Winter school on ultrafast thermodynamics

Abstract booklet

February 19-23, 2024

CHALMERS
UNIVERSITY OF TECHNOLOGY

Scope of the winter school

Ultrashort laser pulses are a powerful tool for controlling and probing materials properties at ultrafast timescales. To fully describe and understand time-dependent phenomena in materials, it is necessary to extend our concepts of thermodynamics beyond classical and equilibrium regimes into the quantum and nonequilibrium domains. This dynamic and challenging research direction has emerged as a vibrant field of study. The winter school aims to train the next generation of scientists by inviting international experts who work in the field of ultrafast thermodynamics to deliver lectures. This event is open to research students and postdocs worldwide, and we are also reserving seats for local participants at Chalmers on all levels. The winter school provides an excellent opportunity for building future research collaborations and disseminating knowledge to the next generation of experts in Sweden and beyond.

Funding sources

The winter school is made possible by generous support of the Carl Trygger Foundation and the Chalmers Area of Advance Nano.

Organizers

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Contents

The winter school - a 3 ECTS course

Quantum materials host a variety of intriguing phenomena, based on many-body interactions or topology. Due to tremendous experimental progress, these phenomena can now be controlled and probed on sub-picosecond time-scales, showing the dynamics of excitations, e.g., in terms of phonons (lattice), magnons (magnetization), excitons (electrons), and phase transitions. This exciting progress requires extending our concepts of thermodynamics beyond classical and equilibrium regimes into the quantum and nonequilibrium domains. As a result, this dynamic and challenging research direction has emerged as a vibrant field of study. To shape this promising research direction, the upcoming winter school aims to bring together experts from the fields of non-equilibrium statistical physics as well as ultrafast dynamics under the umbrella of ultrafast thermodynamics.

Course structure

The winter school is divided in 1 week of on-site lectures (21 h), peer-discussions (5 h), poster preparation and presentation (14 h) as well as one week of self-study (40 h) with selected reading material. In selected cases (e.g. for Chalmers students) an additional oral seminar can serve as an examination.
The expected learning outcomes are a basic familiarity with the following topics:

- Classical and quantum stochastic thermodynamics
- Active crystals
- Stochastic dynamics in quantum materials
- Ultrafast electron spectroscopy
- Nanoscale thermodynamics and quantum transport
- Time-resolved magneto-optical spectroscopy

Selected reading material

The self-study is based on the following reading material, complementary to the lectures provided.

- Caprini, Lorenzo, et al."The entropy production of Ornstein–Uhlenbeck active particles: a path integral method for correlations." *Journal of Statistical Mechanics: Theory and Experiment* 2019.5 (2019): 053203.

- Caprini, Lorenzo, Hartmut Löwen, and R. Matthias Geilhufe. "Ultrafast entropy production in pump-probe experiments." *Nature Communications* 15.1 (2024): 94.

- Bossini, Davide, et al. "Magnetoelectrics and multiferroics: theory, synthesis, characterisation, preliminary results and perspectives for all-optical manipulations." *Journal of Physics D: Applied Physics* 56.27 (2023): 273001.

- K. Macieszczak, M. Guta, I. Lesanovsky, J. P. Garrahan, "Towards a Theory of Metastability in Open Quantum Dynamics", *Physical review letters* 116, 240404 (2016) .

- L. Tesser, J.Splettstoesser, "Out-of-Equilibrium Fluctuation-Dissipation Bounds", *arXiv preprint arXiv*:2309.17422 (2023).

- Aron, Camille, Giulio Biroli, and Leticia F. Cugliandolo. "(Non) equilibrium dynamics: a (broken) symmetry of the Keldysh generating functional." *SciPost Physics* 4.1 (2018): 008.

- Mikaelsson, Sara, et al. "A high-repetition rate attosecond light source for time-resolved coincidence spectroscopy." *Nanophotonics* 10.1 (2020): 117-128.

