Entropy and the Second Law of Thermodynamics – The past, the present, and the future

761. WE-Heraeus-Seminar

July 14 - 17, 2022
Hybrid at the Physikzentrum
Bad Honnef/Germany

WILHELM UND ELSE
HERAEUS-STIFTUNG

Subject to alterations!

Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see https://www.we-heraeus-stiftung.de

Aims and scope of the 761. WE-Heraeus-Seminar

The second law of thermodynamics that characterizes the entropy change of many-body systems is a fundamental law of Nature. Originally formulated by Rudolf Clausius to understand the conversion of heat into work in the context of heat engines, it is now universally used to describe the direction of thermodynamic transformations close and far from equilibrium in physics, chemistry and biology.

In this workshop, we will celebrate Clausius' 200th birthday in 2022 by exploring the recent developments in the experimental and theoretical investigations of the second law in various directions. We aim for an inspiring exchange between researchers from such diverse fields as information theory, cosmology, quantum physics, non-equilibrium thermodynamics, physical chemistry and biophysics under the unifying framework of the second law.

We will, in particular, focus on the intimate interplay between entropy and information, the study of far-from-equilibrium processes in classical and quantum systems, as well as the central role played by entropy in the function of molecular and biological systems. The participants will be both senior and young researchers working in these active fields.

Scientific Organizers:

Prof. Dr. Jens Bredenbeck — Universität Frankfurt, Germany
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Prof. Dr. Eric Lutz — Universität Stuttgart, Germany
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Prof. Dr. Artur Widera — TU Kaiserslautern, Germany
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Introduction

Administrative Organization:

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Registration:

Martina Albert (WE Heraeus Foundation)
at the Physikzentrum, reception office
Thursday (12:00 h – 19:00 h) and Friday morning

Program

Program

Thursday, 14 July 2022

12:00 – 19:00	Registration	
12:30	*LUNCH*	
14:00 – 14:15	Scientific organizers	**Welcome**
14:15 – 14:30	Stefan Jorda (online)	**About the Wilhelm and Else Heraeus Foundation**
14:30 – 15:30	Johannes Orphal	**„Rudolph Clausius (1822-1888) - the discoverer of entropy. What do we know about his life and his ideas?"**
15:30 – 16:00	*COFFEE BREAK*	
16:00 – 16:45	Ken Dill (online)	**The principle of Maximum Caliber for nonequilibrium statistical physics**
	Hot Topic Talks	
16:50 – 17:10	Thomas Busch	**Efficient Quantum Engines in Interacting Ultracold Gases**
17:10 – 17:30	Simone Pezzotti (online)	**Mapping local hydration entropy in biology from THz spectroscopy**
17:30 – 17:50	Jenny Poulton	**Fundamental limits on prediction**
18:30	*DINNER*	

Program

Friday, 15 July 2022

08:00	*BREAKFAST*	
09:00 – 09:45	Yael Roichman	**Active matter information engines**
09:45 – 10:30	Masahito Ueda (online)	**Universal Thermodynamic Uncertainty Relation in Non-Equilibrium Dynamics**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Frank Jülicher	**Active processes in Cells and Tissues**
11:45 – 12:30	Rajibul Islam	**Probing coherent and dissipative dynamics on a trapped ion quantum simulator**
12:30	*LUNCH*	
14:00 – 14:45	Aljaz Godec	**Time-reversal symmetry and dissipation in dynamics with memory**
14:45 – 15:30	Nicolai Kiesel	**Levitated optomechanics and the second law**
15:30 – 16:00	*COFFEE BREAK*	
16:00 – 16:45	Martin Gruebele (online)	**Quantum information Scrambling in Molecules**
16:45 – 18:15	**Poster Session I**	

18:30 *HERAEUS DINNER at the Physikzentrum*

(cold & warm buffet, with complimentary drinks)

Program

Saturday, 16 July 2022

08:00	*BREAKFAST*	
09:00 – 09:45	NN	**tba**
09:45 – 10:30	Massimiliano Esposito	**Towards a Nonequilibrium Thermodynamics of Complex Systems**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Udo Seifert	**From stochastic thermodynamics to thermodynamic inference**
	Hot Topic Talks	
11:50 – 12:10	Mauro Paternostro	**Informational steady-states and conditional entropy production in continuously monitored systems**
12:10 – 12:30	Lingna Wu	**Dynamical phase transition in an open quantum system**
12:30	*LUNCH*	
14:00 – 18:30	**Excursion**	
18:30 – 20:00	*DINNER*	
20:00 – 21:00	**Poster Session II**	

Program

Sunday, 17 July 2022

08:00	*BREAKFAST*	
09:00 – 09:45	Manas Mukherjee	**Single atom heat engine with quantum load**
09:45 – 10:30	Karin Hauser	**The role of entropy in protein folding – insights from IR-spectroscopic studies**
10:30 – 11:00	*COFFEE BREAK*	
11:00 – 11:45	Larissa von Krbek	**Guest recognition in dynamic libraries and spin-crossover cages**
11:45 – 12:30	Dieter Braun	**Non-equilibrium conditions for the Emergence of Life**
12:30 – 12:40	Scientific Organizers	**Closing remarks and poster awards**
12:40	*LUNCH*	

End of seminar and departure

Posters

Posters I

1	Amin Alibakhshi	**On the entropy dilemma: Gibbs paradox revisited**
2	Sinan Altinisik	**Master equation for an arbitrarily quick driven harmonic oscillator**
3	Amy Altshuler	**Starting over without forgetting the past**
4	Julian Arnold	**Entropy production in ticking clocks: Fundamental limits of timekeeping**
5	Faraj Bakhshinezhad	**Master Equation and detailed fluctuation relation in the presence of continuous feedback control**
6	Rick Bebon	**First-passage times in complex energy landscapes: a case study with nonmuscle myosin II assembly**
7	Kristian Blom	**Tuning the Kinetics of Magnetization Reversal in an Irreversible Ising Model**
8	Valentin Boettcher	**Calculating Energy Flows in Strongly Coupled Open Quantum Systems with HOPS**
9	Dmitry Boriskovsky	**An experimental test of a nonlinear fluctuation-dissipation theorem to test Markovianity far from thermal equilibrium**
10	A. Mert Bozkurt	**Topological information device operating at the Landauer limit**
11	Vasco Cavina	**Thermodynamic consistency of quantum master equations**
12	Omer Chor	**Number fluctuations and the Szilard Engine: active matter wins**

Posters I

13	Yurii Dumin (online)	**Spontaneous Temperature Increase in Ultracold Plasmas: Disorder-Induced Heating vs. Virialization**
14	Owen C. Ernst	**Circumventing the second law of thermodynamics by entropy export to generate regular arrays of liquid metal droplets**
15	Julian Feß	**Dynamical phase transition in an open quantum system**
16	Ian Ford	**Entropy production for Brownian trajectories of a reduced density matrix**
17	Klavs Hansen (online)	**Temperature of a finite system and the origin of the Boltzmann factor**
18	Yuchi He	**Conductance of correlated many-fermion systems from bipartite charge fluctuations and entanglement entropies**
19	Miku Ishizaki	**Switching the function of the quantum Otto cycle in non-Markovian dynamics: heat engine, heater and heat pump**
20	Kathrin Laxhuber	**Heat flux in phase-separated systems out of equilibrium**
21	Jing Li	**Quantum heat engine based on a spin-orbit and Zeeman-coupled Bose-Einstein condensate**

Posters II

22	Shishira Mahunta (online)	**Optimization of the performance of the quantum many-body heat engine using CRAB**
23	Arthur Mendonça Faria	**Fluctuation theorems for a quantum Brownian motion due to a disordered environment**
24	Saulo V. Moreira	**Extractable work in a Szilard engine with a finite-size reservoir**
25	Jonathan Pachter (online)	**Non-Equilibrium Statistical Physics Beyond the Ideal Heat Bath Approximation**
26	Tuan Pham (online)	**Stochastic thermodynamics of networked systems without a thermodynamic interpretation**
27	Daniel Pijn	**Detecting Heat Leaks with Trapped Ion Qubits**
28	Gilad Pollack	**Optimizing Information Engines in and out of Equilibrium**
29	Rodolfo Reis Soldati	**Thermodynamics of a minimal algorithmic cooling refrigerator**
30	Paul Riechers	**Initial-state dependence of entropy production for any quantum process**
31	Franklin Rodrigues	**Non-equilibrium thermodynamics of quantum coherence**
32	Projesh Kumar Roy	**Derivation of a statistical model for classical systems obeying the exclusion principle**
33	Sungguen Ryu	**Outperforming Carnot efficiency using periodically driven quantum chiral conductors**

Posters II

34	Dominik Šafránek	**Work Extraction from Unknown Quantum Sources**
35	Finn Schmolke	**Quantum Synchronization of Opposite Heat Flows**
36	Peter Schürger	**Wave packet dynamics in an harmonic potential disturbed by disorder: Entropy, uncertainty, and vibrational revivals[1]**
37	Vahid Shaghaghi (online)	**Extracting work from random collisions: A model of a quantum heat engine**
38	Varinder Singh (online)	**Thermodynamic uncertainty relation in degenerate and nondegenerate maser heat engines**
39	Sergey Sobolev (online)	**Entropy, entropic temperature, second and third laws for far-from-equilibrium 1D system with heat flux**
40	Noah Van Horne	**Single-atom energy-conversion device with a quantum load**
41	Chris Whitty	**Enhanced shortcuts to adiabaticity**
42	Shadab Zakavati Gharagozlou	**Thermodynamic characterization of the stored work and charging power in quantum batteries: An open quantum system analysis**

Abstracts of Lectures

(in alphabetical order)

Non-equilibrium conditions for the Emergence of Life

Dieter Braun

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A way to study the emergence of life is to create a physico-chemical system that is capable of open ended evolution. The aim is to search for most minimal requirements to maximize the probability to find it outside the lab. Starting life with three molecules in a one-pot geological non-equilibrium without human intervention would be a favorable scenario.

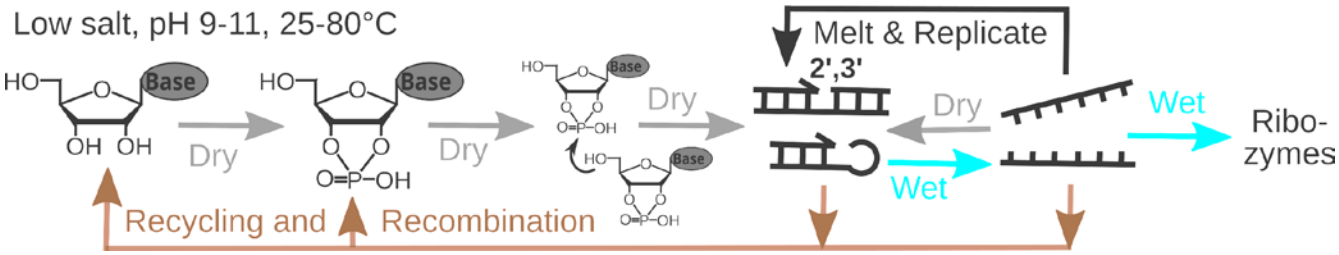
We revisited polymerization and templated ligation of RNA from nucleotides with 2',3' cyclic phosphates. Simple alkaline conditions at pH 9-11 without catalysts or added salts oligomerized the nucleotides up to 10mers over across 25-80°C within a day, both in the 'dry' state or in the wet-dry cycling at a heated air-water interface [1]. The polymerization was dominated by G, but cold and dry conditions, achieved in the planet simulator of McMaster University yielded random sequences of GC or GCAU according to mass spectrometry.

