THIRD WORKSHOP ON STOCHASTIC THERMODYNAMICS (WOST III)

VIRTUAL CONFERENCE PROCEEDINGS

Tutorials: May 26, 2022

Poster session: May 27, 2022

Main conference: May 30 – June 3, 2022

(7 am – 12 pm, Mountain Daylight Time)

Meeting Description

Stochastic thermodynamics has revolutionized our understanding of far-from-equilibrium statistical physics over the last few decades and continues to result in profound, powerful results, ranging from fluctuation theorems to speed-limit theorems to thermodynamic uncertainty relations. With this new series of online workshops, we aim to provide a platform to everyone with an interest in stochastic thermodynamics to present and discuss their current research. We especially welcome junior researchers to submit their work for 10min lightning talks.

Scope

The workshop's primary aim is to have a wide-ranging cross-section of the stochastic thermodynamics community present their current research in one forum. The main topics of the workshop include applications of stochastic thermodynamics to:

- Fundamental Principles
- Physics and Chemistry
- Biophysics and Active Matter
- Quantum Stochastic Thermodynamics
- Computation and Information Processing

Mission

The mission of the WOST workshops is to:
To promote the field of stochastic thermodynamics to a broad range of scientists.
To foster collaboration on stochastic thermodynamics research among communities.
To encourage early-career researchers in the dissemination of their results.
To support academics from under-represented groups working in the field of stochastic thermodynamics or related fields.

Previous Workshops

WOST I was organized by the Complexity Science Hub Vienna. The talks can be found at: https://www.csh.ac.at/event/csh-workshop-stochastic-thermodynamics-complex-systems/.

WOST II was organized by the Santa Fe Institute. The talks can be found at: https://santafe.edu/pages/stochastic-thermodynamics-ii-videos?uid=MzY3&pw=OeW2BfMlCx.

WOST III Organizing committee

Velimir Ilic	*Mathematical Institute of the Serbian Academy of Sciences and Arts*
Christopher Jarzynski	*University of Maryland*
Gülce Kardeş	*University of Leipzig*
Jan Korbel	*Medical University of Vienna*
Tom Ouldridge	*Imperial College London*
Jenny Poulton	*Imperial College London*
Saar Rahav	*Technion - Israel Institute of Technology*
Takahiro Sagawa	*University of Tokyo*
Udo Seifert	*University of Stuttgart*
Henrik Wilming	*Leibniz University Hannover*
David Wolpert	*Santa Fe Institute*
Cigdem Yalcin	*Istanbul University*

IMPORTANT INFORMATION

Zoom

The whole conference will be available through video conferencing software Zoom except for the poster session. The zoom link and the password will be sent to all registered participants.

Talks

There are several types of talks:

- Tutorials (26th May): 1hr introductory talks, accessible to non-experts and students.
- Colloquium talks: 30 min talks describing the current state of art of stochastic thermodynamics research in a range of domains.
- Invited talks: 20 min talks addressing a particular topic in stochastic thermodynamics.
- Lightning talks: 10 min talks mainly by junior researchers, chosen from applications, ranging across all aspects of stochastic thermodynamics.

Note that no questions will be allowed during a talk (Everyone except the speaker will be muted). Instead, all talks will be followed by a short Q&A period.

Poster session (27th May)

Poster session will be available through Microsoft Teams. We will send the invitation email.

Q&A

Participants may ask questions during the Q&A period after each talk. Participants can raise their virtual hand during the talk to indicate that they would like to ask the speaker a question. The session chair will unmute the questioner and they pose the question to the speaker.
Note that after each talk, the first round of questions is dedicated to students.

Recording

All talks will be recorded, and the videos will be published on the workshop YouTube channel.

Discussion

There is one discussion session each day. Discussion sessions will be moderated by the session chair. If you want to contribute to the discussion, please raise your virtual hand to get the attention of the chair. Discussions will not be recorded.

Website

The workshop website is:
http://noneq.c.u-tokyo.ac.jp/Stochastic_Thermodynamics_III/
We will upload all the relevant information there.

Contact information

You can contact the workshop organizers at the following addresses:
stochastic.thermodynamics.iii@gmail.com

Tutorial Speakers:

Thermodynamic uncertainty relations
Andreas Dechant: *Kyoto University*

Thermodynamics of systems with strong coupling
Christopher Jarzynski: *University of Maryland*

Introduction to information geometry
Masafumi Oizumi: *University of Tokyo*

Introduction to stochastic thermodynamics
Simone Pigolotti: *Okinawa Institute of Science and Technology Graduate University*

Invited Speakers:

[Fundamental Principles]

Jordan Horowitz	*University of Michigan*
Sarah Loos	*International Centre for Theoretical Physics (ICTP)*
Patrick Pietzonka	*Max Planck Institute*
Keiji Saito	*Keio University*
Masahito Ueda*	*University of Tokyo*

[Physics and Chemistry]

Gili Bisker	*Tel Aviv University*
Massimiliano Esposito*	*University of Luxembourg*
Nahuel Freitas	*University of Luxembourg*
Jason Green	*University of Massachusetts Boston*

[Biophysics and Active Matter]

Rosalba Garcia Millan	*University of Cambridge*
Thomas Ouldridge	*Imperial College London*
Grant M. Rotskoff	*Stanford University*
Udo Seifert*	*University of Sttutgart*
Yuhai Tu	*IBM*

[Quantum Stochastic Thermodynamics]

Kay Brandner	*University of Nottingham*
Nelly Ng	*Nanyang Technological University*
Juan Parrondo	*Universidad Complutense de Madrid*
Martí Perarnau-Llobet	*University of Geneva*
Takahiro Sagawa*	*University of Tokyo*

*, Colloquium

[Computation and Information Processing]

Jean-Charles Delvenne	*Université catholique de Louvain*
Artemy Kolchinsky	*Santa Fe Institute*
David Limmer	*University of California, Berkeley*
Naoto Shiraishi	*University of Tokyo*
David Wolpert*	*Santa Fe Institute*

*, Colloquium

Lightning Talk Speakers:

Steven Blaber	*Simon Fraser University*
Lorenzo Buffoni	*University of Lisbon*
Sara Dal Cengio	*Liphy-Université Grenoble Alpes*
Cillian Cockrell	*Queen Mary University of London*
Salambô DaGo	*Laboratoire de Physique de l'ENS de LYON*
Aleksander Lasek	*University of Maryland*
Matthew Leighton	*Simon Fraser University*
Christopher Lynn	*Princeton University*
Naruo Ohga	*University of Tokyo*
Riccardo Rao	*Institute for Advanced Study, Princeton*
Paul Riechers	*Nanyang Technological University*
Sungguen Ryu	*Instituto de Física Interdisciplinary Sistemas Complejo*s
Hiroyasu Tajima	*University of Electro-Communications*
Gennaro Tucci	*SISSA*
Kohei Yoshimura	*University of Tokyo*

Poster session:

Miguel Aguilera	*University of Sussex*
Nicholas Anto-Sztrikacs	*University of Toronto*
Aubin Archambault	*ENS de Lyon*
Debankur Bhattacharyya	*University of Maryland*
Avishek Das	*University of California Berkeley*
Mauricio del Razo	*Freie Universität Berlin*
Guilherme de Sousa	*University of Maryland*
Cai Dieball	*Max Planck Institute*
Joshua Eglinton	*University of Nottingham*
Paolo Andrea Erdman	*Freie Universität Berlin*
Adam Frim	*UC Berkeley*
Matthew Gerry	*University of Toronto*
Ashwin Gopal	*University of Luxembourg*
Pedro Harunari	*University of São Paulo*
Kenza Hammam	*Queen's University Belfast*
Hisao Hayakawa	*Kyoto Univeristy*
Ruo Cheng Huang	*Nanyang Technological University*
Felix Hubmann	*IQOQI Vienna*
Miku Ishizaki	*University of Tokyo*
Jordan Juritz	*Imperial College London*
Gülce Kardeş	*University of Leipzig*
Michael Kewming	*Trinity College Dublin*
Anthony Kiely	*University College Dublin*
Daiki Kiyooka	*University of Tokyo*
Nazul Jared López-Alamilla	*University of Otago*
Shayan Majidy	*University of Waterloo*
Sreekanth K Manikandan	*NORDITA*
Atul Tanaji Mohite	*University of Luxembourg*
Anthony Munson	*University of Maryland*
Kazuki Nakamura	*University of Tokyo*
Asawari Pagare	*UNC Chapel Hill*
Andrea Plati	*Sapienza University*
Kacper Prech	*University of Basel*
Onur Pusuluk	*Koç University*
Benjamin Qureshi	*Imperial College London*
Jesús Rubio	*University of Exeter*
Daiki Sekizawa	*University of Tokyo*

Andrea Solfanelli	*SISSA Trieste*
Jeongrak Son	*Nanyang Technological University*
Shesha Gopal Marehalli Srinivas	*University of Luxembourg*
Philip Taranto	*TU Vienna*
Zhongmin Zhang	*UNC Chapel Hill*

Program

Workshop on stochastic thermodynamics III

Note: all times in Mountain Daylight Time (UTC -6h)

Thursday 26th May 2022

Tutorial

Chair: Sagawa / Parrondo

7:00 AM - 7:10 AM			*Opening Remarks*
7:10 AM - 8:30 AM	**Tutorial**	**Simone Pigolotti**	*Introduction to stochastic thermodynamics*
8:40 AM - 10:00 AM	**Tutorial**	**Masafumi Oizumi**	*Introduction to information geometry*
10:10 AM - 11:30 AM	**Tutorial**	**Andreas Dechant**	*Thermodynamic uncertainty relations*
11:40 AM - 1:00 PM	**Tutorial**	**Christopher Jarzynski**	*Thermodynamics of systems with strong coupling*

Friday 27th May 2022
Poster session

1. Fundamental Principles
Cai Dieball, Matthew Gerry, Pedro Harunari, Anthony Kiely, Sreekanth K Manikandan, Atul Tanaji Mohite, Andrea Plati

2. Physics and Chemistry
Aubin Archambault, Miguel Aguilera, Avishek Das, Mauricio del Razo, Adam Frim, Jordan Juritz, Kazuki Nakamura, Benjamin Qureshi, Jesús Rubio, Shesha Gopal Marehalli Srinivas

3. Biophysics & Active Matter
Nazul Jared Lopez-Alamilla, Daiki Sekizawa

4. Quantum Stochastic Thermodynamics
Nicholas Anto-Sztrikacs, Joshua Eglinton, Paolo Andrea Erdman, Guilherme de Sousa, Kenza Hammam, Hisao Hayakawa, Ruo Cheng Huang, Felix Hubmann, Miku Ishizaki, Michael Kewming, Shayan Majidy, Anthony Munson, Kacper Prech, Onur Pusuluk, Andrea Solfanelli, Jeongrak Son, Philip Taranto

5. Computation & Information Processing
Debankur Bhattacharyya, Ashwin Gopal, Gülce Kardeş, Daiki Kiyooka, Asawari Pagare, Zhongmin Zhang

Monday 30th May 2022

Fundamental Principles

Chair: Esposito / Green

7:00 AM - 7:45 AM	**Colloquium**	**Masahito Ueda**	*Universal Thermodynamic Uncertainty Relation in Non-Equilibrium Dynamics*
7:45 AM - 8:15 AM	**invited**	**Keiji Saito**	*Coherence and thermodynamic cost in Landauer erasure*
8:15 AM -8:45 AM	**invited**	**Sarah Loos**	*The role of non-conservative interactions in nonequilibrium systems*
8:45 AM - 9:30 AM	**Discussion**		*Discussion session*
9:45 AM - 10:00 AM	**Lightning**	**Naruo Ohga**	*Legendre duality in stochastic thermodynamics: A construction based on information geometry*
10:00 AM - 10:15 AM	**Lightning**	**Cillian Cockrell**	*Stochastic Thermodynamics of a non-Markovian Dynamical System*
10:15 AM - 10:30 AM	**Lightning**	**Riccardo Rao**	*Evolutionary Dynamics: a Stochastic Thermodynamics perspective*
10:30 AM -11:00 AM	**invited**	**Patrick Pietzonka**	*Classical Pendulum Clocks Break the Thermodynamic Uncertainty Relation*
11:00 AM -11:30 AM	**invited**	**Jordan Horowitz**	*Thermodynamic limits to nonequilibrium response*

Tuesday 31st May 2022

Physics and Chemistry

Chair: Kolchinsky / Millan

7:00 AM - 7:45 AM	**Colloquium**	**Massimiliano Esposito**	*Nonequilibrium Thermodynamics of Complex Systems*
7:45 AM - 8:15 AM	**invited**	**Gili Bisker**	*Inferring entropy production in nonequilibrium systems from partially observed statistics*
8:15 AM - 8:45 AM	**invited**	**Jose Nahuel Freitas**	*An electronic Maxwell demon that can work at macroscopic scales*
8:45 AM - 9:30 AM	**Discussion**		*Discussion session*
9:45 AM - 10:00 AM	**Lightning**	**Kohei Yoshimura**	*Fluctuation and thermodynamic trade-off relations in deterministic chemical reaction networks*
10:00 AM - 10:15 AM	**Lightning**	**Sara Dal Cengio**	*Schnakenberg without Schnakenberg*
10:15 AM - 10:30 AM	**Lightning**	**Steven Blaber**	*Steps minimize dissipation in rapidly driven stochastic systems*
10:30 AM -11:00 AM	**invited**	**Jason Green**	*Speed limits on thermodynamic costs and benefits*
11:00 AM -11:30 AM	**invited**	**Grant M. Rotskoff**	*Energetic costs of nonequilibrium control in active self-assembly*

Wednesday 1st June 2022

Biophysics and Active Matter

Chair: Shiraishi / Loos

7:00 AM - 7:45 AM	**Colloquium**	**Udo Seifert**	*Thermodynamic inference: Principles and applications*
7:45 AM - 8:15 AM	**invited**	**Rosalba Garcia Millan**	*Entropy Production of Non-reciprocal Interactions*
8:15 AM - 8:45 AM	**invited**	**Thomas Ouldridge**	*Avoiding equilibrium in a minimal molecular information-processing system*
8:45 AM - 9:30 AM	**Discussion**		*Discussion session*
9:45 AM - 10:00 AM	**Lightning**	**Matthew Leighton**	*Dynamic and thermodynamic bounds for collective motor-driven transport*
10:00 AM - 10:15 AM	**Lightning**	**Christopher Lynn**	*Decomposing the local arrow of time in interacting systems*
10:15 AM - 10:30 AM	**Lightning**	**Gennaro Tucci**	*Modelling the active oscillations of the hair bundle of the bullfrog*
10:30 AM - 11:00 AM	**invited**	**Yuhai Tu**	*Nonequilibirum Thermodynamics of Coupled Molecular Clocks: The Energy Cost of Synchronization*

Thursday 2nd June 2022

Quantum Stochastic Thermodynamics

Chair: Saito / Freitas

7:00 AM - 7:45 AM	**Colloquium**	**Takahiro Sagawa**	*Three Approaches to Quantum Thermodynamics*
7:45 AM - 8:15 AM	**invited**	**Kay Brandner**	*Thermodynamic Uncertainty Relations for Coherent Transport*
8:15 AM -8:45 AM	**invited**	**Nelly Ng**	*Quantum field thermal machines*
8:45 AM - 9:30 AM	**Discussion**		*Discussion session*

9:45 AM - 10:00 AM	**Lightning**	**Hiroyasu Tajima**	*Superconducting-like heat current: Effective cancellation of current-dissipation trade off by quantum coherence*
10:00 AM - 10:15 AM	**Lightning**	**Sungguen Ryu**	*Beating Carnot efficiency with periodically driven chiral conductors*
10:15 AM - 10:30 AM	**Lightning**	**Aleksander Lasek**	*Experimental observation of thermalisation with noncommuting charges*
10:30 AM - 11:00 AM	**invited**	**Juan Parrondo**	*Scattering and thermalization: wave-particle duality hits quantum thermodynamics*
11:00 AM - 11:30 AM	**invited**	**Martí Perarnau-Llobet**	*Finite-time bounds on the probabilistic violation of the second law of thermodynamics*

Friday 3rd June 2022

Computation and Information Processing

Chair: Ng / Horowitz

7:00 AM - 7:45 AM	**Colloquium**	**David Wolpert**	*STOCHASTIC THERMODYNAMICS OF DISTRIBUTED SYSTEMS*
7:45 AM - 8:15 AM	**invited**	**Artemy Kolchinsky**	*The algorithmic cost of a classical or quantum single-shot computation*
8:15 AM - 8:45 AM	**invited**	**Naoto Shiraishi**	*Undecidability in quantum thermalization*
8:45 AM - 9:30 AM	**Discussion**		*Discussion session*
9:45 AM - 10:00 AM	**Lightning**	**Lorenzo Buffoni**	*Spontaneous fluctuation-symmetry breaking and the Landauer principle*
10:00 AM - 10:15 AM	**Lightning**	**Salambô DaGo**	*When it comes to information processing, fast is hot, and hot is expensive*
10:15 AM - 10:30 AM	**Lightning**	**Paul Riechers**	*Two paradigms for energetically efficient computing*
10:30 AM - 11:00 AM	**invited**	**David Limmer**	TBA
11:00 AM - 11:30 AM	**invited**	**Jean-Charles Delvenne**	*Thermo-Kinetic Relations for elementary computing devices*

ABSTRACTS

Thursday 26th May - Tutorials

Tutorial 1 - Simone Pigolotti

Title: Introduction to stochastic thermodynamics

Abstract: Stochastic thermodynamics has emerged as a theory for the non-equilibrium behavior of mesoscopic systems. Its predictions, most notably fluctuation theorems, have been confirmed in experiments and led to interesting applications. In this tutorial, based on our recent book [1], we will introduce the basic ideas of stochastic thermodynamics. We will use as example what is arguably the simplest possible setting: an overdamped non-equilibrium system, described by a master equation, and in contact with a single heat reservoir. The tutorial will encompass two parts. In the first part, we will use physical considerations to define thermodynamic quantities such as heat, work, and entropy production at the level of individual trajectories. In the second part, we will connect entropy production with statistical irreversibility of trajectories. This connection will permit us to directly derive fluctuation theorems, including the Jarzynski and the Crooks equalities. We will conclude by discussing the relevance of these results.