Lecturers

- **Davide Bossini**, Emmy Noether group leader at University of Konstanz
- **Katarzyna Macieszczak**, Assistant Professor at University of Warwick
- **Janine Splettstösser**, Professor at Chalmers University of Technology
- **Juliette Monsel**, Research Specialist at Chalmers University of Technology
- **Anne-Lise Viotti**, Assistant professor at Lund University
- **Camille Aron**, Visiting professor at École Polytechnique Fédérale de Lausanne, on sabbatical leave from École Normale Supérieure, CNRS
- **R. Matthias Geilhufe**, Assistant Professor at Chalmers University of Technology
- **Lorenzo Caprini**, Assistant Professor at University of Rome

Equality, diversity, and inclusion

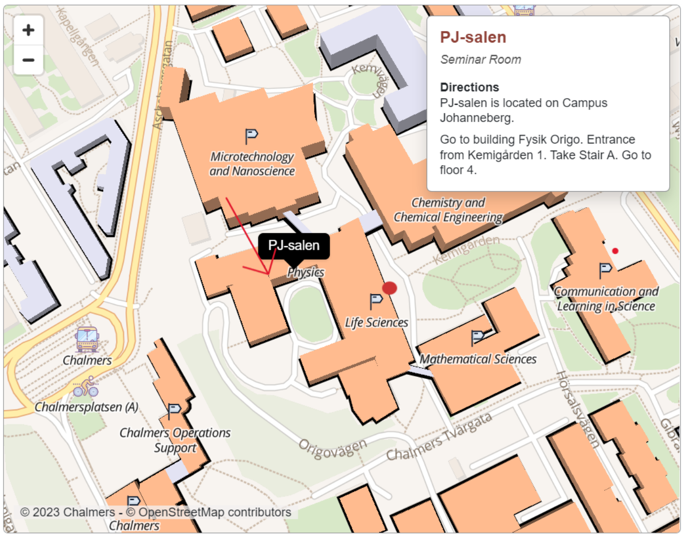
The winter school on Ultrafast thermodynamics is an international event. Diversity includes everyone, irrespective of gender, nationality, physical ability, religion, ethnicity, etc. Every participant is given equal opportunities to learn and always feel safe and included. As a participant it is your responsibility to respect and support diversity, equal opportunity, and inclusion. Any misconduct will result in an exclusion from the event.

Family room

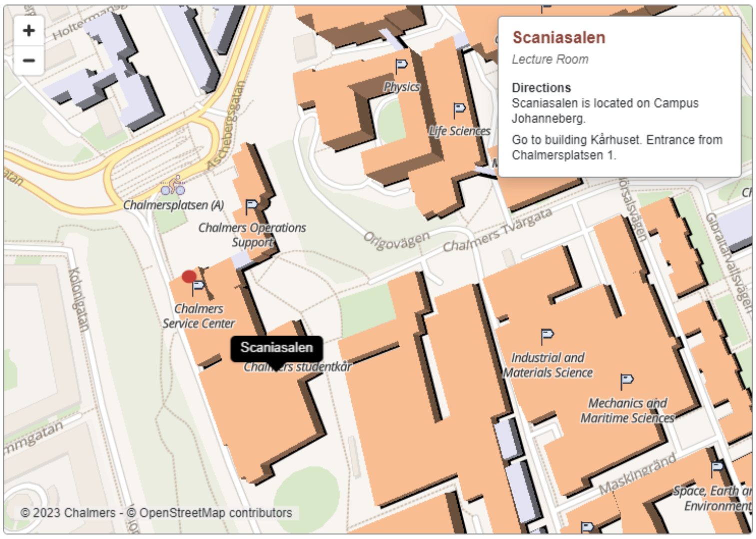
Chalmers is committed to increase the diversity among the participants of the winter school. As one example, we would like to mention the "family room" which might be relevant for young parents. Please contact the organizers if you would like to know more about this or other possible support measures.

Location

The lectures will take place in the PJ lecture hall on Johanneberg Campus. The closest entrance is marked with the red arrow on the map below.



