Foundations and applications of non-equilibrium statistical mechanics

1. Non-equilibrium statistical mechanics

For systems that are in equilibrium with their environment, the knowledge of a small set of parameters characterizing it (temperature, pressure, etc) is sufficient to fully specify the statistical and thermodynamic properties of the system. Under out-of-equilibrium conditions, a description of such generality is not available, basically because the system state depends on the coupling with the environment (e.g. the heath baths), and on the details of the system dynamics. As a consequence, there is no straightforward generalization of the equilibrium thermodynamical potentials describing the state probability distribution of a system out of equilibrium, nor a conclusive understanding of how non-equilibrium phenomena emerge out of the underlying microscopic dynamics.

Nowadays it is clear that molecular fluctuations play a fundamental role in the understanding of systems out of equilibrium, and in recent years some relations of surprising general validity have been derived. These statements are categorized into fluctuation theorems, two remarkable examples being the Gallavotti–Cohen relation and the Jarzynski relation. Their study has developed into a new independent line of research in statistical mechanics. The results thus obtained are distinguished by two common features. Firstly, they are valid even if the system is driven far away from equilibrium. Secondly, they usually connect properties of equilibrium states with the non-equilibrium behaviour of the system.

Whereas most of the studies on fluctuation theorems concentrate on transitions between equilibrium states (during which the system is driven away from equilibrium), a few results have also been obtained for the more general case of transitions between non-equilibrium steady states. In such theories, non-equilibrium steady states are characterized by the flow of stationary currents, in contrast to equilibrium states which are defined by the absence of any currents. This is an extremely active area of research in non-equilibrium statistical physics as well, with manifold applications in biophysics. There are only a few cases where the state or the current probability distribution of out-of-equilibrium systems have been obtained explicitly, mainly for one-dimensional systems. Such explicit solutions provide a valuable means for detailed studies of non-equilibrium features.

A further trend in statistical physics, complementary to the basic research just described, consists in applying methods and techniques from statistical physics to biology or biological-motivated problems. This includes the modelling and analysis of molecular processes in the cell, the development of new methods for interpreting the huge amount of data produced in bioinformatic problems, the modelling of population dynamics or whole ecosystems, and the study of artificial molecular machines. In particular, the biophysical research on the level of single molecules has profited greatly from the increased understanding of fluctuations in non-equilibrium processes. For instance, as an immediate and promising application, the above mentioned work relations are exploited to extract useful equilibrium information from non-equilibrium measurements: the equilibrium mechanical properties of individual bio-molecules can be reconstructed from dynamical single-molecule experiments (e.g. pulling experiments) in the form of free energy landscapes.

2. The scientific programme

Between 19 September and 14 October 2011, the Nordic Institute for Theoretical Physics hosted the scientific programme *Foundations and Applications of Non-Equilibrium Statistical Mechanics* in Stockholm, Sweden. The programme was centred around modern developments in non-equilibrium statistical mechanics with respect to both fundamental aspects, such as fluctuation theorems, entropy production, fluctuation–dissipation theorems, and applications, such as noise-induced phenomena and biophysical problems, to mention but a few. With this aim, the programme was structured in four different weekly focal points:

- fluctuation theorems and work relations;
- transport phenomena;
- exactly solvable models;
- applications.

It attracted over 90 participants, amongst them world-leading experts in the field of non-equilibrium statistical physics, as well as several PhD students and young postdocs.

Motivated by the success of this scientific programme, we present here 16 contributed comments on the physics of non-equilibrium systems.

2.1. Sponsors

This scientific programme and the 16 contributions presented here were made possible by the financial and administrative support of the Nordic Institute for Theoretical Physics (NORDITA) and by the financial support of the European Science Foundation (ESF) through the Research Network 'Exploring the Physics of Small Devices'.

