

Scientific report on the ESF-workshop 2812

Optimization in stochastic nano-systems

10.-13. October 2010, Delmenhorst, Germany

Summary

The workshop was very successful meeting the expectations of speakers, participants, and organizers alike. All talks had a high standard reporting results from the frontier of research in an accessible way. Also the few but high-quality posters presented during the workshop contributed to the fine scientific level of the event. All speakers took part in the meeting and except for one stayed till the end. The intimate atmosphere permitted by the conference venue and the limited number of participants allowed an intense exchange of ideas and stimulated lively discussions. The conference programme with a somewhat longer lunch break and free evenings left ample time for thorough poster presentations and ongoing discussions in smaller groups. As planned the workshop took place at the Hanse-Wissenschaftskolleg in Delmenhorst with its unique combination of modern infra-structure and noble isolation. The local staff at the HWK did a marvelous job in supplying everything that was needed for a smooth course of the workshop.

Description of the scientific content of the workshop

The focus of the workshop was on basic problems related to energy transformation at the nano-scale, a problem of technical relevance as well as fundamental importance. Generators and motors as well as cooling and heating systems of tiny size behave rather differently from their macroscopic, everyday counterparts. The ubiquitous presence of thermal fluctuations with an energy comparable to that of the system itself makes the application of standard thermodynamical methods inappropriate. Instead, tools and techniques from *stochastic thermodynamics* that have been developed in the last 10-20 years are the suitable framework for a quantitative analysis of functionality and efficiency of these devices. In particular all attempts to optimize processes of energy conversion at the nano-scale will be ill-advised if they do not take into account strong fluctuation effects.

The scientific problems discussed at the workshop can be roughly grouped into four, interconnected categories: fundamental problems in stochastic thermodynamics, optimizing the performance of microscopic energy converters, experimental techniques in fluctuating thermodynamics, and concrete projects for stochastic nano-machines.

1. Fundamental problems in stochastic thermodynamics

This topic was in particular represented by the talks of Seifert, Van den Broeck, Nieuwenhuizen and Parrondo. Udo Seifert gave a concise and up-to-date introduction to the whole field of stochastic thermodynamics on the basis of the impressive activity of his group during the last 5-10 years. His talk served as a perfect starting point for most of the other presentations. Chris Van den Broeck presented joint work with Massimiliano Esposito on new aspects of the second law of thermodynamics. Being the central ingredient for the characterization of the efficiency of macroscopic machines the precise meaning of the second law at the nano-level is of particular importance for all problems discussed at the meeting. Juan Manuel Parrondo presented a microcanonical realization of Szilard's version of a Maxwell demon that raised interesting fundamental questions. Finally, Theo Nieuwenhuizen discussed some ideas on Brownian entanglement, a subject that first seemed to be somewhat outside the realm of the meeting but which turned out to be very near to central concepts in stochastic thermodynamics.

2. Optimizing the performance of microscopic energy converters

This subject was mainly covered by the talks of Gaspard, Kawai, and Esposito. Similar as for macroscopic machines practitioners are not so much interested in maximal efficiency alone but at high efficiency at maximum power. Systems that need to run extremely slowly in order to reach their high efficiencies do not match the requirements of most applications. It is hence of foremost interest to find ways to optimize the power output of energy converting devices. With their discussion of different aspects of this problem and the connection to the laws of stochastic thermodynamics the three speakers therefore contributed to the very focus of the workshop.

3. Experimental techniques in fluctuating thermodynamics

This point comprises the talks of Blickle, Ciliberto, Braun, and Grill. Valentin Blickle gave an overview over the experimental methods suitable to characterize the stochastic dynamics of colloidal systems. Several of the central notions and results of stochastic thermodynamics have been verified experimentally with the help of colloidal particles, optical tweezers and advanced video microscopy. Sergio Ciliberto gave an account on the investigations of fluctuation-dissipation relations in non-equilibrium situation performed in his laboratory over the last years. The classical fluctuation-dissipation theorem plays a crucial role in near-equilibrium situations. However, in trying to reach optimal performance of energy converters one often drives the systems strongly

away from equilibrium, well outside the validity of linear response. It is therefore of great importance to monitor the deviations from traditional fluctuation-response relations and to verify the different generalizations that have been put forward in the framework of stochastic thermodynamics. A wide range of fluctuating nano-systems can be found in micro-biology. In fact the very problem of energy conversion in small systems bears directly on several important processes in biological cells. Dieter Braun and Stephan Grill gave with their talks an impressive insight into this fascinating field. As for macroscopic systems there are ample possibilities to learn from biology in order to find clever technical solutions.

