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Fundamental Aspects of Statistical Mechanics and the Emergence of Thermodynamics in Non-Equilibrium Systems

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Abstracts

Thermodynamic Geometry of Microscopic Heat Engines

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ABSTRACT

Friction is a ubiquitous phenomenon that hinders the performance of thermal machines across all length and energy scales. Here, we explore this effect from the perspective of thermodynamic geometry. We develop a general framework that uses the concept of thermodynamic length to quantify friction-like energy losses in microscopic heat engines driven by slow periodic temperature and control-field variations. Covering both the classical and the quantum regime, this approach leads to a universal optimization principle and a new trade-off relation between power and efficiency. These results follow solely from geometric arguments and hold for any thermodynamically consistent microdynamics. Focusing on Lindblad dynamics, we then derive a second bound showing that coherence as a genuine quantum effect inevitably reduces the performance of slow engine cycles regardless of the driving amplitudes. To demonstrate the practical applicability of our theory, we show how it can be used to optimize the performance of a single-qubit heat engine, which lies within the range of current solid-state technologies.

Relaxation theory for perturbed many-body quantum systems

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ABSTRACT

We develop an analytic prediction for the relaxation of isolated many-body quantum systems subject to weak-to-moderate perturbations. Provided that the unperturbed behavior is known, we employ a typicality approach modeling the essential characteristics of the perturbation operator to describe the time evolution of expectation values in the perturbed system. Our theory provides a unified framework for such diverse phenomena as prethermalization, quantum quenches, or the relaxation of system-bath compounds. We demonstrate its wide applicability by comparison with various experimental and numerical results from the literature.

Ordering in non-equilibrium steady states of driven-dissipative quantum systems

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ABSTRACT

Statistical mechanics provides a powerful framework for predicting the equilibrium properties of matter. The lack of such a universal concept for driven many-body systems makes their theoretical treatment difficult; but, at the same time, it also allows for engineering non-equilibrium states of matter with novel properties beyond the strict constraints of thermodynamics. As an example, I will discuss ordering (Bose condensation) in non-equilibrium steady states of systems in thermal environments that are strongly driven by time-periodic forcing [1,2], temperature gradients [1-3], and pumping [4, 5]. Our work predicts robust excited-state and fragmented Bose condensation [1-5], Bose condensation in environments well-above the equilibrium critical temperature [3], and it explains experiments with photons in structured environments [4,5].

[1] D. Vorberg, W. Wustmann, R. Ketzmerick, and A. Eckardt, *Generalized Bose-Einstein condensation into multiple states in driven-dissipative systems*, Phys. Rev. Lett. **111**, 240405 (2013).

[2] D. Vorberg, W. Wustmann, H. Schomerus, R. Ketzmerick, and A. Eckardt, *Non-equilibrium steady states of ideal bosonic and fermionic quantum gases*, Phys. Rev. E **92**, 062119 (2015).

[3] A. Schnell, D. Vorberg, R. Ketzmerick, and A. Eckardt, *High-temperature nonequilibrium Bose condensation induced by a hot needle*, Phys. Rev. Lett. **119**, 140602 (2017).

[4] H. A. M. Leymann, D. Vorberg, T. Lettau, C. Hopfmann, C. Schneider, M. Kamp, S. Höfling, R. Ketzmerick, J. Wiersig, S. Reitzenstein, and A. Eckardt, *Pump-power-driven mode switching in a microcavity device and its relation to Bose-Einstein condensation*, Phys. Rev. X **7**, 021045 (2017).

[5] D. Vorberg, R. Ketzmerick, and A. Eckardt, *A unified theory for excited-state, fragmented, and equilibrium-like Bose condensation in pumped photonic many-body systems*, Phys. Rev. A **97**, 063621 (2018).

Stochastic thermodynamics with hidden degrees of freedom

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ABSTRACT

Stochastic Thermodynamics allows the definition of heat and work for microscopic systems far from thermodynamic equilibrium from observations of their stochastic dynamics. Taking into account thermal fluctuations leads to the so called fluctuation theorems which are useful symmetry relations for the entropy production. However, a complete account of the energetics of small-scale systems necessitates that all relevant degrees of freedom are resolved. In many experimental situations this is not feasible.