[1] L. Peliti, S. Pigolotti, “Stochastic Thermodynamics. An introduction”. Princeton University Press, 2021.

Tutorial 2 - Masafumi Oizumi

Title: Introduction to Information geometry

Abstract: Information geometry is a method to reveal the geometric structure of the manifold of probability distributions. Information geometry, emerging from the studies of statistical inference, has now been broadly used in diverse fields such as machine learning, signal processing, neuroscience, and physics. Recently, information geometry has also been actively used in stochastic thermodynamics, revealing a fundamental link between thermodynamic quantities and information geometric quantities.

In this tutorial, we will introduce the essential concepts of information geometry for those interested in potential applications to stochastic thermodynamics but who do not have any prior knowledge of information geometry. Thus, we will cover only the basics of information geometry. Specifically, we will focus on the exponential family of probability distributions and its geometric structure. In the exponential family, we can introduce a convex function, which corresponds to free energy, and derive a Bregman divergence from the convex function, corresponding to well-known Kullback-Leibler divergence. Then, from the Bregman divergence, we can induce a dually flat Riemannian structure on the manifold of the exponential family. After introducing the basics, we will review several example applications of information geometry to stochastic thermodynamics.

Tutorial 3 - Andreas Dechant

Title: Deriving, Interpreting, and Generalizing the Thermodynamic Uncertainty Relation

Abstract: The thermodynamic uncertainty relation (TUR) is one of the hallmark results of stochastic thermodynamics in recent years and has inspired a huge amount of follow-up research. The TUR relates the averages and fluctuations of stochastic currents to entropy production, resulting in a quantitative version of the second law of thermodynamics for certain types of dynamics.

In this tutorial, we will work our way through a hands-on derivation of the TUR for overdamped Brownian motion. The derivation is based on an information-theoretical result called the Cramer-Rao inequality, which will help us understand how this remarkable relation is related to special symmetries in the dynamics. We will also discuss interpretations of the TUR from the viewpoints of thermodynamics and estimation theory, and how it can be used to estimate entropy production from experimentally accessible quantities. Finally, we will learn about a few generalizations of the TUR and how they differ from the original relation.

Tutorial 4 - Christopher Jarzynski

Title: Thermodynamics of systems with strong coupling

Abstract: Ordinarily, we use the canonical ensemble to represent a system that is in equilibrium with its thermal surroundings. Although familiar macroscopic relations between internal energy, entropy, free energy, heat and work are easily derived from the canonical ensemble, this ensemble does not accurately describe a nanoscale system that is strongly coupled to its surroundings, such as a biomolecule in aqueous solution. I will discuss a modified thermodynamic framework that describes a classical system of arbitrary size that is strongly coupled to its thermal environment. Within this framework, I will show how key thermodynamic quantities are defined microscopically and are shown to obey thermodynamic relations including both the first and second law, as well as nonequilibrium fluctuation theorems. These quantities scale up to their macroscopic values when the system of interest is large. Thus a unifying framework is developed, which encompasses nanoscale, stochastic thermodynamics at one end, and traditional macroscopic thermodynamics at the other. A central element in this approach is a thermodynamic definition of the volume of the system of interest, which converges to the usual geometric definition when the system is large. I will also discuss alternative approaches to this problem.

Monday 30th May - Fundamental Principles

Colloquium - Masahito Ueda

Title: Universal Thermodynamic Uncertainty Relation in Non-Equilibrium Dynamics

Abstract: The conventional thermodynamic uncertainty relations (TURs) suffer two main 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 often only apply to time-antisymmetric observables, which are often thermodynamic observables in nature. 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.

Invited 1 - Keiji Saito

Title: Coherence and thermodynamic cost in Landauer erasure

Abstract: The Landauer principle states that any logically irreversible information processing must be accompanied by dissipation into the environment. In this study, we investigate the heat dissipation associated with finite-time information erasure and the effect of quantum coherence in such processes. By considering a scenario wherein information is encoded in an open quantum system whose dynamics are described by the Markovian Lindblad equation, we show that the dissipated heat is lower-bounded by the conventional Landauer cost, as well as a correction term inversely proportional to the operational time. To clarify the relation between quantum coherence and dissipation, we derive a lower bound for heat dissipation in terms of quantum coherence. This bound quantitatively implies that the creation of quantum coherence in the energy eigenbasis during the erasure process inevitably leads to additional heat costs.

Invited 2 - Sarah Loos

Title: The role of non-conservative interactions in nonequilibrium systems

Abstract: The world that surrounds us, including all living and various artificial systems, mostly operates far from thermal equilibrium. Intensive work is being done in the field of stochastic thermodynamics to unravel the fundamental principles that govern the individual and collective dynamics of nonequilibrium systems. However, there is an important mechanism that has so far received little attention, although it is ubiquitous in biology, chemistry, engineering, and learning, namely the presence of non-conservative interactions, such as time-delayed [1,2] or non-reciprocal [3,4] interactions. Indeed, non-conservative interactions already appear in various models used in the field of stochastic thermodynamics, but their general significance and thermodynamic implications have not been considered from a fundamental perspective. In this talk, I will discuss at a general level the thermodynamic implications of non-conservative interactions using simple stochastic models consisting of few variables. I will also provide a perspective on how non-conservative interactions affect the phase behaviour of large collectives described by many-body models or stochastic field models.

[1] Loos and Klapp, Sci. Rep. 9, 2491 (2019)
[2] Holubec, Geiss, Loos, Kroy, and Cichos, PRL 127, 258001 (2021)
[3] Loos and Klapp, NJP 22, 123051 (2020)
[4] Loos, Hermann, and Klapp, Entropy 23, 696 (2021)

Lightning talk 1 - Naruo Ohga

Title: Legendre duality in stochastic thermodynamics: A construction based on information geometry

Abstract: Despite the usefulness of Legendre transformations in classical equilibrium thermodynamics, its application in stochastic thermodynamics has been limited. Examples of the applications are the definition of nonequilibrium free energy [1] and the transform of large deviation functions [2]. However, these transformations mainly deal with the average values of thermodynamic quantities; they do not treat probability distributions themselves to provide a new theoretical tool for stochastic descriptions.

In this talk, we construct a new Legendre duality of probability distributions for stochastic thermodynamics [3]. For this purpose, we imitate the construction of Legendre duality in information geometry[4]. We perform a Legendre transformation of the total thermodynamic entropy with respect to the probability distributions as coordinates, resulting in a new thermodynamic potential and a new coordinate system. We discuss the following properties: (i) The new coordinate system specifies probability distributions by the thermodynamic forces. (ii) The new potential is equal to the equilibrium free energy of the system with a certain external field applied. The external field is a linear combination of the new coordinates. This interpretation provides a new link between stochastic thermodynamics and equilibrium statistical mechanics. (iii) The new potential monotonically decreases in time, providing a new constraint on time evolution. (iv) Our Legendre duality serves as dual affine coordinates in information geometry, enhancing the connection between stochastic thermodynamics and information geometry. We demonstrate these properties with specific models. If time allows, we also discuss a chemical-thermodynamic counterpart of our results [5].

[1] M. Esposito and C. Van den Broeck, EPL 95, 40004 (2011).
[2] H. Touchette, Phys. Rep. 478, 1 (2009).
[3] N. Ohga and S. Ito, arXiv:2112.11008 (2021).
[4] S.-i. Amari, Information geometry and its applications (Springer, 2016).
[5] N. Ohga and S. Ito, arXiv:2112.13813 (2021).

Lightning talk 2 - Cillian Cockrell

Title: Stochastic Thermodynamics of a non-Markovian Dynamical System

Abstract: The developing field of stochastic thermodynamics extends concepts of macroscopic thermodynamics such as entropy production and work to the microscopic level of individual trajectories taken by a system through phase space, providing a powerful extension of classical thermodynamics to small systems. The scheme involves coupling the system to an environment - typically a source of Markovian noise that affects the dynamics of the system. Markovian noise possesses the qualities we expect from a bath in classical thermodynamics, i.e., it is characterised by one or more static parameters (temperature etc.) and does not change its behaviour due to correlations with the system. These qualities, however, do not apply to an environment which is of comparable size to the system, is strongly coupled to the system, or does not possess a negligible relaxation time compared to the characteristic timescale(s) of the system. In this work we extend the framework of stochastic thermodynamics to consider a non-Markovian environment - one whose dynamics have memory, and which create additional correlations with the system variables. We do this in a analytically and computationally straightforward way via the introduction of an auxiliary system (or reaction coordinate) which is dynamically coupled to a Markovian bath and to the system at interest (which itself is not coupled to the bath). We discuss the statistical mechanics of this technique and how can associate a “Markovian equivalent” to non-Markovian systems using it. We then examine the thermodynamics of such a non-Markovian environment, the auxiliary system plus bath, using a selection of simple examples. Such an environment produces a rich variety of behaviour and interactions with external protocols. In particular, for a case of thermal relaxation, the distributions of entropy produced under the non-Markovian dynamics differ from the equivalent case of Markovian dynamics only by a delay time. When a time-dependent external work protocol is turned on, the system's correlations with the environment can either speed up or slow down its approach to equilibrium and affect its production of entropy, depending on the coupling strength between the system and environment. This is because a non-Markovian environment gives the process of equilibration a characteristic timescale, thereby allowing for an irreversible thermodynamic resonance, an analogue to purely mechanical resonance arising from interacting mechanical timescales.

Links to associated work: https://doi.org/10.48550/arXiv.2202.06912

Lightning talk 3 - Riccardo Rao

Title: Evolutionary Dynamics: a Stochastic Thermodynamics perspective

Abstract: A conventional view of evolutionary dynamics is based on three essential elements: (i) organism reproduction with imperfect heredity; (ii) variations, including mutations, which are typically introduced by the reproduction process; (iii) selection, which acts within a population and allows some variant species to survive and reproduce while eliminating others. These elements shape the “evolutionary forces” that characterize the evolutionary dynamics. In this presentation, we introduce a general model of reproduction–variation–selection dynamics. By treating these dynamics as stochastic thermodynamic processes, we make precise the notion of the forces that characterize evolution. One of these forces, in particular, can make organism reproduction insensitive (robust) to variations. We finally show how some of the detailed predictions of our model are compatible with laboratory experiments of viral evolution.

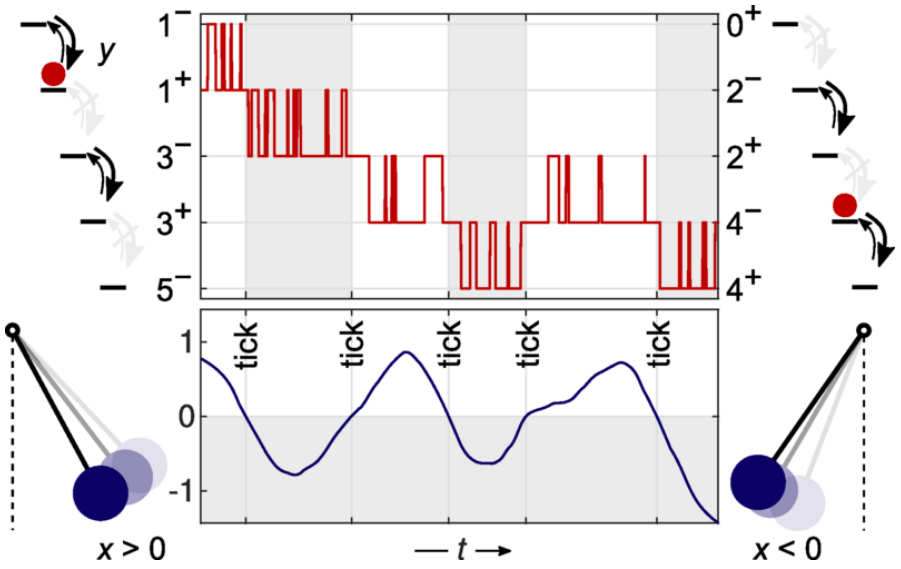
[R. Rao and S. Leibler, “Evolutionary Dynamics, Evolutionary Forces, and Robustness: A Nonequilibrium Statistical Mechanics Perspective”,
bioRxiv (accepted in Proc. Natl. Acad. Sci. U.S.A.) (2021), 2021.10.10.463854]

Invited 3 - Patrick Pietzonka

Title: Classical Pendulum Clocks Break the Thermodynamic Uncertainty Relation

Abstract: The thermodynamic uncertainty relation expresses a seemingly universal trade-off between the cost for driving an autonomous system and precision in any output observable. It has so far been proven for discrete systems and for overdamped Brownian motion. Its validity for the more general class of underdamped Brownian motion, where inertia is relevant, was conjectured based on numerical evidence. We now disprove this conjecture by constructing a counterexample. Its design is inspired by a classical pendulum clock, which uses an escapement to couple the motion of an oscillator to another degree of freedom (a “hand”) driven by an external force. Considering a thermodynamically consistent, discrete model for an escapement mechanism, we first show that the oscillations of an underdamped harmonic oscillator in thermal equilibrium are sufficient to break the thermodynamic uncertainty relation. We then show that this is also the case in simulations of a fully continuous underdamped system with a potential landscape that mimics an escaped pendulum.

Journal Ref.: PRL 128, 130606 (2022)



Invited 4 - Jordan Horowitz

Title: Thermodynamic limits to nonequilibrium response

Abstract: Near thermodynamic equilibrium, the fluctuation-dissipation theorem provides a robust theoretical and experimental tool to determine the nature of response via spontaneous equilibrium fluctuations. Generalizations of the fluctuation-dissipation theorem for arbitrary perturbations around nonequilibrium steady states have offered fundamental theoretical insight, but often include observables that require detailed system-specific knowledge of the system. Here, we suggest that an alternative fruitful method for characterizing nonequilibrium response is to study specific families of perturbations. For these families, we derive equalities and inequalities valid arbitrarily far from equilibrium that constrain the response of nonequilibrium steady states in terms of the strength of nonequilibrium driving. As an illustration, we show how our results rationalize the energetic cost of some common biochemical motifs.

Tuesday 31st May - Physics and Chemistry

Colloquium - Massimiliano Esposito

Title: Nonequilibrium Thermodynamics of Complex Systems

Abstract: 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 (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. Finally, I will briefly describe a novel type of finite-time dynamical phase transition in nonequilibrium relaxation [3].

[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).
[3] J. Meibohm and M. Esposito, Finite-time dynamical phase transition in non-equilibrium relaxation, Phys. Rev. Lett. 128, 110603 (2022).

Invited 1 - Gili Bisker

Title: Inferring entropy production in nonequilibrium systems from partially observed statistics

Abstract: Far-from-equilibrium processes constantly dissipate energy while converting a free-energy source to another form of energy. Living systems, for example, rely on an orchestra of molecular motors that consume chemical fuel to produce mechanical work. Drawing inspiration from biology, where the underlying nonequilibrium activity gives rise to a plethora of emergent collective phenomena, we strive to capture their mechanistic essence in order to mimic life-like behaviour in synthetic systems. Estimating the amount of the free energy budget lost to dissipation is crucial for a deeper understanding of the underlying nonequilibrium dynamics of driven systems, aiming for general design principles for biomimicking custom-made systems.

I will present a recently developed theoretical toolkit for estimating the dissipation from partial information, based on detecting time-irreversibility from asymmetry in waiting time distributions in observed 2nd-order semi-Markov processes. Using the framework of stochastic thermodynamics, bounds on the total entropy production are derived. The results of this work will advance new analytical and numerical approaches for quantifying nonequilibrium dynamics in stochastic systems, when only partial information is available.

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[2] I.A. Martínez, G. Bisker, J.M. Horowitz, J.M.R. Parrondo, Nature communications 2019, 10(1), 1-10
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Invited 2 - Nahuel Freitas

Title: An electronic Maxwell demon that can work at macroscopic scales

Abstract: Maxwell's demons work by rectifying thermal fluctuations. They are not expected to function at macroscopic scales where fluctuations become negligible and dynamics become deterministic. We will discuss an electronic implementation of an autonomous Maxwell's demon that indeed stops working in the regular macroscopic limit as the dynamics becomes deterministic. However, we find that if the power supplied to the demon is scaled up appropriately, the deterministic limit is avoided and the demon continues to work. The price to pay is a decreasing thermodynamic efficiency, which satisfies a simple scaling law. Our work suggests that novel strategies may be found in nonequilibrium settings to bring to the macroscale non-trivial effects so far only observed at microscopic scales.

