DY 49: Statistical Physics: General

Time: Friday 9:30–12:15 Location: H20

DY 49.1 Fri 9:30 H20

Large-Deviation Properties of Non-equilibrium RNA Work Processes — •Peter Werner and Alexander K. Hartmann — Institute of Physics, University of Oldenburg, Germany

The Higgs *RNA model* [1] is one of the few cases of a model with quenched disorder and complex free energy landscape, where *exact* partition function calculation and sampling can be done in polynomial time. Building on previous work [2], non-equilibrium properties of this model are investigated further. Here, we are interested in the case where, by applying an external force, RNAs are stretched or refolded, like it is also done in experiments with real RNA. Such processes are realized by first sampling an RNA secondary structure in equilibrium and subsequently performing a non-equilibrium MC Simulation during which the external force parameter is varied. The performed physical work W and secondary structures are measured during the processes.

By utilizing a *large-deviation algorithm* that is based on biasing random numbers [3], we are able to measure the work distributions $P(W)$ over a wide range of the support down to probabilities such as 10^{-40}. We show how work distributions and the corresponding *large-deviation rate function* behave under an appropriate length variations of various nucleotide sequences, specifically, whether the *large-deviation* principle holds.

[1] P. G. Higgs, Phys. Rev. Lett., **76**, 704 (1996)
[2] P. Werner and A. K. Hartmann, Phys. Rev. E **104**, 034407 (2021)
[3] A. K. Hartmann, Phys. Rev. E **89**, 052103 (2014)

DY 49.2 Fri 9:45 H20

Choosing the right event (in non-reversible event-chain Monte Carlo) — •Philipp Höllmer[1], Nicolas Noirault[2], Botao Li[2], A. C. Maggs[3], and Werner Krauth[2] — [1]University of Bonn, Germany — [2]École normale supérieure de Paris, France — [3]ESPCI Paris, France

The general framework of event-chain Monte Carlo (ECMC) constructs non-reversible Markov chains for continuous statistical-physics models ranging from hard-disk systems to long-range interacting molecular systems. Over recent years, several algorithms from the family of ECMC have been proposed, which, in the event-driven formulation of ECMC, only differ in their treatment of events (e.g., of disk collisions in a hard-disk system). Still, we show that different variants can have widely different performances. As a first example, we consider locally stable sparse hard-disk packings. Using a scaling theory confirmed by simulation results, we obtain two classes for the escape from slightly relaxed hard-disk packings parameterized by a relaxation parameter. In one class, the escape time varies algebraically with the relaxation parameter. In the other class, the escape time only scales as the logarithm of the relaxation parameter. As a second example, we consider integrated autocorrelation times in dense systems of flexible extended hard-disk dipoles. Here, the ECMC variants show order-of-magnitude spreads. We expect the performance differences to carry over to long-range interacting molecular systems, where the choice of the optimal ECMC variant is thus highly important.

DY 49.3 Fri 10:00 H20

The GOE ensemble for quasiperiodic tilings without unfolding: r-value statistics — •Rudolf A. Römer[1] and Uwe Grimm[2] — [1]University of Warwick, Coventry, UK — [2]Open University, Milton Keynes, UK

We study the level-spacing statistics for non-interacting Hamiltonians defined on the two-dimensional quasiperiodic Ammann–Beenker (AB) tiling. When applying the numerical procedure of "unfolding", these spectral properties in each irreducible sector are known to be well-described by the universal Gaussian orthogonal random matrix ensemble. However, the validity and numerical stability of the unfolding procedure has occasionally been questioned due to the fractal self-similarity in the density of states for such quasiperiodic systems. Here, using the so-called r-value statistics for random matrices, $P(r)$, for which no unfolding is needed, we show that the Gaussian orthogonal ensemble again emerges as the most convincing level statistics for each irreducible sector [1]. The results are extended to random-AB tilings where random flips of vertex connections lead to the irreducibility.

[1] U. Grimm, R. A. Römer, Phys. Rev. B **104**(6), L060201 (2021)

DY 49.4 Fri 10:15 H20

Classical density functional theory and the primitive model: beyond the standard mean-field approximation — •Moritz Bültmann and Andreas Härtel — Albert-Ludwigs-Universität Freiburg, Physikalisches Institut

To understand the physics of electrolyte solutions one often uses the *primitive model*, where ions are represented by charged hard spheres in a dielectric background. The powerful theory of density functionals, which is widely known from quantum mechanics, can also be applied to such systems in the context of statistical physics. There, the first order of a functional perturbation yields the *mean-field electrostatic functional*, which also contributes at particle separations that are forbidden due to the hard-core interations.