Interestingly, the same conditions triggered (i) with Trimetaphosphate the specific cyclic phosphorylation and (ii) the templated ligation of oligonucleotides, the latter also under 'dry' conditions. Therefore, we envisage a dry RNA world where exponential replication is driven by long enough polymers, templated ligation and hydrolytic recombination using wet-dry cycles to separate the strands. Short, replicated RNA sequences could enhance their own ligation and start the first cycle of functional RNA evolution.

That CO_2-water interfaces can drive the replication towards sequence lengths of up to 1300mers was demonstrated recently [2]. The accumulation by capillary flow overcame the tyranny of the shortest. The long strands were shown to separate under the pH cycling provided by the Hadean atmosphere of CO_2. While the replication was still implemented by a polymerase to enhance kinetics, the findings indicate that a similar strand separation will be possible for RNA based replication even under intermediate Mg^{2+} concentrations.

[1] doi:10.26434/chemrxiv-2022-zwh2t (2022)

[2] **Nature Physics** doi.org/10.1038/s41567-022-01516-z (2022)



Efficient Quantum Engines in Interacting Ultracold Gases

T. Fogarty, M. Boubakour, T. Keller, and Th. Busch

Quantum Systems Unit, OIST Graduate University, Onna, Okinawa 904-0495, Japan

Thermodynamic cycles using ultra cold and interacting atomic systems can be highly efficient and are able to outperform cycles with non-interaction working media. We will demonstrate this on two systems, each simulating a quantum Otto cycle. The first suggests a work stroke that quenches a trap (changes the volume) while at the same time adjusting the inter particle interactions [1], while the second operates across a quantum critical point [2]. In the latter, the existence of an energy gap at the transition provides a performance boost to the many-body system over a comparable ensemble of single particle engines. If time permits, I will also briefly introduce an engine in which the work stroke is carried out by a Feshbach pulse instead of a change in volume [3].

References

[1] Enhancing a few-body heat engine by driving the interactions, M. Boubakour, T. Fogarty, and Th. Busch, in preparation.

[2] A many-body heat engine at criticality, T. Fogarty and Th. Busch, Quantum Sci. Technol. **6** 015003 (2020).

[3] A Feshbach engine in the Thomas-Fermi regime, T. Keller, T. Fogarty, J. Li, and Th. Busch, Phys. Rev. Research **2**, 033335 (2020).

The principle of Maximum Caliber for nonequilibrium statistical physics

K. Dill and J. Pachter

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Equilibrium statistical thermodynamics draws great power from: (1) its experimental underpinning on the Clausius relationship, a principle of dissipation that describes reversible situations near equilibria, and (2) its ability to predict microscopic probability distributions over microstates using the relationship Delta S = -sum p_i log p_i (eq 1). We have been interested in developing a fuller Nonequilibrium Statistical Physics (NESP) for situations away from equilibria, where neither of these premises applies. We hypothesize that the generalization of the Second Law that applies beyond near-equilibria is Maximum Caliber, an inference procedure in which eq 1 is now expressed in terms of path entropies rather than microstate entropies. Max Cal gives pathways and rate distributions including for processes that are nonlinear, Far-From-Equilibrium, few-particle, or not involving heat baths. It resolves some foundational issues and gives new results such as for gene circuits, traffic, social networks, dissipative systems and others.

Towards a Nonequilibrium Thermodynamics of Complex Systems

Massimiliano Esposito

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I will start by discussing some of the main challenges that one faces when trying to formulate a nonequilibrium thermodynamics of complex systems. I will then discuss how to use stochastic thermodynamics to make progress in that direction by considering systems which display a macroscopic limit and nonequilibrium phase transitions (e.g. chemical reaction networks, nonlinear electric circuits and Potts models). I will discuss in particular how an emergent second law can be used to bound the rate function of nonequilibrium steady states (NESS) using the macroscopic entropy production [1]. I will also describe a novel linear response regime at the level of NESS rate functions [2] and show that it saturates this bound.

References:
[1] N. Freitas and M. Esposito, "Emergent second law for non-equilibrium steady states", arXiv:2109.04906.
[2] N. Freitas, G. Falasco and M. Esposito, "Linear response in large deviations theory: A method to compute non-equilibrium distributions", New J. Phys. 23, 093003 (2021).

Time-reversal symmetry and dissipation in dynamics with memory

David Hartich & Aljaž Godec
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Modern single-molecule experiments and computer simulations track effective, low dimensional "reaction coordinates" projected from the full system phase space as a function of time. Examples are distances between fluorescent labels in FRET spectroscopy, molecular extensions in single-molecule force spectroscopy, or internal distance-coordinates and other coarse-grained observables in molecular dynamics simulations. It is well known that projections that couple to slow hidden degrees of freedom induce memory in the observed dynamics. However, we are only beginning to understand the implications of memory for thermodynamics, in particular in systems that are driven far from thermodynamic equilibrium. I will review our recent efforts on how to understand and describe dissipation (a.k.a. irreversibility) in discrete-state systems where not necessarily slow degrees of freedom are ignored.

References

[1] D. Hartich & A. Godec, *Phys. Rev. X* **11**, 041047 (2021)
[2] D. Hartich & A. Godec, arXiv:2111.14734 (2022)
[3] D. Hartich & A. Godec, arXiv:2112.08978 (2022)

Quantum information Scrambling in Molecules

M. Gruebele[1]

[1]University of Illinois at Urbana-Champaign, USA

Molecules are highly anharmonically coupled systems. In the classical limit, their K-S entropy grows according to a Lyapunov coefficient, but not at the maximum possible speed: there are regular dynamical regions embedded in the overall chaotic phase space. The problem becomes even more interesting in the quantum limit: Herzfeld, Maldacena and others have proposed limits ~kT/h on the scrambling of quantum systems. Scrambling in quantum systems can be due to the analog to classical chaos, but also other phenomena like instabilities in non-adiabatic systems or tunneling that do not occur in classical systems. Here I will discuss some computational work and analysis to show how quantum information is scrambled in molecules, and how this creates a phase diagram for molecular reactivity with 'bottle neck' and 'free reactivity' phases. We also apply regularized out-of-time-order correlators (OTOCs), whose growth is given by the Lyapunov exponent in the classical limit, to molecules and chemicals reactions. We can see how tunneling and other quantum phenomena affect scrambling, and how the so-called Maldacena bound can be reached by molecular systems only in the tunneling limit, not by heating them to high temperature to induce chaos.

References

[1] Chenghao Zhang, Peter G. Wolynes, and Martin Gruebele, **Quantum Information Scrambling in Molecules**, Phys. Rev. A **105**, 033322 (2022)

[2] Chenghao Zhang, Edwin L. Sibert III, and Martin Gruebele, **A phase diagram for energy flow-limited reactivity**, J. Chem. Phys. **154**, 104301 (2021)

The many faces of entropy for thermodynamics and information

Peter Hänggi, Dept. of Physics, University of Augsburg, Germany
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Entropy is a buzzword that is used by all kinds of communities, covering biologists, economists, social scientists and journalists. One of the reasons for the bewilderment of the term *entropy* is the unheralded appearance is the superabundance of situations bearing this expression. Being so, using the term forces one to respect its precise meaning without effusing unnecessarily its wild growth, thereby adding only to confusion rather than to clarity.

The plan is to discuss the precise meaning of these various notions for entropy in different ensembles setups. In particular, let us elaborate on the proper choice of entropy as it depends on the interests of the individual, the particular situations under study (classical or quantum regime), the type of implemented measurement protocols, the precision available and method of the employed description and the overall physical situation; -- such as equilibrium versus non-equilibrium. Moreover, I comment on the thermodynamic entropy for systems of finite size as being of relevance in nanoscience, or when the system under study is interacting strongly with environment(s). In doing so, I point to various subtleties and warn of hidden pitfalls which go with its use and abuse in physics and elsewhere.

A sample of sources for further reading are:

[1] Fabian Immanuel IJpelaar; Univ Groningen: *Entropy in Physics: An Overview of Definitions and Applications in Quantum Mechanics (2021; 155 pages)* https://fse.studenttheses.ub.rug.nl/23834/

[**2**] A. Wherl, *The many facets of entropy*, Rep. Math. Physics 30,119 (1991)

[**3**] A set of inspiring warnings on abuse of entropy are addressed by N. G. Van Kampen, "*Entropie*", IN: PLUS LUCIS **3/97**, p.7-8; https://www.pluslucis.org/ZeitschriftenArchiv/1997-3_PL.pdf

[4] S. Hilbert, P. Hänggi, and J. Dunkel, *Thermodynamic Laws in Isolated Systems*, Phys. Rev. E **90**, 062116 (2014); P. Hänggi, S. Hilbert, and J. Dunkel, *Meaning of temperature in different thermostatistical ensembles*, Phil. Trans. Roy. Soc. A **374**, 20150039 (2016).

[5] P. Talkner and P. Hänggi, *Statistical mechanics at strong coupling: Quantum and Classical*, Rev. Mod. Phys. **92**, 041002 (2020).

The role of entropy in protein folding – insights from IR-spectroscopic studies

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Understanding the molecular mechanisms of protein folding is a very active field in biophysical research and of fundamental importance since misfolded proteins can lose their function or even cause diseases. Much of our knowledge has been derived from *in vitro* studies revealing that protein folding involves several structural transitions including backbone ordering, hydrogen bond formation and side-chains packing. We apply infrared (IR) spectroscopy to analyze protein stability and dynamics. The spectral changes of temperature-dependent measurements under equilibrium conditions provide the melting temperature and the equilibrium constant for the thermal unfolding. Entropic and enthalpic contributions to the standard free-energy change can be derived from a thermodynamic analysis. To study non-equilibrium relaxation dynamics of proteins, we built-up a spectrometer with tunable quantum cascade lasers (QCL) for mid-IR detection combined with a nanosecond laser-excited T-jump. Peptide models and site-specific probes are used to study folding mechanisms at the level of individual amino acids. I will give several examples of our recent studies [1-3]. Mutations can change barriers of the energy landscape and thus affect folding pathways. Furthermore, configurational entropy in the transition state can be responsible for an apparent rate enhancement [4].