Lightning talk 1 - Kohei Yoshimura

Title: Fluctuation and thermodynamic trade-off relations in deterministic chemical reaction networks

Abstract: Universal thermodynamic laws in nonequilibrium systems have long been explored since the equilibrium theory was established. Chemical reactions are one of the typical subjects in the research. In this century, stochastic thermodynamics, where thermally fluctuating systems are of interest, appeared as a nodal point of previous studies. Deterministic chemical reactions can be seen as the average of fluctuating reactions, so the techniques of stochastic thermodynamics are highly suggestive and helpful to understand their nonequilibrium thermodynamic properties. However, due to the nonlinearity represented by mass action law, the analogy between stochastic thermodynamics and chemical thermodynamics has not been understood completely yet.

We prove that thermodynamic trade-off relations—thermodynamic uncertainty relation (TUR) and thermodynamic speed limits—hold in deterministic chemical reaction networks (CRNs) under general settings. While the conventional TURs that hold in stochastic thermodynamics show a trade-off between dissipation and fluctuations evaluated by, e.g., the variance of a current, we formulate a new TUR for deterministic CRNs by using the diffusion coefficient that appears in the chemical Fokker–Planck equation. Although the measure of “fluctuation” derives from the stochastic equation, it can be represented by macroscopic reaction rates only. Moreover, we show a speed limit given by the entropy production and the diffusion coefficient. Because our results offer universal thermodynamic constraints to general chemical reaction networks, we believe that they would help evaluate various CRNs from a coherent point of view.

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[1] K. Yoshimura and S. Ito, Thermodynamic Uncertainty Relation and Thermodynamic Speed Limit in Deterministic Chemical Reaction Networks, Phys. Rev. Lett. 127, 160601 (2021)

Lightning talk 2 - Sara Dal Cengio

Title: Schnakenberg without Schnakenberg

Abstract: Schnakenberg's paper from 1976 [1] has been foundational to the field of network thermodynamics. Exploiting tools from graph theory and circuit analysis, it provides a geometrical framework to identify the fundamental thermodynamic observables in master-equation dynamics. More recently, an algebraic construction for deterministic mass-action kinetics was introduced to build the thermodynamics of chemical reaction networks (CRNs) [2]. In presence of interactions, the geometry of CRNs is encoded not by graphs but hypergraphs - making their understanding more difficult. Here we propose a unified framework which reconciles the algebraic and geometric representations of CNRs, allowing one to identify conservative and driving chemical forces. We apply the proposed tools to study the linear response of complex CRNs.

The work is conducted in collaboration with Vivien Lecomte (Université Grenoble Alpes) and Matteo Polettini (University of Luxembourg) and a paper is in preparation.

[1] J. Schnakenberg, Rev. Mod. Phys. 48, 571 (1976).
[2] M. Polettini and M. Esposito, The Journal of Chemical Physics 141, 024117 (2014)

Lightning talk 3 - Steven Blaber

Title: Steps Minimize Dissipation in Rapidly Driven Stochastic Systems

Abstract: Since its inception nearly 200 years ago, a central theme of thermodynamics has been the design of energetically efficient engines. In our modern world the engines grow ever smaller, down to the micro- and nano-scale of biological molecular machines, where stochastic fluctuations are large. To achieve fast operating speeds, these small-scale machines are driven by rapid changes in control parameters (control protocols). By focusing on the fast limit, we show that for any stochastic system driven sufficiently rapidly, the most energetically efficient driving always consists of jumps at the beginning and end of the protocol, spending the entire duration at the point which optimally balances the relaxation rate with jump size. Our results are of practical use in thermodynamic computing, single-molecule experiments, and free-energy estimation.

Article: https://doi.org/10.1103/PhysRevE.104.L022101

Invited 3 - Jason Green

Title: Speed limits on thermodynamic costs and benefits

Abstract: Biological molecular motors generate mechanical work by quickly adapting to the unsteady states of their environment, dissipating energy as heat in the process. In synthesizing our own molecular machines, the balance between speed and thermodynamic costs is fundamental to understanding this functionality. However, to fully optimize their efficiency, we also need to understand the limits on the speed of delivering mechanical work and how to maximize this thermodynamic benefit, despite inevitable dissipation. In this talk, I will describe some new thermodynamic speed limits for work. These speed limits set upper and lower bounds on the minimum time for an amount of work to be done on or by a system. They are expressed in terms of measurable quantities and a potential route to understanding the performance of dynamical functioning systems, regardless of whether they are living or synthetic.

https://arxiv.org/abs/2204.10368

Invited 4 - Grant M. Rotskoff

Title: Energetic costs of nonequilibrium control in active self-assembly

Abstract: Active biomaterials self-organize into complex and functional structures. The goal of emulating biology has stimulated many investigations into the properties that lead to robust assembly. Many of the works that focus on designing self-assembly have pursued a strategy of tuning the interaction among the various components to stabilize a given target structure. In this talk, I will discuss some work that approaches this problem from a distinct viewpoint, namely, through the lens of nonequilibrium control. I will discuss computational strategies for carrying out an optimization to control the steady state of interacting particle systems using only external fields. In addition, I will introduce a framework to quantify the dissipative costs of maintaining a nonequilibrium steady state that uses average, observable properties alone.

Wednesday 1st June - Biophysics and Active Matter

Colloquium - Udo Seifert

Title: Thermodynamic inference: Principles and applications

Abstract: Thermodynamic inference aims at revealing hidden properties of non-equilibrium systems by using universal results from stochastic thermodynamics. One key quantity of such systems is their entropy production, which is hard to get exactly without having full access to the system. Universal lower bounds can be derived by various types of coarse-graining and optimization approaches. A particularly promising tools is the thermodynamic uncertainty relation (TUR), which, inter alia, yields a model-free lower bound on the efficiency of molecular motors as I will show using experimental data for kinesin. For biochemical oscillations, I will present a conjecture for their universal minimal cost. I will also touch on inference beyond estimating entropy production such as inferring topological properties of biochemical networks. As a step towards developing tools that are applicable to interacting many-particle system, I will present analytical and numerical results for the TUR in driven diffusive multi-particle systems.

Invited 1 - Rosalba Garcia Millan

Title: Entropy Production of Non-reciprocal Interactions

Abstract: Non-reciprocal interactions are very common in natural systems. They can be used to explain the emergence of certain patterns such as bird flocking [1]. Generally, systems with non-reciprocal interactions are out of equilibrium, although they can obey detailed balance under certain conditions [2]. In this talk, I will present a particle model with non-reciprocal pair interactions between two species of drift-diffusive particles, say dogs and sheep. Following a path integral approach, I will discuss the stationary two-point correlation function and the entropy production. Even in the absence of drift, detailed balance is broken by non-reciprocity except for a particular choice of pair interactions.

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[2] S. Loos, S. Klapp, New J. Phys. 22(12), 123051 (2020).

Invited 2 - Thomas Ouldridge

Title: Avoiding equilibrium in a minimal molecular information-processing system

Abstract: The production of sequence-specific copolymers using copolymer templates is fundamental to biology. For example, all three processes in the central dogma of molecular biology fall under this description. Unlike the superficially similar process of self-assembly, however, the development of synthetic analogs of copolymer copying has been challenging. The main difficulty is that successfully-assembled copies are inherently far from equilibrium, due to their low entropy, and we have limited expertise in designing a chemical system to steer clear of the equilibrium ensemble and instead reach a highly specific non-equilibrium state. The practical manifestation of this challenge is the need to overcome product inhibition – or the tendency of products to adhere strongly to their templates – while still allowing for the accurate copying of long sequences. In this talk I first introduce a theoretical model of a minimal copying system that overcomes product inhibition, then discuss our progress in implementing a minimal non-equilibrium copying system in the laboratory.

Lightning talk 1 - Matthew Leighton

Title: Dynamic and thermodynamic bounds for collective motor-driven transport

Abstract: Molecular motors work collectively to transport cargo within cells, with anywhere from one to several hundred motors towing a single cargo. We study the stochastic thermodynamics of general collective-transport systems, using the observation that all components of such systems must “stay together” and Jensen’s inequality to derive a new lower bound on their rate of entropy production. This bound holds for a broad class of systems, is tighter than the second law, and is often tighter than the thermodynamic uncertainty relation (TUR). Our new entropy-production inequality, combined with the TUR, implies new bounds on the velocity, efficiency, and precision of general transport systems; constraining emergent properties of collective systems using only basic properties of individual subsystems. For identical motors we derive a set of analytic Pareto frontiers proving that many pairs of desirable properties, for example high velocity and high efficiency, cannot simultaneously be achieved by any kind of collective-transport system. Finally, numerical simulation of a specific model illustrates our derived bounds and shows conditions sufficient for saturation.

Arxiv Preprint: https://arxiv.org/abs/2202.13992

Lightning talk 2 - Christopher Lynn

Title: Decomposing the local arrow of time in interacting systems

Abstract: We show that the evidence for a local arrow of time, which is equivalent to the entropy production in thermodynamic systems, can be decomposed. In a system with many degrees of freedom, there is a term that arises from the irreversible dynamics of the individual variables, and then a series of non—negative terms contributed by correlations among pairs, triplets, and higher—order combinations of variables. We illustrate this decomposition on simple models of noisy logical computations, and then apply it to the analysis of patterns of neural activity in the retina as it responds to complex dynamic visual scenes. We find that neural activity breaks detailed balance even when the visual inputs do not, and that this irreversibility arises primarily from interactions between pairs of neurons.

Preprint: https://arxiv.org/abs/2112.14721v1

Lightning talk 3 - Gennaro Tucci

Title: Modelling the active oscillations of the hair bundle of the bullfrog

Abstract: Modelling noisy oscillatory Active Matter is one of the current challenges in physics and biology. Among these systems, we are interested in describing the spontaneous oscillations of the hair bundle of the inner ear cells of the bullfrog. The hair bundle is an organelle formed by a cohesive tuft of cylindrical stereocillia that protrude from the apical surface of the namesake hair cells. This receptor cells transduces a mechanical stimulus, such as a sound wave, into a neural signal and thus facilitates hearing and other sensory processes in vertebrates. The oscillatory motion of a hair bundle is powered by an active process, which is essential for the organelle's sensory function, and results in the violation of the fluctuation-dissipation theorem.

Because the microscopic mechanisms governing these type of processes are difficult to model, we propose an effective description based on a stochastic system displaying periodic oscillations. For this purpose, we consider the motion of a Brownian particle in the presence of a harmonic potential whose center switches stochastically between two distinct points. Accordingly, the dynamics of the particle consists of an alternate relaxation towards the two centers of the potential. The resulting oscillatory trajectories are governed by the probability distribution of the waiting time between two consecutive switches: this mechanism makes the evolution of the system non-Markovian. Thanks to the linearity of the model, we derive analytical predictions for its most relevant dynamical and thermodynamic properties for any choice of the waiting-time distribution.

This minimal model describes accurately bistable-like oscillatory motion of hair bundles in bullfrog sacculus. We check this by using the analytical expression of the power spectrum of the model to fit that of the oscillations of the tip of the bullfrog's hair bundle, measured experimentally by A. J. Hudspeth's laboratory (Rockefeller University, NY). In order to characterize the thermodynamic properties of these trajectories, we substitute the inferred parameters of the model into the exact expression of its average stationary power, enabling us to estimate the power required to sustain such active oscillations. In agreement with the active nature of the process and with previous estimates of the entropy production, we find that the predicted average dissipated power per cycle is compatible with the consumption of ~ 10ATP molecules to fuel a single oscillation.

Reference: G. Tucci, É. Roldán, A. Gambassi, R. Belousov, F. Berger, R. G. Alonso, and A. J. Hudspeth, *Modelling Active Non-Markovian Oscillators*, arXiv:2201.12171

Invited 3 - Yuhai Tu

Title: Nonequilibirum Thermodynamics of Coupled Molecular Clocks: The Energy Cost of Synchronization

Abstract: A central problem in biology is how living systems manage to perform vital functions (e.g., replication, development, computing, etc.) accurately by using inherently stochastic biochemical circuits to process highly noisy information. What are the molecular mechanisms to control noise for accurate information processing? What is the energy cost for implementing these molecular mechanisms? In this talk, we will present some of our recent work in addressing these two related general questions in the context of synchronization of molecular oscillators [1].

A model of coupled molecular biochemical oscillators is proposed to study nonequilibrium thermodynamics of synchronization. Under general considerations, we find that chemical interactions within an ensemble of autonomous oscillators break detailed balance and thus cost energy. This extra energy cost, in addition to the energy dissipated for driving each individual oscillator, is necessary to power the coupling interactions, which are responsible for correcting the phase error in each individual noisy oscillator with respect to the collective oscillation of the whole ensemble. By solving the steady-state distribution of the many-oscillator system analytically, we show that the system reaches its synchronized state through a non-equilibrium phase transition as energy dissipation increases. The critical energy dissipation per period depends on both the frequency and strength of the exchange reaction, which reveals an optimal (efficient) design for achieving maximum synchronization with a fixed energy budget. We apply our general theory to the Kai system in the cyanobacterial circadian clock and predict a relationship between the KaiC ATPase activity and synchronization of the KaiC hexamers. The theoretical framework established here can be extended to study thermodynamics of collective behaviors in other non-equilibrium active systems.

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Thursday 2nd June - Quantum Stochastic Thermodynamics

Colloquium - Takahiro Sagawa

Title: Three Approaches to Quantum Thermodynamics

Abstract: Stochastic thermodynamics is quite a successful and promising approach to quantum thermodynamics. For example, the fluctuation theorems for quantum systems have been derived for various setups and revealed the role of quantum information in thermodynamics [1]. Such nonequilibrium relations in stochastic thermodynamics have been experimentally tested not only in the classical but also in the quantum regime. Meanwhile, there are also other approaches to quantum thermodynamics, which have fundamental connections to stochastic thermodynamics. One is resource theory of thermodynamics, developed as a branch of quantum information theory. Another approach is based on quantum many-body physics, including quantum ergodicity and quantum chaos. In this talk, I will review these three approaches and the interplay between them.

I will then briefly talk about some of our recent results related to these approaches: (i) Quantum fluctuation theorem under continuous measurement and feedback control [2], based on the standard approach of stochastic thermodynamics. (ii) Eigenstate fluctuation theorem [3,4], which integrates the ideas of stochastic thermodynamics and the eigenstate thermalization hypothesis of quantum many-body physics. (iii) Emergence of nonequilibrium thermodynamic potentials that completely characterize state convertibility [5,6,7], addressing one of the most fundamental questions in resource theory. (iv) Characterization of symmetry-protected thermal equilibrium in terms of complete passivity [8], which provides a basis for quantum thermodynamics in the presence of symmetries.

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Invited 1 - Kay Brandner

Title: Thermodynamic Uncertainty Relations for Coherent Transport

Abstract: Thermodynamic uncertainty relations (TURs) describe a trade-off between precision and dissipation in non-equilibrium thermodynamic processes. Specifically, such relations put universal lower bounds on the overall dissipation rate of a given process, which depend only on the mean value and fluctuations of a single current. In practice, these bounds can be used, for example, to infer the efficiency of mesoscopic machines, which can be hard to measure directly [1].

Over the last years, TURs have been obtained for large classes of thermodynamic processes that can be described by means of classical models, in particular Markov-jump processes. Moreover, various generalized TURs involving additional quantities, which may be difficult to access in experiments, have been derived for quantum systems. Still, the overall picture is arguably less complete on the quantum than on the classical side.

Coherent conductors provide a powerful platform to explore the impact of quantum effects on the relation between precision and dissipation in thermodynamic processes. Such systems can be described within a simple and transparent theoretical framework based on the Landauer-Büttiker model of non-interacting transport carriers. At the same time, they can be experimentally realized and controlled with a high degree of accuracy using nanoscale structures at millikelvin temperatures.

In this talk, we consider general multi-terminal coherent conductors. As a reference, we first derive a TUR that holds for such systems in absence of time-dependent driving and under the assumption that the transport carriers can be described as classical particles. We then show that this relation breaks down in the quantum regime as a consequence of the Pauli exclusion principle and derive a modified TUR accounting for this effect. This relation holds arbitrary far from equilibrium and, like its classical counterpart, can be used to bound the overall dissipation rate in terms of a single electric current and its fluctuations, both of which are directly measurable quantities. Furthermore, we show that a similar result holds also for coherent conductors that are subject to oscillating driving fields. As an application, we discuss how our TURs for coherent transport could be used to infer bounds on the efficiency of quantum devices such as coherent charge pumps or quantum motors.

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Invited 2 - Nelly Ng

Title: Quantum field thermal machines

Abstract: Recent years have enjoyed an overwhelming interest in quantum thermodynamics, a field of research aimed at understanding thermodynamic tasks performed in the quantum regime. Further progress, however, seems to be obstructed by the lack of experimental implementations of thermal machines in which quantum effects play a decisive role. In this talk, I describe a blueprint of quantum field machines, which fills this gap by constructing several modularized components in one-dimensional ultra-cold atomic gases. These models are derived within Bogoliubov theory, which allows us to study the operational primitives numerically in an efficient way. By composing the numerically modelled operational primitives we design complete quantum thermodynamic cycles that are shown to enable cooling and hence giving rise to a quantum field refrigerator. The active cooling achieved in this way can operate in regimes where existing cooling methods become ineffective. Finally, I describe the consequences of operating the machine at the quantum level, and give an outlook of how this work serves as a road map to explore open questions in quantum information, quantum thermodynamic and the study of non-Markovian quantum dynamics.

