Scientific report

Foundations and Applications of Non-Equilibrium Statistical Mechanics

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Timeslot

from 19 September 2011 to 13 October 2011

Summary

The meeting "Foundations and Applications of Non-Equilibrium Statistical Mechanics" was organized as a Nordita scientific program. A Nordita scientific program is an extended workshop where a limited number of scientists work together on specific topics for a period of 4 to 6 weeks. This program was centered around modern developments in non-equilibrium statistical mechanics both with respect to fundamental aspects as well as applications, and covered 4 weeks of intensive program activities. The main objective was to create a lively and fruitful atmosphere of intensive research and mutual interactions between the participants. Accordingly, we typically had about 3 talks on recent results and developments in a morning session, while the afternoon was reserved for discussion sessions and related project work. This setup attracted over 90 participants, amongst them world-leading experts in the field of non-equilibrium statistical physics, but also a number of PhD students and young postdocs (see Appendix B).

Scientific content

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 properties of the system. Out of equilibrium, 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 nonequilibrium 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: First, they are valid even if the system is driven far away from equilibrium. Second, they usually connect properties of equilibrium states with the non-equilibrium behavior 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. The latter 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 biological or biology-motivated problems. This includes the modeling and analysis of molecular processes in the cell, the developments of new methods for interpreting the huge amount of data produced in bioinformatic problems, the modeling of population dynamics or whole ecosystems, but also the study of artificial molecular machines. In particular the biophysical research on the level of single molecules has profited a lot 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 form of free energy landscapes.

The scientific program was centered around these modern developments in statistical

physics and covered a broad spectrum of topics ranging from fundamental questions to application of statistical mechanics methods to the modeling of ecosystems.

In order to provide a certain level of structuring, we chose "focus themes" for the four different weeks of the program, so that talks, discussions and meetings were primarily around that theme, see Table 1 and also Appendix A.

First week	Fluctuation theorems and work relations
Second week	Transport phenomena
Third week	Exactly solvable models
Fourth week	Applications

Table 1: Focus themes for the different weeks of the program.

The topics covered within the four weeks of the program are well summarized by the following keywords: the second law (extensions to non-equilibrium), entropy production away from equilibrium, fluctuation theorems, fluctuation-dissipation relations properties of non-equilibrium steady states, reconstruction of free energy landscapes, transport away from equilibrium, response behavior to external perturbations, fluctuation induced phenomena, quantum work relations, diffusion under non-equilibrium conditions, large deviation functions, granular motors, information theory, evolutionary biology, population dynamics.

As already mentioned strong emphasis was on informal discussion and working group meetings. This concept worked extremely well. Usually, people started to continue discussing open problems and new ideas already during lunch, and the discussions continued the whole afternoon. This lively exchange between the participants as well as the possibility to immediately work out new ideas in some detail was supported by Nordita in providing office space with whiteboards, internet connection, printing facilities. Moreover, the participants had access to several seminar rooms, which have been used for discussions in small groups of 5-10 persons. These discussions were typically around the topics of the talks during the morning, going much more into detail as it would be possible during a talk, and around questions and problems which were mentioned in these talks or which resulted from critical queries from the audience. Additionally, other recent publications of the speakers and participants were often subject of discussions, so that topics and important results beyond the specific talks were examined as well. Although these discussions were typically led by senior scientists, also younger colleagues were involved and actively participating. In this way, they could introduce their research on the whiteboard to the experts in the field, even if not having had the possibility to talk as an invited speaker.

Assessment of the results

We think that this meeting was very fruitful and successful. The presentations covered a wide spectrum of topics in non-equilibrium statistical mechanics and its applications, in particular to biophysical problems. Concerning the quality of presentation and of the scientific work, the overwhelming majority of the contributions were well beyond the "average" one is used to from other large conferences. Therefore, the participants could gain a comprehensive overview of the state-of-the-art in the field.

However, a large part of the success of the meeting is due to the discussion sessions in the afternoon. The resonance of the participants on that concept was very enthusiastic and positive. In an evaluation, which Nordita performs as a standard procedure after a workshop in order to improve quality, participants called this meeting "one of the best in statistical physics they ever attended" (the results of the evaluation may be provided upon request). During the workshop it was mentioned that open problems could be solved as a result from the interaction between participants, and that new collaborations were initiated.

Motivated by the success of the meeting we, the organizers, have evaluated the possibility of publishing proceedings-type articles in a peer-reviewed journal in order to summarize, review and critically discuss the research topics covered during the program. We found such a possibility in the Comments section of Physica Scripta (IOP Science), where current thinking of leading researchers on outstanding problems, discussion of open questions, important new applications, new theoretical or experimental approaches, or predictions of future developments are published. We believe that this constitutes a perfect platform for summarizing our Nordita program. Projecting the responses of the participants, we got so far concerning a contribution to this collection of Comments, we expect that around 15 articles will be published as a direct outcome of this meeting.