4. Concrete projects for stochastic nano-machines

This most applied subtopic of the workshop was covered by the talks of Linke and Rurali. Heiner Linke discussed general considerations for the setup of a synthetic protein motor. Riccardo Rurali presented results on the experimental realization of a linear motor based on carbon nano-tubes. Both contributions showed that the technical application of many of the ideas discussed during the workshop are indeed within reach of modern technology.

Connecting all of the above topics the talk by Christopher Jarzynski discussed possibilities to control and guide artificial molecular machines in their action. Inspired by examples from biological molecular complexes he used results from the theory of stochastic processes to give conditions for the occurrence of directed currents of energy or matter in general reaction networks and analyzed how these can be optimized by controlling external parameters.

Assessment of the results

Probably the most important result of the workshop was the intense exchange of ideas in the lively discussions during the whole course of the event. The field of stochastic thermodynamics is still young and may not yet be in its final form. At such times it is extremely important to bring together the leading experts of the field to compare and elucidate their different opinions and ways of thinking. Moreover some of the talks and posters concerned work that is not yet published and the authors have benefited from the feedback obtained in the various discussions. Of course also new scientific acquaintanceships were made and older ones were renewed. The workshop hence contributed to a strengthening of the scientific community in stochastic thermodynamics in Europe and beyond. Also, the concept of fellowships of the Hanse-Wissenschafts-Kolleg was introduced to some of the speakers and the organizers are quite optimistic that some of them will come back to Delmenhorst for between 3 and 12 months to study problems related to energy conversion at the nano-scale, together with their colleagues from Oldenburg, Osnabrück and Bremen.

Final programme of the meeting

Sunday, October 10

Arrival, gathering of participants in the hotel

Monday, October 11

09:15 – 09:45	Welcome
09:45 – 10:45	Udo Seifert: Optimization in stochastic thermodynamics
10:45 – 11:15	<i>coffee break</i>
11:15 – 12:00	Sergio Ciliberto: Fluctuation-dissipation in out-of-equilibrium systems
12:00 – 12:45	Pierre Gaspard: From loose to tight coupling between fluctuating transport processes
13:00 – 14:00	<i>lunch</i>
14:00 – 15:30	posters and discussion
15:30 – 16:00	<i>coffee break</i>
16:00 – 16:45	Valentin Blickle: Colloidal particles as probes for stochastic thermodynamics
16:45 – 17:30	Christian Van den Broeck: The three faces of the second law in stochastic thermodynamics

Tuesday, October 12

09:00 – 10:00	Dieter Braun: Biomolecules in temperature gradients: From biotechnology to Darwinian evolution
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10:00 – 10:45	Stephan Grill: Active forces and flows that drive cellular polarization
10:45 – 11:15	<i>coffee break</i>
11:15 – 12:00	Heiner Linke: Optimizing the design of a synthetic protein motor
12:00 – 12:45	Riccardo Rurali: Thermal nanomotor based on carbon nanotubes
13:00 – 14:00	<i>lunch</i>
14:00 – 15:30	posters and discussion
15:30 – 16:00	<i>coffee break</i>
16:00 – 16:45	Theo Nieuwenhuizen: Brownian entanglement: Entanglement in classical Brownian motion
16:45 – 17:30	Massimiliano Esposito: Optimization of efficiency, Onsager symmetry, and the fluctuation theorem
19:00	<i>conference dinner</i>

Wednesday, October 13

09:00 – 10:00	Christopher Jarzynski: Guiding the motion of artificial molecular machines
10:00 – 10:45	Juan Manuel Parrondo: Cooling classical particles with a microcanonical Szilard engine
10:45 – 11:15	<i>coffee break</i>
11:15 – 12:00	Ryoichi Kawai: Efficiency at maximum power in weak dissipation regimes
13:00 – 14:00	<i>lunch</i>
	Departure

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