Lightning talk 1 - Hiroyasu Tajima

Title: Superconducting-like heat current: Effective cancellation of current-dissipation trade off by quantum coherence

Abstract:

[Topics] Quantum Stochastic Thermodynamics

[Paper link] Phys. Rev. Lett. **127**, 190604 (2021).

[Background and summary] Quantum coherence is a useful resource for increasing the speed and decreasing the irreversibility of quantum dynamics. Due to this feature, coherence is used to enhance the performance of various quantum information processing devices beyond the limitations set by classical mechanics. However, when we consider thermodynamic processes, such as energy conversion in nano-scale devices, it is still unclear whether coherence provides similar advantages. Here we give general three rules clarifying how coherence affects on the trade-off relation between the heat current and the entropy production in open quantum systems. Our results show that if the amount of coherence is large enough, the energy loss in the heat current becomes virtually zero, realizing a “dissipation-less” heat current. By using the dissipation-less heat current, we construct a quantum heat engine cycle that effectively attains the Carnot efficiency with finite power in fast cycles.

[Formulation] We consider a system connected to a heat bath whose inverse temperature is β obeying the quantum master equation: $\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}[H, \rho] + D[\rho]$. Here *H* is the Hamiltonian of the system which may have degeneracy, and *D* is the dissipation term (For other details including multi-bath case, see the paper link).

As a key quantity, we introduce a ratio between the heat current *J* and the entropy production $\dot{\sigma}$: $r(\rho) := J^2(\rho)/\dot{\sigma}(\rho)$. Here, the heat current is defined as $J(\rho) := Tr[H\partial_t \rho]$, and the entropy production is defined as $\dot{\sigma}(\rho) := \dot{S}(\rho) - \beta J(\rho) \geq 0$ where, $\dot{S}(\rho) = \mathrm{Tr}[\partial_t \rho \log \rho]$. This quantity is the inverse of the strength of the loss in heat current. We remark that the ratio is similar to the inverse of the resistance of electric current. In fact, Joule’s law in electric conduction shows $R = W/I^2$.

To evaluate the effect of coherence on the ratio *r*, we denote the energy eigenstates of the Hamiltonian as $|e, j\rangle$, where *e* is the energy eigenvalue and *j* is introduced to label degenerate states. We introduce two diagonalized states $\rho_{\mathrm{bd}} := \sum_e \prod_e \rho \prod_e$ and $\rho_{sd} := \sum_{e,j} \prod_{e,j} \rho \prod_{e,j}$, where $\prod_e = |e,j\rangle\langle e,j|$ and $\prod_e = \sum_i \prod_{e,j}$ is the projection to the eigenspace of *H* whose eigenvalue is e. In the state ρ_{bd}, coherence between degenerate energy eigenstates is kept, but coherence between different energy eigenspaces is lost. To measure of coherence remained in ρ_{bd}, we introduce the l_1-norm of coherence, a standard resource measure in the resource theory of coherence [1]: $C_1(\dots) := \sum_{(e,j)\neq(e',j')} |\langle e,j|\rho|e',j'\rangle|$. By looking at $C_{l_1}(\rho_{pd})$, we can find the amount of coherence between degeneracies that *ρ* has.

Results: Our results can be summarized the following three rules:

Quantum friction: Coherence between different energy eigenspaces does not enhance the current dissipation ratio: $J(\rho)^2/\dot{\sigma}(\rho) \leq J(\rho_{bd})^2/\dot{\sigma}(\rho_{bd})$. In other words, coherence between different energy enhances friction.

Quantum lubrication: Coherence between degeneracies does enhances the ratio $J^2/\dot{\sigma}$. In other words, coherence between degeneracies reduces friction:

$$\frac{J^2(\rho_{bd})}{\dot{\sigma}(\rho_{bd})} \leq \frac{A_{\mathrm{cl}}}{2}, \frac{J^2(\rho_{bd})}{\dot{\sigma}(\rho_{bd})} \leq \frac{A_{\mathrm{cl}}+A_{\mathrm{qm}}}{2}. \qquad (1)$$

Here A_{cl} and A_{qm} are non-negative quantities. We remark the following three points: 1. A_{qm} is proportional to $C_{l_1}(\rho_{bd})$. Therefore, we can interpret A_{qm} as the term of coherence effect. 2. Due to $J(\rho)^2/\dot{\sigma}(\rho) \leq J(\rho_{bd})^2/\dot{\sigma}(\rho_{bd})$ and (1), $J(\rho)^2/\dot{\sigma}(\rho) \leq (A_{cl} + A_{qm})/2$ also holds. 3. by coherence effect, $J(\rho)^2/\dot{\sigma}(\rho)$ can be strictly larger than $A_{\mathrm{cl}}/2$ in supperradiance qubit model. See the figure 3 in the paper link.

Dissipation-less current: When there is the coherence between degeneracies much enough, the friction can be effectively zero. This is implied by (1). Suppose that

Aqm be $O(N^2)$, where $2N$ is the number of degeneracy in the system Hamiltonian. Then, the upper bound of the ratio $J(\rho)^2/\dot{\sigma}(\rho)$ becomes $O(N^2)$, which allows the following scaling

$$J(\rho) = O(N), \dot{\sigma} = O(1). \qquad (2)$$

In other words, our inequality (1) implies that large non-diagonal elements might cause macroscopic current without macroscopic dissipation. And we show that the scaling (2) can be realized in a concrete model using a $2N$-state Hamiltonian $H = \sum_{j=1}^{N} \hbar\omega_0 |\mathrm{e}, j\rangle\langle \mathrm{e}, j|$, where $|\mathrm{g}, j\rangle$ and $|\mathrm{e}, j\rangle$ are the j-th degenerate ground state and excited state, respectively. Using this "dissipation-less" current, we construct an heat engine cycle that effectively cancels the power-efficiency trade-off relation [2]:

$$P = O(N), \ \eta = \eta_{Car} - O(1/N). \qquad (3)$$

where P is power and η is efficiency, and η_{Car} is the Carnot efficiency.

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Lightning talk 2 - Sungguen Ryu

Title: Beating Carnot efficiency with periodically driven chiral conductors

Abstract: Classically, the power generated by an ideal thermal machine cannot be larger than the Carnot limit. This profound result is rooted in the second law of thermodynamics. A hot question is whether this bound is still valid for microengines operating far from equilibrium. Here, we demonstrate [1] that a quantum chiral conductor driven by AC voltage can indeed work with efficiencies much larger than the Carnot bound. The system also extracts work from common temperature baths, violating Kelvin-Planck statement. Nonetheless, with the proper definition, entropy production is always positive and the second law is preserved. Our results are relevant in view of recent developments that use small conductors to test the fundamental limits of thermodynamic engines.

Our pump engine [see Fig. 1(a)] 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 [see Fig. 1(b)]. This completely avoids any AC input power, allowing a high efficiency of the quantum engine, in contrast to nonchiral cases. Under these circumstances caution is needed in the thermodynamical description that has to be adapted for a nonthermal bath. We adopt the Floquet scattering matrix approach for electric and heat currents and also a generalized definition of entropy production based on Shannon formula for the incoming and outgoing electron distributions in each terminal [2]. We find that the engine efficiency exceeds the Carnot limit when the entropy production is deviated from the Clausius relation due to the energy uncertainty induced by the AC driving. The role of the AC driving can be interpreted as a nonequilibrium demon [3] as the driving induces additional entropy production by rearranging the electron energy distribution in a more uncertain way, while injecting no energy.

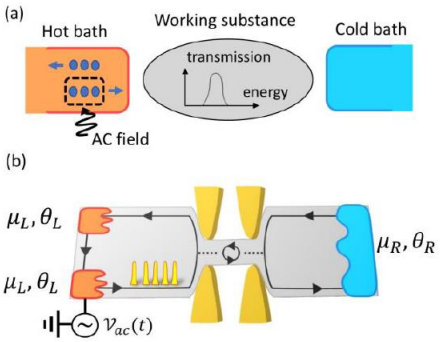

FIG. 1 (a) Schematic of periodically driven chiral engine. (b) An implementation using a chiral conductor.

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Lightning talk 3 - Aleksander Lasek

Title: Experimental observation of thermalisation with noncommuting charges

Abstract: Noncommuting charges have recently emerged as an area at the intersection of quantum thermodynamics and quantum information. There is a flurry of papers being published in this rapidly developing subfield. Often, the global energy and particle number are conserved, and the system is prepared with a well-defined particle number. However, quantum evolution can also conserve quantities, or charges, that fail to commute with each other. As noncommutation underlies quantumness, such systems are of particular interest. Quantum simulators have recently enabled experimental observations of quantum many-body systems' internal thermalisation. We initiate the experimental testing of its predictions with a trapped-ion simulator. We initialize 6–15 qubits in an approximate microcanonical subspace, a recently theorized generalisation of the microcanonical subspace for accommodating noncommuting charges. The noncommuting charges are the three spin components. We report the first experimental observation of an equilibrium state predicted within quantum-information thermodynamics in 2016: the non-Abelian thermal state. Despite the threat of decoherence breaking multiple conservation laws, thanks to our use of dynamical decoupling, our many-body system is shown to exhibit quantum-thermodynamical effects only described in theory until now. This work initiates the experimental testing of a recently emerged subfield that has so far remained theoretical.

Arxiv preprint "Experimental observation of thermalisation with noncommuting charges" available at: https://arxiv.org/abs/2202.04652

Invited 3 - Juan Parrondo

Title: Scattering and thermalization: wave-particle duality hits quantum thermodynamics

Abstract: An interesting class of open quantum systems is defined by the so-called repeated interaction scheme, where the system interacts sequentially with small and fresh subsystems or units coming from the reservoir. The interaction is unitary and relatively easy to analyze. However, it must be switched on and off, and this action introduces or extracts energy in many cases of interest, performing work and preventing thermalization. As a consequence, the repeated interaction scheme cannot be used to model thermostats in quantum thermodynamics.
We partly overcome this problem by considering collisional reservoirs where the units are particles that collide with the system. The whole setup is autonomous and, if the units are in thermal equilibrium, the work to switch on and off the interaction becomes heat, and thermalization is recovered in most cases.

Invited 4 - Martí Perarnau-Llobet

Title: Finite-time bounds on the probabilistic violation of the second law of thermodynamics

Abstract: Jarzynski's equality sets a strong bound on the probability of violating the second law of thermodynamics by extracting work beyond the free energy difference [1]. Recently, Cavina, Mari and Giovannetti developed a work-extraction protocol that saturates this bound, but however requires infinite time [2]. In this talk, I will explain how to construct optimal protocols for this task in finite time. This will lead us to finite-time refinements to Jarzynski's bound, derived in the context of driven systems interacting with a thermal Markovian environment. The finite-time bound will be expressed through the geometric notion of thermodynamic length, thus building a connection between thermodynamic geometry and higher order statistical properties of work [3]. Finally, I will also explain how to minimize work fluctuations in driven quantum systems through geometric methods [4].

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Friday 3rd June - Computation and Information Processing

Colloquium - David Wolpert

Title: STOCHASTIC THERMODYNAMICS OF DISTRIBUTED SYSTEMS

Abstract: To date stochastic thermodynamics has (mostly) been applied to systems with only a few subsystems, and only a few degrees of freedom. Here I present some results concerning stochastic thermodynamics of distributed systems with multiple, heterogenous subsystems. I focus on how the interaction network among the subsystems affects thermodynamic behavior of the full system. I first review results concerning (loop-free) Boolean circuits, and then extend those results to the case of arbitrary Bayes nets. I then present results concerning composite processes, which are a generalization of multipartite processes, to allow more than one subsystem to change state at a given moment. These results start to lay the foundation for the thermodynamic analysis of distributed computational systems, ranging from brains to concurrent processors to digital circuits.

Invited 1 - Artemy Kolchinsky

Title: The fundamental cost of a single-shot classical or quantum computation: stochastic thermodynamics meets algorithmic information theory

Abstract: We consider the thermodynamic cost of a single-shot computation, which may be classical or quantum, in which some particular input x is transformed into a particular output y. Using techniques from stochastic thermodynamics and algorithmic information theory, we demonstrate that the conditional Kolmogorov complexity of the input given the output, $K(x|y)$, is a fundamental cost of any such computation. Our approach builds on ideas developed by Zurek in the 1980s, who used an informal argument to suggest that $K(x|y)$ bounds the heat generated by a classical deterministic computation. We provide a fully rigorous derivation of Zurek's bound, generalize it to arbitrary (noisy and / or quantum) computations, and highlight several implicit assumptions. We also show that the fundamental cost $K(x|y)$ can be paid for via some combination of heat, non-determinism (noise), and driving protocol complexity, implying a tradeoff between these resources.

Invited 2 - Naoto Shiraishi

Title: Undecidability in quantum thermalization

Abstract: If we leave an isolated quantum many-body system at a nonequilibrium initial state, it will relax to the unique equilibrium state, which is called thermalization. Almost all physical quantum many-body systems are considered to show thermalization, while some quantum many-body systems including integrable systems do not thermalize. One of the central problems in quantum thermalization is to find the conditions determining whether thermalization occurs in a given system. Despite vast literature in this field, this problem has still been left as an open problem.
We tackle this problem with a completely different approach. Applying the viewpoint of theoretical computer science, we clarify the hardness of the problem of quantum thermalization. Surprisingly, we find that the decision problem of thermalization is undecidable [1]. Our result is still valid even when the system is one-dimensional, Hamiltonian is shift-invariant and nearest-neighbor interaction, the initial state is a product state, and the observable is a shift-sum of a one-body observable. Our result also shows that thermalization is Turing complete, which implies that thermalization is much more complicated phenomena than expected.

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Lightning talk 1 - Lorenzo Buffoni

Title: Spontaneous fluctuation-symmetry breaking and the Landauer principle

Abstract: We will present a novel approach to the problem of the energetic cost of information erasure by looking at it through the lens of the Jarzynski equality. We will point out in what sense the Landauer principle can be distinguished from the second law of thermodynamics. The Landauer bound, $\langle W \rangle \geq kT\ln 2$, on average dissipated work $\langle W \rangle$ associated to an erasure process, literally emerges from the underlying second law bound as formulated by Kelvin, $\langle W \rangle \geq 0$, as consequence of a spontaneous breaking of the Crooks-Tasaki fluctuation-symmetry, that accompanies logical irreversibility. The latter does not generally hold true when absolute irreversibility is present, just like the Gibbs distribution becomes inappropriate for describing, e.g., ferromagnets below the critical temperature. While the second law is a direct consequence of the fluctuation relation, the Landauer principle is a direct consequence of its breakdown. We illustrate and corroborate this insight with numerical simulations of the process of information erasure performed on a 2D Ising ferromagnet.

Preprint: https://arxiv.org/abs/2106.07570

Lightning talk 2 - Salambô Dago

Title: When it comes to information processing, fast is hot, and hot is expensive.

Abstract: The Landauer principle states that at least $k_B T \ln 2$ of energy is required to erase a 1-bit memory, with $k_B T$ the thermal energy of the surrounding thermostat. We study the effects of inertia on this bound using as one-bit memory an underdamped micro-mechanical oscillator confined in a tunable double-well potential created by a feedback loop [3]. Contrary to most experiments using over-damped systems, the underdamped regime, minimizing the dissipation, allows to cut the energetic cost and speed up the operation time: we reached the Landauer's bound with 1% uncertainty, with protocols as short as 100 ms [1].

Besides, we show experimentally and theoretically that for such underdamped systems, faster erasures induce a heating of the memory: the work influx is not instantaneously compensated by the inefficient heat transfert to the thermostat. The rising temperature of the memory rules the information processing cost, now scaling as $k_B T_{\mathrm{eff}} \ln 2$ [2], with T_{eff} the average (using a proper weighting) temperature of the memory during erasure. We therefore extend Landauer's bound from the isothermal to the adiabatic case (in the sense of low heat exchanges allowed with the thermostat) and demonstrate, with results from experiment, simulation and from our theoretical model, that the work required to erase 1-bit tends to $k_B T$ in the adiabatic limit. Our model covering all damping regimes paves the way to new optimisation strategies in information processing, based on the thorough understanding of the energy exchanges.

References

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Lightning talk 3 - Paul Riechers

Title: Two paradigms for energetically efficient computing

Abstract: We reconsider the thermodynamics of computation in light of new advances in stochastic thermodynamics developed here. Many recent works have identified why computation can be inefficient—practically desirable traits like speed, modularity, time-symmetric driving, and precision all incur dissipation within at least some regimes. Our current work corroborates and contextualizes these results in a more general framework. However, there has not been much guidance to directly assert how to achieve thermodynamically efficient computing—except for these warnings of what not to do. Indeed, it is now widely appreciated that logical reversibility is neither necessary nor sufficient for thermodynamic reversibility. Our main objective is more constructive: we identify how practical computation can finally be made efficient.