Furthermore, during the Nordita program several manuscript have been finalized or initiated:

1. D J Evans, S R Williams, D J Searles
   On the entropy of relaxing deterministic systems
   J. Chem. Phys. 135, (2011) 194107

2. E Aurell, C Mejia-Monasterio, P Muratore-Ginanneschi
   Boundary layers in stochastic thermodynamics
   arXiv:1111.2876

3. H Fogedby, A Imparato
   Heat flow in driven chains
   arXiv:1112.3945v1 (submitted to J. Stat. Mech.)

4. D Boyer, D Dean, C Mejia-Monasterio, G Oshanin
   Single particle trajectories - making the most out of bad statistics
   (submitted to PNAS)

5. C Mejia-Monasterio, P Muratore-Ginanneschi
   A non-perturbative renormalization group study of the stochastic
   Navier-Stokes equation
   (to be submitted to PRE)

6. T Mattos, C Mejia-Monasterio, G Oshanin
   Geometrical effects on the first passage times in bounded domains
   (to be submitted to JSTAT)

7. S Bo, E Aurell, R Eichhorn, A Celani
   Optimal stochastic transport in general diffusive media
   (to be submitted to EPL)

Remarks on the budget

When applying for funding of the meeting at ESF, we mentioned that Nordita has already granted 230,000 SEK (ca. 24,700 EUR) (for travel of about 25 speakers, program dinners, receptions and other social activities), and that housing will be provided for up to 20 participants at a time. The total expenditure as well as the contribution by Nordita (co-sponsorship) as indicated in the online form are considerably higher than the numbers given in the original proposal, because the expenses for accommodation are explicitly included.

The amount given as "local administrative costs" mainly covers the rent for seminar rooms, which we needed to book in the main AlbaNova building (in the immediate neighborhood of the Nordita main building), because the number of participants exceeded the capacity of the Nordita seminar room.

The Scientific Organizers

Ralf Eichhorn, Alberto Imparato, Hans Fogedby, Carlos Mejia-Monasterio

Appendix A: Program of the meeting

Appendix B: List of participants

NORDITA

FOUNDATIONS AND APPLICATIONS OF NON-EQUILIBRIUM STATISTICAL MECHANICS

19 September — 14 October 2011

TIMETABLE

Monday, 19 September 2011

10:00 - 10:15   **Welcome and Opening Remarks**
(FA32, AlbaNova)

10:15 - 11:00   *Denis Evans*
Dissipation and the foundations of classical statistical mechanics
(FA32, AlbaNova)

11:00 - 11:45   *Peter Talkner*
Quantum fluctuation theorems
(FA32, AlbaNova)

Tuesday, 20 September 2011

10:00 - 10:45   *Sergio Ciliberto*
Heat flux and the violation of Fluctuation Dissipation theorem during aging
(Nordita Seminar Room (132:028))

10:45 - 11:30   *Michael Lässig*
The arrow of time in evolutionary biology
(Nordita Seminar Room (132:028))

Wednesday, 21 September 2011

10:00 - 10:45   *Udo Seifert*

Stochastic thermodynamics of non-equilibrium steady states: From the FDT to efficient nano-machines
(Nordita Seminar Room (132:028))

10:45 - 11:30   *Frederic Van Wijland*

Field theoretic formulation of a mode coupling equation for colloids
(Nordita Seminar Room (132:028))

Thursday, 22 September 2011

10:00 - 10:45   *Bernard Derrida*

Current fluctuations in non-equilibrium systems
(Nordita Seminar Room (132:028))

10:45 - 11:30   *Felix Ritort*

Recent advances in free energy recovery of molecular structures
(Nordita Seminar Room (132:028))

14:00 - 14:45   *Peter Reimann*

Equilibration and thermalization under realistic preparation and measurement conditions
(Nordita Seminar Room (132:028))

Friday, 23 September 2011

10:00 - 10:45   *Andreas Engel*

Asymptotics of work distributions in Langevin systems
(Nordita Seminar Room (132:028))

10:45 - 11:30   *Ryoichi Kawai*

Physics and Information Theory: Landauer's principle and beyond
(Nordita Seminar Room (132:028))

Monday, 26 September 2011

10:00 - 10:45   *Jorge Kurchan*

An infinite set of Second Law-like inequalities
(Nordita Seminar Room (132:028))

10:45 - 11:30   *Lamberto Rondoni*

Initial growth of Boltzmann entropy and chaos in a large assembly of weakly interacting systems

(Nordita Seminar Room (132:028))

14:00 - 14:45   *Angelo Vulpiani*

On anomalous diffusion and the out of equilibrium response function in one-dimensional models

(Nordita Seminar Room (132:028))

Tuesday, 27 September 2011

10:00 - 10:45   *Herbert Spohn*

The motion of 1D driven interfaces: exact solutions of the KPZ equation

(Nordita Seminar Room (132:028))

10:45 - 11:30   *Christian Maes*

Nonequilibrium heat capacities

(Nordita Seminar Room (132:028))

14:00 - 14:45   *Gleb Oshanin*

Mean first passage times: Meaningful or meaningless?