The location of the poster session is Scania hall shown on the map below.



To find your way around Campus you may find this web page useful: https://maps.chalmers.se/. Alternatively, you can download Find Your Way on Campus app on App Store or GooglePlay.

Schedule

Monday, Feb 19th

09:00-09:30	Registration	PJ lecture hall
09:30-10:00	Introduction	PJ lecture hall
10:00-11:00	*Lorenzo Caprini* - Stochastic Thermodynamics and active crystals	PJ lecture hall
11:00-12:00	*Davide Bossini* - Ultrafast THz Spectroscopy	PJ lecture hall
12:00-14:00	Lunch	
14:00-15:00	*R. Matthias Geilhufe* - Ultrafast phononics	PJ lecture hall
15:00-16:00	*Katarzyna Macieszczak* - Metastability in Open Quantum Systems	PJ lecture hall

Tuesday, Feb 20th

10:00-11:00	*Davide Bossini* - Ultrafast THz Spectroscopy	PJ lecture hall
11:00-12:00	*Lorenzo Caprini* - Stochastic Thermodynamics and active crystals	PJ lecture hall
12:00-14:00	Lunch	
14:00-15:00	*Davide Bossini* - Ultrafast THz Spectroscopy	PJ lecture hall
15:00-16:00	*R. Matthias Geilhufe* - Ultrafast phononics	PJ lecture hall
17:00-20:00	Poster session	Scania hall

Wednesday, Feb 21st

10:00-11:00	*Lorenzo Caprini* - Stochastic Thermodynamics and active crystals	PJ lecture hall
11:00-12:00	*R. Matthias Geilhufe* - Ultrafast phononics	PJ lecture hall
12:00-14:00	Lunch	
14:00-15:00	*Janine Splettstösser* - Nanoscale thermodynamics - role of fluctuations	PJ lecture hall
15:00-16:00	*Anne-Lise Viotti* - Experimental methods for ultrafast photoelectrons	PJ lecture hall
16:00-17:00	*Katarzyna Macieszczak* - Metastability in Open Quantum Systems	PJ lecture hall

Thursday, Feb 22nd

10:00-11:00	*Anne-Lise Viotti* - Experimental methods for ultrafast photoelectrons	PJ lecture hall
11:00-12:00	*Janine Splettstösser* - Nanoscale thermodynamics - role of fluctuations	PJ lecture hall
12:00-14:00	Lunch	
14:00-15:00	*Anne-Lise Viotti* - Experimental methods for ultrafast photoelectrons	PJ lecture hall
15:00-16:00	*Camille Aron* - Introduction to Quantum Stochastic Thermodynamics	PJ lecture hall
17:00-20:00	Dinner speakers & organizers	

Friday, Feb 23rd

10:00-11:00	*Juliette Monsel* - Tutorial: Nanoscale thermodynamics	PJ lecture hall
11:00-12:00	*Camille Aron* - Introduction to Quantum Stochastic Thermodynamics	PJ lecture hall
12:00-14:00	Lunch	
14:00-15:00	*Janine Splettstösser* - Nanoscale thermodynamics - role of fluctuations	PJ lecture hall
15:00-16:00	*Camille Aron* - Introduction to Quantum Stochastic Thermodynamics	PJ lecture hall

Lecture abstracts

Introduction to stochastic thermodynamics: from single-particle dynamics to collective excitations