I will present three example systems which illustrate the influence of unobserved slow degrees of freedom on the energetics of small-scale systems. The first is a simple microswimmer model for which the observation of its movement alone does not suffice to correctly assess its energy dissipation [1]. With the help of a second model of a driven process, I show that mapping the observed dynamics to a Markov process, while being a promising first attempt, results in the breaking of fluctuation theorems, which quickly exposes this flawed description [2]. Finally, for the setting of a masked Markovian kinetic network, I show a more promising approach, which is to consider the full non-Markovian statistics of the observed data and to try to find an underlying hidden Markov model responsible for generating them.

[1] J. Ehrich and M. Kahlen, Phys. Rev. E **99**, 012118 (2019).

[2] M. Kahlen and J. Ehrich, J. Stat. Mech. 063204 (2018).

Conservation Laws in Nonequilibrium Thermodynamics

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ABSTRACT

Conservation laws play a key role in shaping dissipation in nonequilibrium thermodynamics by identifying conservative and nonconservative thermodynamic forces as well as the right nonequilibrium potential. I will first demonstrate this finding using stochastic thermodynamics and then deterministic open chemical reaction networks. Various applications will then be presented.

[1] R. Rao and M. Esposito, *Conservation Laws shape Dissipation*, New J. Phys. **20**, 023007 (2018).

[2] R. Rao and M. Esposito, *Conservation Laws and Work Fluctuation Relations in Chemical Reaction Networks*, J. Chem. Phys. **149**, 245101 (2018).

[3] R. Rao and M. Esposito, *Nonequilibrium Thermodynamics of Chemical Reaction Networks: Wisdom from Stochastic Thermodynamics*, Phys. Rev. X **6**, 041064 (2016).

Eigenstates of many-body systems as random-matrix states

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ABSTRACT

Quantum dynamics is reconciled with statistical mechanics through the eigenstate thermalization hypothesis (ETH). ETH relies on the idea that high-energy eigenstates of complex quantum systems are effectively "random". By considering different properties of many-body eigenstates, I will examine the validity and limitations of this idea.

Many-body localization dynamics and time crystals protected by gauge invariance

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ABSTRACT

In this talk I will show how lattice gauge theories can display many-body localization dynamics in the absence of disorder as a consequence of local constraints induced by gauge invariance. The starting point is the observation that, for some generic homogeneous initial conditions, the time-evolved state can be decomposed into different superselection sectors as a consequence of Gauss law in such a way that it realizes an effective disorder average. By carrying out extensive exact simulations on the real-time dynamics of a lattice Schwinger model, describing the coupling between $U(1)$ gauge fields and staggered fermions, it is shown that the dynamics can become nonergodic leading to a slow, double-logarithmic entanglement growth. Further, it will be shown how the nonergodic behavior induced by this localization mechanism can give rise to eigenstate phases in homogeneous systems. Specifically, I will introduce a model for a "gauge time crystal" breaking spatiotemporal symmetries.

Tripartite information and scrambling in quantum spin systems

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ABSTRACT

The delocalization of information and scrambling are of fundamental interest for the characterization of dynamics in quantum many-body systems. Out-of-time-order correlators constitute a possible probe of this behavior, but a more general observable-independent measure is given by scrambling as quantified by the tripartite information. In this talk I show results for the dynamics of the tripartite information in quantum lattice models with tuneable integrability breaking. One can see that non-integrable systems scramble information very efficiently (Haar limit) irrespective of the chosen partitioning of the Hilbert space.

Thermalization properties of a system with topological flat bands and impurities

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ABSTRACT

Topological insulators posses edge states, which are gapless in contrast to the bulk states. Bi_2Se_3 is of particular interest, because of its relatively simple Hamiltonian and most importantly under the influence of a Zeeman field flat bands appear in thin stripes of this material [1].

Due to the zero group velocity of electrons in flat bands there is no thermalization for a localized initial state. The question arises how this non-thermalization behaviour and the localization changes in the presence of impurities. In this work we focus on disorder, which modifies the on-site energy of the material. The influence of this disorder is investigated numerically using time evolution. The observable of interest is a quantity which is related to the localization of the wavepacket. The behaviour of this observable under change of strength and number of impurities is compared to a situation without a flat band. To investigate the question of thermalization it is probed whether the eigenstate thermalization hypothesis holds. To do this we employ a method suggested by Steinigeweg et al. [2] This method uses random state vectors and scaling behaviour to decide this matter.

[1] T. Paananen and T. Dahm, *Magnetically robust topological edge states and flat bands*, Phys. Rev. B **87**, 195447 (2013).

