DY 15: Statistical Physics far from equilibrium

Time: Wednesday 9:30–13:30 Location: MA 004

Invited Talk DY 15.1 Wed 9:30 MA 004

Fluctuations and State Variables in Driven Granular Materials — •Karen Daniels — Dept. of Physics, North Carolina State University, Raleigh, NC, USA — MPI for Dynamics and Self-Organization, Göttingen

Statistical mechanics has provided a powerful tool for understanding the states of thermodynamic matter, and it is intriguing to investigate whether these successes are also relevant to non-equilibrium systems such as granular materials. I will describe experiments on a two-dimensional dense granular gas of disks suspended on a horizontal air table and agitated at the boundaries. We measure both bulk and particle-scale dynamics, and find a number of thermal-like behaviors including diffusive dynamics, a granular Boyle's law with a van der Waals-like equation of state, and energy equipartition for rotational and translational degrees of freedom. However, the scarcity of free volume provides a crucial control on the dynamics, and each of the above thermal-like behaviors is accompanied by interesting caveats.

DY 15.2 Wed 10:00 MA 004

Spin Glass to Ferromagnet: Ageing Simulations on GPUs — •Markus Manssen[1], Martin Weigel[2], and Alexander K. Hartmann[1] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — [2]Applied Mathematics Research Centre, Coventry University, England

The dynamics of spin glasses, frustrated magnetic systems, have been extensively studied [1] with computer simulations [2]. We broaden our view to the phase transition to the ferromagnet with the aid of Graphics Processing Units (GPUs) for long time simulations [3]. We focus on the three-dimensional binary Edwards-Anderson model and examine spatial and temporal correlations trying to explain them in terms of a growing dynamical correlation length.

[1] Naoki Kawashima and Heiko Rieger. Recent Progress in Spin Glasses. In Hung T. Diep, editor, *Frustrated Spin Systems*, pages 491–596. World Scientifc, 2004.

[2] Alexander K. Hartmann, *Practical Guide to Computer Simulations*, World Scientific, 2009

[3] Martin Weigel. Simulating spin models on GPU. *Computer Physics Communications*, 182(9): 1833–1836, 2010.

DY 15.3 Wed 10:15 MA 004

Microscopic Scattering Theory for Interacting Bosons in a Random Potential — Tobias Geiger, •Thomas Wellens, and Andreas Buchleitner — Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg

We microscopically derive a theory for scattering of N atoms – with all atoms initially prepared in the same single-particle momentum eigenstate – from a three dimensional random disorder potential in the presence of two-body interactions. Starting from an exact diagrammatic expansion of the N-particle scattering amplitude, we identify those combinations of diagrams which – in the case of a weak random potential (mean free path much larger than wavelength) – survive the disorder average, and sum up the remaining series of ladder and crossed diagrams non-perturbatively in the strength of the particle-particle interaction [1]. We show that the latter leads to a relaxation of the individual particles' energies towards a Maxwell-Boltzmann distribution as the particles diffuse throughout the random potential. As interferential correction to diffusive transport, we furthermore consider the phenomenon of coherent backscattering and analyze how this coherent effect is modified by interactions.

[1] T. Wellens and B. Grémaud, Phys. Rev. Lett. **100**, 033902 (2008).

DY 15.4 Wed 10:30 MA 004

Pressure fluctuations lead to assembly of smectic domains — •Marco Mazza[1] and Martin Schoen[1,2] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany — [2]Department of Chemical and Biomolecular Engineering, North Carolina State University, 911 Partners Way, Raleigh, NC 27695, U.S.A.

The interplay of geometry and directional interactions generates myriad different equilibrium phases in liquid crystal materials. However, comparatively little is known of their nonequilibrium behavior, especially in the case of nanoscopic confinement. Here, we perform nonequilibrium computer simulations of a system of prolate mesogens confined to a nanoscopic slit-pore. We apply a time-dependent surface anchoring at the walls. A steady state arises consisting of a smectic domain. We study the behavior of these smectic domains as temperature and frequency are varied.