We establish general principles for thermodynamically efficient computing, from a very general framework that accommodates many diverse approaches to computing. We find that density reversibility—the recoverability of probability density within each contracting memory class, via local time reversal—is the key to thermodynamically reversible computing. It is a necessary condition that places useful constraints on efficient design. When this condition is not fulfilled, we provide novel lower bounds on the requisite dissipation, both in general and in the limit of nearly deterministic computations.

Density reversibility suggests at least two distinct paradigms for energetically efficient computing: metastable and inertial. Metastable computing is most familiar within the framework of stochastic thermodynamics. However, intertial computing unlocks new opportunities while challenging some of the traditional assumptions of stochastic thermodynamics. We find that the time-reversal symmetries of memory elements play a prominent role in determining density reversibility in each of these paradigms. Aspects of both paradigms will be discussed.

Invited 3 - David Limmer

Title:

Abstract:

Invited 4 - Jean-Charles Delvenne

Title: Thermo-Kinetic Relations for elementary computing devices

Abstract: Landauer's theorem, in its original and more modern forms, states the minimal cost of a computational device. It can be reached in principle through underdamped processes, or overdamped processes at very slow speed.

Unfortunately most computational devices today are overdamped, and are not meant to proceed infinitely slowly, quite the contrary. This results in overhead costs making Landauer's cost largely irrelevant for current technologies.

In this talk we attempt to bridge the gap between Laudauer's optimistic bound and thermodynamic cost of real-word device through various assumptions on the system at hand, resulting in various trade-offs between speed, cost and reliability.

In order to do so we derive novel Thermo-Kinetic Relations. These relations, linking thermodynamic quantities such as entropy production with kinetic features encompass in particular (strengthened forms of) Thermodynamic Uncertainty Relations and Classical Speed Limits.

Our main example is the fundamental building block of modern computing devices: the NOT gate, also called the inverter.

ABSTRACTS (Poster session: Friday 27th May)

[Poster] Fundamental Principles

P#1.01 - Cai Dieball

Title: Coarse graining Empirical Densities and Currents in Continuous Space

Abstract: We will present general results on fluctuations and spatial correlations of the coarse-grained empirical density and current of Markovian diffusion in equilibrium or non-equilibrium steady states on all time scales. The results unravel a deep connection between the fluctuations of empirical currents and a generalized time-reversal symmetry, providing a deeper understanding of time-averaged observables, and highlight the essential role of coarse-graining in space. The spatial coarse-graining ensures mathematical consistency and is required to uncover salient features of currents due to broken detailed balance. Moreover, the variation of the coarse-graining scale can improve the accuracy of inferring dissipation. Notably, the fluctuations of empirical density and current defined without coarse graining are proven to diverge on all time scales in dimensions higher than one, suggesting that the commonly used definitions in large deviation theory require a revision. Our findings provide a deeper understanding of time-averaged observables, give insight into the necessity of coarse graining, and may allow for a more reliable analysis of single-molecule and particle-tracking experiments.

Link to pre-print: https://arxiv.org/abs/2105.10483

P#1.02 - Matthew Gerry

Title: Bounds on fluctuations of continuous machines in stochastic thermodynamics

Abstract: Thermal machines (heat engines and refrigerators) may be described at the nanoscale, with stochastic processes underlying the exchange of heat with thermal baths and the input or output of work. As a result, heat and work are represented by stochastic variables exhibiting fluctuations which often play a significant role in evaluating device performance, particularly at small scales. In this talk, I will focus on classical and quantum *continuous* thermal machines: those whose operation is characterized by steady-state energy currents through an open system away from equilibrium. Recently, a set of bounds has been identified, involving the ratio of fluctuations in a continuous thermal machine's output current to those in its input current. Namely, this ratio is bounded from below by the square of the machine's efficiency (or coefficient of performance), and from above by the square of the relevant Carnot bound, set by the temperatures of the baths. This amounts to a novel, tighter-than-Carnot bound on efficiency in such machines. These results have been proven universally for continuous machines operating close to equilibrium, in the regime of linear response. I will discuss this proof and relate it to basic models of continuous thermal machines. I will proceed to describe various analytic and computational approaches that have been taken towards extending these results to the far-from-equilibrium regime.

Links to associated work:
https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.127.190603
https://arxiv.org/abs/2109.03526

P# 1.03 - Pedro E. Harunari

Title: Inferences from Statistics of a Few Observable Transitions

Abstract: The rapidly growing field of Stochastic Thermodynamics relies on the mathematics of Markov processes to assess Statistical Physics concepts outside of thermal equilibrium, it thrives under the full knowledge of the microscopic dynamics via master or Fokker-Planck equations. However, in most realistic settings, part of the information is hidden, what in fact distinguishes Statistical Mechanics from Thermodynamics is that for the latter only macroscopic phenomena are available.

Some recent works address the issue of partial information by considering a specific set of observable states [1,2]. Conversely, in this work we consider that a set of transitions are the only observables. Molecular machines represent one of the biggest examples of such setting [3], their internal state and most transitions are hidden (e.g. dynein's consumption of one ATP), however some specific transitions are observable (e.g. dynein's steps along a microtubule).

From first-passage-time techniques we derive analytical expressions for probability of sequence of transitions and the time intervals between them, which describe data from molecular motor simulations [4]. We address how the observer can make inferences about irreversibility, disorder and topology of an underlying process from the collected partial information and apply the framework to biophysical models.

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P# 1.04 - Anthony Kiely

Title: Entropy production in quantum control

Abstract: Protocols for non-adiabatic quantum control invariably involve the use of time varying classical fields. Assessing the thermodynamic cost of such protocols, however, is far from trivial, with several non-equivalent measures proposed in the literature. In this work we study the irreversible entropy produced by the classical apparatus generating the control fields. This associates the cost of a given control protocol with the dissipation. We focus, in particular, on the case of time-dependent magnetic fields and shortcuts to adiabaticity. We show-case our results with two examples: a Landau-Zener model of a spin 1/2 particle in a magnetic field and an ion confined in a Penning trap.

P# 1.05 - Sreekanth K Manikandan

Title: Non-monotonic skewness of currents in non-equilibrium steady states

Abstract: Measurements of any property of a microscopic system are bound to show significant deviations from the average, due to thermal fluctuations. For time-integrated observables such as heat, work or entropy production in a steady-state, it is in fact known that there will be long stretches of fluctuations both above as well as below the average, occurring equally likely at large times. In this paper we show that for any finite-time measurement in a non-equilibrium steady state – rather counter-intuitively - fluctuations below the average are more probable; there is even an optimal time for time-integrated current fluctuations to most likely lie below the average. We demonstrate that these effects are a consequence of the non-monotonic skewness of current fluctuations in non-equilibrium stationary states. We also provide evidence that our findings are easily observable in experiments.

Links to associated work: arXiv:2201.06563, submitted to PRL

P# 1.06 - Atul Tanaji Mohite

Title: Optimising Energetics of Field Theories: Pareto Front and Phase Transitions

Abstract: Understanding finite time optimal processes is a frontier of non-equilibrium statistical physics. Phase transitions are ubiquitous in Physics with many applications. Field theories have been extremely successful in characterizing the universal properties of various phase transitions, and in delineating a few canonical models which capture the essential Physics at play in a large class of systems [1-3]. Interestingly, a generic framework for optimizing the energetic cost associated with the finite-time driving of such systems is still largely missing. What is the optimal process for a change of phase in finite time?

Here, building on recent advances in stochastic thermodynamics and optimal transport theory [4-7], we show how to analytically derive the optimal driving protocols that minimizes work for a finite driving time, which we apply to cases with either conserved or non-conserved scalar order parameter in the weak noise regime. We compute exact closed form analytical expressions for the optimal driving protocols and the optimum energy cost associated with it. Moreover, we formulate a numerical multi-optimization problem to simultaneously optimize the mean and variance of work, leading to revealing a first-order phase transition in the corresponding Pareto front, which features the coexistence of multiple optimal protocols. Overall, our results elucidate how to drive field theories to minimize the average and fluctuations of energy cost, with the potential to be deployed to a broad class of systems.

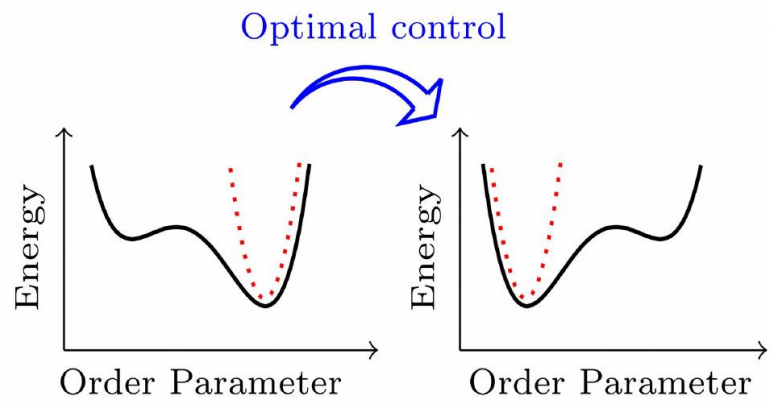

Fig. 1: Free energy landscape is denoted by the solid black line. Changing control parameters exchanges the stability of the landscape minima, thus undergoing a change of phase. In small noise limit, the initial and final Gaussian probability distribution around the stable minima is denoted by dotted red line. We compute the optimal protocol and the energy cost for the finite-time driving of scaler field from the initial to the final phase.

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P# 1.07 - Andrea Plati

Title: Thermodynamic bound on anomalous diffusion arising from memory effects

Abstract: An intriguing connection between Thermodynamic Uncertainty Relations (TUR) and anomalous diffusion has been recently highlighted [1].

Here we address this issue in the case of anomalous diffusion of a tracer described by a generalized Langevin equation with exponential memory kernels. We show that, for this class of models, one can derive an underdamped TUR where specific contributes of the entropy production rate are relevant. This leads to a tighter bound with respect the general one. We apply our analytical results to experimental data for the diffusion of a tracer in a dense vibro-fluidized granular medium where the crossover between different non diffusive regimes seems to be linked to this thermodynamic bound.

[1]: David Hartich and Aljaž Godec Phys. Rev. Lett. 127, 080601 (2021)

[Poster] Physics & Chemistry

P# 2.01 - Aubin Archambault

Title: Calibrated force measurement in Atomic Force Microscopy using the Transient Fluctuation Theorem

Abstract: In my talk I will present how the Transient Fluctuation Theorem is used to calibrate an Atomic Force Microscope by measuring the fluctuations of the work performed by a time dependent force applied between a colloïdal probe and the surface. From this measure one can easily extract the value of the interaction force and the relevant parameters of the measuring cantilever. The results of this analysis are compared with those obtained by standard calibration methods.

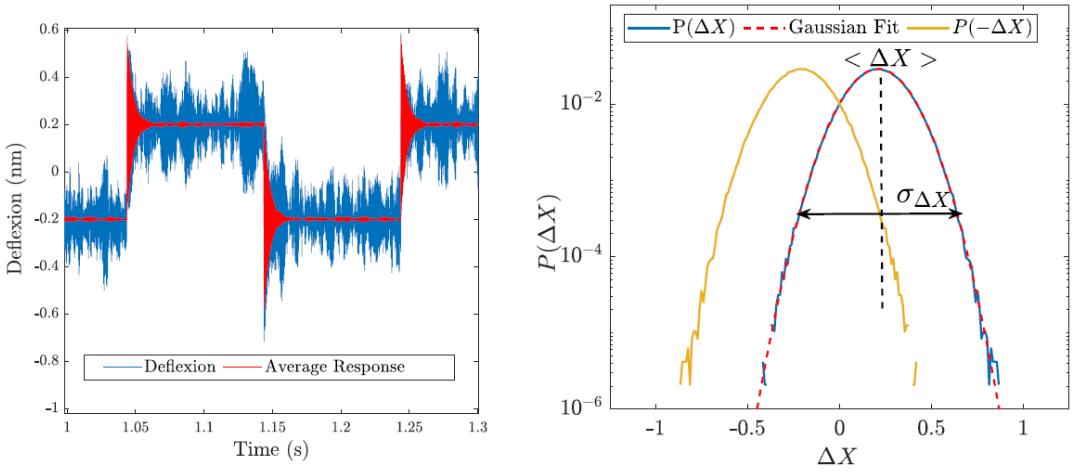

Illustration of the presented technique : A square wave force is applied to the cantilever and the deflection ΔX of the micro-cantilever is measured (left figure: result of one experiment in blue, average in red). The work received by the system is then $W = F\Delta X$, and its probability distribution is obtained easily from the distribution of deflection ΔX (right figure: $\mathcal{P}(\Delta X)$). The probability distributions are gaussian, which allows us to write the Transient Fluctuation Theorem as $F = 2k_BT\frac{\langle\Delta X\rangle}{\sigma^2_{\Delta X}}$, where $\sigma^2_{\Delta X}$ is the variance of ΔX. This gives us a calibration free force measurement. From this measurement, one can extract the stiffness k of the cantilver using that $k = \frac{F}{<\Delta X>} = \frac{2k_BT}{\sigma^2_{\Delta X}}$.

Refences

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P# 2.02 - Miguel Aguilera

Title: Stochastic thermodynamics of a non-equilibrium Sherrington-Kirkpatrick model

Abstract: Stochastic thermodynamics unveils the exchange of energy and matter in physical, chemical, and biological processes with the environment. Furthermore, it elucidates the information-theoretic bounds of different thermodynamics quantities. However, when system's elements are numerous, it becomes challenging to characterize nonequilibrium states due to the expansion of the state space. Conceived as a model of magnetic materials, the disordered Ising or Sherrington-Kirkpatrick model has been a standard tool to study interacting systems such as neural networks in the thermodynamic limit, revealing rich repertoires of equilibrium dynamics, including the celebrated spin-glass phases and transitions between them. Nevertheless, researchers have not yet theoretically underpinned the nonequilibrium properties of spin kinetics caused by asymmetric, heterogeneous connectivities of the Ising model with large system size.

Here, we study the kinetics of asymmetric Sherrington-Kirkpatrick systems as a prototypical model of nonlinear and nonequilibrium processes. We apply a path integral approach to calculate exactly a generating functional over the system's trajectories capturing the system's sufficient statistics as well as quantities related with its nonequilibrium thermodynamics. As a result, we derive the exact solutions of the order parameters (means and correlations) of the system, the conditional entropy of the dynamics, and the entropy flow of the system (equivalent to the entropy production in steady state conditions) in the limit of infinitely large networks. Unlike the replica method, the path integral approach for fully asymmetric networks gives the exact solutions in thermodynamic limit without additional ansatzes such as the analytic continuation and replica symmetry breaking.

As expected, the order parameters reveal that the kinetic model exhibits order-disordered nonequilibrium phase transitions analogous to the paramagnetic-ferromagnetic phase transitions in the equilibrium systems but no dynamics akin to the spin-glass phases (which vanish due to coupling asymmetry). In addition, we show that the entropy production is maximized near the nonequilibrium phase transition points, being the first derivative discontinuous at phase transitions (Fig. 1C, dashed line). However, the entropy production can be more prominent outside the critical regime, especially in the disordered systems with low entropy rates, i.e., if the connections are heterogeneous and strong enough to make the dynamics disordered but highly deterministic (Fig. 1C, top right).

Our results indicate that a non-smooth change of the entropy flow or entropy production can be a useful indicator for nonequilibrium phase transitions. At the same time, our results suggest that, even if the system shows large entropy flow/production, it does not necessarily indicate the system is near a phase transition. Instead, a combination of the order parameters, entropy rate and entropy production yield a more precise picture of the behaviour of complex, disordered systems and its phase transitions.

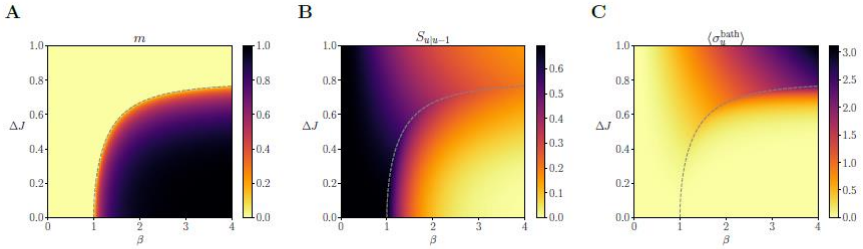

Figure 1: **Analytical results of the behaviour of the asymmetric, kinetic SK model.** Analytical solution of a system with asymmetric couplings following a distribution $J_{ij} \sim \mathcal{N}(\frac{1}{N}, \frac{\Delta J^2}{N})$ and no internal fields, showing the mean magnetization (**A**), conditional entropy (**B**) and entropy production (**C**).

