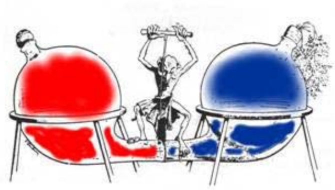
kT LOG 2 '09
COMPUTING MATTERS



kT log 2 '09: Computing Matters
Physics of Information

A workshop supported by the European Science Foundation
under the Programme EPSD
Toledo, Spain, October 22nd-24th, 2009

SCIENTIFIC REPORT

Summary

The mini-workshop has addressed different topics related to dissipation, heat, work, and information. We have been able to bring together theoretical groups from different disciplines (non equilibrium statistical mechanics, mesosocopic transport, quantum information) as well as experimentalist working in energetic aspect of small devices.

The Workshop also included the participation of several PhD students and Posdocs who gave short talks about their work.

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

Scientific content

The first session of the conference (Thursday morning) explored different aspects of the energetic of processes far from equilibrium. **Pierre Gaspard** presented results relating fluctuation theorems and response far from equilibrium as well as the energetic of polymerization. **Christian van den Broeck** further explored the information and energetic consequences of polymerization using linear irreversible thermodynamics. **Parrondo** discussed some issues on the Second Law applied to microcanonical ensembles, and **Izumida** also applied linear irreversible thermodynamics to study a Brownian Carnot engine.

In the second session (Thursday evening), **Michele Campisi** presented quantum versions of work theorems developed by the Ausburg group. **Benjamin López** reported on experiment of feedback controlled ratchets, in which information about the position of particles is used to modify the potential experimented by the particles. **Koji Maruyama** reviewed fundamental aspects of quantum information processing and storage and **Edgar Roldán** applied work theorems to the estimation of entropy production using stationary trajectories.

The third session (Friday morning) was devoted mainly to quantum systems. **Heiner Linke** explained his last experimental results on thermo-electrical devices. Similar effects were discussed theoretically by **Ryoichi Kawai** and **Fernando Sols**. **David Sánchez** adopted a different approach, from the field of mesoscopic transport, to fluctuation theorems and linear response. Finally, **Massimiliano Esposito** gave an interesting proposal for a general definition of entropy production valid for systems arbitrarily far from equilibrium.

In the fourth session (Saturday morning) **Udo Seifert** discussed fluctuation dissipation theorems far from equilibrium and **Karoline Weisner** gave a very general approach to the concept of information processing. **Nathan Kawada** presented the basic lines of an ambitious project for the construction of artificial molecular motors based on DNA proteins. Finally, **Takahiro Sagawa** presented a generalization of the Landauer's principle based on incomplete and/or asymmetric erasure.

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.

The main aim of our Workshop was to put together three different fields: work theorems and energetics of small systems, computation and information processes, and non equilibrium response. Many of the speakers and groups involved in the workshop are actually working in several or even the three fields together, combining applications to both quantum and classical systems. We have seen in many talk an increasing use of the of relative entropy or Kullbak-Leibler distance between states or between forward and backward processes, a concept form information theory that allows one to quantify the difference between two probability distributions or quantum states. It is likely that a general framework for thermodynamics of computation will be based on this type of concept.

Another topic which drawn much attention along the conference and raised different discussion and potential collaborations was response and transport theory applied to electronic transport and thermoelectric devices. In this respect, the workshop has included very different viewpoint from experimentalist to theoretician coming from different disciplines: statistical mechanics (Seifert, Gaspard), condensed matter (sols) and mesoscopic systems (Sánchez).

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Toledo, October 22-24, 2009

	Thursday	Friday	Saturday
9:00-9:30	Gaspard	Linke	Seifert
9:30-10:00			
10:00-10:30	Van den Broeck	Kawai	Weisner
10:30-11:00			
11:00-11:30	Coffee break		
11:30-12:00	Parrondo	Sols	Kawada
12:00-12:30			Sagawa
12:30-13:00	Izumida	Sánchez	
13:00-13:30		Esposito	
13:30-15:00	Lunch	Free discussions, visit to Toledo, etc	
15:00-15:30	Campisi		
15:30-16:00			
16:00-16:30	López		
16:30-17:00	Coffee break		
17:00-17:30	Maruyama		
17:30-18:00			
18:00-18:30	Roldán		
20:30-22:00		Dinner	

Invited talks

Fluctuation and work theorems for open quantum systems

Michele Campisi, University of Augsburg, Germany

Fluctuation and work theorems have first been known as exact relations between equilibrium and non-equilibrium properties of isolated or open classical systems and have later been generalized to closed quantum systems [1] and quantum systems staying in weak interaction with their environment [2]. Only recently it was shown that fluctuation and work theorems also hold for quantum systems in strong contact with their environment [3]. This though requires a proper description of the thermodynamics of small open quantum systems which may show unusual properties such as negative specific heats [4].