In this talk I summarize our findings from the article [J. Phys.: Condens. Matter **34** 235101], where we modified the mean-field functional such that the occuring pair potential is constant for distances smaller than hard-core contact. The resulting formalism involves weighted densities similar to the ones used in most hard-sphere functionals. Comparing different functionals and result from MD simulations, we analyze density profiles, direct and total correlation functions, and thermodynamic sum rules. Thereby, we found that the modifications improved the predictions compared to the standard mean-field functional significantly. Finally, I report on recent findings of the modified mean-field functional e.g. concerning the decay behavior of total correlation functions.

DY 49.5 Fri 10:30 H20

Recoil experiments determine the eigenmodes of viscoelastic fluids — Karthika Krishna Kumar[1], Félix Ginot[1], •Juliana Caspers[2], Luis Reinalter[1], Matthias Krüger[2], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, Germany — [2]Institute for Theoretical Physics, Georg-August Universität Göttingen, Germany

Probing viscoelastic media using colloidal particles reveals their complex relaxation processes at the microscopic level. Unlike Newtonian fluids, viscoelastic fluids can store and dissipate energy on much longer timescales because of their microstructure, therefore, these materials play a significant role in many technical applications. In this work, we perturb a viscoelastic fluid by driving a colloidal particle through the fluid using an optical tweezer. On deforming the viscoelastic matrix, the fluid tries to relax back by pushing the particle to recoil when the trap is turned off. The trajectory of such a recoiling particle exhibits a bi-exponential behavior indicating two distinct relaxation processes of the fluid. Detailed investigation shows that a microscopic model, with two fictitious bath particles connected to the probe particle via harmonic springs, explains the observed behavior. The analytical solution to the model also reveals two more timescales corresponding to the relaxation of the bath particles when the probe is fixed. The need for two bath particles to explain the results can be justified by considering the fluid as a glassy system, however, further experiments are required to confirm this.

15 min. break

DY 49.6 Fri 11:00 H20

FIPS: A generic framework for many-particle simulations focusing on efficiency and reliability* — •Julian Jeggle and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Numerical calculation of particle trajectories in many-particle systems is an important class of molecular dynamics (MD) simulations that has been implemented in well-known MD packages such as GROMACS, HOOMD-blue, and LAMMPS. Recently, efforts have been made to develop more flexible data models for this task with the help of modern programming techniques. In this talk, we present further advancements into this direction in the form of FIPS, the *flexibly integrating particle simulator*. This tool enables the simulation of many-particle systems and their dynamics described by a domain specific language heavily inspired by GPU shaders. Unlike traditional MD packages, we utilize just-in-time compilation and shared-state concurrency to achieve a high degree of efficiency. To increase resilience towards pro-

gramming errors, our implementation is tightly coupled to Rust, a novel systems programming language with a focus on reliability, in particular for concurrent applications.

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DY 49.7 Fri 11:15 H20

The reversible heat production during the electric double layer buildup: Analysis with an extension of the primitive model by hydration shells — •Philipp Pelagejcev, Fabian Glatzel, and Andreas Härtel — Albert-Ludwigs-Universität Freiburg

The reversible heat production during the electric double layer (EDL) buildup was measured experimentally [Janssen et al., Phys. Rev. Lett. 119, 166002 (2017)] and in theoretical work [Glatzel et al., J. Chem. Phys. 154, 064901 (2021)], it was found that steric interactions of ions with the flat electrodes, which result in the so-called Stern layer, are sufficient to explain the experimental results. In the latter only symmetric ion sizes in a restricted primitive model were examined.

In this work, I present the impact of ion asymmetry on the reversible heat production for each electrode separately. Additionally, an extension of the primitive model where hydration shells of ions can evade in the vicinity of the electrodes is discussed. With this extended model one can describe situations where one electrode is heated and the other electrode is cooled simultaneously during charging, while both electrodes together behave similarly to the already mentioned experimental results.