We find that, although pressure and temperature are too low to form a smectic state, pressure fluctuations in the nonequilibrium steady state match the pressure fluctuations in equilibrium. Our calculations demonstrate in principle a novel method of manufacturing materials with a high degree of molecular order.

DY 15.5 Wed 10:45 MA 004

How to capture self-propelled particles — •Andreas Kaiser, Henricus H. Wensink, and Hartmut Löwen — Heinrich-Heine-Universität Düsseldorf

For many applications, it is important to catch collections of autonomously navigating microbes and man-made microswimmers in a controlled way. Here we design an efficient trap to capture rod-like elf-propelled particles collectively. By computer simulations in two dimensions, a V-shape is found to be the optimal boundary for a trapping device. The efficiency of catching can be largely tuned by the opening angle α of the trap. For increasing α, there is a sequence of three emergent states corresponding to partial, complete, and no trapping.

DY 15.6 Wed 11:00 MA 004

Experimentally realizable control functions: optimal control with arbitrary basis functions — •Selina Rohrer, Joachim Ankerhold, and Jürgen Stockburger — Institut für Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

Optimal control theory aims at driving a dynamical system towards a final state that minimizes a figure of merit and at finding the required time-dependent controls. Using the Moore-Penrose Pseudoinverse [1] we are able to find optimal control functions, not in the whole control space, but in a subspace, which is spanned by arbitrary, not necessarily orthogonal basis functions. This optimization technique allows us to take into account limitations of experimental set-ups, such as, eg., a finite rise time of the control pulses. To illustrate this optimization technique with different sets of basis functions, we study a harmonic oscillator as model system, which is coupled to a thermal environment. For all presented sets of basis functions, we are able to cool the system below the temperature of the coupled bath.

[1] R. Penrose, A generalized inverse for matrices. Proceedings of the Cambridge Philosophical Society 51, S. 406-413, 1955

15 min. break

DY 15.7 Wed 11:30 MA 004

Quantum cold ion heat engine at maximal efficiency — •Obinna Abah[1], Sebastian Deffner[2], Georg Jakob[3], Johannes Rossnagel[3], Kilian Singer[3], Ferdinard Schmidt-Kaler[3], and Eric Lutz[1,4] — [1]Department of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742 USA — [3]Institut für Quantenphysik, Universität Mainz, D-55128 Mainz, Germany — [4]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, D-14195 Berlin-Dahlem, Germany

We propose an experimental realizable quantum Otto heat engine working with a single ion in a segmented linear Paul trap. We analyze the theoretical efficiency at maximum power for adiabatic and nonadiabatic processes, both in the limit of high and low temperatures. We moreover present results from numerical simulations with realistic parameters.

DY 15.8 Wed 11:45 MA 004

Counting statistics of an electronic Maxwell's demon — •Gernot Schaller, Clive Emary, Gerold Kiesslich, and Tobias Brandes — Institut für Theoretische Physik, Technische Universität Berlin, Berlin

A single-electron transistor (SET) that is continuously monitored by a quantum point contact may function as Maxwell's demon when closed-loop feedback operations are applied as time-dependent modifications of the tunneling rates across its junctions. The device may induce a current across the SET even when no bias voltage or thermal gradient is applied. For sufficiently strong feedback, it is also possible to transport electrons against an existing voltage (or thermal) gradient. We compare the generated power for different feedback schemes with the heat arising from Landauers principle and find no violation of the second law.

G. Schaller *et al.*, Phys. Rev. B **84**, 085418 (2011).

DY 15.9 Wed 12:00 MA 004

Current fluctuation theorems under incomplete monitoring — •Thilo Krause, Gernot Schaller, and Tobias Brandes — Institut für Theoretische Physik, Technische Universität Berlin, Berlin

We demonstrate the validity of the fluctuation theorem for a double quantum dot surrounded by four terminals within the Born-, Markov- and secular approximations beyond the Coulomb-blockade regime. The electronic tunneling to two fermionic contacts conserves the total number of electrons, and the internal tunneling is phonon-assisted by two bosonic baths. Adapted choice of thermodynamic parameters between the baths may drive a current against an existing electric or thermal gradient. We study the apparent violation of the fluctuation theorem when only some of the energy and matter currents are monitored.