[1] P. Talkner, E. Lutz, P. Hanggi, Phys. Rev E 75, 050102(R) (2007).
[2] P. Talkner, M. Campisi, P. Hanggi, J. Stat. Mech. Theor. Exp. P02026 (2009).
[3] M. Campisi, P. Talkner, P. Hanggi, Phys. Rev. Lett. 102, 210401 (2009).
[4] G.-L. Ingold, P. Hanggi, P. Talkner, Phys. Rev. E 79, 0611505 (2009).

Finite time thermodynamics of a quantum tunneling junction and quantum heat engine

Ryoichi Kawai, University of Alabama, USA

We investigate finite time thermodynamics of a single quantum state interacting with a metallic environment through a tunneling junction. This simple model is analytically tractable and can be a useful toy model of open quantum systems. We first discuss how to raise or lower the quantum level with minimum work. The optimal protocols involve singularities similar to the classical cases. We extend our investigation to a single quantum state interacting with two reservoirs with different temperature through tunneling junctions. Such a system can work as a quantum heat engine. We attempt to find the efficiency of the engine at the highest power.

Highly-efficient thermoelectric energy conversion using quantum-dot energy filter

Heiner Linke, Lund University, Sweden

Experiments will be reported on the use of heterostructure, group III/V nanowires as model systems to understand how electronic properties of a device should be designed to optimize the efficiency of thermal-to-electric power conversion. Specifically, I will review the theory underlying concepts for highly efficient thermal-to-electric energy conversion using sharp features of the electronic density of states, and will report the near-Carnot efficient energy conversion using a quantum dot embedded into a nanowire, as demonstrated by an electronic ZT >> 1 (neglecting phonon-mediated heat flow). Theoretical results concerning the efficiency at maximum power of idealized, low-dimensional thermoelectric devices will also be reported.

Out-of-equilibrium directionality and information processing at the nanoscale

Pierre Gaspard, Université Libre de Bruxelles, Belgium.

Systems maintained in nonequilibrium steady states are described by an invariant probability distribution which typically breaks the time-reversal symmetry at the statistical level of description in consistency with the microreversibility of the motion of electrons and nuclei. This has for consequence new relationships for the large-deviation properties of nonequilibrium fluctuations, such as the fluctuation theorem for currents [1,2] as well as relations between the thermodynamic entropy production and quantities characterizing temporal disorder and information dynamics at the nanoscale [3,4]. These latter relations show that the fluctuations of nonequilibrium systems, such as driven Brownian particles or RC electric circuits, bear the signature of the aforementioned time-reversal symmetry breaking down to the nanoscale [5]. These results provide a general understanding of the directionality which manifests itself out of equilibrium, for instance, in the motion of molecular motors [4]. This nonequilibrium directionality is also at the origin of information processing in copolymerizations with or without a template, such as DNA replication [6,7].

[1] M. Esposito, U. Harbola, and S. Mukamel, Nonequilibrium fluctuations, fluctuation theorems, and counting statistics in quantum systems, Rev. Mod. Phys. (2009).
[2] D. Andrieux, P. Gaspard, T. Monnai, and S. Tasaki, The fluctuation theorem for currents in open quantum systems, New. J. Phys. 11 (2009) 043014.
[3] P. Gaspard, Time-reversed dynamical entropy and irreversibility in Markovian random processes, J. Stat. Phys. 117 (2004) 599.
[4] P. Gaspard, Temporal ordering of nonequilibrium fluctuations as a corollary of the second law of thermodynamics, Comptes Rendus Physique 8 (2007) 598-608.
[5] D. Andrieux, P. Gaspard, S. Ciliberto, N. Garnier, S. Joubaud, and A. Petrosyan,
Thermodynamic time asymmetry in non-equilibrium fluctuations, J. Stat. Mech.: Th. & Exp. (2008) P01002.
[6] D. Andrieux and P. Gaspard, Nonequilibrium generation of information in copolymerization processes, Proc. Natl. Acad. Sci. USA 105 (2008) 9516-9521.
[7] D. Andrieux and P. Gaspard, Molecular information processing in nonequilibrium copolymerizations, J. Chem. Phys. 130 (2009) 014901.