(Nordita Seminar Room (132:028))

Wednesday, 28 September 2011

10:00 - 10:45   *Shin-Ichi Sasa*

Thermodynamic formula for the cumulant generating function of time-averaged current

(Nordita Seminar Room (132:028))

10:45 - 11:30   *Pierre Gaspard*

Microreversibility, current fluctuations, and nonlinear responses in nonequilibrium systems

(Nordita Seminar Room (132:028))

14:00 - 14:45   *David Dean*

Out of equilibrium fluctuation induced forces

(Nordita Seminar Room (132:028))

15:00 - 15:45   *Ken Sekimoto*

Momentum transfer in non-equilibrium steady states

(Nordita Seminar Room (132:028))

Thursday, 29 September 2011

10:00 - 10:45   *Giovanni Jona-Lasinio*

Lagrangian phase transitions in nonequilibrium thermodynamic systems

(Nordita Seminar Room (132:028))

10:45 - 11:30   *Keiji Saito*

Additivity Principle in High-dimensional Deterministic Systems

(Nordita Seminar Room (132:028))

14:00 - 14:45   *Abhishek Dhar*

Large deviation functions and fluctuation theorems in heat transport

(Nordita Seminar Room (132:028))

Friday, 30 September 2011

10:00 - 10:45   *Stefano Lepri*

A stochastic model of anomalous heat conduction

(Nordita Seminar Room (132:028))

10:45 - 11:30   *Massimiliano Esposito*

Nonequilibrium fluctuations and thermodynamics for electron transport through small devices

(Nordita Seminar Room (132:028))

Monday, 3 October 2011

10:00 - 10:45   *Tobias Ambjörnsson*

First-passage times for single-file diffusion and fractional Langevin dynamics

(Nordita Seminar Room (132:028))

10:45 - 11:30   *Cedric Bernardin*

Anomalous diffusion for a class of Hamiltonian systems with two conserved quantities

(Nordita Seminar Room (132:028))

Tuesday, 4 October 2011

10:00 - 10:45   *Anatoly Kolomeisky*

Mechanisms of Formation of Signaling Molecules Concentration

Profiles
(Nordita Seminar Room (132:028))

10:45 - 11:30   *Joachim Krug*

Record statistics in time series with drift: Theory and applications
(Nordita Seminar Room (132:028))

Wednesday, 5 October 2011

10:00 - 10:45   *Vivien Lecomte*

Current fluctuations: mapping non-equilibrium to equilibrium
(Nordita Seminar Room (132:028))

10:45 - 11:30   *Jani Lukkarinen*

Nonequilibrium Stationary States of Harmonic Chains with Bulk Noises
(Nordita Seminar Room (132:028))

Thursday, 6 October 2011

10:00 - 10:45   *Pascal Viot*

Asymmetric granular motors: Does the ratchet effect persist in the presence of friction?
(Nordita Seminar Room (132:028))

10:45 - 11:30   *Tomaz Prosen*

Exact nonequilibrium steady state of a strongly driven open XXZ chain
(Nordita Seminar Room (132:028))

Friday, 7 October 2011

10:00 - 10:45   *Martin Evans*

Diffusion with stochastic resetting
(Nordita Seminar Room (132:028))

10:45 - 11:30   *Raphael Lefevere*

Large deviations of the current in collisional dynamics
(Nordita Seminar Room (132:028))

Monday, 10 October 2011

10:00 - 10:45   *Michael A. Lomholt*

Motion in an aging environment
(Nordita Seminar Room (132:028))

10:45 - 11:30   *Namiko Mitarai*

Ecosystems with mutually exclusive interactions
(Nordita Seminar Room (132:028))

Tuesday, 11 October 2011

10:00 - 10:45   *David Lacoste*

Modified fluctuation-dissipation theorem near non- equilibrium states and applications
(Nordita Seminar Room (132:028))

10:45 - 11:30   *Felipe Barra*

Conductance of quasi one-dimensional periodic systems and current in a one-dimensional non equilibrium quantum system
(Nordita Seminar Room (132:028))

Wednesday, 12 October 2011

10:00 - 10:45   *Ralf Metzler*

Single particle trajectories and time averages in ageing systems with weak ergodicity breaking
(Nordita Seminar Room (132:028))

10:45 - 11:30   *Bernhard Mehlig*

Metapopulation dynamics
(Nordita Seminar Room (132:028))

Thursday, 13 October 2011

10:00 - 10:45   *Christophe Texier*

Sinai diffusion with weakly concentrated absorbers
(Nordita Seminar Room (132:028))

10:45 - 11:30   *Giacomo Gradenigo*

Fluctuating hydrodynamics for a driven granular fluid: out of equilibrium correlations
(Nordita Seminar Room (132:028))

Friday, 14 October 2011

10:00 - 10:45   *David Mukamel*

Long-range correlations in driven, nonequilibrium systems
(Nordita Seminar Room (132:028))

Foundations and Applications of Non-Equilibrium Statistical Mechanics

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