P# 2.03 - Avishek Das

Title: Reinforcement learning, control and design of diffusive nonequilibrium trajectories

Abstract: The control and design of functional nonequilibrium molecular dynamics is rendered difficult by the breakdown of detailed balance. Driving nonequilibrium systems with an additional force can in principle make an otherwise rare fluctuation, typical. We have developed a numerical technique for computing the optimal driving force in generic many particle Langevin dynamics simulations, by exploiting a variational principle that relates the rate of the rare fluctuation to the probability cost in trajectory space. This approach uses explicit gradients of trajectory probabilities to solve the variational problem and learn the optimal force within a chosen basis set. Additional reinforcement learning tools have been developed to improve the computational efficiency of the gradient-based optimization algorithm by multiple orders of magnitude. In my talk I will describe our recent applications of this algorithm for the inverse design of targeted self-assembly in DNA-labeled colloids in a shear flow, towards nano-clusters of pre-specified shape and size.[1] I will also talk about sampling rare diffusive barrier-crossing trajectories with multiple reaction paths, and a new paradigm we have developed for computing reaction rates in far-from-equilibrium systems and active matter, called Variational Path Sampling (VPS).[2,3]

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P# 2.04 - Mauricio J. del Razo

Title: Stochastic thermodynamics of reaction-diffusion processes

Abstract: Reaction-diffusion processes are key to model biochemical processes at the scale of a living cell, and thus fundamental to understand gene regulation, cell sensing and cell signaling among many other processes essential for life. Recent work presented a stochastic description of open reaction-diffusion processes in the form of a master equation [1], termed chemical diffusion master equation (CDME). At the particle resolution, chemical reactions can change the number of particles in the system, and diffusion can modify their distribution in space. Thus, the CDME and the system configuration must include both the number of particles of each species (discrete), as well as their distribution in space (continuous). Due to the combination of discrete and continuous degrees of freedom, the probability distribution of the system lives in a family of symmetrized multidimensional spaces, the so-called Fock space. To derive a stochastic thermodynamics framework for reaction-diffusion processes, we first define the stochastic entropy in this setting, and we derive the main thermodynamic relations. We further develop the concept of stochastic trajectories for reaction-diffusion processes, as well as their entropy.

Further results might be available by the time of the presentation of this work at the workshop.

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[2] del Razo, Mauricio J “Stochastic thermodynamics of reaction-diffusion processes” (in preparation)

P# 2.05 - Adam G. Frim

Title: A geometric bound on the efficiency of irreversible thermodynamic cycles

Abstract: Stochastic thermodynamics has revolutionized our understanding of heat engines operating in finite time. Recently, numerous studies have considered the optimal operation of thermodynamic cycles acting as heat engines with a given profile in thermodynamic space (e.g. $P-V$ space ijn classical thermodynamics), with a particular focus on the Carnot engine. In this talk, I will use the lens of thermodynamic geometry to explore the full, unconstrained space of non-equilibrium thermodynamic cycles in search of optimally shaped cycles. By applying classical isoperimetric inequalities, I derive a universal geometric bound on the efficiency of any irreversible thermodynamic cycle and explicitly construct efficient heat engines operating in finite time that nearly saturate this bound for a parametric harmonic oscillator, a central model system that has also been the focus of experimental study. Given the bound, these optimal cycles perform more efficiently than all other thermodynamic cycles operating as heat engines in finite time, including notable cycles, such as those of Carnot, Stirling, and Otto. For example, in comparison to recent experiments, this corresponds to orders of magnitude improvement in the efficiency of engines operating in certain time regimes. Our results suggest novel design principles for future mesoscopic heat engines and are ripe for experimental investigation.

Links to associated preprint: arXiv:2112.10797.

P# 2.06 - Jordan Juritz

Title: Minimal mechanism for cyclic templating of length-controlled copolymers under isothermal conditions

Abstract: Sequence-based copying of copolymer templates is fundamental to the synthesis of biological molecules and is a promising framework for artificial life and life-like system. Previous work demonstrated that creating accurate copies of template sequences necessitates generating a low entropy ensemble of products, and hence is a highly non-equilibrium process [10.1103/PhysRevX.7.021004, 10.1073/pnas.1808775116]. An underappreciated fact is that reliably producing copies of a certain length also necessitates operating far from equilibrium. In this talk I will demonstrate that the phenomenon of product inhibition (the tendency of long molecules to adhere to their template) is the main challenge for length control – the practical manifestation of the conceptual challenge of creating a system that converges to a far-from-equilibrium state. I will then demonstrate minimal mechanisms which may achieve length control for templates of arbitrary length, using a series of coarse-grained models of templated copolymerisation. I will describe the landscape these models generate through kinetic and thermodynamic analysis supported by stochastic simulations. At the core of these mechanisms is a requirement that the chemical free energy transduced in the extension of polymers is coupled to their detachment from the template. Our models predict that reliable copying with a high yield of full-length, sequence-matched products is possible over experimentally accessible regions of the parameter space, opening the way to the engineering of synthetic copying and, looking forward, self-replicating systems that operate autonomously.

This talk will contain results presented in our recent paper:
https://aip.scitation.org/doi/full/10.1063/5.0077865

P# 2.07 - Kazuki Nakamura

Title: Universal Relation between Entropy Production, Accuracy, and Phase Sensitivity in General Chemical Oscillators

Abstract: Mesoscopic chemical oscillations are subject to fluctuations due to the system size and the period of the oscillation fluctuates. Recently, it has been shown that the period can be made accurate by increasing the energy consumption for three specific models of biochemical reaction and the Stuart-Landau oscillator [1]. It was also suggested that even both accuracy and phase sensitivity can be increased by the increase of energy consumption [2]. In spite of this progress, a unified relation that includes the entropy production, accuracy, and phase sensitivity at the same time has yet been obtained. Here, we have derived the unified relation for the chemical oscillations described by the following stochastic Stuart-Landau equation (SSLE) [3]:

$$\frac{dr}{dt} = \sigma r + C_r r^3 + \frac{\varepsilon}{\sqrt{V}}\xi_r(t),\ \frac{d\theta}{dt} = \omega + C_i r^2 + \frac{\varepsilon}{r\sqrt{V}}\xi_\theta(t), \qquad (1)$$

where V is the system size, $C_r < 0$ and C_i are parameters of the system, and ξ_r and ξ_θ are white Gaussian noises with $\langle \xi_l(t) \rangle = 0$ and $\langle \xi_l(t)\xi_{l'}(t') \rangle = \delta_{ll'}\delta(t-t')$ $(l, l' = r, \theta)$. We define the correlation time as $\tau_c \equiv 2/D_\phi$, where D_ϕ is the phase diffusion constant. The accuracy of the oscillation for the SSLE is defined as $R \equiv \tau_c/T$, where T is the mean value of the period. If the system size is sufficiently large, the following relation is derived as the main result [4]:

$$\beta Q_{cyc}^{SSLE} = 4\pi^2 \chi_m^2 R, \qquad (2)$$

where β is the inverse temperature of the environment, Q_{cyc}^{SSLE} is the energy dissipation in one cycle for the SSLE, and $\chi m \equiv \sqrt{(C_i/C_r)^2 + 1}$ is the normalized phase sensitivity.

The second main result is associated with the thermodynamic uncertainty relation (TUR). By formulating the TUR for the SSLE, we obtain the inequality:

$$\beta Q_{cyc}^{SSLE} \geq 4\pi^2 R, \qquad (3)$$

We have shown that the equality condition of the TUR [5] for the SSLE is satisfied when the normalized phase sensitivity takes the lower limit. In particular, the equality condition in a nonequilibrium steady state is satisfied in no phase-radius coupling limit $C_i \rightarrow 0$.

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[2] C. Fei, Y. Cao, Q. Ouyang, and Y. Tu, Nat. Commun. 9, 1434 (2018).
[3] T. J. Xiao, J. Ma, Z. Hou, and H. Xin, New J. Phys. 9 403 (2007).
[4] K. Nakamura, Y. Izumida, and H. Kori, in preparation.
[5] Y. Hasegawa and T. Van Vu, Phys. Rev. E, 99, 062126 (2019).

P# 2.08 - Benjamin Qureshi

Title: A Universal Method for Analysing Copolymer Growth

Abstract: In this talk, I will introduce a generalised method for analysing copolymerisation processes, applicable to both free and templated copolymerisation. In contrast to prior methods, our method can be applied to microscopically reversible models (enabling thermodynamic analysis); the reaction rates may be conditional on prior monomers in the chain and template sequences (which introduce correlations in the sequence of copolymer produced); and monomer inclusion steps may be given by arbitrarily complex underlying reaction networks. The method allows for straightforward, analytical extraction of quantities related to copolymerisation processes such as: the probability of inclusion of a certain monomer type; time taken to complete polymerisation; the free energy exchange due to the copolymerisation; and the free energy transduced in internal cycles. I will outline the method and then apply it to generalised model of kinetic proofreading with N activation stages. Many of the techniques presented in this talk, such as spanning tree methods and self-avoiding walks on graphs, also have further reaching applications for Markovian processes in general.

Links to associated work: https://www.overleaf.com/read/gptcffmdbfnq

P# 2.09 - Jesús Rubio

Title: Fluctuation relations as a predictive tool for redox potentials

Abstract: The tunable design of redox potentials could open a range of applications in biotechnology and catalysis. This talk introduces a new method to predict redox potentials by combining fluctuation relations, Bayesian inference and molecular dynamics (MD) simulations. Reduced and oxidised states are first simulated, followed by the conversion between them. Energy differences are then calculated using the Kubo-Onsager approach. Such energies are finally processed into efficient estimates for the redox potentials by means of a detailed fluctuation relation. This is tested on several proteins whose experimentally measured redox potentials vary over a range of 60 mV. When compared with standard techniques, our stochastic-thermodynamic method is found to perform reliably, having a moderately strong correlation (~ 0.7) with experimental data.

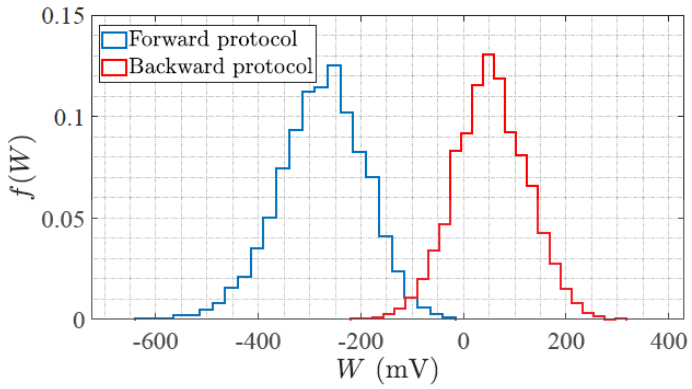

Figure 1: Forward/reduction (blue) and backward/oxidation (red) work histograms for a four-helix bundle heme protein.

A. S. F. Oliveira, J. Rubio et al, in preparation (2022)

P. Maragakis, F. Ritort et al, J Chem Phys 129, 024102 (2008)

G. Ciccotti, M. Ferrario, Mol Simul 42, 1385-1400 (2016)

P# 2.10 - Shesha Gopal Marehalli Srinivas

Title: Growth in Linear Reaction Networks: A Thermodynamic Perspective

Abstract: We investigate how the long-time dynamics and thermodynamics of open chemical reaction networks change depending on the exchange mechanism with the environment. By focusing on (pseudo) linear re-action networks, we analytically prove that they must relax towards a steady state when some species are exchanged via chemical reactions. This happens because in the long time limit the work performed by the environment is fully dissipated. On the other hand, the concentrations of the chemical species continuously grow when some species are exchanged at constant influxes and outfluxes. In this regime, only a fraction of the work performed by the environment is dissipated in the long time limit, while the remaining powers growth. We further show that the dissipation decays with time, implying that chemical reaction networks approach a growing equilibrium.

[Poster] Biophysics and Active Matter

P# 3.01 - Nazul Jared López-Alamilla

Title: Virial-like Thermodynamic Uncertainty Relation in the Tight-Binding Regime

Abstract: The thermodynamic uncertainty relation (TUR) provides a trade-off $\sigma \times (\hat{D}/\hat{v}^2) \geq k_B$ between the cost σ (entropy generation) and the precision of the system $\hat{D}/\hat{v}^2$ [1, 2]. The TUR can be used to provide a lower bound 'σ_{TUR}' for
the entropy generation of this system $\sigma \geq \sigma_{TUR}$. However, experiments and analytic studies show that this bound is rather a loose bound in many regimes $\sigma \gg \sigma_{TUR}$ [3, 4]. Here, we present a methodology to approximate the entropy production for Brownian motion in a tilted periodic potential $V(x) = V_{per}(x) - \hat{f}x$. The approximation stems from
the well known thermodynamic uncertainty relation. By applying a virial-like expansion, we provided a tighter lower limit solely in terms of '$\hat{v}$' the drift velocity and '$\hat{D}$' diffusion

$$\sigma \geq \sigma_{TUR}^{N-th} = k_B \sum_{n=1}^{N} \frac{\hat{v}^{2n}}{2^{2n-2}(2n-1)\hat{D}^{2n-1}}. \qquad (1)$$

This expression is systematically analysed in the tight-binding regime [5]. In this regime Eq. (1) converges to the actual value of the entropy generation in the system for increasing N values, see Figure 1. We also discuss the implications of our results outside the tight-binding regime [5] (full preprint available at arxiv.org: 2202.10526).

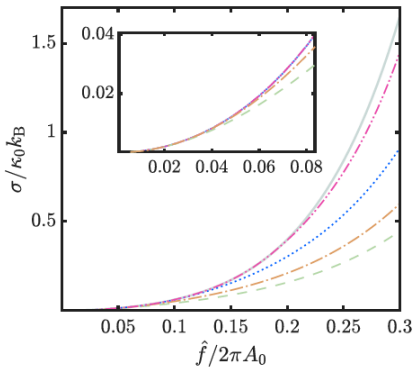

Figure 1. Steady-state entropy production as function of tilting force for Brownian motion over a tilted periodic potential $V(x)/k_BT = A_0\cos(2\pi x) - \hat{f}x$. Plots correspond to (solid) full entropy σ, (dashed) $\sigma_{TUR} = k_B\hat{v}^2/\hat{D}$, (dash-dotted) Eq. (1) 2-nd order, (dotted) Eq. (1) 7-th order, (dash-dot-dot-dashed) Eq. (1) 29-th order.

[1] A. C. Barato and U. Seifert, Phys. Rev. Lett. 114, 158101 (2015).

[2] P. Pietzonka, A. C. Barato, and U. Seifert, J. Stat. Mech: Theory Exp. 2016, 124004 (2016).

[3] Y. Song and C. Hyeon, J. Phys. Chem. Lett. 11, 3136 (2020).

[4] M. W. Jack, N. J. López-Alamilla, and K. J. Challis, Phys. Rev. E 101, 062123 (2020).

[5] N. J. López-Alamilla and R. U. L. Cachi, "Virial-like thermodynamic uncertainty relation in the tight-binding regime," (2022), arXiv:2202.10526.

P# 3.02 - Daiki Sekizawa

Title: Information-Thermodynamic Cost and Speed Limit in High-dimensional Neural Dynamic

Abstract: The brain enables various information processing by flexibly transitioning to different brain states. Since transitioning between states involve a transition cost, quantifying the cost can reveal the characteristics of information processing in the brain in terms of which transitions are easy or difficult. For this purpose, several methods for quantifying transition costs have been proposed. However, considering situations biological systems face with where state transitions must be performed as quickly as possible within limited resources, simply quantifying the costs is not sufficient. In addition to that, it will be important to evaluate how efficiently the consumed costs are converted to realizing the state transitions. Here, we propose a framework to quantify the efficiency of the state transitions in the brain based on stochastic thermodynamics. Recently, Nakazato & Ito (2021) derived the cost-speed trade-off inequality, which states that the maximum speed of a transition a system can attain is bounded by the consumed cost, where the cost is entropy production and the speed is a traveled path length in the L^2-Wasserstein space in a fixed duration. Based on this theory, we can define the efficiency η ($0 \leq \eta \leq 1$) as the ratio of the consumed cost converted to the speed of the travel. If η is large, it means that the transition is close to the speed limit under the consumed cost. We applied this framework to the human electrocorticography (ECoG) data set (Miller, 2019), and evaluated the efficiency of the state transitions during a simple visual task and a working memory task. We regarded the time course of the probability distribution of the event-related potentials (ERP) as the traveled path in the L^2-Wasserstein space and computed the efficiency. To capture the characteristics of high-dimensional brain dynamics, we evaluated how the estimated efficiency η changes as the number of electrodes for the analysis (dimension) is increased. We found that irrespective of subjects and tasks, the efficiency η is about 0.8 in lower dimensions, and converges to about 0.5 as dimension increases. We expect our framework offers a novel perspective to assess how efficiently the brain performs various functions through state transitions under limited resources.

[Poster] Quantum Stochastic Thermodynamics

P# 4.01 - Nicholas Anto-Sztrikacs

Title: Effects of strong coupling in quantum thermodynamics with the reaction coordinate method

Abstract: At the nanoscale, strong system-reservoir interactions are ubiquitous and could potentially play a large role in the development of novel nanoscale quantum machines. As a result, a complete formulation of thermodynamics which is valid in the quantum regime must incorporate the effects of strong system-reservoir couplings. The reaction coordinate (RC) mapping is emerging as a significant method in the fields of open quantum systems and quantum thermodynamics, allowing one to go beyond the standard Born-Markov approximation and tackle the strong coupling regime. In this technique, the system-environment boundary is reshaped to include a collective degree of freedom from the environment, resulting in an enlarged system comprising of the original system and the extracted bath mode. Following the RC mapping, standard Born-Markov treatments are permissible on the enlarged system, where strong degrees of correlations are maintained throughout the dynamical evolution between the extracted collective degree of freedom and the original system. As a result, the reaction coordinate mapping provides a numerically cheap approach capable of accurate predictions in studies of strongly coupled open quantum systems.

