kT log 2: Fluctuation Theorems and the Physics of Information

A workshop supported by the European Science Foundation
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Segovia, Spain, May 3rd-5th, 2007

SCIENTIFIC REPORT

Summary

The mini-workshop has addressed different topics related to dissipation, heat, work, and information. We have been able to bring together theoretician and experimentalists working in different fields related with these topics: micro- and mesoscopic refrigerators, molecular and protein motors, foundations of statistical mechanics, and dissipation theorems.

The format of the conference has allowed participants to give very detailed talks which prompted several and fruitful scientific discussions.

We were forced to change the location from Chinchón to Segovia, due to a lack of availability of rooms in Chinchón. The hotel in Segovia has the same characteristics as the one that we have in mind in Chinchón (they belong to the same company) and Segovia has been an excellent and attractive location for our meeting.

Scientific content

The first session of the conference (Thursday morning) explored different ways of using fluctuations to induce thermal effects, such as refrigeration. **Jukka Pekola** presented recent experiments in microscopic refrigeration coupling semiconductors and superconductors. **Christian van den Broeck** showed the theory of Brownian refrigerators. **Ricardo Brito** presented a novel theoretical idea which can provide the simultaneous cooling or heating of two systems without any energy supply and **Bart Cleuren** discussed effusion in black body radiation. The session combined theoretical and experimental talks, giving the opportunity of interesting discussions and the creation of new collaborations.

In the second session (Thursday afternoon) we also combine one experiments and theory in the field of protein motors. **Stephan Grill** discussed some recent single-molecule experiments with the RNA polymerase, the protein responsible of DNA transcription and **Ken Sekimoto** presented a unified mechanism for protein motors such as kinesins and myosins, based on logical and control gates. In both talks, information play a relevant role, since RNA polymerase is able to copy and proofread genetic information, whereas the mechanism proposed by Sekimoto can be expressed in terms of information flows. These two talks are important insights on how information is used by biological process and what are the implications for the energetics of such processes.

The third session (Thursday evening) was devoted to control protocols in physics and also to some results on dissipation theorems. **Udo Seifert** discussed the two topics both from a theoretical and experimental point of view. He presented his concept of entropy associated to single trajectories and also recent results on the protocols minimizing the dissipated heat in a given isothermal process.

Luis Dinís tackled the problem of feedback control in a flashing ratchet, this time with the aim of maximizing the current.

In the fourth session (Friday morning) we had two interesting talks about foundations of statistical mechanics. **Sandu Popescu** presented a new idea to objectivize probabilities in statistical mechanics by using quantum entanglement between a system and the rest of the universe. **Peter Reimann** explored the generality of this idea studying general combination of pure quantum states.

In the fifth session (Friday morning) we had several talks on a recently discovered relationship between irreversibility and dissipation. **Ryoichi Kawai** explained and tderived this general results, and **Juan MR Parrondo** applied it to information processing and logical irreversibility. Finally, **Alex Gómez-Marín** applied the same results to a Brownian particle in a moving harmonic potential.

The sixth session (Friday afternoon) consists of a single talk by **David Leigh**, where he made a review of the experiments done in his laboratory with rotaxenes. His group has been able to create chemical switches and motors. He also presented one of his last and remarkable achievements: a chemical reaction sensitive to the position of one chemical ring inside a molecule. They have been able to create a system resemble a pressure Maxwell demon, which can pump particles (in this case, rotaxenes) from one side to the other side of a molecular complex.

Finally, in the last session (Saturday morning) we had three interesting talks on work theorems. **David Andrieux** explained how Kolmogorov entropy can be related with dissipation in general stochastic dynamical systems, **Alejandro B. Kolton** discussed the application of work theorems to disordered systems, and **Teruhisa Komatsu** presented a generalization of some of this theorems to systems in contact with several thermal baths at different temperatures.

We did not include a poster session which is often reserved for contributions of junior scientists and doctoral students. Instead we provided several of them (Cleuren, Kolton, Dinis, Andrieux) with the opportunity to present a talk.