2.2. Invited lectures

1. Tobias Ambjörnson, Lund University, Sweden
   First-passage times for single-file diffusion and fractional Langevin dynamics
2. Felipe Barra, University of Chile, Chile
   Conductance of quasi one-dimensional periodic systems and current in a one-dimensional non equilibrium quantum system
3. Cedric Bernardin, ENS Lyon, France
   Anomalous diffusion for a class of Hamiltonian systems with two conserved quantities
4. Sergio Ciliberto, ENS Lyon, France
   Heat flux and the violation of fluctuation dissipation theorem during aging
5. David Dean, University Paul Sabatier, France
   Out of equilibrium fluctuation induced forces
6. Bernard Derrida, ENS, France
   Current fluctuations in non-equilibrium systems
7. Abhishek Dhar, Raman Research Institute, India
   Large deviation functions and fluctuation theorems in heat transport
8. Andreas Engel, University of Oldenburg, Germany
   Asymptotics of work distributions in Langevin systems
9. Massimiliano Esposito, Université Libre de Bruxelles, Belgium
   Nonequilibrium fluctuations and thermodynamics for electron transport through small devices
10. Denis Evans, Australian National University, Australia
    Dissipation and the foundations of classical statistical mechanics
11. Martin Evans, University of Edinburgh, UK
    Diffusion with stochastic resetting
12. Pierre Gaspard, Université Libre de Bruxelles, Belgium
    Microreversibility, current fluctuations, and nonlinear responses in nonequilibrium systems

13. Giacomo Gradenigo, National Institute of Nuclear Physics, Italy
Fluctuating hydrodynamics for a driven granular fluid: out of equilibrium correlations
14. Giovanni Jona-Lasinio, National Institute of Nuclear Physics, Italy
Lagrangian phase transitions in nonequilibrium thermodynamic systems
15. Ryoichi Kawai, University of Alabama at Birmingham, AL, USA
Physics and information theory: Landauer's principle and beyond
16. Anatoly Kolomeisky, Rice University, TX, USA
Mechanisms of formation of signaling molecules concentration profiles
17. Joachim Krug, University of Cologne, Germany
Record statistics in time series with drift: theory and applications
18. Jorge Kurchan, ESPCI, France
An infinite set of second law-like inequalities
19. David Lacoste, ESPCI, France
Modified fluctuation–dissipation theorem near non-equilibrium states and applications
20. Vivien Lecomte, University of Paris VII, France
Current fluctuations: mapping non-equilibrium to equilibrium
21. Raphael Lefevere, University of Paris VII, France
Large deviations of the current in collisional dynamics
22. Stefano Lepri, CNR Institute for Complex Systems, Italy
A stochastic model of anomalous heat conduction
23. Michael A Lomholt, University of Southern Denmark, Denmark
Motion in an ageing environment
24. Jani Lukkarinen, University of Helsinki, Finland
Nonequilibrium stationary states of harmonic chains with bulk noises
25. Michael Lässig, University of Cologne, Germany
Heat flux and the violation of fluctuation dissipation theorem during aging
26. Christian Maes, Katholieke Universiteit Leuven, Netherlands
Nonequilibrium heat capacities
27. Bernhard Mehlig, University of Gothenburg, Sweden
Metapopulation dynamics
28. Ralf Metzler, TU Munich, Germany
Single particle trajectories and time averages in ageing systems with weak ergodicity breaking
29. Namiko Mitarai, Niels Bohr Institute, Denmark
Ecosystems with mutually exclusive interactions
30. David Mukamel, Weizmann Institute, Israel
Long-range correlations in driven, nonequilibrium systems
31. Gleb Oshanin, LPTMC, France
Mean first passage times: meaningful or meaningless?
32. Tomaz Prosen, University of Ljubljana, Slovenia
Exact nonequilibrium steady state of a strongly driven open XXZ chain
33. Peter Reimann, University of Bielefeld, Germany
Equilibration and thermalization under realistic preparation and measurement conditions
34. Felix Ritort, University of Barcelona, Spain
Recent advances in free energy recovery of molecular structures
35. Lamberto Rondoni, Turin Polytechnic, Italy
Initial growth of Boltzmann entropy and chaos in a large assembly of weakly interacting systems
36. Keiji Saito, University of Tokyo, Japan
Additivity principle in high-dimensional deterministic systems
37. Shin-Ichi Sasa, University of Tokyo, Japan
Thermodynamic formula for the cumulant generating function of time-averaged current
38. Udo Seifert, University of Stuttgart, Germany
Stochastic thermodynamics of non-equilibrium steady states: from the FDT to efficient nano-machines