T. Krause, G. Schaller, and T. Brandes, Phys. Rev. B **84**, 195113 (2011).

DY 15.10 Wed 12:15 MA 004

Thermodynamics of genuine non-equilibrium states under feedback control — •David Abreu and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

The work extracted from a thermodynamic system can exceed the free energy difference between final and initial states if feedback control is implemented. For transitions between equilibrium states, Sagawa and Ueda showed that the Jarzynski equality - and therefore the second law of thermodynamics - can be generalized to take into account the information obtained through measurements [1].

In the case of transitions between genuine non-equilibrium states that even at fixed external control parameter exhibit dissipation, we extend the Hatano-Sasa equality to processes with feedback control [2]. The resulting bound on the maximal extractable work is substantially sharper than what would follow from applying the Sagawa-Ueda equality to transitions involving such states. For repeated measurements at short enough intervals, the power thus extracted can even exceed the average cost of driving as demonstrated explicitly with a simple, analytically solvable example.

[1] T. Sagawa and M. Ueda. Phys. Rev. Lett. 104, 090602 (2010).
[2] D. Abreu and U. Seifert. arXiv: 1109.5892 (2011).

DY 15.11 Wed 12:30 MA 004

Information free energy for nonequilibrium states — Sebastian Deffner[1] and •Eric Lutz[2] — [1]Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742 — [2]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin

We introduce an information free energy for thermodynamic systems driven by external time-dependent parameters. We show that the latter is a nonequilibrium state function and that it is a natural generalization of the usual equilibrium free energy. We discuss its importance for the maximum work theorem, the Jarzynski relation in the presence of feedback, and the relaxation to nonequilibrium steady states.

DY 15.12 Wed 12:45 MA 004

The thermodynamic cost of measurements — •Léo Granger and Holger Kantz — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The measurement of thermal fluctuations provides information about the microscopic state of a thermodynamic system and can be used in order to extract work from a single heat bath in a suitable cyclic process. We present a minimal framework for the modeling of a measurement device and we propose a protocol for the measurement of thermal fluctuations. In this framework, the measurement of thermal fluctuations naturally leads to the dissipation of work. We illustrate this framework on a simple two states system inspired by the Szilard's information engine.

Topical Talk DY 15.13 Wed 13:00 MA 004

Impact of interaction effects on hopping transport in driven systems — •Mario Einax — Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück, Germany

Particle transport in low-dimensional biological, chemical and physical systems is of vital importance for many applications and has hence attracted much attention in recent years. Prominent examples are Brownian motors and ratchets, photovoltaic cells, and electron transport in the incoherent limit in molecular wires. A one-dimensional hopping motion is also the decisive transport mechanism in ion conduction through membrane channels and in unidirectional motion of motor proteins along filaments. Driven lattice gases offer a promising approach for studying the role of interaction effects between transported particles in such systems. In this talk I will review how by using the time-dependent density functional theory (TDFT) for lattice systems a systematic method is provided that allows one to treat the kinetics of driven lattice gases with interactions. To demonstrate its effectiveness, I will consider the motion of interacting particles through an open channel under peristaltic driving [1] and a totally asymmetric site exclusion process (TASEP) with nearest-neighbor interactions [2,3].

[1] M. Einax, G. C. Solomon, W. Dieterich, and A. Nitzan, J. Chem. Phys. **133**, 054102 (2010).
[2] M. Dierl, P. Maass, and M. Einax, Europhys. Lett. **93**, 50003 (2011).
[3] M. Dierl, P. Maass, and M. Einax, Phys. Rev. Lett., in Press (2012).