References

[1] H.-W. Siu, B. Heck, M. Kovermann, K. Hauser, Chem. Sci., 2021, **12**, 412 (2021)

[2] D. Scheerer, H. Chi, D. McElheny, T.A. Keiderling, K. Hauser, Chem Eur J, **26**, 3524 (2020)

[3] A. Popp, D. Scheerer, B. Heck, K. Hauser, Spectrochim Acta. A Mol. Biomol. Spectrosc., **181**, 192 (2017)

[4] A. Popp, L. Wu, T.A. Keiderling, K. Hauser, J. Phys. Chem. B, **118**, 14234 (2014)

Probing coherent and dissipative dynamics on a trapped ion quantum simulator

Rajibul Islam

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Trapped ions are among the most advanced technology platforms for quantum simulation [1] of many-body spin systems. When laser-cooled close to absolute zero temperature, atomic ions form a Coulomb crystal with micron-scale spacings in a radio-frequency ion trap. Spin-1/2 levels, encoded in hyperfine energy states of each ion, can be initialized, manipulated, and detected optically with high precision. Laser fields can also couple the spin states to collective phonon modes of ions, creating programmable spin Hamiltonians. This talk will give an overview of the capabilities of trapped ion quantum simulators to investigate spin dynamics where coherence and site-selective dissipation or measurement compete. Techniques from holographic optical engineering [2] to machine learning [3] can be combined to program such a simulator to probe non-trivial many-body physics processes such as reservoir engineering and measurement-induced quantum phase transitions [4]. Controls at the level of single atoms will allow direct measurement of in situ probes, such as local order parameters and (Renyi) entanglement entropy.

References

[1] C. Monroe *et al*, Reviews of Modern Physics **93**, 025001 (2021)
[2] C.-Y. Shih *et al*, npj Quantum Information **7**, 57 (2021)
[3] Y. H. Teoh *et al,* Quantum Science and Technology **5,** 024001 (2020)
[4] S. Czischek *et al,* Physical Review A **104**, 062405 (2021)

Active Processes in Cells and Tissues

Frank Jülicher

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Living matter is highly dynamic and organizes in complex patterns and spatial structures. Cells and tissues are driven far from thermodynamic equilibrium by a supply of chemical energy via metabolic processes. I will discuss how active processes drive cells away from thermodynamic equilibrium and I will present general concepts from irreversible thermodynamics that capture the physics of active processes. Fluid flows generated by material contraction driven by active mechanical stresses provide a general mechanism for cell polarity establishment. Phase separated droplets form small compartments in cells that organize biochemistry. Such biological condensates motivate the physical study of chemically active droplets that exhibit nonequilibrium states and that can imitate cell like behaviors such as spontaneous division. Active droplets can also serve as simple physical models of protocells that operate away from equilibrium. Finally, at larger scales, many cells organize collectively during the morphogenesis of organisms. These examples show that living matter is a form of active matter governed by nonequilibrium physics. To advance our understanding of principles that underlie the emergence of complex biological structures far form thermodynamic equilibrium will remain a challenge for future research.

Levitated optomechanics and the second law

N. Kiesel[1]

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Optical levitation of nanoparticles can provide a versatile experimental platform for spatiotemporal control of one or eventually few mechanical degrees of freedom and their environment. It provides the natural extension of colloidal, overdamped systems to the underdamped and eventually the quantum regime.
I will present our recent experiments that exploit harmonically trapped, underdamped nanoparticles to shed light on the non-equilibrium statistical properties of the work and of the entropy production under the influence of fast temperature changes [1] and time-delayed feedback [2,3] control.
To conclude, I will demonstrate how we will investigate actual spatio-temporal control with nonlinear potentials in the future, as illustrated by our recent experiment on memory erasure and Landauer's bound with non-equilibrium initial states [4].

References

[1] M. Rademacher., Phys. Rev. Lett. **128**, 070601 (2022)
[2] M. Debiossac et al., Nat. Comm. **11**, 1360 (2020)
[3] M. Debiossac et al., Phys. Rev. Lett. **128**, 200601 (2022)
[4] M. Ciampini et al., arXiv:2107.04429 (2021)

Single atom heat engine with quantum load

N. Van Horne, D. Yum, T. Dutta, P. Hänggi, J. Gong, D. Poletti, M. Mukherjee
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Abstract: Ion trap technology is a forerunner in quantum computing, simulation, sensing and clocks. The versatile application of ion trap setups stem from their ability to control and manipulate single or multiple ions in a near isolated environment with negligible kinetic energy. Therefore, using this device we demonstrated [1] the behaviour of an isolated thermodynamic work fluid represented by a single atom when subjected to cyclic evolution. The fluid is prepared in a quantum state such that we could infer the non-classical outcomes of the cycle. We studied its entropy and ergotropy as a function of the number of operated cycles both in forward as well as reverse operations. We will discuss the experiment and the theory as well as provide some insight on quantumness of the system.
.

References:

[1] N. Van Horne, D. Yum, T. Dutta, G. Jiangbin, P. Hanggi, D. Poletti and M. Mukherjee, Single-atom energy-conversion device with a quantum load, *npj Quantum Information volume 6, Article number: 37 (2020)*.

„Rudolph Clausius (1822-1888) - the discoverer of entropy. What do we know about his life and his ideas?”

Johannes Orphal

Karlsruhe Institute of Technology , Head of Division 4,
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Rudolph Clausius was one of the leading physicists in the 19th century. His famous paper of 1850, where he united Carnot’s and Joule’s conceptions of the generation of work in the steam engine, by introducing both the 1st and - for the first time - the 2nd principles of thermodynamics, is astoundingly clear and modern in its logical and mathematical form. How was this possible? How did he conceive the concept of entropy in 1865? And what else did this man discover? - This talk will show some material from historic archives in Europe, that the author has collected over more than 35 years, in order to provide a more complete picture of this nearly forgotten genius.

Informational steady-states and conditional entropy production in continuously monitored systems

A. Belenchia[1,2], G. T. Landi[3], and M. Paternostro[2]

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[2]Centre for Theoretical Atomic, Molecular, and Optical Physics, School of Mathematics and Physics, Queens University, Belfast BT7 1NN, United Kingdom
[3]Instituto de Fisica da Universidade de Sao Paulo, 05314-970 Sao Paulo, Brazil

I will put forth a unifying formalism for the description of the thermodynamics of continuously monitored systems, where measurements are only performed on the environment connected to a system. I will show, in particular, that the conditional and unconditional entropy production, which quantify the degree of irreversibility of the open system's dynamics, are related to each other by the Holevo quantity. This, in turn, can be further split into an information gain rate and loss rate, which provide conditions for the existence of informational steady-states, i.e. stationary states of a conditional dynamics that are maintained owing to the unbroken acquisition of information. I will illustrate the applicability of our framework through several examples, including the modelling of a recent experiment in the field of cavity optomechanics

References

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Mapping local hydration entropy in biology from THz spectroscopy

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Hydration free energies are dictated by a subtle balance of hydrophobic and hydrophilic interactions, which involves compensating entropic and enthalpic terms. Evaluating such balance requires a local mapping of hydrophilic and hydrophobic hydration entropy and enthalpy, which remains a challenge for both theory and experiments. From the experimental side, these contributions are notoriously difficult to probe and cannot be dissected by standard calorimetry approaches.

I will present here a spectroscopic approach,[1] which gives direct access to the two main contributions only based on experimental quantities: Using THz-spectroscopy to probe the frequency range of the intermolecular stretch (150–200 cm^{-1}) and the hindered rotations (450–600 cm^{-1}), the local contributions due to cavity formation and hydrophilic interactions can be traced back. We show that via THz-calorimetry these fingerprints can be correlated 1:1 with local solvation entropy and enthalpy. This allows to deduce separately the hydrophobic (i.e. cavity formation) and hydrophilic contributions to thermodynamics, as shown for hydrated alcohols as a case study. Accompanying molecular dynamics simulations quantitatively support our experimental results. In the future our approach will allow to dissect hydration contributions in inhomogeneous mixtures and under non-equilibrium conditions, paving the way toward the tuning of solvation free energies in biological processes from THz screening.

As a proof of principle, I will briefly illustrate some recent results[2] where we used THz-screening to rationalize hydration contributions to liquid-liquid phase separation, i.e. the biological phenomenon observed for some families of disordered proteins, which spontaneously condensate in aqueous solutions to form a dilute and a protein-rich phase. Such reversible, membrane-less separation can be induced by minute changes in adjustable parameters, such as temperature and concentration. Understanding how to rationally tune these parameters is expected to bring major advances in both medical and biological applications.

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Fundamental limits on prediction

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The ability to predict the future is beneficial to many biological systems. For example, some organisms can react to an environment without glucose by making a costly adaptation to allow processing different types of sugars such as xylose. However, this is only worth doing if the cell can predict that glucose is unlikely to return. Alternatively, in bacterial chemotaxis, the cell must detect the gradient of resources it has experienced to predict whether an area of high resource density lies ahead.
To make good predictions, a system must collect information about the current and past state of the environment and this information gathering also costs resources. In this talk we first ask, what are the optimal statistics to collect about the environment? We then calculate the fundamental limits on the cost of extracting these statistics consider simple systems able to reach these limits. We discuss how a system can exploit correlations within the environment to reduce the costs of information gathering, and what the consequences are if the system has made an incorrect guess about the statistics of the environment.

Active matter information engines

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The relation between information and thermodynamics remains a fundamental thought-provoking issue since the days of Maxwell. The most effective platforms used to explore this relation are information machines: processes that convert measured information about a system to extractable work. A crucial question that goes beyond the currently explored regime in the field is how information machines perform out of equilibrium, namely when not in equilibrium with a thermal bath. This is the general scenario of relevance to biological systems and stands at the focus of this presentation. In this talk, I will discuss several experimental realizations of information engines operating on driven and active systems with different geometries and compare their operation to equivalent engines working on equilibrated system.

From stochastic thermodynamics to thermodynamic inference

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Stochastic thermodynamics provides a universal framework for analyzing nano- and micro-sized non-equilibrium systems. Prominent examples are single molecules, molecular machines, colloidal particles in time-dependent laser traps and biochemical networks. Thermodynamic notions like work, heat and entropy can be identified on the level of individual fluctuating trajectories. They obey universal relations like the fluctuation theorem [1].

Thermodynamic inference as a general strategy uses consistency constraints derived from stochastic thermodynamics to infer otherwise hidden properties of non-equilibrium systems [2]. As a paradigm for thermodynamic inference, the thermodynamic uncertainty relation provides a lower bound on the entropy production through measurements of the dispersion of any current in the system [3]. Likewise, it provides a model-free bound on the thermodynamic efficiency of molecular motors. Inference from waiting-time distributions between consecutive transitions yields further information about topological aspects of the underlying network [4]. For coherent oscillations, I will present a conjecture on their universal minimal cost.

