DY 28: Statistical Physics far from Equilibrium

Time: Thursday 10:15–13:15 Location: HÜL 186

DY 28.1 Thu 10:15 HÜL 186

Nonequilibrium steady states in contact: Approximate thermodynamic structure and zeroth law for driven lattice gases — •Punyabrata Pradhan, Christian Amann, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

We explore a class of nonequilibrium systems, called driven lattice gases, for the existence of an intensive thermodynamic variable which could determine "equilibration" between two such nonequilibrium systems kept in weak contact [1]. We numerically check that there exists an intensive thermodynamic variable, like equilibrium chemical potential, which equalize in the final "equilibrated" steady state when two initially separated driven lattice gases are brought into contact and allowed to exchange particles with total number of particles conserved. We find that these systems satisfy surprisingly simple thermodynamic laws, such as the zeroth law and the fluctuation-response relation between the particle-number fluctuation and the corresponding susceptibility remarkably well. However at higher densities, small but observable deviations from these laws occur due to nontrivial contact dynamics and the presence of long-range spatial correlations.

Reference: [1] P. Pradhan, C. P. Amann and U. Seifert, Phys. Rev. Lett. **105**, 150601 (2010).

DY 28.2 Thu 10:30 HÜL 186

Crooks fluctuation theorem for the fluctuating lattice-Boltzmann model — •Léo Granger[1], Markus Niemann[2], and Holger Kantz[1] — [1]Max Planck Institut für Physik komplexer Systeme, Dresden, Germany — [2]Carl von Ossietzky Universität Oldenburg, Institut für Physik, Oldenburg, Germany

We probe the validity of Crooks' fluctuation relation on the fluctuating lattice-Boltzmann model (FLBM), a highly simplified lattice model for a thermal ideal gas. Crooks' relation is one of the only rigorous results known about non-equilibrium thermodynamics. It links a dynamic quantity, the probability to perform a certain amount of work during a non quasi-static process, to a thermodynamic quantity, the difference in equilibrium free energy between the initial and the final states.

We simulate am ideal gas submitted to a force field. By gradually switching on and off the force field, we drive the system frome one thermondynamic equilibrium state to another, performing some work on the gas. By comparing the distributions of the work performed during the forward driving and time reversed driving, we show that the system satisfies Crooks' relation.

DY 28.3 Thu 10:45 HÜL 186

Investigations of unconventional quantum statistics in isolated spin clusters — •Kai Ji and Boris Fine — Institute for Theoretical Physics, University of Heidelberg, Philosophenweg 19, 69120 Heidelberg, Germany

Quantum micro-canonical (QMC) ensemble refers to an isolated quantum system with fixed average energy but unrestricted participation of eigenstates. The QMC ensemble reveals marked deviation from the conventional Boltzmann-Gibbs (BG) statistics [1]. In this work, based on an anisotropic Heisenberg model, we perform numeral investigations on the statistics of QMC ensemble and discuss the physical realization of it in isolated spin clusters. The exploration for superpositions of quantum states in the Hilbert space is proposed to be driven by strong perturbations with a series of magnetic pulses. It is demonstrated that starting from a BG distribution, the occupation numbers universally evolve to the distribution obtained in Ref. [1] before reaching the infinite temperature limit, indicating the onset of QMC ensemble. Possible ways for detecting the established QMC ensemble is to be addressed as well.

[1] B.V. Fine, Phys. Rev. E 80, 051130 (2009).

DY 28.4 Thu 11:00 HÜL 186

Nonequilibrium entropy production for open quantum systems — •Sebastian Deffner and Eric Lutz — Department of Physics, University of Augsburg, D-86135 Augsburg, Germany

We consider a driven quantum system weakly coupled to a thermal environment. We provide a microscopic expression for the irreversible entropy production for general far from equilibrium processes and show that it fulfills an integral fluctuation theorem. Our derivation is solely based on thermodynamic arguments and does not rely on master equations or quantum trajectories.