Lorenzo Caprini - University of Rome

Several physical or biological systems across different length scales are characterized by stochastic equations of motion dominated by fluctuations. At the micron-scale, this is the standard scenario for colloids and microswimmers, such as bacteria and Janus particles, but stochastic equations are common also at the nano-scale, for example to describe the effective dynamics of phonons. In these lectures, we review stochastic thermodynamics [1], i.e. the thermodynamics theory which applies to small systems governed by stochastic equations of motion. We discuss the concept of heat, work, and entropy production generated by a fluctuating trajectory and link these concepts with the standard thermodynamics theory describing macroscopic systems. After commenting on the stochastic version of the second thermodynamics law, we focus on theoretical tools to practically calculate entropy production and heat generated by stochastic dynamics. In particular, we focus on path-integral techniques that are discussed with several examples [2]. These theoretical tools allow us to calculate the energetics of single particles, such as colloids or microswimmers, but also heat and entropy production emerging from collective excitations, such as phonons driven by external forces. Within our theory, we also investigate and interpret the collective excitations of active solids, i.e. crystals consisting of particles intrinsically out of equilibrium that continuously consume energy and thus generate entropy on their own. In the absence of external forces, the spectrum of active solids is formed by the superposition of standard phonons with thermal origin and additional, collective excitations with non-equilibrium origin. These second excitations are called entropons because each of them represents a mode of the spectral entropy production of the system [3].

Introduction on stochastic thermodynamics [1]

-Introduction on stochastic thermodynamics: the role of fluctuations.
-Stochastic Langevin equation and Brownian motion. Examples: colloids and bacteria at the micron-scale, but also effective dynamics of phonons at the nanoscale scales.
-Heat, work and entropy production. Connection with standard thermodynamics.
-Entropy production of the medium and entropy production of the system.

-Second law of thermodynamics in stochastic thermodynamics.

Path-integral techniques and stochastic thermodynamics [2]

-Path-integral techniques: how can we calculate entropy production in stochastic systems?
-Examples of entropy production: Brownian particles subject to an external driving force.
-Path-integral in Fourier space: spectral entropy production.

Active systems and novel collective excitations producing entropy [3]

-Brief Introduction on active matter: systems that produce entropy by their own.
-Active crystals: crystals consisting of active particles.
-Entropy production in active crystals.
-Harada Sasa relation and novel collective excitations in active crystals

Literature:
[1] U Seifert, *Reports on progress in physics* 75 (12), 126001, 3129, (2012)
[2] L Caprini, UMB Marconi, A Puglisi, A Vulpiani, *Journal of Statistical Mechanics: Theory and Experiment*, 2019 (5), 053203, (2019)
[3] (Letter): L Caprini, U Marini Bettolo Marconi, A Puglisi, H Löwen. *The Journal of Chemical Physics* 159 (4), (2023), (Long paper): L Caprini, UMB Marconi, H Löwen. *Physical Review E* 108 (4), 044603, (2023)

Ultrafast spin dynamics

Davide Bossini - University of Konstanz

Lecture 1: Fundamentals of spin dynamics in magnetic materials

In my first lecture I will address the basic aspects of collective spin dynamics in magnetic solids. In particular, I will introduce the concept of spin wave, or magnon, deriving the dispersion relation in both a classical and quantum mechanical formalism. A discussion of the main approximations and limitations of linear spin wave theory and of the semiclassical Landau-Lifschitz-Gilbert equations of motion will conclude this lecture.

Literature:
[1] J. Stöhr, H.C. Siegmann *Magnetism: From Fundamentals to Nanoscale Dynamics,* Springer
[2] C. Kittel *Introduction to solid state physics,* Wiley John & sons

[3] C. Kittel *Quantum theory of solids,* Wiley

Lecture 2: Excitation and detection mechanisms of ultrafast collective spin dynamics

The second lecture will provide an introduction to the main processes allowing to drive and detect collective magnetic excitations, in particular in a coherent fashion. I will first discuss resonant mechanisms, such as the Zeeman torque, magnetoelastic coupling and exciton-magnon transition. The non-resonant approach, based on inelastic lightscattering, will be then extensively discussed. I will also comment on the applicability of all these excitation mechanisms to magnons both in the center and near the edges of the Brillouin zone. In conclusion, I will derive the key connection between the optical excitation of spins ("opto-magnetism") and the optical detection of spins ("magnetooptics"), showing that do share the same microscopic origin.