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Universal Thermodynamic Uncertainty Relation in Non-Equilibrium Dynamics

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The conventional thermodynamic uncertainty relations (TURs) suffer two major limitations. Firstly, the entropy production diverges when either the forward probability or the backward probability vanishes for some trajectory, which makes the conventional TUR inapplicable to situations in which the initial state is far from equilibrium, absorbing states exist, or the underlying process relies on chemical catalysis whose reverse process is forbidden. Secondly, the previous TURs usually apply only to time-antisymmetric observables, which are often thermodynamic observables in nature such as a current. These limitations hinder our understanding of a general nonequilibrium process. In this talk, we derive a universal TUR applicable to an arbitrary system with or without absolute irreversibility and to an arbitrary observable. Based on our general result, we make two new findings: (1) for an arbitrary out-of-equilibrium system, the imbalance between the entropy production and the degree of non-stationarity is required to bound the strength of a thermodynamic current; (2) by removing the antisymmetric constraint on observables, the TUR in physics and a fundamental inequality in theoretical-finance are united in a single framework. Our result thus greatly expands the scope of application of the TUR.

This work is done in collaboration with Ziyin Liu.

Guest recognition in dynamic libraries and spin-crossover cages

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Spin-crossover (SCO) metal-organic cages are capable of switching between high-spin and low-spin states, which enables these molecular containers to be used as magnetic sensors and switches. A SCO tetrahedral Fe^{II} cage is capable of encapsulating various guests, which stabilize different cage spin states depending on guest size (Figure 1a). Conversely, the SCO tetrahedron exhibits different affinities for the guests in different spin states, which is inferred to result from the subtle structural differences of the cavity caused by the change in metal centre spin state.[1]
A dynamic library of metallo-supramolecular assemblies formed from a bis-urea-functionalized subcomponent reconfigured in response to the addition of monosaccharide derivatives, which served as guests for specific library members (Figure 1b). The (*P*) enantiomer of the Fe^{II}_2L3 helical structure bound β-D-glucose selectively over α-D-glucose. As a consequence, the library collapsed into the (*P*)-$Fe^{II}_2L_3$ helicate following glucose addition.[2]

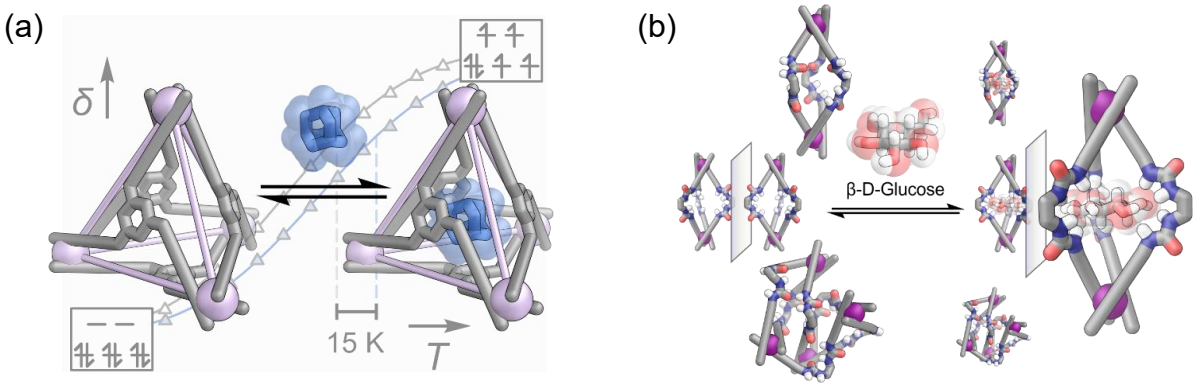

Figure 1. (a) A spin crossover Fe^{II} tetrahedron in which the low-spin or high-spin states are stabilized by guests (blue) of suitable sizes. **(b)** A dynamic library of cages (an irregular $Fe^{II}_4L_6$ structure, $Fe^{II}_2L_3$ left- and righthanded helicates and a meso-structure) capable of selectively recognizing β-D-glucose over its α-anomer.

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Dynamical phase transition in an open quantum system

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As discovered recently, the nonequilibrium dynamics of isolated quantum systems can undergo dynamical phase transitions, with *time* being the control parameter rather than, e.g., temperature. We demonstrate that dynamical phase transitions occur also in open systems. We measure the spin dynamics of individual Caesium atoms, induced by the dissipative coupling to an ultracold Rubidium cloud. For initial states far from equilibrium, the spin entropy is observed to peak in time, long before reaching its thermal value. This behavior indicates a prethermal loss of the system's memory of its initial state. Finite-size scaling analyses based on numerical simulations reveal that it corresponds to a continuous phase transition in the large-system limit and provide a universal critical exponent for the associated divergence of a localization length.

Abstracts of Posters

(in alphabetical order)

On the entropy dilemma: Gibbs paradox revisited

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Although the initially described statistical thermodynamics interpretation of entropy seemed to be clear and easy to understand, a paradox resulted by the initially proposed interpretation as pointed out by Gibbs in his pioneering book [1] which later on became famous as Gibbs paradox, has resulted in numerous debates on the topic within the past century. The most widely accepted resolution to the Gibbs paradox requires inclusion of a $1/N!$ factor on the estimated total number of microstates. Nevertheless, justifications for such ad-hoc treatment itself has been a controversial topic in the field and is not still quite clear.

The main aim of the present study is to shed a new light on the statistical thermodynamical interpretation of entropy and its connection with classical thermodynamics by theoretical arguments which has not been considered thus far, the consequences of inclusion of the $1/N!$ factor, and providing experimental evidences to support the proposed arguments.

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Master equation for an arbitrarily quick driven harmonic oscillator

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We derive a Redfield master equation for an arbitrarily quick driven harmonic oscillator that generates a CPTP-map due to the choice of the interaction Hamiltonian. Afterwards we solve the master equation for arbitrary Gaussian initial states and calculate the mean energy, the entropy and a coherence measure for Gaussian states from the solutions. Finally, we compare our results with the adiabatic master equation and with the O'Connell master equation and find good agreement with the adiabatic master equation in the slow driving regime.

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Starting over without forgetting the past

Amy Altshuler[1,2], Ofek Lauber Bonomo[1,2], Nicole Gorohovsky[3], Shany Marchini[3], Eran Rosen[1], Ofir Tal-Friedman[3,2], Shlomi Reuveni[1,2], and Yael Roichman[1,2,3]

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Abstract

In the past decade, resetting of random processes has been studied extensively, being relevant to natural processes. Under resetting, a random process can reach a stationary steady state that may reduce the average time it takes to reach a target. A resetting process generally includes cycles of a period of random motion followed by a period of return to the origin. When the random process is reset, the entire system starts from the same initial conditions as in the previous cycle. Inspired by scent trails left by ants, we study the case where the random motion leaves a mark on the environment. Namely, after resetting the system, the environment retains some memory of previously used paths. We implement this process using a self-propelled bristle robot moving within an arena filled with mobile obstacles. We return the bristle robot to the origin at constant time intervals. Surprisingly, we find that the propagator of motion is Gaussian in our experiments. We find that environmental memory increases the width of the steady state distribution. We observe that memory expedites the search in our setup.

Entropy production in ticking clocks: Fundamental limits of timekeeping

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The concept of time and its role in physics, in particular quantum theory, remains an active field of research. The process of timekeeping is linked to the usage of clocks as reference systems. Thus, many open questions about time can be addressed through the study of these devices. Ticking clocks provide information about the flow of time in terms of discrete ``ticking'' events. In this project, we studied autonomous ticking clocks based on a model derived from axiomatic principles [1]. We tried to answer the question whether the theory of quantum information imposes any constraints on the relation between the entropy production per tick of a ticking clock and its accuracy. Here, the entropy production serves as a measure for the exchanged information between a ticking clock and its environment. We find that there exist quantum ticking clocks with coherent internal dynamics that approach infinite accuracy at zero entropy production per tick. In contrast, ticking clocks whose state remains incoherent at all times must produce a minimal amount of entropy in each tick that increases with increasing accuracy. For such classical clocks the entropy production per tick acts as a fundamental resource for measuring time.

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Master Equation and detailed fluctuation relation in the presence of continuous feedback control

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Measurement and feedback control are essential features of quantum science, with applications ranging from quantum technology protocols to information-to-work conversion in quantum thermodynamics. Theoretical descriptions of feedback control are typically given in terms of stochastic equations requiring numerical solutions, or are limited to linear feedback protocols. Here we present a formalism for continuous quantum measurement and feedback, both linear and nonlinear. Our main result is a quantum Fokker-Planck master equation describing the joint dynamics of a quantum system and a detector with finite bandwidth. For fast measurements, we derive a Markovian master equation for the system alone, amenable to analytical treatment. We illustrate our formalism by investigating two basic information engines, one quantum and one classical.

First-passage times in complex energy landscapes: a case study with nonmuscle myosin II assembly

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Complex energy landscapes arise in biological systems, e.g. for protein folding, biochemical reactions, or intracellular transport processes. The physical effects emerging from these landscapes are frequently reflected in their first-passage times (FPTs). However, their calculation is challenging and it is typically difficult to identify key features of a given energy landscape. Here we show how this can be achieved by coarse-graining continuous-state overdamped Langevin dynamics to a Markov jump process described by a Master equation which allows us to decompose its mean first-passage time in an iterative process. We apply this method to the electrostatic interaction between two rods of nonmuscle myosin II (NM2), which is the main motor for force generation in nonmuscle cells. Energy landscapes are computed directly from the amino acid sequences. Our approach allows us to identify the most relevant energy barriers for their self-assembly into NM2 minifilaments and by computing the mean first-passage times we find that antiparallel configurations are more stable than parallel ones.

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Tuning the Kinetics of Magnetization Reversal in an Irreversible Ising Model

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The Ising model is a cornerstone in the theory of cooperative phenomena. Since the seminal works by Glauber [1] and Kawasaki [2] the reversible kinetics of the Ising model has gained considerable attention from a variety of fields, including mathematics, physics, and econophysics.

Here we are interested in an irreversible two-dimensional Ising model undergoing single spin-flip dynamics with an external driving that breaks detailed-balance while preserving the Z_2-symmetry. Particularly, we focus on the magnetization reversal time, which is the first passage time to flip all spins in the system.

Recently it has been shown that for reversible dynamics in the thermodynamic limit there exists a dynamical phase transition where the average magnetization reversal time attains a minimum [3]. Here we show that by breaking time-reversal symmetry we can drive the system below this threshold and find a new universal minimum where magnetization reversal is the fastest.