Impact and results

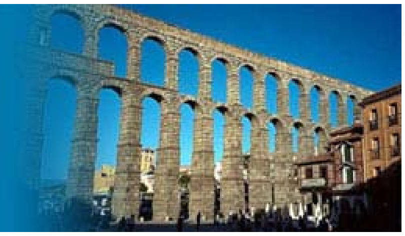
The meeting has been an outstanding success. Participants come from very different fields and the meeting has been a new but also fruitful experience, as most of them have reported to us.

We think that Statistical Mechanics is facing a new era, where novel techniques, such as single-molecules experiments, optical tweezers, and synthetic chemistry, can help us to understand better the role of fluctuations in nature, and how these fluctuations can be used for energy transduction and information processing. Similarly to new quantum technologies, we are now witnessing taht fundamental problems of Statistical Mechanics, such as the Maxwell demon, become closely related to problems with technological relevance, such as refrigeration, control devices, and information processing and storage.

This conference has contributed to link these fundamental and applied aspects of fluctuations and to create new contacts between theoretical and experimental groups from different disciplines.

kT log 2

Fluctuation Theorems and the Physics of Information



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Organizers: Juan MR Parrondo, Chris van den Broeck, Ryoichi Kawai.

1 Program

	Thursday 3	Friday 4	Saturday 5
9:00-9:30	*Presentation*	Popescu	
9:30-10:00	Pekola		Andrieux
10:00-10:30		Reiman	Kolton
10:30-11:00	*Coffee break*		Komatsu
11:00-11:45	Van den Broeck	Kawai	*Coffe break*
11:45-12:15	Brito	Parrondo	*Final remarks*
12:15-12:30	Cleuren		
12:30-12:45		Gomez Marín	
12:45-13:00			
13:00-15:30	*Lunch*		
15:30-16:15	Grill	Leigh	
16:15-16:30	Sekimoto		
16:30-17:00		*Coffe break*	
17:00-17:30	*Coffee break*		
17:30-18:15	Seifert		
18:15- 18:45	Dinis		

2 Abstracts

Irreversibility, information, and fluctuations in nonequilibrium systems

David Andrieux
Université Libre de Bruxelles

We investigate the time-reversal symmetry in nonequilibrium fluctuations. Their dynamical randomness can be characterized in terms of the standard and time-reversal entropies per unit time of dynamical systems theory. In particular, we present experimental results for a Brownian particle in a moving trap, showing that their difference equals the thermodynamic entropy production. Such concepts enlight the physics of information, such as Landauer's principle, with new understandings.

Heating without heat

Ricardo Brito
Universidad Complutense de Madrid

Two systems at different temperatures are put in contact by means of a passive energy filter. By an appropriate choice of the filter, the two systems can heat up or cold down simultaneously without any energy input.

Effusion of Photons and the Fluctuation Theorem

Bart Cleuren
Universiteit Hasselt

Effusion is the motion of a gas through a small opening. The discrete nature of the particles involved and their thermal motion, naturally leads to fluctuations in the outcoming flux of particles. These fluctuations, which are irrelevant in most situations, have rather intricate properties and obey the so called fluctuation theorem. We demonstrate these properties, first for an classical ideal gas, and then for a gas of photons. In the latter, the validity of the symmetry relation requires a fully quantum mechanical description of the photons which takes into account the effect of photon bunching.

Control and optimization in a collective flashing ratchet

Luis Dinis
Universidad Complutense de Madrid

Rectification of thermal fluctuations is becoming a major topic in non equilibrium statistical mechanics, with applications in biology, condensed matter and nanotechnology. Most Brownian rectifiers work by introducing an external time-dependent perturbation, usually either a periodic or a random one, in an asymmetric equilibrium system. In this talk, I will review our results on applying external perturbations that depend on the state of the system, that is, feedback controlled perturbations, to an ensemble of Brownian particles. Two types of control protocols were studied with the aim of maximizing the flow of particles in the steady state. In the first one, the instant velocity of the center of mass is maximal at any time. This protocol is optimal for one particle but, surprisingly enough, yields worse results than a periodic or random one for large ensembles. The second protocol utilizes two control parameters and performs well for either small or large ensembles. Both protocols make use of information of the state of the system to better take advantage of fluctuations.