I will describe our efforts to apply the RC method to a range of problems in quantum transport and thermodynamics in the strong coupling regime. Such applications range from the investigation of the suppression of thermal current at strong coupling, the emergence of inter-bath transport mechanisms enabled by strong coupling, and finally, the performance of quantum absorption refrigerators where we report a shift in the cooling window in the strong coupling regime relative to weak coupling treatments. Lastly, I will show our efforts to extend the reaction coordinate method to create effective models, where the aforementioned impacts of strong system-reservoir coupling can be interpreted analytically.

Papers of the work:
Strong coupling effects in quantum thermal transport with the reaction coordinate method – IOPscience
[2111.05302] Strong system-bath coupling reshapes characteristics of quantum thermal machines (arxiv.org)

P# 4.02 - Joshua Eglinton

Title: Geometric Bounds on the Power of Adiabatic Thermal Machines

Abstract: The laws of thermodynamics put fundamental bounds on the efficiencies of thermal machines such as heat engines or refrigerators. However, these Carnot bounds can typically be attained only if the machine is operated quasi-statically, which leads to vanishing power output. How this trade-off between power and efficiency can be captured quantitatively for meso- and micro-scale thermal machines is a question that has attracted significant attention over the last years. Here we use the methods of thermodynamic geometry to analyze the performance of slowly driven meso- and micro-scale devices that operate between two thermal baths with small temperature difference.

Using Onsager's symmetry relations and general scaling argument, we show that the efficiency of such devices reaches the Carnot bound only if heat-leaks between the baths can be fully suppressed. Furthermore, we find that their power is in fact determined by second-order terms in the temperature difference between the two baths, which are neglected in standard linear-response theory. These additional contributions lead to a new family of power-efficiency trade-off relations that imply a quadratic rather than a linear decay of power at Carnot efficiency.

Notably, these relations depend only on geometric quantities such as the thermodynamic length of the driving cycle. Our bounds can be asymptotically saturated in the quasi-static limit if the driving protocols are suitably optimized and the temperature difference between the baths goes to zero with the driving frequency. They hold for essentially any thermodynamically consistent micro-dynamics such as classical Markov-jump processes, adiabatic Lindblad dynamics or coherent transport. To illustrate our general theory, we investigate two models representing two different classes of systems, a qubit-refrigerator working in a two-stroke cycle and a coherent charge pump operating as cooling devices.

[1] Joshua Eglinton and Kay Brandner. Geometric Bounds on the Power of Adiabatic Thermal Machines. 2022. arXiv: 2202.08759 [cond-mat.stat-mech].

P# 4.03 - Paolo Andrea Erdman

Title: Identifying optimal cycles in quantum thermal machines with reinforcement-learning

Abstract: Driven thermal machines, such as heat engines and refrigerators, allow us to control the conversion between heat and work through time-dependent controls that are periodically driven to implement thermodynamic cycles.

The performance of stochastic/quantum thermal machines is mainly characterized by power, efficiency, and power fluctuations. However, optimizing such quantities is an extremely challenging task: in finite-time, the state can be driven far from equilibrium, and cycle optimization is a search over the exponentially large space of all possible time-dependent controls. While general results have been found in the slow [1] and fast [2] driving regime – general finite-time optimization schemes are currently lacking.

We introduce a general framework based on Reinforcement Learning (RL) to discover optimal cycles that maximize the power of quantum thermal machines [3]. Our method makes no assumptions on the shape or speed of the cycle. Rather, the RL agent is free to arbitrarily couple the quantum system to any bath, and to arbitrarily manipulate the controls.

We apply our method, based on state-of-the-art RL algorithms, to three systems: a benchmark two-level system heat engine, where we find the known optimal cycle [4]; a refrigerator based on a superconducting qubit, where we find a non-intuitive control sequence that outperforms previous proposals; a heat engine based on a quantum harmonic oscillator, where we find an elaborate cycle that outperforms Otto cycles. We show that such cycles mitigate the detrimental effect of generation of coherence [5].

At last, I briefly discuss extensions of our method to:
- optimize the full trade-off between power, efficiency, and fluctuations [6]. We apply such method to a quantum dot-based engine and test the validity of the thermodynamic uncertainty relations [7] in finite-time driven engines.
- Identify optimal cycles only observing the heat currents, thus potentially applicable to experimental devices [8].

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[7] A.C. Barato and U. Seifert, Phys. Rev. Lett. 114, 158101 (2015).
[8] P.A. Erdman and F. Noé, in preparation (2022).

P# 4.04 - Guilherme de Sousa

Title: Quantum harmonic oscillator under measurement and feedback

Abstract: In order to control and manipulate quantum systems it is often necessary to apply measurement and feedback. Applications of quantum technology depend on these features and a theoretical understanding is necessary to correctly simulate quantum dynamics. Recently a Quantum Fokker-Planck Master Equation (QFPME) was derived for the joint distribution of system and detector (Annby-Andersson et al, arXiv:2110.09159). This generalized master equation contains the feedback dynamics for the system of interest but also distributions of detector variable for many realizations of the experiment. The main ingredients are the measurement backaction that disturbs the system and the detector bandwidth that accounts for how fast the measurement apparatus can keep up with system dynamics. For a generic system, the QFPME is only suitable for numerical solutions; for the specific case of separation of time scales, when the detector is very fast compared to the internal dynamics of the system, one can derive an effective master equation for the system alone. Here we apply this formalism to the quantum harmonic oscillator. Results were derived for arbitrary values of the parameters, without relying on the assumption of separation of timescale. We found analytical results for the position measurement and cooling protocol. The optimal protocol depends on a precise choice of the ratio between the measurement strength and detector lag. That indicates a trade-off between measurement disturbance and how much information one can collect and process to correctly apply the feedback. Our results provide intuition into quantum measurement and feedback and illustrate how to apply this new master equation for continuous quantum systems.

P# 4.05 - Kenza Hammam

Title: Optimizing autonomous thermal machines powered by energetic coherence

Abstract: The characterization and control of quantum effects in the performance of thermodynamic tasks may open new avenues for small thermal machines working in the nanoscale. In our work [1], by using a quantum collision model framework, we study the impact of coherence in the operation of a small thermal machine which can act either as a heat engine or as a refrigerator. We show that input coherence may enhance the machine's performance and allows it to operate in otherwise forbidden regimes. Moreover, our results also indicate that, in some cases, coherence may also be detrimental, rendering optimization of particular models a crucial task for benefiting from coherence-induced enhancements.

Reference

[1] K. Hammam, Y. Hassouni, R. Fazio and G. Manzano, Optimizing autonomous thermal machines powered by energetic coherence, (2021), New J. Phys. 23 043024.

P# 4.06 - Hisao Hayakawa

Title: Geometrical Maxwell's demon

Abstract: We theoretically study an entropy production and a work extracted from a system connected to two reservoirs by periodic modulations of chemical potentials of the reservoirs and one parameter in the system Hamiltonian under an isothermal condition. We find that the modulation of parameters can drive the geometrical state, which is away from nonequilibrium steady state. As a result, the driven system cannot reach the nonequilibrium steady state at which the relative entropy takes the minimum value. With the aid of this property, we construct Maxwell's demon in which the relative entropy increases with time and we can extract the work, if we begin with the nonequilibrium steady state without modulations of parameters. We employ the Anderson model to demonstrate that the relative entropy can increase with time. Figure 1 is the plot of the time evolution of the relative entropy which can increase with time, and Figs. 2 are schematics of parameter controls and the BSN curvature, which is the origin of the geometrical Maxwell's demon. This work is a natural extension of our previous works [1-4].

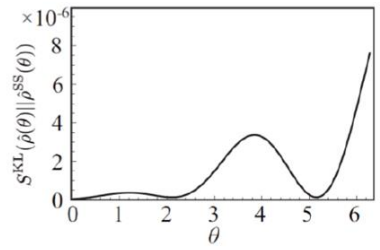

Fig.1: Time evolution of the relative entropy.

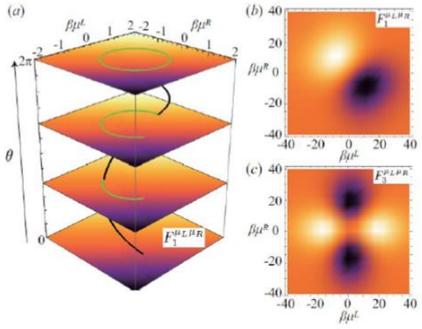

Fig.2: (a) Schematics of a contour of the integral, where the black solid line is the trajectory of the parameters. The color scale and (b) & (c) express the BSN curvature.

[1] K. Takahashi, K. Fujii, Y. Hino and H. Hayakawa, PRL **124**, 150602 (2020).
[2] Y. Hino and H. Hayakawa, PRR **3**, 013187 (2021).
[3] H. Hayakawa, V. M. M. Paasonen, and R. Yoshii, arXiv:2112.12370.
[4] R. Yoshii and H. Hayakawa, arXiv:2203.***.

P# 4.07 - Ruo Cheng Huang

Title: Work extraction from quantum systems with complex temporal correlations

Abstract: Quantum information-processing techniques enable work extraction from a system's inherently quantum features, in addition to the classical free energy it contains. Meanwhile, the science of computational mechanics affords tools for the predictive modelling of non-Markovian classical and quantum stochastic processes.

We combine tools from these two sciences to develop a theoretical prototype for a predictive quantum engine: a machine that charges a battery by feeding on a multipartite quantum system whose parts are temporally correlated via a classical stochastic process. We also test the engine on simple models to benchmark the performance of our engine against various alternatives, including one without coherent quantum information-processing and one without predictive functionality; our predictive quantum engine is shown to outperform these alternatives in terms of work output.

Finally, we evaluate the engine's performance on fuel processes with different degrees of temporal correlations and find the work yield to increase with such correlations. Our results also suggest that any process with a parametric family of quantum outputs exhibits a phase boundary between parametric regions where memory of past observations can and cannot enhance the work yield. Our work opens the prospect of machines that harness environmental free energy in an essentially quantum, essentially time-varying form.

P# 4.08 - Felix Hubmann

Title: Open quantum evolution from thermodynamic collision models

Abstract: Thermal operations are those that can be realised by coupling a system of interest to a thermal bath and performing an energy-conserving unitary. These provide a viable tool to understand which transformations between pairs of states are possible within the resource theory of athermality. Such operations are an important subset of those possible within the general theory of open quantum evolutions. Here, by invoking the Born-Markov approximation, one can describe the continuous-time evolution of the system in terms of a master equation. Particular properties of the master equation arise when thermodynamic assumptions (such as strict energy conservation) are further imposed. A priori, it is not clear that invoking thermodynamic assumptions before and after the Born-Markov approximations lead to the same description. In this work, we begin with a collision model based on sequences of thermal operations and take the continuous-time limit to yield a master equation, which we show to have similar properties as that derived in the work of others[1]. An advantage of our approach is the ability to compute properties in terms of relevant Hamiltonians. This offers additional insights on how thermodynamic processes can be tuned. One of these properties are decay rates, which can be set in ratio, resulting in a detailed balance condition. By that, our approach also allows for expressing the found detailed balance condition in terms of these relevant Hamiltonians. This additional insight further enables us to find certain conditions under which detailed balance implies strict energy conservation and vice versa.

1. R. Dann, R. Kosloff, ”Open system dynamics from thermodynamic compatibility”, 2020- arXiv:2011.03504

P# 4.09 - Miku Ishizaki

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

Abstract: 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].

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 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].

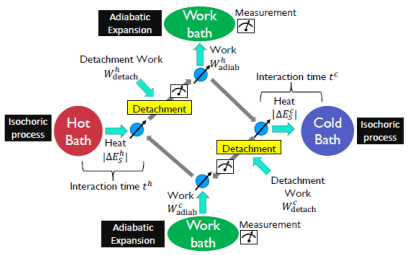

Figure 1: Quantum Otto Cycle. A qubit absorbs or emits heat from or to the bath in each isochoric process and does work to the outside in the adiabatic processes. After each isochoric process, we need detachment work to separate a qubit from the bath. We also perform indirect measurement in order to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

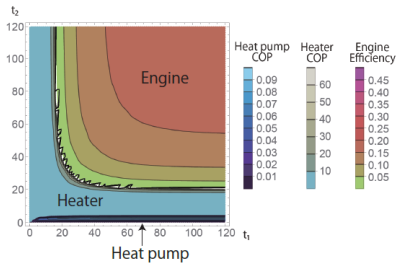

Figure 2: Work, heat, efficiency η and COP (Coefficient of performance), which is the heat absorbed from the cold bath divided by the work acquired from the external system. The parameters are set to $\omega_c/\omega_h = 0.5$ and $T_c/T_h = 0.2$ for the interaction times t^h and t^c, where ω_h and ω_c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

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[2] Miku Ishizaki, Hiroyasu Tajima, Naomichi Hatano, in preparation.

[3] Yuji Shirai, Kazunari Hashimoto, Ryuta Tezuka, Chikako Uchiyama, Naomichi Hatano, Phys. Rev. Research 3, 023078 (2021)

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P# 4.10 - Michael Kewming

Title: Entropy Production at Zero Temperature

Abstract: Fluctuation theorems allow one to make generalised statements about the behaviour of thermodynamic quantities in systems that are driven far from thermal equilibrium. In this talk, I'll present our recent results where we use Crooks' fluctuation theorem to understand the entropy production of a continuously measured, zero-temperature quantum system; namely an optical cavity measured via homodyne detection.

At zero temperature, if one uses the classical definition of inverse temperature then the entropy production becomes divergent. Our analysis shows that the entropy production can be well defined at zero temperature by considering the entropy produced in the measurement record. We link this result to the Cramer-Rao inequality and show that the product of the Fisher information in the work distribution with the entropy production is bounded below by the square of the inverse energy fluctuations. This inequality indicates that there is a minimal amount of entropy produced in acquiring information about the work done to a quantum system driven far from equilibrium via quantum measurement.

In this talk, I will present a pedagogical derivation of this result and argue that thermodynamics quantities should be best understood through the lens of quantum measurements, and the associated fluctuations in these quantum measurement records.

Reference

1. M. Kewming, S. Shrapnel, “Entropy Production at Zero Temperature” arXiv:2109.01998 (2022)

P# 4.11 - Shayan Majidy

Title: How to build Hamiltonians that transport noncommuting charges in quantum thermodynamics

Abstract: Noncommuting conserved quantities have recently launched a subfield of quantum thermodynamics. In conventional thermodynamics, a system of interest and an environment exchange quantities—energy, particles, electric charge, etc.—that are globally conserved and are represented by Hermitian operators. These operators were implicitly assumed to commute with each other, until a few years ago. Freeing the operators to fail to commute has enabled many theoretical discoveries—about reference frames, entropy production, resource-theory models, etc. Little work has bridged these results from abstract theory to experimental reality. This paper provides a methodology for building this bridge systematically: we present a prescription for constructing Hamiltonians that conserve noncommuting quantities globally while transporting the quantities locally. The Hamiltonians can couple arbitrarily many subsystems together and can be integrable or nonintegrable. Our Hamiltonians may be realized physically with superconducting qudits, with ultracold atoms, and with trapped ions.

P# 4.12 - None

P# 4.13 - Anthony Munson

Title: Resource theory of quantum uncomplexity

Abstract:

■ **Introduction**. Quantum complexity—the difficulty of preparing a quantum state from a simple tensor-product state—is an essential subject in quantum computation with a wealth of recent applications to many-body physics and stochastic thermodynamics [1–6]. Importantly, under random dynamics, a system's quantum complexity increases linearly up to times exponential in the system's size, long after most physical observables have thermalized [6]. The observation that complexity saturation is a late stage of quantum thermalization suggests that a state's lack of complexity, or "uncomplexity," is a useful resource for quantum computation [7]: Much as a system far from thermal equilibrium can serve as a resource in thermodynamic and information-processing tasks, a state with high uncomplexity—i.e., a low-complexity state such as $|0^w\rangle$—can be utilized as "blank scrap paper" for quantum computers. It is natural, therefore, to view uncomplexitythrough the lens of a resource theory. In a resource theory, an agent can perform any operation subject toa fixed set of simple rules, and can identify which tasks are achievable under these rules and which tasks require additional resources. Resource theories have successfully characterized many phenomena in quantum information theory and thermodynamics, such as optimal protocols for single-shot work extraction [8–12]. In the influential Ref. [7], Brown and Susskind conjectured that a resource theory of uncomplexity exists.

■ **Results.** (i) We define a resource theory of uncomplexity; (ii) construct protocols in the resource theory for extracting uncomplexity from a state and for expending uncomplexity to imitate a state, and thereby provide a quantification of the resource requirements for one-shot thermodynamic erasure [13, 14] (Landauer erasure) under computational limitations; and (iii) show that a new quantity, the complexity entropy, quantifies the efficiencies with which we can perform uncomplexity extraction and expenditure, and therefore establish a direct connection between complexity and entropy.