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Calculating Energy Flows in Strongly Coupled Open Quantum Systems with HOPS

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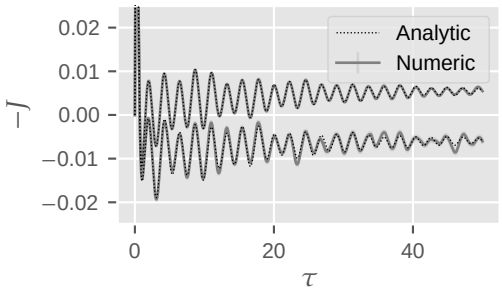
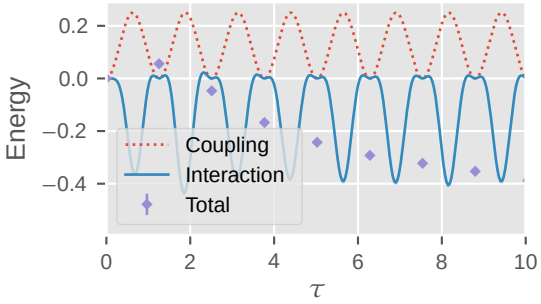
The hierarchy of pure states (HOPS [1, 2]) is a general purpose stochastic numerical framework for the exact simulation of non-Markovian strongly coupled open systems. Without modification of the core method, it is possible to calculate the interaction energy and the bath energy change. This is due to HOPS' foundation on the global dynamics of the system and the bath in contrast to master-equation methods. We extended the result in [3] for the Hierarchical Equations Of Motion method to arbitrary modulations of system and coupling inheriting all the advantages of the HOPS method.

We present the basic theory and its application to simple driven spin-boson like systems, as well as a comparison with an exact solution for a quantum Brownian motion like model.



a) Comparison of the bath energy change $J_i = -\partial_t \langle H_{B,i} \rangle$ for two harmonic oscillators coupled to two baths and each other.



b) Total energy and interaction energy for a qubit coupled to a bath with long correlation time under fast modulation.

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An experimental test of a nonlinear fluctuation-dissipation theorem to test Markovianity far from thermal equilibrium

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Fluctuation-Dissipation-Theorems connect the internal spontaneous fluctuations of a system with its response to an external perturbation. The classic version can be used to test whether a system operates in equilibrium and a generalized version for non-equilibrium systems can be used to determine an effective temperature. However, the physical meaning and predictive power of the effective temperature are, in general, unclear. Here, we propose a generalized non-linear fluctuation dissipation theorem that should hold true for any Markovian system even if it is far from thermal equilibrium, and even if the perturbation is not small. We test this new non-linear fluctuation-dissipation theorem on an experimental system consisting of a Styrofoam ball in a harmonic gravitational potential well and subjected to collisions with macroscopic self-propelled bristle-bots. A mechanical perturbation is applied on the Styrofoam ball by an air stream. By tracking the position sequences of the tracer, transient behavior can be observed as the system transitions between two non-equilibrium steady states (with and without wind). We find that the new non-linear relation holds for various conditions including strong perturbation with no fitting parameters. For a constructed non-Markovian process, the theorem is violated, and a quantitative measure to evaluate the degree of violation of the theorem is suggested.

Topological information device operating at the Landauer limit

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(Dated: June 27, 2022)

We propose and investigate a novel Maxwell's demon implementation based on the spin-momentum locking property of topological insulators. We use the nuclear spins as a memory resource provides the advantage of the scalability to our device, which we call topological information device. We show that the topological information device can ideally operate at the Landauer limit; the heat dissipation required to erase one bit of information stored in the demon's memory approaches $k_B T \ln 2$. Furthermore, we demonstrate that all energy stored in Maxwell's demon memory, $k_B T \ln 2$ per one bit of information, can be extracted in the form of electrical work. Finally, we find that the current-voltage characteristics of the topological information device satisfies the conditions of an ideal memristor.

Thermodynamic consistency of quantum master equations

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Starting from a microscopic system-baths description, we derive the general conditions for a time-local quantum master equation (QME) to satisfy the first and second law of thermodynamics at the fluctuating level. Using counting statistics [1], we show that the fluctuating second law can be rephrased as a Generalized Quantum Detailed Balance condition (GQDB), i.e., a symmetry of the time-local generators which ensures the validity of the fluctuation theorem.

When requiring in addition a strict system-bath energy conservation at the fluctuating level, the GQDB reduces to the usual notion of detailed balance which ensures QMEs with Gibbsian steady states. However, if energy conservation is required only on average, QMEs with non Gibbsian steady states can still maintain a certain level of thermodynamic consistency.

Applying our theory to commonly used QMEs, we show that the Redfield equation breaks the GQDB, and that recently derived approximation schemes based on the Redfield equation (which hold beyond the secular approximation and allow to derive a QME in the Lindblad form) satisfy the GQDB and the average first law.

We find that secular and degenerate QMEs are the only ones ensuring the first and second law at the fluctuating level.

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Number fluctuations and the Szilard Engine: active matter wins

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An information machine is a device that converts information to mechanical work using a feedback loop. We realize such a device which is macroscopic and contains interacting self-propelled particles. We find that giant number fluctuations can be exploited to extract more work from a generalized active-matter Szilard's engine compared to a system that operates the same protocol on an ideal gas.

Spontaneous Temperature Increase in Ultracold Plasmas: Disorder-Induced Heating vs. Virialization

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A well-known phenomenon in the ultracold plasmas, studied in the magneto-optical traps, is a sharp spontaneous increase of temperature immediately after its formation, which is often qualitatively explained by the so-called “disorder-induced heating” (DIH) [1]. Unfortunately, this concept is poorly consistent with the 2nd law of thermodynamics, because it assumes evolution of the system from the disordered to a more ordered state. Besides, a straightforward simulation of some particular cases of heating the ions demonstrates that the DIH mechanism, in principle, operates but has a quite limited efficiency [2]. An alternative explanation of the sharp temperature increase can be based on the effect of “virialization” [3, 4], which was well known for a long time in astrophysical plasmas and seems to be in a better agreement with the fundamental principles of thermodynamics.

The aim of the present report is to investigate what is the prevailing mechanism of heating in the case of electrons, which have received much less attention in the previous studies. So, we perform a straightforward numerical simulation of relaxation of the electron velocities—taken initially in the strongly overcooled state—amid a variety of ionic backgrounds with different arrangement of particles [5]. Surprisingly, it was found that a subsequent establishment of the electron temperature is almost independent of the degree of disorder in the distribution of ions. Consequently, its interpretation in terms of the disorder-induced heating turns out to be not applicable at all. Therefore, the only reasonable mechanism for the spontaneous electron heating seems to be the concept of “virialization” of the electron velocities, whose application to the expanding ultracold plasmas was already demonstrated about a decade ago [4].

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Circumventing the second law of thermodynamics by entropy export to generate regular arrays of liquid metal droplets

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The thermodynamics of forming and growing particles on surfaces is characterised by two theories: the classical nucleation theory and the classical de-wetting theory. From the formation of nanoscopic droplets to the formation of microcrystallites and the growth of bulk crystals, almost all material formation processes can be explained by these approaches.[1]

However, both theories only apply under ideal conditions, i.e. in thermodynamic equilibrium of a closed system. Under real conditions material structures can form which, according to classical nucleation and de-wetting, should actually never occur. The reason for this lies in the way systems may deal with the internally produced entropy: By exporting entropy out of the system, it is possible to reach states of order that would be forbidden in equilibrium thermodynamics. Thus, some open, i.e. real, systems evade the second law of thermodynamics.

Indium micro- and nanostructures on polycrystalline molybdenum surfaces exemplifies this phenomenon. These structures serve as precursor frameworks in novel solar cell designs and can be sufficiently described neither by the principles of classical nucleation theory nor classical de-wetting theory. For this reason, de-wetting theory was extended by the principles of non-equilibrium thermodynamics, in particular by the rules of dissipative structure formation. This results in a possibly new mechanism of structure formation: dissipative de-wetting. Dissipative de-wetting leads to a reduction of the area-normalised Helmholtz energy by forming different subsystems of different indium layer thickness. These subsystems are in constant material exchange with each other and their behaviour can be predicted by the entropy production rate. This not only allows the formation of surface particles where none should be according to classical theory, but even the arrangement of these particles in the shape of regular arrays.

In this way the indium frameworks on molybdenum used in solar cell development can be grown directly, i.e. bottom-up, and complex lithographic top-down etching is no longer necessary.

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Dynamical phase transition in an open quantum system

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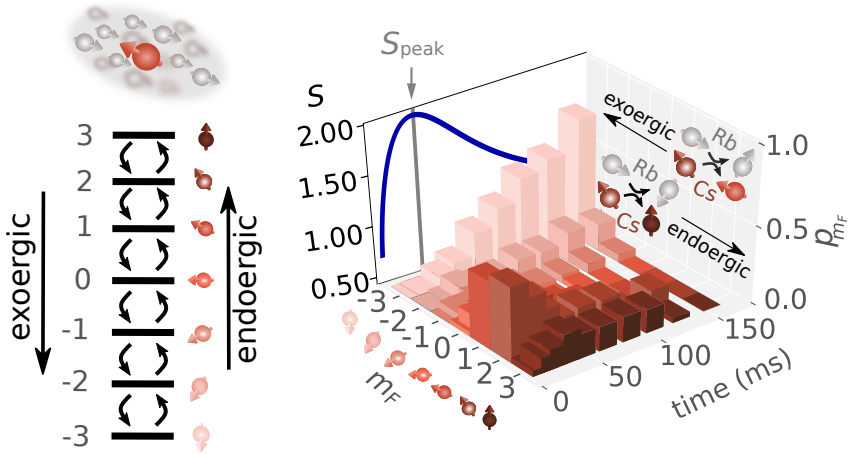
Phase transitions correspond to the singular behavior of physical systems in response to continuous control parameters like temperature. Recently, dynamical quantum phase transitions have been observed in the non-equilibrium dynamics of isolated quantum systems, with time playing the role of the control parameter. However, signatures of such dynamical phase transition in open systems, whose dynamics is driven by the dissipative contact to an environment, were so far elusive. Here, we demonstrate that dynamical phase transitions with respect to time can also occur in open quantum systems described by mixed states. We experimentally measure the relaxation dynamics of the large atomic spin of individual Caesium atoms induced by the dissipative coupling via spin-exchange processes to an ultracold Bose gas of Rubidium atoms. For initial states far from equilibrium, the entropy of the spin state is found to peak in time, transiently approaching its maximum possible value, before eventually relaxing to its lower equilibrium value. Moreover, a finite-size scaling analysis based on numerical simulations shows that it corresponds to a dynamical phase transition of the dissipative system in the limit of large system sizes. Our results show that dynamical phase transitions are not restricted to occur in isolated systems, but, surprisingly, are possible also during the dissipative evolution of open quantum systems.