DY 28.5 Thu 11:15 HÜL 186

Absence of Boltzmann-Gibbs equilibrium in an isolated quantum system with fixed energy and unrestricted participation of eigenstates. — •Boris Fine — Institute for Theoretical Physics, University of Heidelberg, 69120 Heidelberg, Germany

Usual approach to the foundations of quantum statistical physics is based on conventional micro-canonical ensemble as a starting point for deriving Boltzmann- Gibbs (BG) equilibrium. It leaves, however, a number of conceptual and practical questions unanswered. Here we discuss these questions, thereby motivating the study of a natural alternative known as Quantum Micro-Canonical (QMC) ensemble. The QMC ensemble includes all possible superpositions of eigenstates of a large isolated quantum system provided all these superpositions have the same energy expectation value. We obtain analytically the statistics associated with the QMC ensemble for both the entire system and its small subsystem[1]. In a significant departure from the BG statistics, the average occupation numbers of quantum states exhibit in the present case weak algebraic dependence on energy. In the macroscopic limit, this dependence is routinely accompanied by the condensation into the lowest-energy quantum state. The above unconventional kind of equilibrium may be realizable after strong perturbations in small isolated quantum systems having large number of levels. We further suggest that the reason, why BG equilibrium commonly occurs in nature rather than the QMC-type equilibrium, has something to do with the notion of quantum collapse. [1] B.V. Fine, Phys. Rev. E v.80, p. 051130 (2009).

DY 28.6 Thu 11:30 HÜL 186

Monte-Carlo sampling of energy-constrained quantum superpositions in high-dimensional Hilbert spaces — •Frank Hantschel and Boris Fine — Institute for Theoretical Physics, Heidelberg, Germany

The quantum microcanonical (QMC) ensemble is an alternative to conventional statistical ensembles, which results in a deviation from the usual Gibbs distribution. The resulting statistics is computed by performing a Monte-Carlo simulation on high-dimensional Hilbert space.

A straightforward Monte-Carlo routine would enclose the energy constrained manifold within a larger manifold, which is easy to sample, e.g., a hypercube. We observed that the efficiency of such a sampling routine decreases exponentially with the increase of the dimension of the Hilbert space, because the volume of the enclosing manifold becomes exponentially larger than the volume of the manifold of interest. This fact imposes a problem, because it strongly limits the size of the system of interest.

The talk explores the ways to optimize the above routine by varying the shapes of the manifolds enclosing the energy-constrained manifold. The resulting improvement in the sampling efficiency is about a factor of five for a 14-dimensional Hilbert space. The advantage of the above algorithm is that it does not compromise on the rigorous statistical nature of the sampling outcome and hence can be used to test other more sophisticated Monte-Carlo routines. The present attempts to optimize the enclosing manifolds also bring insights into the geometrical properties of the energy-constrained manifold itself.

15 min. break.

DY 28.7 Thu 12:00 HÜL 186

Non-perturbative renormalization of a diffusion-limited decay process — •Anton Winkler and Erwin Frey — Arnold Sommerfeld Center and CeNS, Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, 80333 München, Germany

Many quantitative results for stochastic processes are restricted to one dimension, where a plethora of methods is available. However, in higher dimensions they often fail. Furthermore, the major part of renormalization group analysis focuses on low dimensions, i.e. lower than or equal to the upper critical dimension. For magnetic $O(n)$ models this is of course very reasonable since in this case the upper critical dimension is four.

In our work we have studied the decay process $A + A \rightarrow 0$ in the framework of reaction diffusion processes. The critical dimension of our decay process is two. In three dimensions, fluctuations are not strong enough to obliterate the microscopic structure of space and the shape of the particles. This poses a problem to the usual perturbative approach because it works best for studying universal features.

