroscopic ion transport.

This study is part of a collaboration aiming to bridge experimental observations and theoretical models. Initially, we simulate hectorite systems as realistically as possible to compare the simulation results with experimental results. Subsequently, we investigate artificial systems to systematically analyze the role of specific parameters, such as layer charge. In doing so, we vary the interlayer spacing, solvent composition, and ion concentration.

Our goal is to develop an understanding of the relation between local interactions and dynamics with the long-range transport in confined electrolyte systems. These insights provide valuable contributions to the development of more efficient electrochemical systems, e.g., devices for energy storage and conversion.

DY 22.25 Wed 10:00 P3

Phase transitions in mesoporous solids with structural disorder — •Ali Alzaidi[1], Georgiy Baroncha[1], Dirk Enke[1], Eustathius Kikkinides[2], and Rustem Valiullin[1] — [1]Leipzig University, Leipzig, Germany — [2]Aristotle University of Thessaloniki, Thessaloniki, Greece

Phase transitions within the pore spaces of structurally disordered porous solids exhibit complex behavior with many aspect remaining poorly understood. This complexity arises from cooperative effects emerging during first-order phase transitions in pore networks. Building on the microscopic mechanisms of phase transitions occurring in single pores and between neighboring pores, we propose a statistical thermodynamic model to describe phase transitions in pore networks driven by two competing mechanisms: invasion and nucleation. We solve this model for two types of statistically disordered pore networks, linear pore chains and Bethe lattices, and correlate the results with experimental data on gas-liquid and solid-liquid equilibria in disordered porous glasses.

DY 22.26 Wed 10:00 P3

Cluster Formation and Phase Transitions Induced by Non-Reciprocal Interactions — •Thomas Richard Ullmann and Klaus Kroy — Institute for Theoretical Physics, Leipzig University, 04103 Leipzig, Germany

The emergence of cluster formation in a two-dimensional lattice spin system driven by non-reciprocal interactions (NRI) is investigated. The development of a novel phase, characterized by clusters distinct from the quasi-long-range order (QLRO) state of the conventional XY model, is unveiled through the use of a tunable non-reciprocal parameter. Cluster formation is shown to result from particular local spin alignment due to non-reciprocal coupling, which dynamically reshapes the stability landscape of defects and topological structures. The stability of the system is analyzed using nearest-neighbour interactions and stochastic dynamics, and critical points are identified indicating phase transitions associated with clustering. The stability and evolution of defects and structures within this regime are further examined, providing insights into the interplay between non-reciprocity and the dynamics of spin textures. Broader implications for understanding collective behaviour in non-equilibrium systems are suggested, offering a framework for exploring non-reciprocity-induced phases and their stability in both physical and biological contexts.

DY 22.27 Wed 10:00 P3

Criticality and Percolation in the Off-Lattice XY Model — •Manthan Chattopadhyay, Thomas Richard Ullmann, and Klaus Kroy — Institute for Theoretical Physics, Leipzig University, 04103 Leipzig, Germany

We investigate the critical behavior of the 2D XY model with quenched positional disorder by distributing spins randomly via a spatial Poisson point process. This off-lattice approach allows us to study how quenched disorder affects phase transitions and critical phenomena, with the primary focus being the critical power-law scaling between the Kosterlitz-Thouless transition temperature T_c and the mean spin density $\langle\rho\rangle$. Using both a homogeneous coarse-graining method and percolation theory, we derive predictions for the scaling $T_c \propto (\langle\rho\rangle - \langle\rho_c\rangle)^{\zeta}$. By considering the fractal nature of the spin network near the percolation threshold, characterized by the fractal dimension D_f, the exponent is estimated. Simulation results confirm the existence of a percolation threshold with an exponent obtained from simulations similar to those of our analytic work, aligning closely with theoretical prediction. The fractal nature of the spin network near $\langle\rho_c\rangle$ is validated through the box-counting method, which is consistent with the value for 2D percolation. At high densities well above the percolation threshold, critical exponents approach expected values of the XY universality class, and the magnetization exponent β conforms to empirical observations in ultrathin magnetic films.

DY 22.28 Wed 10:00 P3

The random-field Ising model and two-phase flow in disordered media — •Peter Henning and Martin Weigel — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Two-phase flow in disordered media exhibits a rich phenomenology of behaviors with manifold applications for example in oil extraction [1]. A simplified model for such flows might be provided by the zero-temperature dynamics of the random-field Ising model (RFIM) that

exhibits interfaces between the pure phases that propagate through avalanches and show a roughening transition as a function of disorder strength. In the present study we focus on several properties of the interface between the phases such as its fractal geometry which can be characterized by critical exponents [2]. Furthermore we investigate abrupt changes in the propagation of the interface also known as crackling noise. By applying the RFIM to this problem we hope to gain insights into the underlying mechanisms of two-phase flow in disordered media and to provide a framework for interpreting experimental observations.

[1] R. Holtzman, M. Dentz, R. Planet and J. Ortin, *Commun Phys.* **3**, 222 (2020).
[2] B. Drossel and K. Dahmen, *Eur. Phys. J. B* **3**, 485 (1998)

DY 22.29 Wed 10:00 P3

Relating Thermodynamics and Dynamics in a Trap-like Model of Supercooled Liquids — •Simon Kellers, Anshul D. S. Parmar, and Andreas Heuer — Institute of Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster, Germany

Previous studies on 2D non-network glass formers utilized the million-fold acceleration of Swap Monte-Carlo and potential energy landscape (PEL) analysis to establish a connection between deviations from Gaussian behavior of the inherent structure (IS) density function, Fragile-to-Strong-Crossover [1] and a low-energy depletion regime. In recent work [2] a specific low-temperature behavior for thermodynamical (IS-energy) and dynamical (apparent activation energy) observables could be observed with basically the same onset temperature. To understand the physical background we investigate various model IS distributions in a trap-like picture and their derived dynamic and thermodynamic properties. Indeed, for different realizations of non-Gaussianity in the PEL strong correlations between the respective onset temperatures are observed as well, suggesting indeed a strong correlation between thermodynamics and dynamics. These results contribute to our understanding of the PEL picture of glass formers.

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