Entropy production for Brownian trajectories of a reduced density matrix

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The reduced density matrix of an open quantum system is primarily regarded as a device for computing probabilities for the outcomes of projective measurements of observables. But we might go beyond this interpretation and consider it to be a specification of real-world physical attributes analogous to classical coordinates. If the environment to which the system is coupled has many underspecified degrees of freedom, the reduced density matrix of the system would then naturally evolve in a pseudorandom fashion, rather like the motion of a classical Brownian particle.

The uncertain evolution of the state of any system is accompanied by the production of stochastic entropy, a measure of irreversibility, and it is of interest to compute this quantity for Brownian trajectories of a reduced density matrix. It is more usual in studies of open quantum system evolution to take an average, effectively, over an ensemble of such trajectories and to disregard this entropy production.

We use the framework of quantum state diffusion to generate continuous stochastic trajectories of a reduced density matrix. Various coupling scenarios correspond to system thermalisation or to weak measurement: the selection of an eigenstate of an observable without discontinuous jumps. Interpretational issues that often distinguish thermalisation and measurement can be avoided.

We study simple systems undergoing deterministic Hamiltonian evolution together with stochastic environmental disturbance. The dynamics are used to demonstrate a Zeno effect, where measurement slows down the natural evolution of a quantum system. Furthermore, values of noncommuting observables can coexist in this framework, with specific statistical correlations with one another.

We compute the distribution of associated stochastic entropy production for these cases. The mean stochastic entropy production satisfies the second law of thermodynamics and is a more fine-grained descriptor of irreversibility in quantum systems than the more familiar von Neumann entropy.

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Temperature of a finite system and the origin of the Boltzmann factor

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Temperature is often considered a given quantity, with no need for any definition. This approach encounters serious difficulties when used on phenomena for which the number of degrees of freedom is limited and where the thermodynamic limit does not exist. This is seen very clearly in the thermal behavior of microcanonical nanoparticles and clusters [1].
We define temperature by coupling a system to a heat bath, as the logarithmic derivative of the level density, the microcanonical partition function, of the heat bath with respect to energy. The definition is consistent with the description of a fixed temperature for canonical and grand canonical systems. It also produces the Boltzmann factor with no further ado [2]. An important side result is the clarification that temperature fluctuations is not a meaningful concept. For finite and isolated systems, a microcanonical temperature can be defined and used for activated processes [1]. It has however different properties from a true canonical value, with one obvious difference that it does not determine energy fluctuations.

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Conductance of correlated many-fermion systems from bipartite charge fluctuations and entanglement entropies

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We put forward a relation between the static charge fluctuations and the conductance of correlated many-fermion systems at zero temperature, avoiding the use of time-dependent fluctuations as in the fluctuation-dissipation theorem. Static charge fluctuations can efficiently be computed for low-dimensional systems using tensor network approaches, while the conductance is often significantly more difficult to obtain, requiring a challenging low-frequency linear response computation or an explicit time evolution. We put this relation to the test for quantum dot and quantum point contact setups, where in limiting cases, exact results are known. Our study includes systems in which the one-dimensional reservoirs are interacting. We reveal the conductance can also be fit from the entanglement entropy data.

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Switching the function of the quantum Otto cycle in non-Markovian dynamics: heat engine, heater and heat pump

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Keywords: Quantum stochastic thermodynamics

Quantum thermodynamics explores novel thermodynamic phenomena that emerge when interactions between macroscopic systems and microscopic quantum ones go into action. Among various issues, quantum heat engines, in particular, have attracted much attention as a critical step in theoretical formulation of quantum thermodynamics and in investigation of efficient use of heat by means of quantum resources [1].

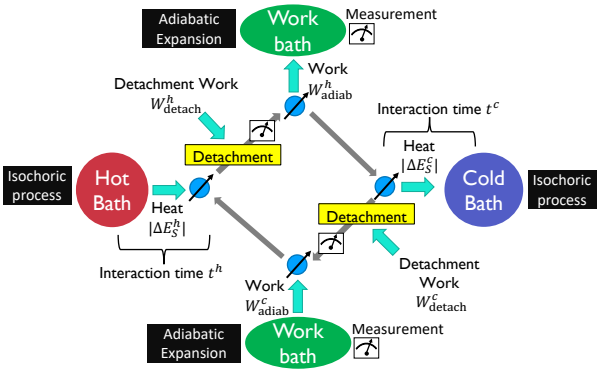

Figure 1: Quantum Otto Cycle. A qubit absorbs or emits heat from or to the bath in each isochoric process and does work to the outside in the adiabatic processes. After each isochoric process, we need detachment work to separate a qubit from the bath. We also perform indirect measurement in order to quantify the extracted work.

In the present research, we focus on heat absorption and emission processes as well as work extraction processes of a quantum Otto cycle (Fig. 1) [2]. We describe the former as non-Markovian dynamics [3], and thereby find that the interaction energy between a macroscopic heat bath and a microscopic qubit is not negligible. In particular, we reveal that the interaction energy is divided into the system and the bath in the short interaction time and remains negative in the long time. We quantify these two effects by defining an index of non-Markovianity in terms of the energy division of the interaction energy. Thanks to this behavior

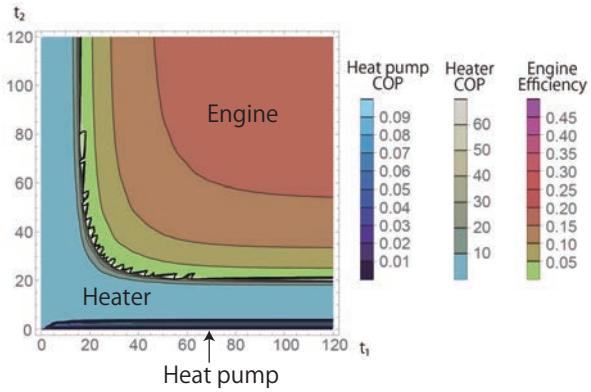

Figure 2: Work, heat, efficiency η and COP (Coefficient of performance), which is the heat absorbed from the cold bath divided by the work acquired from the external system. The parameters are set to $\omega_c/\omega_h = 0.5$ and $T_c/T_h = 0.2$ for the interaction times t^h and t^c, where ω_h and ω_c indicates the frequency of the qubit when it interacts with hot and cold baths, respectively, while T_h and T_c are the temperatures of the hot and cold baths, respectively.

of the interaction energy, our non-Markovian quantum Otto cycle switch functions, such as an engine as well as a heater or heat pump, by controlling the interaction time with the heat bath (Fig. 2). In addition, the qubit itself loses its energy if we shorten the interaction time; in other words, the qubit is cooled through the cycle [3]. This property produces a possibility of being utilized for cooling qubits in quantum computing.

We also describe the work extraction from the microscopic system to a macroscopic system like us humans as an indirect measurement process by introducing a work storage as a new reservoir [4].

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Heat flux in phase-separated systems out of equilibrium

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Phase-separated multi-component systems with chemical reactions have become of wide interest in recent years, as they show interesting behaviors of non-equilibrium systems. Much work has been done on the particle concentration dynamics at constant temperature. We extend the existing framework to non-isothermal systems and study the heat dynamics that arises. Thereby, we obtain the full entropy production when driving the system out of equilibrium by fueling reactions or via baths at the boundaries.

Specifically, we consider continuity equations for the chemical composition and energy. In systems with multiple coexisting phases, the coupling of these equations can depend strongly on the phase. Using a lattice model with hopping of particles and energy, we gain an understanding of how heat and particle flow couple. For this, we write an entropy-driven Metropolis scheme. We observe that, depending on the particle-heat coupling, a phase boundary can act as a heat source or sink. A kinetic Monte Carlo simulation allows us to obtain the stochastic trajectories.

The established framework should, in future work, allow insights into the effects of reaction heat on phase-separated systems. Particular interest is in applying this to understand the energetics of biological cells and organisms.

Quantum heat engine based on a spin-orbit and Zeeman-coupled Bose-Einstein condensate

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We explore the potential of a spin-orbit coupled Bose-Einstein condensate for thermodynamic cycles. For this purpose we propose a quantum heat engine based on a condensate with spin-orbit and Zeeman coupling as a working medium. The cooling and heating are simulated by contacts of the condensate with an external magnetized media and demagnetized media. We examine the condensate ground state energy and its dependence on the strength of the synthetic spin-orbit and Zeeman couplings and interatomic interaction. Then we study the efficiency of the proposed engine. The cycle has a critical value of spin-orbit coupling related to the engine maximum efficiency.

Optimization of the performance of the quantum many-body heat engine using CRAB.

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One of the major aims of the field of quantum technologies is designing optimal quantum thermal machines through quantum control. We aim to focus on this problem, by engineering high-performing single and many-body continuous quantum heat engines through the chopped random basis (CRAB) numerical optimization algorithm[1][2]. The continuous heat engines are one in which the working medium(WM) is simultaneously coupled to a hat and cold bath at all times, while its Hamiltonian is continuously modulated[3][4][5]. Such heat engines have been studied using a two-level system(TLS) working medium, as well as non-interacting multi-spin working mediums, in which the spins are collectively coupled to the hat and the cold bath[6][7]. Optimization of the many-body quantum heat engine using the quantum control technique can be expected to take a lang time owing to the large dimension of the corresponding Hilbert space. So we first optimize a minimal quantum heat engine with a periodic modulated WM. The cost function that is to be optimized is the power output of the engine which depends on the shape of the periodic external pulse when we fix the parameter like the bath temperature, bare transition frequency of the working medium, and modulation time period. Using CRAB we find the best possible shape of the periodic pulse which would maximize the power of the minimal engine. Then we study the possibility of improving the performance of the multi-spin heat engine by using the optimal pulse obtained in the case of a minimal quantum heat engine. We show that using the optimal pulse of the single spin heat engine the performance of the many-body heat engine improves significantly.

heat engine. We show that using the optimal pulse of the single spin heat engine the performance of the many-body heat engine improves significantly.

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Fluctuation theorems for a quantum Brownian motion due to a disordered environment

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Microscopic models for quantum Brownian motion usually consider a particle interacting with several modes representing the influence of the heat bath. However, the interaction between these modes and the particle is often taken as unlimited in space and free of spatial fluctuations. In this work, we elaborate on a previously proposed microscopic model that takes these aspects into account. In particular, we focus on the strong damping limit of the corresponding high-temperature master equation and show that it leads to non-Gaussian statistics. Our results reduce to the well-known Smoluchowski equation in the appropriate limit, which involves the spatial correlation length of the fluctuating interaction. We also derive the corresponding steady state considering a motion under a harmonic potential and the fluctuation theorems for work and entropy production given a protocol.