[2] R. Steinigeweg, A. Khodja, H. Niemeyer, C. Gogolin, and J. Gemmer, *Pushing the limits of the eigenstate thermalization hypothesis towards mesoscopic quantum systems*, Phys. Rev. Lett. **112**, 130403 (2014).

Time-dependent generalized Gibbs ensembles in open quantum systems

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ABSTRACT

Equilibrium description in terms of temperature and chemical potential is an extremely economical way to characterize otherwise complicated many-particle systems. Simplicity lies in the fact that one can specify the state of the system in terms of a few parameters only. I will show that if we allow for time dependent temperature and chemical potential, such description applies also to weakly open and driven interacting systems [1].

Above formalism, based on existence of approximate conservation laws, can be easily extended to nearly integrable models by using extensively many Lagrange parameters, corresponding to additional conservation laws. While generalized Gibbs ensembles have been proposed as steady state of quenched integrable models, I will argue that they approximately describe also steady state and slow relaxation in nearly integrable models that are weakly driven and couple to (non-)equilibrium baths. As an example I will consider a Heisenberg model coupled to Markovian baths and show that evolution of Lagrange parameters is determined by the environment [2].

[1] Z. Lenarčič, F. Lange, and A. Rosch, Phys. Rev. B **97**, 024302 (2018).

[2] F. Lange, Z. Lenarčič, and A. Rosch, Phys. Rev. B **97**, 165138 (2018).

Non-equilibrium steady states and phase transitions in single-file Brownian motion through periodic potentials

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ABSTRACT

Single-file Brownian motion in periodic structures is an important process in nature and technology, which becomes increasingly amenable for experimental investigation under controlled conditions. To explore and understand basic features of this motion, the Brownian asymmetric simple exclusion process (BASEP) was recently introduced [1]. In this BASEP, particles with hardcore interaction are driven by a constant drag force through a periodic potential. We discuss general properties of the collective dynamics in the BASEP and related systems and give a complete description of currents in steady states for all particle densities and diameters [2,3]. For open systems coupled to particle reservoirs, we demonstrate the occurrence of nonequilibrium phase transitions predicted by extremal current principles.

[1] D. Lips, A. Ryabov, and P. Maass, Phys. Rev. Lett. **121**, 160601 (2018).

[2] A. Ryabov, D. Lips, and P. Maass, J. Phys. Chem. C **123**, 5714 (2019).

[3] D. Lips, A. Ryabov, and P. Maass, arXiv:1906.08493 (2019).

Nonequilibrium steady states in weakly dissipative macroscopic quantum systems

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ABSTRACT

In recent years, ultra-cold atomic experiment enables us to control and manipulate the dissipation, and therefore nonequilibrium dynamics and steady states of macroscopic open quantum systems have paid much attention. I talk about our recent work on steady states of macroscopic open quantum systems under weak dissipation [1]. I show that the weak-dissipation perturbation expansion and the eigenstate thermalization hypothesis, which is recognized as a key property for thermalization of isolated quantum systems, leads us to the conclusion that the steady state is described by a Gibbs state even if the environment is out of equilibrium and the detailed balance condition is violated. I then discuss the validity of the perturbation expansion for macroscopic open quantum systems, which is a highly nontrivial problem since its convergence radius is known to shrink exponentially as the system size increases. By analyzing concrete models, I show that the perturbation theory is valid for some models and therefore the Gibbs state is a good description of the steady state, while the perturbation theory does not work for other models.

[1] T. Shirai and T. Mori, arXiv:1812.09713

Similarities and differences between non-equilibrium steady states and time-periodic driving

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ABSTRACT

A system that violates detailed balance evolves asymptotically into a non-equilibrium steady state with non-vanishing currents. Analogously, when detailed balance holds at any instant of time but the system is driven through time-periodic variations of external parameters, it evolves toward a time-periodic state, which can also support non-vanishing currents. In both cases the maintenance of currents throughout the system incurs a cost in terms of entropy production. We compare these two scenarios in two settings: discrete state Markovian dynamics, and one dimensional diffusion dynamics.