Literature:
[1] P.A. Fleury and R. Loudon *Phys. Rev.* 166, 514 (1968).
[2] T. Moriya, Y. Tanabe and S. Sugano *Phys. Rev. Lett.* 15, 1023 (1965)
[3] R. Loudon *Advances in Physics* 17, 243 (1968).

Lecture 3: Experimental state-of-the-art and perspectives

In the final lecture I will first briefly describe the experimental methods required to investigate ultrafast spin dynamics. Subsequently I will show how these techniques have been employed to demonstrate and implement the theoretical concepts introduced during the first two lectures. A discussion of some open fundamental questions and possible future research directions will conclude my series of lectures..

Literature:
[1] A. Kirilyuk et al *Rev. Mod. Phys.* 82, 2731 (2010).
[2] D. Bossini and Th. Rasing *Phys. Scripta* 92, 024002 (2017).
[3] P. Nemec et al *Nature Physics* 14, 229 (2018).
[4] D. Bossini et al *J. Phys. D. Appl. Phys.* 56, 273001 (2023).

Ultrafast phononics

R. Matthias Geilhufe - Chalmers University of Technology

Phonons are collective excitations of the crystalline lattice. Using THz laser pulses, individual phonon modes can be excited in a controlled manner, opening the perspective of tuning material properties on ultrashort time-scales. I will give an introduction into the classical equations of motion describing phonons in strong electric fields [1]. I will continue by introducing chiral phonons and phonon angular momentum and discuss the induction of magnetism in the context of ultrafast phonomagnetism [2-3]. Finally, I will discuss the ultrafast thermodynamics of phonons [4]. Here, we discuss phonons in the presence of a stochastic noise and use stochastic thermodynamics to describe the entropy production of laser driven optical phonons.

Literature:

[1] W. Hergert, R. M. Geilhufe, *Group Theory in Solid State Physics and Photonics: Problem Solving with Mathematica*, Wiley-VCH, (2018)
[2] R. M. Geilhufe, *et al.*, *Phys. Rev. Research*, 3, L022011, (2021)
[3] R. M. Geilhufe, W. Hergert, *Phys. Rev. B*, 107, L020406, (2023)
[4] L. Caprini, H. Löwen, R. M. Geilhufe, *Nat. Commun.*, 15, 94 (2024)

Metastability in Open Quantum Systems

Katarzyna Macieszczak - University of Warwick

In these lectures, we will be exploring Markovian open quantum system focusing on the dynamical phenomenon of timescale separation known as metastability, which, among others, arises in proximity to dissipative phase transitions. After familiarising ourselves with master equations governing such systems, we will learn about conditions needed for the metastability to occur in their dynamics and how their long-lived states can be uncovered in numerical simulations. We will then discuss how those states could be analysed in terms of classical and quantum degrees of freedom and what experimental signatures follow from that characterisation. We will finish by considering possible applications of metastability in quantum technologies.

Literature:

[1] K. Macieszczak, M. Guta, I. Lesanovsky, J. P. Garrahan, *Phys. Rev. Lett.* 116, 240404 (2016)

Nanoscale thermodynamics - the role of fluctuations

Janine Splettstösser - Chalmers University of Technology

One of the main differences in the thermodynamic description of small-scale devices compared to their macroscopic counterparts lies in the role of fluctuations. While macroscopic systems are often well described by observable averages, the fluctuation in small-scale devices can be of the same importance as the actual expectation value. To cast the properties of fluctuations, fluctuation theorems are a powerful tool. This lecture set will reach from a short introduction to equilibrium fluctuation theorems to out-of-equilibrium fluctuation relations. I will highlight famous and topical relations like the Crooks fluctuation theorem and the Jarczinsky equality as well as the thermodynamic uncertainty relation. I will show how such fluctuation relations are impacted when considering nonequilibrium, quantum effects and information.

Literature:

[1] L. Tesser, J.Splettstoesser, *arXiv preprint arXiv*:2309.17422 (2023).