39. Ken Sekimoto, ESPCI, France
    Momentum transfer in non-equilibrium steady states
40. Herbert Spohn, TU Munich, Germany
    The motion of 1D driven interfaces: exact solutions of the KPZ equation
41. Peter Talkner, University of Augsburg, Germany
    Quantum fluctuation theorems
42. Christophe Texier, University of Paris-Sud 11, France
    Sinai diffusion with weakly concentrated absorbers
43. Frederic van Wijland, University of Paris Diderot, France
    Field theoretic formulation of a mode coupling equation for colloids
44. Pascal Viot, LPTMC, France
    Asymmetric granular motors: does the ratchet effect persist in the presence of friction?
45. Angelo Vulpiani, National Institute of Nuclear Physics, Italy
    On anomalous diffusion and the out of equilibrium response function in one-dimensional models

2.3. List of participants

- Paolo Adamo, Turin Polytechnic, Italy.
- Mikko Alava, Aalto University, Finland.
- Tobias Ambjörnson, Lund University, Sweden.
- Erik Aurell, KTH, Sweden.
- Felipe Barra, University of Chile, Chile.
- Cedric Bernardin, ENS Lyon, France.
- Stefano Bo, University of Torino, Italy.
- Eliran Boksenbojm, Katholieke Universiteit Leuven, Belgium.
- Giulio Casati, University of Insubria, Italy.
- Sergio Ciliberto, ENS Lyon, France.
- Matteo Colangeli, Turin Polytechnic, Italy.
- Wojciech De Roeck, University of of Heidelberg, Germany.
- David Dean, University Paul Sabatier, France.
- Bernard Derrida, ENS, France.
- Abhishek Dhar, Raman Research Institute, India.
- Irene Donato, Turin Polytechnic, Italy.
- Ralf Eichhorn, Nordita, Sweden.
- Andreas Engel, University of Oldenburg, Germany.
- Massimiliano Esposito, Université Libre de Bruxelles, Belgium.
- Denis Evans, Australian National University, Australia.
- Martin Evans, University of Edinburgh, UK.
- Hans Fogedby, University of Aarhus, Denmark.
- Pierre Gaspard, Université Libre de Bruxelles, Belgium.
- Natalia Golubeva, University of Aarhus, Denmark.
- Mieke Gorissen, Hasselt University, Belgium.
- Giacomo Gradenigo, National Institute of Nuclear Physics, Italy.
- Jordan Horowitz, Complutense University, Spain.
- Alberto Imparato, University of Aarhus, Denmark.
- Stefano Iubini, University of Florence , Italy.
- Giovanni Jona-Lasinio, National Institute of Nuclear Physics, Italy.
- Christian Karlewski, University of Bielefeld, Germany.
- Ryoichi Kawai, University of Alabama at Birmingham, AL, USA.
- Anatoly Kolomeisky, Rice University, TX, USA.
- Supriya Krishnamurthy, Stockholm University, Sweden.
- Joachim Krug, University of Cologne, Germany.
- Anupam Kundu, International Centre for Theoretical Sciences, India.
- Antti Kupiainen, University of Helsinki, Finland.
- Jorge Kurchan, ESPCI, France.
- David Lacoste, ESPCI, France.
- Vivien Lecomte, University of Paris VII, France.
- Raphael Lefevere, University of Paris VII, France.

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- Jani Lukkarinen, University of Helsinki, Finland.
- Michael Lässig, University of Cologne, Germany.
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- Oksana Manyuhina, Nordita, Sweden.
- Thiago Mattos, Max-Planck-Institute for Intelligent Systems, Germany.
- Bernhard Mehlig, University of Gothenburg, Sweden.
- Carlos Mejia-Monasterio, University of Helsinki, Finland.
- Ralf Metzler, TU Munich, Germany.
- Namiko Mitarai, Niels Bohr Institute, Denmark.
- David Mukamel, Weizmann Institute, Israel.
- Paolo Muratore-Ginanneschi, University of Helsinki, Finland.
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- Daniel Nickelsen, University of Oldenburg, Germany.
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- Ivan Georg Szendro Teran, University of Cologne, Germany.
- Peter Talkner, University of Augsburg, Germany.
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