Tackling quantum many-body dynamics by typicality, numerical linked cluster expansion, and projection operator techniques

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ABSTRACT

The dynamics of spatio-temporal correlations and current autocorrelation functions is studied in quantum spin models with chain or ladder geometry. For nonintegrable models, we demonstrate the occurrence of genuine spin diffusion based on the combination of (i) Gaussian density profiles, (ii) time-independent diffusion coefficients, (iii) exponentially decaying density modes, and (iv) Lorentzian line shapes of the dynamical structure factor [1,2]. Employing a combination of dynamical quantum typicality and numerical linked cluster expansions [3], we moreover show that high-temperature spin transport in the (integrable) isotropic Heisenberg chain is superdiffusive, as indicated by a power-law growth of the time-dependent diffusion coefficient with exponent 1/3. Eventually, upon comparing the decay of currents in chains and ladders, we unveil that the latter is to good quality determined by an exponential damping of the former. In particular, this finding is corroborated by theoretical arguments based on projection-operator techniques for random-matrix models [4].

[1] J. Richter, F. Jin, H. De Raedt, K. Michielsen, J. Gemmer, and R. Steinigeweg, Phys. Rev. B **97**, 174430 (2018).

[2] J. Richter, F. Jin, L. Knipschild, J. Herbrych, H. De Raedt, K. Michielsen, J. Gemmer, and R. Steinigeweg, Phys. Rev. B **99**, 144422 (2019).

[3] J. Richter and R. Steinigeweg, Phys. Rev. B **99**, 094419 (2019).

[4] J. Richter, F. Jin, L. Knipschild, H. De Raedt, K. Michielsen, J. Gemmer, and R. Steinigeweg, in preparation.

Second law and eigenstate thermalization in isolated quantum many-body systems

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ABSTRACT

In recent years, the fundamental mechanism of thermalization of isolated many-body quantum systems has attracted renewed attentions, in light of quantum statistical mechanics, quantum information theory, and quantum technologies. In particular, it has been recognized that the eigenstate thermalization hypothesis (ETH) plays a crucial role in understanding the mechanism of thermalization, which states that even a single energy eigenstate is thermal if the system is quantum chaotic.

In this talk, I will discuss our recent results on the second law of thermodynamics for pure quantum states [1]. In our setup, the entire system obeys unitary dynamics, where the initial state of the heat bath is not the Gibbs ensemble but a single energy eigenstate. Our proof is mathematically rigorous, and the Lieb-Robinson bound plays a crucial role. In addition, I will talk about our numerical result on large deviation analysis of the ETH [2], which directly evaluates the number of athermal energy eigenstates and validates the ETH. Our results would reveal a general scenario that thermodynamics emerges purely from quantum mechanics.

[1] E. Iyoda, K. Kaneko, and T. Sagawa, Phys. Rev. Lett. **119**, 100601 (2017).

[2] T. Yoshizawa, E. Iyoda, and T. Sagawa, Phys. Rev. Lett. **120**, 200604 (2018).

Time Scales and Self-Averaging in Many-Body Quantum Dynamics

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ABSTRACT

Despite its importance to experiments, numerical simulations, and the development of theoretical models, self-averaging in many-body quantum systems out of equilibrium remains under-investigated. Usually, in the chaotic regime, self-averaging is taken for granted. The numerical and analytical results presented here force us to rethink these expectations. They demonstrate that self-averaging properties depend on the quantity and also on the time scale considered. We show analytically that the survival probability in chaotic systems is not self-averaging at any time scale, even when evolved under full random matrices. We also analyze the participation ratio, Rényi entropies, the spin autocorrelation function from experiments with cold atoms, and the connected spin-spin correlation function from experiments with ion traps. We find that self-averaging holds at short times for the quantities that are local in space, while at long times, self-averaging applies for quantities that are local in time. Various behaviors are revealed at intermediate time scales.

Superconducting quantum devices under frequency modulation

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ABSTRACT

When the transition frequency of a quantum system is modulated, several interesting phenomena can be observed, such as Landau–Zener–Stückelberg–Majorana interference, motional averaging and narrowing, geometric phases, and the formation of dressed states with the appearance of sidebands in the spectrum. In recent years, an exquisite experimental control in the time domain was gained through the parameters entering the Hamiltonian, and high-fidelity readout schemes allowed the state of the system to be monitored non-destructively. These developments were made in the field of quantum devices, especially in superconducting quantum devices, as a well as in ultracold gases. As a result of these advances, it became possible to demonstrate many of the fundamental effects that arise in a quantum system when its transition frequencies are modulated. The focus of the talk will be in reviewing advances [1-3] and future directions, especially related on many-body physics, with superconducting quantum devices under frequency modulation.