Tutorial session: Nanoscale thermodynamics - the role of fluctuations

Juliette Monsel - Chalmers University of Technology

In this session, you will gain hands-on experience and put into practice the notions and concepts about fluctuations in nanoscale systems learned during the lesson. You will receive an exercise sheet and some exercises will be covered during the session. The solutions to all the exercises will be handed out at the end.

Experimental methods for ultrafast photoelectrons

Anne-Lise Viotti - Lund University

Following our human intuition, small things are fast and big things are slow. Thus, to understand and explore our world from its smallest parts, scientist often look at electrons, particles that move on the time scale of attoseconds. We are currently able to produce light pulses with similar temporal durations, the so-called attosecond pulses (very popular now after the Nobel Prize in Physics 2023), which are produced by state-of-the-art high-intensity laser systems.

What is the point though of being able to generate absurdly short light pulses? Measuring electron dynamics, such as the initial steps during the formation or the break of a chemical bound, will maybe one day lead to the possibility of controlling such an important biological process. One can also study more fundamental questions by

entering the realm of quantum mechanics where electrons behave like waves, can be in different places at once, can be entangled and correlated in non-intuitive ways.
Easier to grasp is maybe the opportunity to develop the next-generation transistors, the miniaturized building blocks of our laptops and smartphones. By creating nanometer scale structures we can fit billions of such devices in our pockets. However, those nanostructures are so small that a conventional light microscope will only offer blurry images in which all the interesting information is hidden. Thus, one usually turns to electron microscopy instead to form images.
In this series of three lectures, heavily oriented towards experimental tools and instruments, we will look first at ultrafast light sources, which are essential for studying fast moving electrons. An overview of the ultrafast lasers landscape will be presented, together with a short introduction to attosecond pulse generation. In a second time, we will focus on experimental methods to explore the process of photoionization in a spectroscopic manner and with up to attosecond time resolutions. And finally, we will think about how we can create high-resolution images of nanostructures using electrons and how we can follow ultrafast mechanisms in such materials manipulated at the nanoscale. In the end, everything is about understanding how light interacts with matter!

Literature:

[1] H. Fattahi, H. G. Barros, and M. Gorjan et al. *Optica* 1(1), 45–63 (2014).
[2] Rocío Borrego-Varillas et al *Rep. Prog. Phys.* 85 (6): 066401 (2022).
[3] M. Isinger et al., *Science* 358(6365), 893-896 (2017).
[4] Schmidt, O., Bauer, M., Wiemann, C. et al. *Appl Phys B* 74, 223–227 (2002).

Introduction to Quantum Stochastic Thermodynamics

Camille Aron - EPFL

Stochastic thermodynamics, which analyzes quantities such as heat, work, and entropy production at the level of individual trajectories, has achieved a solid understanding in classical systems. However, delving into the quantum realm poses intriguing challenges, especially given the absence of a straightforward notion of trajectory. These lectures aim to bridge the classical and quantum worlds, offering insights into the field of quantum stochastic thermodynamics and its implications for experimental platforms in cold-atom and quantum-optic physics.

Lecture 1: Introduction to Lindblad Master Equation

-Challenges of extending classical stochastic thermodynamics to the quantum domain.
-Introduction to the Lindblad master equation for studying the dynamics of open quantum systems.
-Discussion of its relevance in various experimental platforms.

Lecture 2: Continuously Monitoring Quantum Trajectories

-Continuous monitoring of a quantum system and its interpretation in terms of quantum trajectories.
-Post-selection protocols and their role in effectively modifying the quantum dynamics.
-Stochastic thermodynamics on quantum trajectories.

Lecture 3: Quantum Stochastic Thermodynamics via Feynman Path Integrals

-Feynman-Keldysh path-integral representation of quantum dynamics.
-Fundamental symmetry of thermal equilibrium dynamics and fluctuation-dissipation theorem.
-Non-equilibrium dynamics, symmetry breaking, and quantum fluctuation relations.