Coarse-graining in time and space: an analytical prediction of dissipation bounds due to information loss

Alex Gómez-Marín
Universitat de Barcelona

For a purely nonequilibrium mechanical system we show analytically and explicitly that the coarse-grained relative entropy provides a lower bound for the total dissipated work [1]. The expression found does not coincide with the exact calculated dissipation because only partial information about all the degrees of freedom of the system (nor the complete time history of the stochastic dynamics) is known. The sudden quench and the quasistatic limits are satisfactorily recovered by performing the nonequilibrium excursion infinitely fast and slow, respectively.

[1] "Dissipation: The Phase-Space Perspective", R. Kawai, J. M. R. Parrondo and C. Van den Broeck, Phys. Rev. Lett. 98, 080602 (2007).

Transcription by RNA Polymerase II

Stephan Grill
Max Plank Institute, Dresden

RNA polymerase II (RNAP II) is responsible for transcribing all mRNAs in eukaryotic cells in a highly regulated process that serves as a central control point for cellular function. We have investigated the transcription dynamics of single RNAP II molecules against force in the presence and absence of TFIIS, a transcription elongation factor that enables the enzyme to remove copy errors. Using a single- molecule dual-trap optical-tweezers assay, we found that the response of RNAP II to force is entirely determined by enzyme backtracking. We show that backtrack pause durations follow a $t^{-3/2}$ power law, implying that during backtracking RNAP II performs a random walk in discrete base-pair steps and suggesting that backtracks may account for most of RNAP II pauses. Unexpectedly, we find the polymerase to be naturally biased in the downstream direction while backtracked, possibly due to transient secondary structures that form behind the polymerase within the RNA transcript. Finally, we propose that this intrinsic force bias is a novel mechanism that is central to transcription and that acts to prevent the occurrence of fatally long pauses.

Dissipation Revealed in Phase Space

Ryoichi Kawai
University of Alabama

We show that an exact expression of the average dissipation, upon perturbing a Hamiltonian system arbitrarily far out of equilibrium in a transition between two canonical equilibrium states is given by $\langle W_{diss} \rangle = \langle W \rangle - \Delta F = kT\, D(\rho|\rho^*) = kT \langle \ln (\rho/\rho^*) \rangle$, where ρ and ρ* are the phase space density of the system measured at the same intermediate but otherwise arbitrary point in time, for the forward and backward process, respectively. $D(\rho|\rho^*)$ is the relative entropy of ρ versus ρ*. This expression is valid both in classical and quantum systems. This result also implies general inequalities, which are significantly more accurate than the second law.

Nonequilibrium steady states maintained by multiple heat baths

Teruhisa Komatsu
The University of Tokyo

We have studied a class of heat engines including Feynman's ratchet, which exhibits a directed motion of a particle in nonequilibrium steady states maintained by two heat baths. We have measured heat transfer from each heat bath separately, and found that heat transfer can be a key quantity to describe phenomena in nonequilibrium states. In this talk, we aim more general consideration about steady states of the system maintained by multiple heat baths. Starting from the frame of fluctuation theorem, we will discuss the relation between heat transfer and steady state distribution.

Excess heat in a driven disordered Langevin system

Alejandro B. Kolton
Universidad Complutense de Madrid

We study numerically the heat fluctuations of a Brownian particle driven in a random potential, by solving simultaneously the steady-state Fokker-Planck equation and the overdamped Langevin dynamics. The total interchanged heat in a time interval, $Q_{tot}=Q_{hk}+Q_{ex}$, is analyzed in terms of the house-keeping heat Q_{hk}, needed to maintain detailed balance violation in a given steady state, and the excess heat Q_{ex} generated by arbitrarily changing some of the control parameters. In the steady-states we verify integral and detailed fluctuation theorems. By perturbing a steady state with a change of the control parameters and then by letting the system completely relax to the new (or the same) steady state, we verify the generalization of the second law $-Q_{ex} \leq T\Delta S$ for isothermal transitions between non-equilibrium steady states. Here ΔS is the Shannon entropy difference between the final and initial steady states and the equality holds only for an adiabatic change of the control parameters. We show that disorder plays a crucial role at low temperatures in determining how slow a process must be to be considered "adiabatic".