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Extractable work in a Szilard engine with a finite-size reservoir

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The Szilard engine is a paradigmatic protocol in thermodynamics when it comes to the question of how much work can be extracted from a system coupled to a single thermal reservoir, by means of performing measurement and feedback. Originally conceived as a thought experiment by Szilard [1], experimental realizations of the engine have been implemented over the last few years, for example in the context of nanodevices such as quantum dots [2,3]. In an ideal Szilard engine, in which the system is coupled to an infinite-size bath at constant temperature, the extractable work has an upper bound, reaching k_BT ln 2 for a quasi-static, large amplitude cycle.
Here, we investigate how the extraction of work in a Szilard engine is impacted by finite-size reservoirs. We focus on a system constituted of a quantum dot, which is, in turn, coupled to a finite-size fermionic reservoir. Due to the exchange of heat between the quantum dot and the reservoir, the temperature of the reservoir develops fluctuations in time. We find that the maximum amount of work that can be extracted is always lower than in the ideal Szilard engine, with infinite size reservoirs. Furthermore, in the limit of large but finite-size reservoirs, the difference in extractable work is inversely proportional to the heat capacity of the reservoir.
Moreover, we compare our results with previously derived upper bounds for the extractable work derived for finite-size reservoirs [4,5], and show that our results are consistent with these bounds.

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Non-Equilibrium Statistical Physics Beyond the Ideal Heat Bath Approximation

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Important models of nonequilibrium statistical physics (NESP) are limited by a commonly used, but often unrecognized, near-equilibrium approximation. Fokker-Planck and Langevin equations, the Einstein and random-flight diffusion models, and the Schnakenberg model of biochemical networks suppose that fluctuations are due to an ideal equilibrium bath. But far from equilibrium, this perfect bath concept does not hold. A more principled approach should derive the rate fluctuations from an underlying dynamical model, rather than assuming a particular form. Here, using Maximum Caliber as the underlying principle, we derive corrections for NESP processes in an imperfect - but more realistic - environment, corrections which become particularly important far from equilibrium. Beyond characterizing a heat bath by the single equilibrium property of temperature, we must also consider finite bath size and finite bath speed to fully describe dynamics further from equilibrium.

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Stochastic thermodynamics of networked systems without a thermodynamic interpretation

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Stochastic thermodynamics has recently emerged as a powerful new approach toward out-of-equilibrium physical mesoscopic systems. However, a stochastic thermodynamics treatment of a much broader scope of phenomena, ranging from social to economic and biological, remains sparse. This is partially because the coarse-grained level at which many of these systems are modeled cannot be described in terms of physical energy levels. Despite the non-physical nature of such systems, we show how to use the full power of stochastic thermodynamics to understand dynamical properties of any system that can be modeled as a continuous-time Markov chain (CTMC), whether or not those systems have energetic descriptions. In particular, we focus on those systems that can be represented as a directed network of interdependent and co-evolving subsystems, such as social networks of voters, where directed links (non-reciprocal social ties) indicate who follows whom, or gene regulatory networks, where directed links indicate which genes regulate which other genes. We show how dynamical properties of these systems are affected by the degree of non-reciprocity in the structure of the network representation of system interdependencies. For example, in the context of social networks, our results suggest that a system's dynamics will become less reversible as the fraction of individuals who unidirectionally pay attention to their peers increases. Additionally, we show how stochastic thermodynamics allows us to bound the speed with which an opinion network can change its distribution, or the precision of the amount of consensus throughout the network.

References

Detecting Heat Leaks with Trapped Ion Qubits

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The concept of *passivity* has been conceived to set bounds on the evolution of microscopic systems initialized in thermal states. We experimentally demonstrate the utility of two frameworks, global passivity [1] and passivity deformation [2], for the detection of coupling to a hidden environment. We employ a trapped-ion quantum processor [3], where system qubits undergoing unitary evolution may optionally be coupled to an unobserved environment qubit, resulting in a heat leak. Evaluating the measurement data from the system qubits only, we show that *global passivity* can verify the presence of a heat leak, which is not detectable by a microscopic equivalent of the second law of thermodynamics. Furthermore, we experimentally show that *passivity deformation* allows for even more sensitive detection of heat leaks, as compared to global passivity, and detect a heat leak with an error margin of 5.3 standard deviations, in a scenario where other tests fail. [4]

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Optimizing Information Engines in and out of Equilibrium

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Information engines use measurement and feedback to extract work from a system as described by the idea of “Maxwell’s demon” and later by Szilard’s engine. As such engines become experimentally viable, we seek to find protocols that optimize power output or efficiency. This work focuses on optimizing the work obtained per measurement, which we denote as $\bar{W}$. As our model system, we use colloidal particles in a box, and a protocol that utilizes information to compress the particles in the box without performing direct work on them. Using computer simulations and analytical results, we explore the performance of such engines for systems in thermal equilibrium, and for two distinct nonequilibrium variants - athermal colored noise, and active Brownian particles. We find that equilibrium systems show distinct universal features, most notably that the maximal $\bar{W}$ is the same for any equilibrium system. For nonequilibrium systems, we analyze the engine performance as we vary the strength of the nonequilibrium driving (denoted by the system's Peclet number). Our results show a clear qualitative and quantitative difference between the two nonequilibrium variants, demonstrating the utility of information engines for characterizing nonequilibrium systems

Thermodynamics of a minimal algorithmic cooling refrigerator

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We investigate, theoretically and experimentally, the thermodynamic performance of a minimal three-qubit heat-bath algorithmic cooling refrigerator. We analytically compute the coefficient of performance, the cooling power and the polarization of the target qubit for an arbitrary number of cycles, taking realistic experimental imperfections into account. We determine their fundamental upper bounds in the ideal reversible limit and show that these values may be experimentally approached using a system of three qubits in a nitrogen-vacancy center in diamond.

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Initial-state dependence of entropy production for any quantum process

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Combining the tools of quantum information and nonequilibrium thermodynamics, we identify the initial-state dependence of entropy production for any quantum process.

We first find that entropy production can always be expressed as the change in correlation between system and environment, plus the change in relative entropy between the actual and reference states of the environment. This shows that entropy production can be negative, even on average—if the system and environment are initially correlated, or if the environment begins out of local equilibrium. This, in turn, clarifies the assumptions required for the validity of the Second Law of thermodynamics, which states that entropy production is non-negative on average.

We then find an elegant expression for the initial-state dependence of entropy production for any quantum process. Any process will have a minimal amount of entropy production incurred by the minimally dissipative state. We find that the entropy production from any other initial state is quantified exactly by the contraction of the quantum relative entropy between the actual and minimally-dissipative states over the course of the process. This implies that nonunitary processes cannot be thermodynamically optimized for all inputs simultaneously. In particular, this implies the impossibility of Landauer's bound for almost every input to any reliable reset device. This rewrites the relationship between energy and information, ousting the idea of a simple exchange rate between the two.

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Non-equilibrium thermodynamics of quantum coherence

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The thermodynamic properties of quantum heat engines are stochastic owing to the presence of thermal and quantum fluctuations. We here experimentally investigate the efficiency and non-equilibrium entropy production statistics of a spin-1/2 quantum Otto cycle. We first study the correlations between work and heat within a cycle by extracting their joint distribution for different driving times. We show that near perfect anti-correlation, corresponding to the tight-coupling condition, can be achieved. In this limit, the reconstructed efficiency distribution is peaked at the macroscopic efficiency and fluctuations are strongly suppressed. We further test the second law in the form of a joint fluctuation relation for work and heat. Our results characterize the statistical features of a small-scale thermal machine in the quantum domain and provide means to control them.

Derivation of a statistical model for classical systems obeying the exclusion principle

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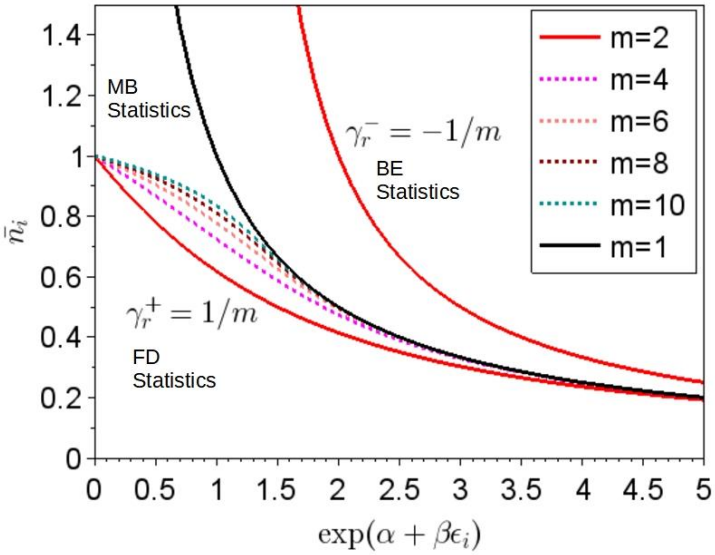

Fractional Exclusion Statistics[1,2] (FES) models allow multiple-but-finite occupancy in different states of a quantum system and are shown to be intermediate between Bose-Einstein (BE) and Fermi-Dirac (FD) statistics. An alternative FES model can be derived using classical tools which show quantum features such as exclusion, without any *a-priory* assumption of the validity of the exclusion principle[3]. The difference between the BE statistics and the Maxwell-Boltzmann (MB) statistics is understood in terms of a separable quantity, namely the degree of indistinguishability. Starting from the usual MB microstate counting formula, a special restriction related to the degree of indistinguishability is incorporated using Lagrange multipliers to derive the probability distribution function at equilibrium under NVE conditions. It is found that the resulting probability distribution function generates real positive values within the permissible range of parameters[3,4]. For a dilute system, the probability distribution function is intermediate between the FD and BE statistics and follows the exclusion principle. Properties of various variables of this novel statistical model are studied and possible application to the classical thermodynamics is discussed[3,5].

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Outperforming Carnot efficiency using periodically driven quantum chiral conductors

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We demonstrate [1] that a quantum chiral conductor driven by AC voltage can work with efficiencies much larger than the Carnot bound. Our pump engine consists of a scatterer of arbitrary energy-dependent transmission tunnel coupled to electronic hot and cold reservoirs in the presence of an external AC bias voltage. An AC driving typically generates a finite input power that diminishes the efficiency. Our key idea to overcome this difficulty is to selectively apply an AC external field to the electrons depending on the direction, which can be implemented using a chiral conductor such as those created with topological matter. This completely avoids any AC input power, allowing a high efficiency of the quantum engine, in contrast to nonchiral cases. We adopt the Floquet scattering matrix approach for electric and heat currents and also a generalized definition of entropy production based on Shannon formula [2] for the incoming and outgoing electron distributions in each terminal. We find that the engine efficiency exceeds the Carnot limit when the entropy production is deviated from the Clausius relation due to the nonequilibrium induced by the AC driving. Such effect can be understood by the fact that the AC driving effectively increases the temperature [3] of the incoming electrons by rearranging the energy distribution in a more uncertain way, while injecting vanishing net energy. Our results are relevant in view of recent developments that use small conductors to test the fundamental limits of thermodynamic engines.