Thus, in experiments the heat production should be measured for each electrode separately. By this, the importance of certain ingredients for a primitive model based electrolyte could be evaluated experimentally, finally leading to a deeper understanding of EDLs. (Reference: [Pelagejcev et al., J. Chem. Phys. 156, 034901 (2022)])

DY 49.8 Fri 11:30 H20

Uncovering broken detailed balance hidden by unknown degrees — •Gabriel Knotz, Till moritz Münker, Timo Betz, and Matthias Krüger — Fakultät für Physik, Georg-August-Universität, Göttingen, Germany

The complex nature of non equilibrium systems remains a challenging task in statistical physics, but especially for living matter. A major experimental problem is, that often some relevant degrees cannot be observed (are hidden) which complicates theoretical analysis. We study a non-equilibrium model with two degrees of freedom. If both degrees are observed, the breaking of detailed balance can easily be quantified. However, by treating one of the degrees as hidden, the trajectory of the other is time reversal symmetric. To still detect the breakage of detailed balance we can use a new quantity, the mean backward relaxation (MBR), that measures the relaxation of displacements caused by the fluctuating forces. By deriving rigorous statements for equilibrium in general and calculating the MBR for the non-equilibrium system, we show that the MBR reveals that the system breaks detailed balance even though one degree is hidden. Further we are able to relate the deviation of the MBR compared to an equilibrium system to an effective energy. This analysis adds a new approach to systems that deal with unknown, but relevant non-equilibrium degrees of freedom.[1]

[1] Till M. Muenker, Gabriel Knotz, Matthias Krüger and Timo Betz. *Onsager regression characterizes living systems in passive measurements.* bioRxiv: 2022.05.15.491928

DY 49.9 Fri 11:45 H20

Generalized hydrodynamics description of the classical Toda lattice and high-low pressure domain wall initial conditions — •Christian Mendl and Herbert Spohn — Technische Universität München (TUM)

We review and discuss generalized hydrodynamics applied to the classical Toda lattice, a paradigmatic example for an interacting integrable system. One first identifies the Lax matrix of the system, which is closely related to the microscopic conservation laws. For the Toda lattice, the free energy can be expressed in terms of the eigenvalue spectrum of the Lax matrix. One finally arrives at semi-analytic formulas for dynamical correlation functions in equilibrium, which show good agreement with molecular dynamic simulations.

In the second part, we focus on domain wall initial conditions, for which the left and right half lattice are in thermal equilibrium but with distinct parameters. The particular case of interest is a jump from low to high pressure at uniform temperature and zero mean velocity, whereby the scaling function for the average stretch is forced to change sign. The hydrodynamic equations seem to be singular at zero stretch, but nevertheless the self-similar solution exhibits smooth behavior.

[1] C. B. Mendl, H. Spohn, High-low pressure domain wall for the classical Toda lattice, SciPost Phys. Core 5, 002 (2022)

[2] H. Spohn, Hydrodynamic equations for the Toda lattice, arXiv:2101.06528

[3] H. Spohn, Generalized Gibbs ensembles of the classical Toda chain, J. Stat. Phys. 180, 4 (2020)

DY 49.10 Fri 12:00 H20

The square-lattice Ising model on the rectangle — •Fred Hucht — Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg

For the square-lattice Ising model, the universal critical Casimir potential and force scaling functions can be calculated exactly for many geometries and boundary conditions. We present a recent exact solution of the square lattice Ising model on the $L \times M$ rectangle, with open boundary conditions in both directions [1], in terms of the determinant of a $M/2 \times M/2$ Hankel matrix $\mathbf{H}$. The $M-1$ independent matrix elements of $\mathbf{H}$ are Fourier coefficients of a certain symbol function, which is given by the ratio of two characteristic polynomials. These polynomials are associated to the different directions of the system, encode the respective boundary conditions, and are directly related through the symmetry of the considered Ising model under exchange of the two directions. This representation is a major simplification of earlier results [2,3].

[1] A. Hucht, *J. Phys. A: Math. Theor.* **54**, 375201 (2021). arXiv:2103.10776.
[2] A. Hucht, *J. Phys. A: Math. Theor.* **50**, 065201 (2017). arXiv:1609.01963, erratum [4].
[3] A. Hucht, *J. Phys. A: Math. Theor.* **50**, 265205, (2017). arXiv:1701.08722.
[4] A. Hucht, *J. Phys. A: Math. Theor.* **51**, 319601 (2018).