Exercising Demons: Synthetic Molecular Motors and Machines

David Leigh
University of Edinburgh

An exciting contemporary area of chemistry is making molecules with moving parts, with the goal that they can function as nanoscopic machines capable of performing physical tasks. We will discuss some of the latest developments from our group on the introduction of ratchet principles into synthetic molecular structures, including the experimental realisation of both energy ratchets and information ratchets.

For some recent papers from the Leigh group see: *Nature*, **424**, 174-179 (2003); *Science*, **299**, 531 (2003); *Science*, **306**, 1532-1537 (2004); *Proc Natl Acad Sci USA*, **102**, 13378-13382 (2005); *Nature Mater*, **4**, 704-710 (2005); *Proc Natl Acad Sci USA*, **103**, 17650-17654 (2006); *Nature*, **440**, 286-287 (2006); *Nature*, **445**, 523-527 (2007). For a recent review on synthetic molecular motors and machines, see: *Angew Chem Int Ed*, **46**, 72-191 (2007);

Probabilistic Arrows of Time

Juan M.R. Parrondo
Universidad Complutense de Madrid

Irreversibility is often thought by playing movies forward and backward in time. If one can clearly distinguish between the two, the processes in the movie are irreversible. Here we will show processes where the distinction is not so clear and can be made only in probabilistic terms. We prove that this processes are accompanied by microscopic dissipation (of order kT) and discuss their relation with the thermodynamics of computations and the Szilard engine.

Refrigeration, energy relaxation and thermometry in electronic mesoscopic structures

Jukka Pekola
Helsinki University of Technology

Metallic nanostructures at low temperatures provide a rich variety of systems where intriguing thermal and thermodynamic phenomena can be investigated [1]. Of particular interest are hybrid systems where one can combine nanoscale superconductors and usual metals, tunnel barriers and direct metallic contacts. Thermal properties of such structures are determined by the various relaxation mechanisms, for instance by electron-electron, electron-phonon, and electron-photon rates in comparison to external operation frequencies. I will discuss our earlier efforts on standard electronic refrigeration [1,2] and thermometry [1,3], and then I move to our more recent work on quantized thermal conductance [4], cyclic single-electron refrigeration [5,6] and on a Brownian refrigerator of electrons [7].

[1] F. Giazotto, T.T. Heikkilä, A. Luukanen, A.M. Savin, and J.P.Pekola, Rev. Mod. Phys. 78, 217 (2006).
[2] M.M. Leivo, J.P. Pekola, and D.V. Averin, Appl. Phys. Lett. 68, 1996 (1996).
[3] J.P. Pekola, K.P. Hirvi, J.P. Kauppinen, and M.A. Paalanen, Phys. Rev. Lett. 73, 2903 (1994).
[4] Matthias Meschke, Wiebke Guichard, and Jukka P. Pekola, Nature (London) 444, 187 (2006).
[5] Jukka P. Pekola, Francesco Giazotto, and Olli-Pentti Saira, Radio-frequency single-electron refrigerator, Phys. Rev. Lett. 98, 037201 (2007).
[6] Olli-Pentti Saira, Matthias Meschke, Francesco Giazotto, Alexander M. Savin, Mikko Möttönen, and Jukka P. Pekola, cond-mat /0702361.
[7] J.P.Pekola and F.W.J. Hekking, cond-mat/0702233.