Thermodynamics of quantum information storage

Koji Maruyama, RIKEN, Japan

The generality of thermodynamics enables us to understand a broad spectrum of phenomena from physics to information science or even to biology. Over the past few decades, it has been realised that information storage and processing based on quantum mechanics can be much more efficient than their classical counterpart. What general bound on storage/acquisition of quantum information does thermodynamics imply? We show that thermodynamics implies a weaker bound than the quantum mechanical one (the Holevo bound). In other words, if any post-quantum physics should allow more information storage, it could still be under the umbrella of thermodynamics.

Cooling classical particles with a microcanonical Szilard engine

Juan MR Parrondo, Universidad Complutense, Spain

We show that it is possible to extract energy from a single isolated system if its initial energy is known. We construct an explicit example based on the celebrated the Szilard engine. Our microcanonical version of the engine allows extraction of energy without the need of any measurement. The extraction possible by a cyclic protocol which reduces the energy of a single particle by increasing the uncertainty of its energy, a mechanism that could be in principle extended to systems with several degrees of freedom.

Quantum cooling in electron and atom systems

Fernando Sols, Universidad Complutense de Madrid, Spain

We investigate a mechanism for extracting heat from metallic conductors based on the energy-selective transmission of electrons through a spatially asymmetric resonant structure subject to ac driving. This quantum refrigerator can operate at zero net electronic current as it replaces hot by cold electrons through two energetically symmetric inelastic channels. We present numerical results for a specific heterostructure and connect them to general questions of quantum cooling. Inelastic reflection is shown to contribute to heating if the external driving signal is time-symmetric. The quantum of cooling power, $\pi^2 k_B^2 T^2/6h$, is shown to be an upper limit to the cooling rate per transport channel in the presence of an arbitrary driving signal. The quantum limit to bulk atom cooling is also discussed. Within the electron tunneling limit, it is shown that electron cooling still occurs if the coherent ac source is replaced by a sufficiently hot thermal bath. A comparison with related refrigeration setups is presented.

1. M. Rey, M. Strass, S. Kohler, P. Hänggi, F. Sols, "Nonadiabatic electron heat pump", Phys. Rev. B 76, 085337 (2007).
2. F. Sols, "Aspects of quantum cooling in electron and atom systems", Physica E, in press (FQMT08 Proceedings).

Non-equilibrium steady states in stochastic thermodynamics: Entropy production and the general fluctuation-dissipation theorem.

Udo Seifert, University of Stuttgart, Germany

In a non-equilibrium steady state (NESS), the external driving leads to permanent entropy production. If identified properly along individual trajectories as stochastic entropy, the distribution of the total entropy production obeys a detailed fluctuation theorem for finite length of trajectories [1]. In the long time limit, this distribution can be written in the form of a large deviation function. I will present simple examples which share a remarkable structure of this large deviation form [2,3]. The stochastic entropy also features prominently in the general fluctuation-dissipation theorem for such NESSs which we derived very recently [4]. I will clarify the a priori remarkable freedom exhibited by different variants of this FDT. Where possible I will illustrate our theoretical results with measurement of driven colloidal particles [5,6].

[1] U.S., Phys. Rev. Lett., 95: 040602/1-4, 2005.
[2] J. Mehl, T. Speck and U.S., Phys. Rev. E, 78 : 011123, 2008.
[3] T. Speck, J. Mehl, an U.S., Phys. Rev. Lett., 100: 178302, 2008.
[4] U.S. and T. Speck, submitted to EPL, arXiv.org: 0907.5478, 2009.
[5] V. Blickle et al, Phys. Rev. Lett., 98: 210601/1-4, 2007.
[6] T. Speck et al, EPL, 79: 30002, 2007.

Extracting energy by growing disorder.

Christian Van den Broeck, Hasselt University, Belgium

We consider the efficiency of energy extraction from the environment by the entropy-driven growth of a copolymer made of two constitutional units. We show that the standard linear thermodynamics argument, predicting an efficiency at maximum power of 1/2, is inappropriate, because the regime of maximum power is either located outside the linear regime or on a separate bifurcated branch, the latter being due to the specific nonlinearities associated to the Shannon entropy.

Information-processing efficiency of complex systems

Karoline Wiesner, University of Bristol, UK

Complex systems are found in most branches of science. It is still argued how to best quantify their complexity and to what end. We will discuss prominent measures of complexity and show how they are linked by the concept of information erasure. Out of this arises an information-processing efficiency parameter. We find a bound to this information-processing efficiency in analogy to the second law of thermodynamics.