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Work Extraction from Unknown Quantum Sources

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We ask whether, and how much energy we can extract from a completely unknown source of quantum states, assuming we have only a single type of coarse-grained measurement that we can perform, and unitary extraction operations that do not allow access to the inner structure of macrostate, by transforming its constituent microstates. We find that even under these harsh and restricted situations, energy can be extracted in some situation. This defines an alternative notion of coarse-grained ergotropy. It shows that the amount of energy that is possible to extract in this situation is implicitly given by observational entropy. This gives an operational interpretation to this quantity and demonstrates its practical relevance, not only as a descriptive, but also as a predictive figure of merit.

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Quantum Synchronization of Opposite Heat Flows

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In the presence of initial correlations the second law of thermodynamics does no longer hold and entropy may spontaneously decrease in a closed system as the correlations degrade. This could be demonstrated in a thermal two-qubit system with initial correlations where the direction of heat flow was shown to be reversed, i.e. energy is transferred from the colder to the hotter qubit [1].

Here, we build on this work and couple two such systems, one with and one without initial correlations where the composite four-qubit system has thus competing directions of heat flow.

First, we provide bounds for the heat flow of an uncorrelated system and express the total heat flow in terms of entropic quantities. We furthermore extract the only negative contribution responsible for violating the bounds.

In order to establish a definite direction of the heat flow of the two bipartite systems, we use the mechanism of noise-induced quantum synchronization.

To this end, white noise is applied to the chain leading to a Lindblad equation for the average density matrix.

Depending on the location of the noise in the chain and the interaction strength between the two subsystems, (anti-)synchronization may be induced [2]. More specifically, we find one such configuration where, additionally, the total heat flow retains its anomalous feature, exceeding the bounds for an uncorrelated system and also find a second configuration where the total heat flow is not reversed and stays thus in-between the bounds.

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Wave packet dynamics in an harmonic potential disturbed by disorder: Entropy, uncertainty, and vibrational revivals[1]

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We investigate the quantum and classical wave packet dynamics in an harmonic oscillator that is perturbed by a disorder potential. This perturbation causes the dispersion of a Gaussian wave packet, which is reflected in the coordinate-space and the momentum-space Shannon entropies, the latter being a measure for the amount of information available on a system. Regarding the sum of the two quantities, one arrives at an entropy that is related to the coordinate–momentum uncertainty. Whereas in the harmonic case, this entropy is strictly periodic and can be evaluated analytically, this behavior is lost if disorder is added. There, at selected times, the quantum mechanical probability density resembles that of a classical oscillator distribution function, and the entropy assumes larger values. However, at later times and dependent on the degree of disorder and the chosen initial conditions, quantum mechanical revivals occur. Then, the observed effects are reversed, and the entropy may decrease close to its initial value. This effect cannot be found classically.

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Extracting work from random collisions: A model of a quantum heat engine

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We study the statistical distribution of the ergotropy and of the efficiency of a single-qubit battery ad of a single-qubit Otto engine, respectively fueled by random collisions. The single qubit, our working fluid, is assumed to exchange energy with two reservoirs: a nonequilibrium "hot" reservoir and a zero-temperature cold reservoir. The interactions between the qubit and the reservoirs are described in terms of a collision model of open system dynamics. The qubit interacts with the nonequilibrium reservoir (a large ensemble of qudits all prepared in the same pure state) via random unitary collisions and with the cold reservoir (a large ensemble of qubits in their ground state) via a partial swap. Due to the random nature of the interaction with the hot reservoir, fluctuations in ergotropy, heat, and work are present, shrinking with the size of the qudits in the hot reservoir. While the mean, "macroscopic" efficiency of the Otto engine is the same as in the case in which the hot reservoir is a thermal one, the distribution of efficiencies does not support finite moments, so that the mean of efficiencies does not coincide with the macroscopic efficiency.

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Thermodynamic uncertainty relation in degenerate and nondegenerate maser heat engines

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In this work, we investigate the thermodynamic uncertainty relation, which represents a trade-off between entropy production rate and relative power fluctuations, for non-degenerate three-level and degenerate four-level maser heat engines. For the non-degenerate case, we study two slightly different configurations of three-level maser engine and compare degree of violation of thermodynamic uncertainty relation in both models. We highlight that in the high temperature regime, conventional thermodynamic uncertainty relation is always violated in three-level maser heat engine. We also show that the thermodynamic uncertainty relation remains invariant when we scale the matter-field coupling constant and system-bath coupling constants by the same factor. Further, for the degenerate four-level engine, we study the effects of noise-induced coherence on the thermodynamic uncertainty relation. We show that depending on the parametric regime of operation, the phenomenon of noise-induced coherence can either enhance or suppress the relative power fluctuations.

Entropy, entropic temperature, second and third laws for far-from-equilibrium 1D system with heat flux

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We use the Shannon (information) entropy to define an “entropic” nonequilibrium temperature from the generalized Gibbs relation [1-4]. The extended nonequilibrium variables, namely, entropy, entropic temperature, thermal conductivity, and heat capacity demonstrate a third-law-like behavior at high deviation from equilibrium when the heat flux tends to its maximum value, even at nonzero value of the kinetic temperature. Moreover, the entropic temperature controls the energy exchange with surroundings, which guaranties validity of the second law of thermodynamics in a sense that heat flow direction is from the hotter to the colder region. The difference between the entropic temperature and the kinetic one is proportional to the non-thermalized fraction of the local energy density due to the ordered motion of energy carriers which can be converted into work. However, the gradient of the kinetic controls the value and direction of the heat flux inside the system, which nondimensional value plays a role of an order parameter – it varies from zero in the completely disordered equilibrium state to unity in the completely ordered nonequilibrium state. We demonstrate that there are some analogies between the behavior of the nonequilibrium systems in the maximum heat flux limit and equilibrium quantum system in the low temperature limit, which arise due to the breakdown of the equipartition in both cases [3].

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Single-atom energy-conversion device with a quantum load

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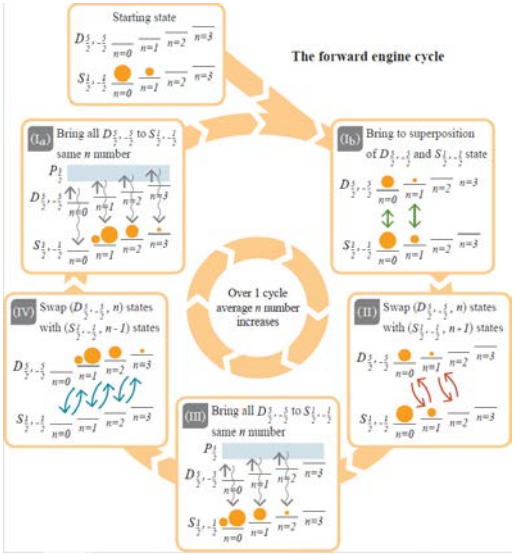
We study a single atom energy-conversion device coupled to a quantum load. The "working fluid" consists of the two optical levels of an ion, while the load is one of its vibrational modes, cooled down to the quantum regime. The protocol implemented presents two distinctive features: (i) the presence of a strong generic coupling interaction between the engine and load which can induce correlations between them; (ii) setting to a superposition state in each cycle. We examine the ergotropy of the load, which indicates the maximum amount of energy of the load extractable using solely unitary operations. We show that ergotropy rises with the number of engine cycles despite an increase in the information entropy of the load. Thus, the protocol used leads to a shift in the phonon distribution away from a thermal-type distribution. The increase of ergotropy of the load points to the possibility of using the phonon distribution of a single atom as a form of quantum battery.



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Enhanced Shortcuts to Adiabaticity

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Shortcuts to Adiabaticity (STA) are a collection of quantum control techniques that allow perfect state transfer for certain quantum systems. They have been successfully applied both theoretically and experimentally to a wide variety of quantum control tasks, for a review see [1]. In this work we develop and apply a new analytic extension to existing Shortcuts to Adiabaticity (STA) techniques, called enhanced Shortcuts to Adiabaticity (eSTA) [2]. This method extends STA methods to systems where STA cannot be applied directly, by creating an analytic correction to existing STA schemes. This correction can be easily calculated and the resulting protocols may even be outside the original class of STA schemes. We have shown that eSTA can improve fidelity and robustness simultaneously [3], and we have demonstrated the effectiveness of eSTA using several examples: population transfer in two-level systems beyond the rotating wave approximation, robustness of optical lattice transport, anharmonic trap expansion and two (Coulomb interacting) ion transport in non-harmonic traps [2-4]. There have already been furhter applications of eSTA to atom transport in optical conveyor belts and double-well lattices [5, 6].

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Thermodynamic characterization of the stored work and charging power in quantum batteries: An open quantum system analysis

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The study of the thermodynamic behavior of quantum systems in the context of quantum thermodynamics requires the derivation of a consistent formulation for the desired thermodynamic quantities from acknowledged quantum principles. Heisenberg's uncertainty relation as an intrinsic time-scale of state transportation, also known as quantum speed limit, has been broadly exploited to characterize quantum dynamics. Considering this notion and from a geometric viewpoint, fundamental constraints to minimize the charging time and maximize the associated power of a quantum battery set can be investigated. Also, concerning the fragile nature of all quantum systems, it sounds plausible that the batteries may interact with the surrounding environment, leading to the dissipation of the stored energy. Motivated by the considerations, we investigate the charging process of quantum batteries in the framework of open system analysis. Due to the fact that every system out of equilibrium in contact with a thermal bath contains an amount of free energy that can do work, an *activity operator*, which quantifies how far the state of the system distances from equilibrium, is defined. A tight upper bound on charging power is proposed in terms of quantum Fisher information and the variance of the activity operator. The former describes the speed of evolution, and the latter may be interpreted as a generalized thermodynamic force. The thermodynamic interpretation of the upper bound is discussed in detail. By applying the notion of the extended quantum Fisher information, the speed of evolution is divided into the classical and quantum parts, based on more physically meaningful contributions. Moreover, the tightness of the proposed bound, and the role of dissipation effects and the backflow of information on both the stored work and the charging power of the battery are investigated in two examples.

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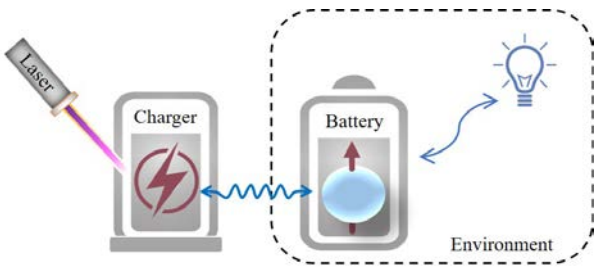

Figure 1. Schematic diagrams of an open quantum battery.