Entanglement and the foundations of statistical mechanics

Sandu Popescu
University of Bristol

Statistical mechanics is one of the most successful areas of physics. Yet, almost 150 years since its inception, its foundations and basic postulates are still the subject of debate. Here we suggest that the main postulate of statistical mechanics, the equal a priori probability postulate, should be abandoned as misleading and unnecessary. We argue that it should be replaced by a general canonical principle, whose physical content is fundamentally different from the postulate it replaces: it refers to individual states, rather than to ensemble or time averages. Furthermore, whereas the original postulate is an unprovable assumption, the principle we propose is mathematically proven. The key element in this proof is the quantum entanglement between the system and its environment. Our approach separates the issue of finding the canonical state from finding out how close a system is to it, allowing us to go even beyond the usual boltzmannian situation.

Microcanonical typicality, the role of entanglement, and the classical limit

Peter Reimann
Universität Bielefeld

It is shown that the majority of pure states within the quantum mechanical energy shell yield expectation values for a given observable with bound spectrum which are almost indistinguishable from the microcanonical expectation value. It is argued that the basic reason behind this result is the high dimensionality of the Hilbert space describing the energy shell, while entanglement plays no significant role. In the classical limit the definition of a pure state disagrees with the one used in classical statistical mechanics, hence the above microcanonical typicality property does not apply any more classically.

Stochastic thermodynamics: Fluctuation theorems, optimal finite-time processes and generalized Einstein relation.

Udo Seifert
Universität Stuttgart

Stochastic thermodynamics provides a conceptual framework for describing small systems embedded in a heat bath and mechanically or chemically driven to non-equilibrium. Both the first law and entropy production can be consistently defined along single trajectories. An infinity of integral fluctuation theorems hold, among which the Jarzynski relation and the one on total entropy production are prominent ones [1]. After briefly reviewing and illustrating these foundations, I will present within this scheme our recent work concerning (i) optimal finite-time processes [2] and (ii) generalized Einstein relations [3,4].

The optimal protocol of an external control parameter minimizes the mean work required to drive the system from one given equilibrium state to another in a finite time. Explicite solutions both for a moving laser trap and a time-dependent strength of such a trap show finite jumps of the optimal protocol to be typical both at the beginning and the end of the process.

The Einstein relation connecting diffusion constant and mobility is violated beyond the linear response regime. We have recently derived and measured an additive correction term which involves an integral over measurable correlation functions.

[1] U. Seifert, PRL 95: 040602/1-4, 2005.
[2] T. Schmiedl and U. Seifert, PRL 98: 108301/1-4, 2007.
[3] T. Speck and U. Seifert, EPL 74: 391-396, 2006.
[4] V. Blickle et al, submitted.

From Maxwell demon to Brownian chirality

Christian Van den Broeck
Universiteit Hasselt

The second law of thermodynamics precludes the transformation by a single heat bath of heat into work. In the presence of two heat baths at different temperature, the rectification, even of Brownian fluctuations, becomes possible.

We present a microscopic description of such a Brownian motor. By invoking Onsager symmetry, every such motor can be transformed into a Brownian refrigerator. A rotational version of such a construction allows to define the concept of thermodynamic chirality.

C. Van den Broeck, R. Kawai and P. Meurs, Phys Rev Lett 93, 090601 (2004) C. Van den Broeck, P. Meurs and R. Kawai, New J Phys 7, 10 (2005) C. Van den Broeck and R. Kawai, Phys Rev Lett 96, 210601 (2006) M. Van den Broeck and C. Van den Broeck, Thermodynamic Chirality, unpublished.

Information processing in a protein motor head

Ken Sekimoto
Université Paris 7

The goal to understand the physical process of protein motors is to relate the 3D structure of their heads with their functions. For this purpose, we propose a viewpoint of ``bidirectional control'' based on the allosteric linkages between the detection and gating within a single motor head. The application to myosin and kinesin reveals that, despite the apparent large disparity of their chemo-mechanical cycles, these motors use a very similar working principle. The finding supports further the hypothesis of the common ancestors in both structural and functional contexts.

3 Participants

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