Short talks

Linear irreversible thermodynamics and a Brownian Carnot cycle

Yuki Izumida, Hokkaido University, Japan

In recent years there has been renewed interests in an old problem: the fundamental limit of efficiency at maximum power for non-equilibrium heat engines. The celebrated Curzon-Ahlborn (CA) efficiency, which has been conjectured as a universal formula for general heat engines working at maximum power, was proved to be the upper limit at least in the linear-response regime in 2005 by Van den Broeck by using linear irreversible thermodynamics. In this workshop, we analyze a Brownian Carnot cycle introduced by Schmiedl and Seifert in 2008 by using linear irreversible thermodynamics. We will clarify why the efficiency at the maximal power of this cycle attains the CA efficiency by calculating the Onsager coefficients of this system explicitly.

Simulation and design of synthetic, diffusional molecular motors

Nathan Kuwada, Lund University, Sweden

Though the biological function of many natural molecular motors is fairly well established, many structural and functional details responsible for motor performance remain vague or unknown completely. Recently, we have undertaken a new bottom-up approach to understanding structure-function relationships in natural molecular motors by designing and building a synthetic, protein-based molecular motor dubbed the Tumbleweed (TW) (Bromley, et al, HFSPJ 3, 204 (2009)). The TW is a purely diffusive motor construct consisting of three DNA-binding proteins attached to a designed, protein-based central hub, where directional stepping along a DNA track is maintained by a temporally periodic external chemical supply. To better understand important design and performance characteristics of the TW, coarse-grained Langevin Dynamics (LD) simulations and numerical solutions to the Master Equation (ME) were carried out. The LD approach, which is a single motor simulation, is particularly suitable for exploring the diffusional behavior of the system, where the ME approach, which models an ensemble of motor states, is best suited for statistically exploring the parameter space of the system and the interaction of processes at different time scales. We present results from these two theoretical approaches that illuminate not only important design and experimental considerations, such as motor geometry and track spacing, but also produce unexpected diffusional behavior. Of particular interest is that the addition of certain internal symmetric potentials can actually increase motor performance. For example, the addition of a non-specific binding potential, which is symmetric about the DNA track, can double motor speed by replacing some of the 3D diffusional search of the protein feet by a relatively fast 1D diffusional slide along the DNA. This, and other symmetric potential inputs that increase motor performance by subtly amplifying asymmetries in the system, are not only fundamentally interesting but also may be applicable to any molecular motor that incorporates a diffusional search in its stepping cycle.

Experimental Realization of a Feedback-Controlled Flashing Ratchet

Benjamin Lopez, Lund University, Sweden

A flashing ratchet is a Brownian motor that rectifies thermal fluctuations of diffusive particles through the use of a time-dependent, periodic, and asymmetric potential. It has been predicted that a feedback-controlled flashing ratchet has a center of mass speed as much as one order of magnitude larger than the optimal periodically flashing ratchet [1]. For dimeric molecular motors, feedback control mechanisms are likely to be crucial to achieve processivity and can help explain experimental data [2]. We have successfully implemented the first experimental feedback ratchet [4], and observed the predicted order of magnitude increase in velocity when we use the originally predicted feedback scheme based on maximizing the instantaneous particle velocity (MIV). In addition, we also implemented a novel maximum net displacement feedback scheme (MND) [3] that predicts for small N to provide an even larger center of mass velocity than the MIV. We experimentally compare these two feedback algorithms for small particle numbers, and find good agreement with Langevin dynamics simulations. All feedback schemes suffer from finite feedback delay times, but we also find that existing algorithms can be improved to be more tolerant to feedback delay times. In our experiment a scanning line optical trap setup is used to transport micron-sized particles using a feedback controlled Brownian ratchet. This system can create potential energy landscapes that realize the steps of a Brownian ratchet process. Currently, we have a scan line 18 μm in length that stably traps 0.9 μm silica spheres. A flat potential with variations on the order of kT, and a ratchet potential with 1.8 μm periods and an asymmetry of 0.35 have been realized. A ratchet depth of up to 40 kT has been measured. Real time particle tracking at 130 Hz is achieved through software based video analysis. To see a significant effect for small N the feedback delay time must be less than the time scale for bead diffusion over a distance of aL, where L is the ratchet period length and a is the asymmetry of the ratchet shape. With current experimental parameters this value is about 300 ms. In this setup, feedback has a minimum implementation delay of 5 ms, and feedback effects are experimentally observable. We will present ratchet velocity for different feedback algorithms, particle numbers, and ratchet potential depths, and compare these to modeling results.