■ **The resource theory of uncomplexity.** The complexity $C(|\psi\rangle)$ of an n-qubit pure state is a measure of the difficulty of preparing a desired n-qubit state $|\psi\rangle$ from the reference state $|0^n\rangle$. For example, one measure of a pure state's complexity is its exact circuit complexity, which is defined as the least number of gates required to prepare the state from $|0^n\rangle$. The uncomplexity of $|\psi\rangle$ is the difference $C_{max} - C(|\psi\rangle)$, which resembles a free-energy difference. To model the noise that occurs in the implementation of real-world gates, we allow the agent in the resource theory to carry out for free any fuzzy gate: Any 2-qubit gate U the agent carries out is accompanied by a small amount of noise, resulting in a randomly chosen unitary $\widetilde{U} \approx U$ being applied. A parameter $\epsilon > 0$ quantifies the fuzziness, with $\left\|\widetilde{U} - U\right\|_\infty \leqslant \epsilon$. Fuzzy operations are arbitrary compositions of fuzzy gates; they form the resource theory's allowed operations and model a phenomenon characteristic of chaotic systems: the accumulation of large errors from a succession of smaller ones.

■ **The complexity entropy.** If one performs a local measurement on a complex pure state $|\psi\rangle$, the measurement outcomes are highly random (e.g., [15, 16]). Despite its being pure, $|\psi\rangle$ looks like it has high entropy. The complexity entropy quantifies this apparent randomness. To define the complexity entropy, we only consider measurements that can be implemented as follows: an experimenter first performs at most r gates, with $r \geqslant 0$ fixed, and then performs a very simple measurement, such as a tensor-product projector.

■ **Uncomplexity extraction and uncomplexity expenditure.** We study two tasks in the resource theory of uncomplexity, the extraction and the expenditure of uncomplexity, and show that their optimal efficiencies are quantified

with the complexity entropy. For both tasks, the agent is effectively restricted to performing at most r gates: The gates' fuzziness otherwise causes the state to become too noisy to be useful. Uncomplexity extraction from ρ consists of applying at $|0^w\rangle$most r gates, such that the w qubits chosen by the agent are δ-close to the state for some given $\delta \geqslant 0$. For example, uncomplexity extraction connects to Landauer erasure: since erasing a qubit costs, on average, $kBT\ln 2$ units of work, quantifying the optimal efficiency for the extraction of w qubits close to $|0^w\rangle$ quantifies the average work required for such an extraction. Given the fundamental trade-off between information and work extraction given by Landauer's principle, uncomplexity extraction is a task of natural importance to researchers interested in thermodynamics and information.

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P# 4.14 - Kacper Prech

Title: Entanglement and TUR violations - two manifestations of quantum coherence

Abstract: Entanglement, a form of correlation that is stronger than what classical systems are capable of, is a prominent manifestation of quantum coherence. Recently, a different manifestation of coherence has been discovered: systems exhibiting quantum coherence have been found to violate inequalities that bound the signal-to-noise ratio of any current in classical systems, so-called thermodynamic uncertainty relations (TUR) [1]. We systematically analyze the relation between these two different manifestations of coherence in a serial double quantum dot. In this system, entanglement can be generated by driving a charge current through the double dot [2]. That same current may exhibit a suppression of fluctuations due to quantum coherence, allowing for TUR violations. We find that TUR violations and entanglement are present for the same range of tunnel-couplings. However, while TUR violations require small bias voltages (keeping dissipation small), entanglement is maximized in the large bias limit. Increasing the bias voltage, we observe a cross-over from TUR violations to entanglement with the window of co-existence for intermediate voltages. We include Coulomb interaction and the spin degree of freedom in our calculations, as these are often unavoidable ingredients in an experimental setup. For large inter-dot Coulomb interaction and in the large bias limit, we find an amount of entanglement that exceeds the results of previous studies.

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P# 4.15 - Onur Pusuluk

Title: Thermocoherent effect: Generalization of Onsager’s reciprocity relations for heat and quantum correlations

Abstract: Although thermoelectric effects were experimentally discovered by (Seebeck and Peltier) between 1821–34, the underlying theory remained immature until Lars Onsager published his famous reciprocal relations between heat and charge in 1931 [1]. Onsager’s paper was built on a paper of Lord Rayleigh [2], in which he focused for the first time on the whole dynamical process by which a thermodynamic steady state is attained. He captured the essential physics by developing a simplified collision model, which in turn allowed him to reveal the role of the environment's initial conditions in heat conduction.

In this talk, we will follow Lord Rayleigh and Lars Onsager's footsteps to systematically establish quantum reciprocal relations between heat and quantum coherence and correlations, for which we introduce the term “thermocoherent effect” [3]. We’ll explore Rayleigh's dynamical problem to equilibration in the quantum regime. For arbitrary collision times and initial states, we’ll develop the quantum master and Fokker-Planck equations. By identifying the quantum version of Rayleigh's heat conduction equation, we’ll show that quantum discord and entanglement can contribute to genuine heat flow only when they are associated with so-called heat-exchange coherences. Analogous to Onsager's use of Rayleigh's principle of least dissipation of energy, we’ll use the entropy production rate to identify the coherence current. We’ll write both coherence and heat flows in the form of quantum Onsager relations, from which we predict coherent Peltier and coherent Seebeck effects. Finally, we’ll discuss some of the possible experimental realizations and technological applications of the thermocoherent phenomena in different platforms.

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P# 4.16 - Andrea Solfanelli

Title: Experimental verification of fluctuation relations with a quantum computer

Abstract: Inspired by the idea that quantum computers can be useful in advancing basic science, we use a quantum processor to experimentally validate a number of theoretical results in non-equilibrium quantum thermodynamics, that were not (or were very little) corroborated so far. In order to do so, we first put forward a novel method to implement the so called two-point measurement scheme, which is at the basis of the study of non-equilibrium energetic exchanges in quantum systems. Like previously established methods, our method uses an ancillary system, but at variance with them, it provides direct access to the energy exchange statistics, and is, accordingly more effective, at least when applied to small quantum systems. Using a quantum computer as a remotely programmable experimental platform, we first validate our ancilla-assisted two-point measurement scheme, and then apply it to i) experimentally verify that fluctuation theorems are robust against projective measurements, a theoretical prediction which was not validated so far, ii) experimentally verify the so called heat engine fluctuation relation, by implementing a SWAP quantum heat engine. iii) experimentally verify that the heat engine fluctuation relation holds for measurement-fuelled quantum heat engines, by implementing the design at the basis of the so called quantum-measurement-cooling concept. Our experiments constitute an experimental basis for the understanding of the non-equilibrium energetics of quantum computation and for the implementation of energy management devices on quantum processors.[1]

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P# 4.17 - Jeongrak Son

Title: Catalysis in Action via Elementary Thermal Operations

Abstract: Catalysts are auxiliary states that interact with the system of interest during a process, and recover their original state afterwards. The benefit of appending such an ancilla has been reported in many frameworks, including quantum thermodynamics. Nevertheless, current results focus mainly on conditions for catalytic advantage, and sometimes constructions of catalytic states. In contrast, the dynamics of catalytic processes have remained unexplored, even theoretically. Moreover, the existing results on state transition conditions that rely on initial and final states, washes out what happens in a continuous-time setting, preventing us from gleaning insight into the potential mechanisms that make a catalyst useful. Motivated by the status quo, we study catalysis in elementary thermal operations (ETO), an experimentally motivated subset of thermal operations, and show that catalysis enhances ETO, which was previously unknown. The structure of ETOs furthermore allow us to naturally trace intermediate steps between the initial and the final states, enabling a study on how system and catalyst explicitly interact with each other during the process. A critical tool we develop is the strengthening of existing upper bounds of computational cost for ETOs, which leads to 1) a full characterization of allowed transitions for three-dimensional systems, and 2) computationally tractable numerics for higher dimensions. Interestingly, non-trivial catalyses with exact recovery are found even in the simplest case of a qutrit system and qubit catalyst, fostering experimental implementation together with straightforward operational recipes provided by ETO. Finally, we capture “snapshots” of the catalysis at work, by tracking the changes in local free energy of the system-catalyst during evolution. We observed that the system free energy, which always decrease after each application of ETO, can increase momentarily during the catalytic processes by borrowing catalyst free energies. Our work provides the first analysis of catalysis mechanism occurring in practicable setup, paving the way for a more in-depth understanding of catalytic processes.

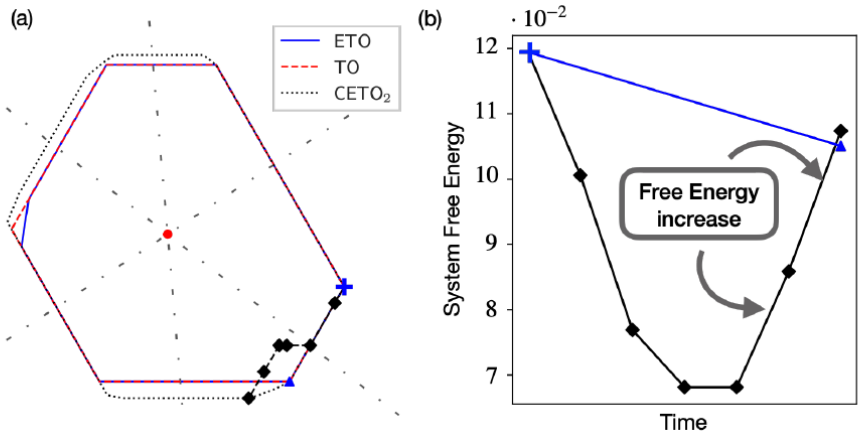

Figure 1: (a): set of final states reachable via ETO, thermal operations (TO), and catalytic ETO with a qubit catalyst ($CETO_2$). Black dotted lines outside of red and blue lines evince the existence of the catalytic advantage. Diamond symbols track the path a catalytic process take in the $CETO_2$ evolution. (b): system local free energy changes during a $CETO_2$ process (black diamonds) and a non-catalytic ETO (blue triangle) are plotted.

P# 4.18 - Philip Taranto

Title: Landauer vs. Nernst: What is the True Cost of Cooling a Quantum System?

Abstract: Thermodynamics connects our knowledge of the world to our capability to manipulate and thus to control it. This crucial role of control is exemplified by the third law of thermodynamics, Nernst's unattainability principle, stating that infinite resources are required to cool a system to absolute zero temperature [1–5]. But what are these resources? And how does this relate to Landauer's principle that famously connects information and thermodynamics [6]? We answer these questions by providing a framework for identifying the resources that enable the creation of pure quantum states. We show that perfect cooling is possible with Landauer energy cost given infinite time or control complexity. Within the context of resource theories of quantum thermodynamics, we derive a Carnot-Landauer limit, along with protocols for its saturation. This generalises Landauer's principle to a fully thermodynamic setting, leading to a unification with the third law and emphasising the importance of control in quantum thermodynamics.

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[Poster] Computation and Information Processing

P# 5.01 - Debankur Bhattacharyya

Title: A network-based stochastic modeling approach for a double quantum dot information ratchet

Abstract: There are two primary paradigms for describing Maxwell's demons: feedback-controlled models and memory-tape models (information ratchets). We present a simple strategy for constructing a memory-tape model of Maxwell's demon, starting from a feedback-controlled model. We illustrate this approach by converting the Annby-Andersson (AA) model [Phys. Rev. B 101,165404 (2020)], a feedback-controlled model in a double quantum dot system, to a memory tape model. In the original AA model, the energy configuration is the control parameter, and the occupation state of the double quantum dot is the stochastic dynamic variable. In our model, energy configuration becomes a dynamic variable on the same footing as the occupation state. We explore the underlying network structure of the AA model to design a set of bit coupling rules that converts the model to an information ratchet. Our model is analytically solvable for the long bit-interaction time intervals. For finite-time interaction, phase diagrams of operational modes are obtained numerically. In summary, this study explores the connection between the feedback-controlled paradigm and the information ratchet paradigm of Maxwell's demons through an illustrative example.

P# 5.02 - Ashwin Gopal

Title: Large deviations theory and thermal noise in non-linear electronic circuits: a case study.

Abstract: We show how to apply the theories of large deviations and stochastic thermodynamics to correctly describe thermal noise in non-linear electronic circuits, both at the level of state and current observables. As a case study, we consider a low-power CMOS inverter, or NOT gate, which is a basic primitive in electronic design. Starting with a thermodynamically consistent description in terms of jump processes at the single-electron level, we consider a macroscopic limit in which the thermal fluctuations satisfy a Large Deviations Principle. Crucially, this limit becomes essentially exact already in settings involving a few tens of electrons, as we show by comparing the analytical results with Gillespie simulations and spectral methods. We also do a comparison with the results obtained from the widespread diffusive approximation leading to Langevin and/or Fokker-Planck equations, highlighting the limitations and problems of such approaches. Finally, we discuss under which conditions a coarse-grained effective model of a given device can be provided, while still correctly describing the current fluctuations.

P# 5.03 - Gülce Kardeş

Title: Inclusive thermodynamics of arbitrary computational machines

Abstract: Every computational system in the Chomsky hierarchy consists of two or more interacting sub-systems: a computational machine (e.g., a deterministic finite automaton (DFA), a Turing machine (TM), etc.) and a sequence of inputs into the machine and / or outputs produced by the machine. While the initial state of the computational machine is generally fixed, the sequence of inputs is typically random, generated by some (perhaps implicit) distribution. Here we lower bound the dissipated thermodynamic work that occurs in a complete cycle of any physical process that implements such a computational system. For a particular computational system it is given in toto by the dynamics of the computational system, as specified in its abstract, computer science definition. It turns out that this lower bound on dissipated work is formally identical to the irreversible entropy production arising in Hamiltonian formulations of stochastic thermodynamics. We exploit this to derive an integral fluctuation theorem (IFT) for the dissipated work of an arbitrary computational system. We illustrate this IFT for the case of a DFA; a Markov information source; and a communication channel. Building on this, we present rate-distortion theory involving thermodynamic distortion functions. We conclude our work with an analysis relating dissipated work to the computational size complexity of a DFA, where we prove that minimal size complexity results in minimal dissipation.

P# 5.04 - Daiki Kiyooka

Title: Quantifying the cost of maintaining a brain state based on stochastic thermodynamics

Abstract: In our daily lives, we perform various tasks with different levels of cognitive demands. To successfully perform these tasks, the brain needs to control its activity and make its state appropriate for each task. Previous studies have utilized control theory and information theory, and have proposed a framework for quantifying the cost of “transitioning” between different task states. However, few studies have quantified the cost of “maintaining” a brain state for performing a particular task. Here, based on information theory and stochastic thermodynamics, we propose a novel framework to quantify the cost of maintaining a target state given a baseline uncontrolled brain dynamics. To this end, we introduce a quantity which is equipped with clear information-theoretic and stochastic-thermodynamic interpretation; minus the change rate of the Kullback-Leibler divergence from a target probability distribution under a baseline dynamics to its equilibrium distribution (Horowitz, Zhou & England, 2017; Horowitz & England, 2017). This quantity not only reflects the intuition that it costs more to maintain a brain state farther from its baseline dynamics but also corresponds to the entropy production, which is a thermodynamic cost. As a proof of concept, we applied the framework to fMRI data of a resting state and task states from the Human Connectome Project (HCP). We use a pairwise maximum entropy model to estimate probability distributions of brain activity patterns during each state. We set resting state as a baseline and each task state as a target, and compute the maintenance cost. We found that the cost of maintaining a cognitively demanding task state was larger than that of a cognitively easier task state. The results suggest that our framework serves as a general theoretical tool for investigating the brain state from the perspective of maintenance cost.

P# 5.05 - Asawari Pagare

Title: Can a single ligand-receptor sensor simultaneously measure multiple environmental properties?

Abstract: Yes. Cell receptor sensors are subject to randomness due to thermal fluctuations and yet they provide a ubiquitous example of information transduction from the outside of the cell to the inside. Previous studies on cellular sensing have focused on minimizing the impact of noise on the concentration sensing abilities of a ligand receptor sensor. However, we discovered that the presence of thermal noise allows a sensor to simultaneously receive multiple channels of information from the environment (e.g., concentration, temperature, and flow speed). This novel behavior is demonstrated by a set of minimal models simulated with Langevin dynamics in environments that are thermally equilibrated or driven out of equilibrium. Moreover, we applied the theory of maximum likelihood estimation and analyzed the maximum number of environmental information that a ligand-receptor could sense. These results provide insights on design principles of novel microscopic sensors that operates in realistic and complex environments.

P# 5.06 - Zhongmin Zhang

Title: The nonequilibrium dynamics of a temporally responsive, single-molecule automaton

Abstract: Molecules with multiple meta-stable configurations on rough energy landscapes could demonstrate complex hysteresis responses to various temporally changing environments. We argue that such nonequilibrium hysteresis responses could allow a molecule to recognize, memorize, and respond specifically to temporal patterns of a changing environment. Moreover, such molecules could be steered into far-from-equilibrium configurations if the environment is programmed to change according to specific protocols. We demonstrate both behaviors in a simple solvable model of a linear polymer chain with a temporally controlled end-to-end distance λ(t). A polymer consisting of N foldable segments is modeled by a novel dual-rate master equation over the 2N possible configurations. With an asymmetric energy landscape for folding/unfolding, we designed a polymer that can function as a molecular timer and temporal pattern recorder. Moreover, we discovered that the evolution of the dominant configuration of the molecule acts like an automaton, which allows us to design driving protocols to steer the molecule into nonequilibrium distributions dominated by any desired configuration.