Our non-perturbative approach is known to cope also with non-universal properties. It allowed us to tackle the intriguing question of how the microscopic structure enters the dynamics of the process in three and higher dimensions by providing exact results for the non-equilibrium Gibbs energy.

DY 28.8 Thu 12:15 HÜL 186

The influence of temperature gradients on protein folding — •Bernhard Reuter[1], Pedro Ojeda-May[2], and Martin E. Garcia[1] — [1]Universität Kassel, Fachbereich Naturwissenschaften, Institut für Theoretische Physik, Heinrich-Plett-Straße 40, 34132 Kassel, Germany — [2]Institute for Computational Physics, Universität Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany

Using Monte Carlo techniques in the framework of the lattice model we addressed the folding of proteins under extreme temperature gradients.

This analysis is inspired by the recent work of Zia [Zia et al., EPL, 89 (2010) 50001] in which a 2D Ising model with two different temperature regions was studied and the presence of persistent currents at the interface between the temperature regions was observed. The relevant fact is that no gravity and no shear forces are necessary to induce those nonequilibrium effects but only the temperature gradient.

In the present work we aim at determining if temperature gradients are also capable of inducing nonequilibrium patterns in more sophisticated models such as proteins in a lattice. We analyze the influence of the magnitude of the temperature difference on the attained protein conformations. Also we compare the so obtained structures with those of the thermodynamic equilibrium.

DY 28.9 Thu 12:30 HÜL 186

Analysis of non-equilibrium fluctuations of quantum mechanical expectation values — •Christian Bartsch and Jochen Gemmer — Fachbereich Physik, Universität Osnabrück, Barbarastrasse 7, D-49069 Osnabrück, Germany

For certain abstract, closed quantum systems the dynamics of expectation values, obtained by exact diagonalization, may be interpreted as a composition of some "regular" dynamics, e.g., an exponential decay into equilibrium, and some "irregular" part, which we call fluctuations. We numerically find that the latter may typically be regarded as Gaussian white noise in good approximation. Furthermore, we analyze particularly the non-equilibrium fluctuations on the basis of a Langevin-type equation describing the time evolution of the expectation value, where the fluctuations are incorporated as a stochastic force. We moreover define an entropy as a function of the analyzed expectation value, similar to the common von Neumann-entropy. As long as the fluctuations correspond to a stochastic Gaussian variable, the entropy production over time may as well be viewed as a Gaussian stochastic variable, for which then the fluctuation theorem holds. Additionally, we analyze the scaling of the fluctuations with fundamental system parameters.

DY 28.10 Thu 12:45 HÜL 186

Energy current magnification in coupled oscillator loops. — •Rahul Marathe — Max Planck Institute for Colloids and Interfaces, 14476, Potsdam, Germany.

Motivated by studies on current magnification in quantum mesoscopic systems, we consider sound and heat transmission in classical models of oscillator chains. A loop of coupled oscillators is connected to two leads through which one can either transmit monochromatic waves or white-noise signal from heat baths. We look for the possibility of current magnification in this system due to some asymmetry introduced between the two arms in the loop. We find that current magnification is indeed obtained for particular frequency ranges. However, the integrated current shows the effect only in the presence of a pinning potential for the atoms in the leads. We also study the effect of anharmonicity on current magnification.

DY 28.11 Thu 13:00 HÜL 186

Endoreversible Modeling using the example of fuel cells — •Katharina Wagner and Karl Heinz Hoffmann — Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany

In endoreversible thermodynamics irreversible processes and systems are split into reversible subsystems and interactions in between them. Subsystems can either be reservoirs storing energy and extensive quantities or engines transferring energy between different extensive quantities. The irreversibilities of the system are completely described by the interactions between the reversible subsystems. This separation leads to a block of balance equations, which characterize the reversible subsystems, and transport equations, which describe the interactions. The entropy production can thus be localized within the whole system. Using the formalism of endoreversible thermodynamics a PEM fuel cell is modeled and the power output as well as the efficiency are investigated.