[1] F.J. Cao, L. Dinis, and J.M.R. Parrondo, Phys. Rev. Lett. 93, 040603 (2004).
[2] M. Bier, BioSystems 88, 301 (2007).
[3] E.M. Craig, N. Kuwada, B. Lopez, H. Linke, Ann. Der Phys. 17, 115 (2008).
[4] B. J. Lopez, N.J. Kuwada, E.M. Craig, B.R. Long, and H. Linke, Phys. Rev. Lett. 101, 220601 (2008)

Entropy production as correlation between system and reservoir

Massimilano Esposito, Free University of Brussels, Belgium

We derive an exact (classical and quantum) expression for the entropy production of a finite system placed in contact with one or several finite reservoirs each of which is initially described by a canonical equilibrium distribution. Whereas the total entropy of system plus reservoirs is conserved, we show that the system entropy production is always positive and is a direct measure of the system-reservoir correlations and/or entanglements. Using an exactly solvable quantum model, we illustrate our novel interpretation of the Second Law in a microscopically reversible finite-size setting, with strong coupling between system and reservoirs. With this model, we also explicitly show the approach of our exact formulation to the standard description of irreversibility in the limit of a large reservoir.We consider a linear chain of independent single level quantum dots. The dots state can be modified by a tip whose chemical potential and speed along the chain are externally controlled. Given an initial probability distribution for the dot to be occupied by an electron, we calculate the entropy change associated to the process of emptying all dots from their electrons. If done very slowly the Landauer result is recovered. We explore the finite time effects of this erasure process.

Estimating Dissipation from single stationary trajectories

Edgar Roldán, Universidad Complutense, Spain

The relationship between dissipated work and irreversibility has been recently established in the context of fluctuation and work theorems, using the relative entropy or Kullback-Leibler divergence as a measure of the arrow of time. We use this relationship to estimate dissipation from single stationary trajectories in a discrete and in a continuous flashing ratchet.

Information Thermodynamics

Takahiro Sagawa, University of Tokyo, Japan

I'd like to talk about the fundamental lower bounds on the thermodynamic energy cost of measurement, information erasure, and feedback control by "Maxwell's demon." The lower bound on the erasure validates Landauer's principle for a symmetric memory; for other cases, the bound indicates the breakdown of the principle. Our results constitute the second law of "information thermodynamics," in which information content and thermodynamic variables are treated on an equal footing.

Onsager asymmetries and nonlinear fluctuation-dissipation relations in mesoscopic conductors

David Sánchez, Universidad de les Illes Balears, Spain

In the nonlinear regime of electron transport, screening effects can lead to a breakdown of microreversibility in mesoscopic systems. The nonequilibrium response of the potential landscape along the system is, quite generally, an uneven function of the magnetic field, implying a magnetoasymmetry of the differential conductance [1]. This effect has been observed in many different phase-coherent conductors [2]. Recent theoretical developments relate the asymmetry of the noise to the asymmetry of the differential conductance in the leading order of a voltage expansion [3,4]. As a consequence, a higher-order fluctuation dissipation relation (FDR) is established between the two magnetoasymmetries even when fluctuation theorems are not obeyed. Here, we discuss the magnetoasymmetries arising in the current fluctuations of quantum dots with strong Coulomb correlations and explicitly demonstrate the validity of nonlinear FDRs when interactions are treated beyond the mean field approximation.

[1] D. Sanchez and M. Buttiker, Phys. Rev. Lett. 93, 106802 (2004)
[2] J. Wei, M. Schimogawa, Z. Whang, I. Radu, R. Dormaier, and D.H. Cobden, Phys. Rev. Lett. 95, 256601 (2005); D. M. Zumbuhl, C. M. Marcus, M. P. Hanson, and A. C. Gossard, Phys. Rev. Lett. 96, 206802 (2006); C. A. Marlow, R. P. Taylor, M. Fairbanks, I. Shorubalko, and H. Linke, Phys. Rev. Lett. 96, 116801 (2006); R. Leturcq, D. Sanchez, G. Gotz, T. Ihn, K. Ensslin, D. C. Driscoll, and A. C. Gossard, Phys. Rev. Lett. 96, 126801 (2006).
[3] H. Forster and M. Buttiker, Phys. Rev. Lett. 101, 136805 (2008).
[4] D. Sanchez, Phys. Rev. B 79, 045305 (2009).