[1] M. P. Silveri, J. A. Tuorila, E. V. Thuneberg, and G. S. Paraoanu, Rep. Prog. Phys. **80**, 056002 (2017).

[2] M. P. Silveri, K. S. Kumar, J. Tuorila, J. Li, E. V. Thuneberg, and G. S. Paraoanu, New J. Phys. **17**, 043058 (2015).

[3] J. Li, M. P. Silveri, K. S. Kumar, J.-M. Pirkkalainen, A. Vepsäläinen, W. C. Chien, J. Tuorila, M. A. Sillanpää, P. J. Hakonen, E. V. Thuneberg, and G. S. Paraoanu, Nat. Commun. **4**, 1420 (2013).

From integer and fractional plateaus to directional locking in colloidal ratchet currents

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ABSTRACT

In this talk I will describe experiments based on investigating the collective transport properties of paramagnetic colloidal particles driven above a magnetic bubble lattice. Such lattice generates a 2D periodic potential and it is composed by a triangular array of uniformly magnetized ferromagnetic domains [1]. Application of an external rotating magnetic field modulates such potential and produces a traveling wave ratchet that propels the particles the particles at a constant and frequency tunable speed. We measure a direct ratchet current which rises in integer and fractional steps with the field amplitude. The stepwise increase is caused by excluded volume interactions between the particles, which form composite clusters above the bubbles with mobile and immobile occupation sites. Transient energy minima located at the interstitials between the bubbles cause the colloids to hop from one composite cluster to the next with synchronous and period doubled modes of transport. The colloidal current may be polarized to make selective use of type up or type down interstitials [2,3]. Further we observe directional locking and transversal current when larger particles are driven along a direction that intersects two crystallographic axis of the lattice. We find that, while single particles show no preferred direction, at high density collective effects induce a bifurcation in the density velocity curve which appear due to spontaneous symmetry breaking.

[1] P. Tierno, T. H. Johansen, T.M. Fischer, Phys. Rev. Lett. **99**, 038303 (2007).

[2] P. Tierno, T.M. Fischer, Phys. Rev. Lett. **112**, 048302 (2014).

[3] P. Tierno, T.M. Fischer, Applied Physics Letters **104**, 174102 (2014).

Probing Quantum Dynamics in Strongly Driven Optical Lattices

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ABSTRACT

Degenerate lithium in modulated optical lattices makes a near-ideal testbed for the experimental study of quantum matter driven far from equilibrium. I will present results from a sequence of experiments, starting with the first experimental realization of a relativistic harmonic oscillator, moving on to Floquet engineering of band structure and transport properties, and concluding with a detailed experimental mapping of the properties of prethermal Floquet matter and ergodicity breaking in a rapidly driven interacting gas.

Boosting the precision of single-atom quantum probes by nonequilibrium spin dynamics

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ABSTRACT

Quantum probes are atomic-sized probes mapping and storing information of their environment, e.g. temperature, onto quantum states. Exploiting the quantum character of the probe has been shown to improve probing accuracy while minimizing the perturbation of the environment probed, forming a central asset for quantum technologies.

I will report about our experimental realization of individual quantum probes by immersing single Cesium atoms into an ultracold cloud of Rubidium. Controlling atomic-collision properties with unprecedented accuracy, we use inelastic spin-exchange processes to map information about gas temperature or local magnetic field onto the probeś quasi-spin population. We find that the steady-state spin distribution of the probe allows for absolute thermometry. Moreover, tracing the spin dynamic before reaching steady-state allows to maximize the information obtained about the system after only three inelastic collisions, boosting the sensitivity of the probe beyond standard quantum bounds. Our results pave the way for new optimization strategies of quantum probing using nonequilibrium dynamics.

Poster

Tjark Heitmann:
Density dynamics in the imbalanced Hubbard model

Robin Heveling:
Impact of pertubations on expectation value dynamics

Sreekanth Kizhakkumpurath Manikandan:
Efficiency fluctuations in microscopic machines

Stefan kleine Brüning:
ETH in a system with topological flat bands and impurities

Fengping Jin:
Quantum annealing with anneal path control and catalyst Hamiltonian

Dominik Lips:
Simulation of experimental setups for Brownian single-file motion in periodic potentials

Jonas Richter:
Combining dynamical quantum typicality and numerical linked cluster expansions

Dennis Schubert:
Classical and quantum dynamics in strongly interacting spin systems

Patrick Vorndamme:
Decoherence of a singlet-triplet superposition state