DY 11: Focus Session: Thermodynamics and Statistical Physics of Small Systems

Time: Tuesday 10:00–13:15 Location: HÜL 186

Invited Talk DY 11.1 Tue 10:00 HÜL 186
Doing small systems: Concepts, Role of Ensembles, Thermalization and Fluctuation Theorems — •Peter Hänggi — Universität Augsburg, Institut für Physik, Universitätsstr. 1, 86135 Augsburg

This symposium is aimed at highlighting issues that relate of doing thermodynamics and statistical physics of finite size systems. This theme gained considerable importance in view of fascinating advances in nanotechnology and system biology. While the fathers of thermodynamics developed the famous Laws having in mind macroscopic systems these grand concepts need to be inspected anew in view of the fact that the fluctuations grow with decreasing size to a level where they even may play the dominant role.– The symposium touches upon several timely issues in designing, measuring and operating systems at the submicron scale, both IN and also FAR AWAY from thermal equilibrium. With this introduction I discuss subtleties related to thermodynamics of small systems, such as (i) the role of finite size for quantities such as (in some cases negative-valued) heat capacitance [1], (ii) the role of entropy and temperature in these small systems, or (iii) the issue of thermalization. Moreover, a key role in doing statistical physics of submicron systems relates to (iv) the choice of the ensemble description and the inter-relationships between the sizable fluctuations of measures like work, heat & heat flow and thermodynamic equilibrium quantifiers such as free energy changes or changes of entropy. [1] P. Hänggi, et al., Finite quantum dissipation: the challenge of obtaining specific heat, New J. Phys. 10, 115008 (2008); in addition see also: G. Ingold, et al., Phys. Rev. E 79, 061105 (2009) .

Invited Talk DY 11.2 Tue 10:30 HÜL 186
Microcanonical singularities in finite systems — •Jörn Dunkel[1] and Stefan Hilbert[2] — [1]Department of Applied Mathematics and Theoretical Physics, Centre for Mathematical Sciences, University of Cambridge, Wilberforce Road, Cambridge CB3 0WA, UK — [2]Instititut für Astronomie, Universität Bonn, Auf dem Hügel 71, 53121 Bonn, Germany

The microcanonical equations of state of a finite isolated system can exhibit a substantially more complex structure than their canonical counterparts [1,2]. Prominent examples are singularities and oscillations in the caloric temperature curves, corresponding to regions of negative specific heat, which reflect structural changes in the microscopic properties of the underlying Hamiltonian system as the energy control parameter is varied. After taking a brief look at the virtues and drawbacks of competing microcanonical entropy definitions, we will illustrate the aforementioned phenomena by means of an exactly solvable 1D dissociation model [1]. Although the model is relatively simple, it suggests an interesting general connection between the microscopic temperature oscillations in a finite microcanonical system and macroscopic canonical phase transitions in the corresponding infinite system.

[1] S. Hilbert and J. Dunkel, Phys. Rev. E 74: 011120, 2006
[2] J. Dunkel and S. Hilbert, Physica A 370(2): 390, 2006

Invited Talk DY 11.3 Tue 11:00 HÜL 186
Recent progress in fluctuation theorems and free energy recovery — •Felix Ritort — Departament de Fisica Fonamental, Facultat de Fisica, Universitat de Barcelona, Diagonal 647, 08028 Barcelona (Spain)

Recent developments in micro and nanotechnologies enable the manipulation of single molecules one at a time. Single molecule experiments make possible to resolve energy processes with unprecedented detail at the level of 1 kT, the typical energy scale of Brownian fluctuations.* Fluctuation theorems establish relations governing energy exchange processes at this level and provide a new methodology to obtain equilibrium information from non-equilibrium experiments. In this talk I will show applications to free energy recovery* in single molecule experiments obtained in our laboratory (Small biosystems lab, Barcelona, Spain) in unzipping experiments carried out on DNA, RNA and proteins. The range of applications covers free energy recovery of molecular native states, intermediate states and misfolded states. I will also show how fluctuation relations can be applied to recover base pairing free energies in RNA, essential to improve free energy prediction of RNA secondary structures.

15 min. break

Invited Talk DY 11.4 Tue 11:45 HÜL 186
Efficiencies and fluctuations in small out-of-equilibrium devices — •Massimiliano Esposito — Center for Nonlinear Phenomena and Complex Systems, Université Libre de Bruxelles, Campus Plaine CP 231, Brussels B-1050, Belgium.

Small systems undergo strong fluctuations and can easily be driven far from their thermodynamic equilibrium. A stochastic description of their dynamics combined with very few physical assumptions and the correct identification of entropy production provide a consistent nonequilibrium thermodynamic description of these small systems. I will show that such description enables the study of finite-time efficiencies and nonequilibrium fluctuations in various small devices such as thermoelectric quantum dots and photoelectric cells.

Invited Talk DY 11.5 Tue 12:15 HÜL 186
Quantum Fluctuation Theorems — •Michele Campisi — Pisa, Italy — Institute for Physics, University of Augsburg, Germany

The second law of thermodynamics poses a stringent constraint on the direction that physical processes may take in macroscopic systems. As their size shrinks, processes taking the opposite direction, apparently defying the second law, become possible and the fluctuation theorems quantify the likelihood of their occurrence. We will address the following issues concerning quantum fluctuation theorems i) the problem of gauge freedom affecting the definitions of work and free energy, ii) the notions of inclusive, exclusive and dissipated work [1], iii) the absence of a work operator in quantum mechanics and the notion of two-point quantum observable iv) the difficulties related to the experimental verification of quantum fluctuation theorems and the possibility to overcome them [2].

[1] M. Campisi et al. “Quantum Bochkov-Kuzovlev work fluctuation theorem” arXiv:1003.1052.
[2] M. Campisi, et al. “Fluctuation theorems for continuously monitored quantum fluxes” Phys. Rev. Lett. 105, 104601 (2010)

Invited Talk DY 11.6 Tue 12:45 HÜL 186
Time-reversal symmetry relations: From the multibaker map to open quantum systems — •Pierre Gaspard — Université Libre de Bruxelles, Brussels, Belgium

On the basis of microreversibility, symmetry relations have been established for the counting statistics of different currents flowing through classical, stochastic, or quantum systems sustaining nonequilibrium steady states in the absence or presence of an external magnetic field. Recently, it has been shown that these relations have consequences on the nonlinear-response properties of the system, extending linear-response Onsager reciprocity relations. These results apply to nonequilibrium processes such as chemical reactions, molecular motors, or electron transport in quantum dots.

References:

- S. Tasaki and P. Gaspard, Fick’s Law and Fractality of Nonequilibrium Stationary States in a Reversible Multibaker Map, J. Stat. Phys. 81 (1995) 935.
- P. Gaspard, Fluctuation theorem for nonequilibrium reactions, J. Chem. Phys. 120 (2004) 8898.
- D. Andrieux and P. Gaspard, Fluctuation theorem and Onsager reciprocity relations, J. Chem. Phys. 121 (2004) 6167.
- D. Andrieux and P. Gaspard, A fluctuation theorem for currents and non-linear response coefficients, J. Stat. Mech. (2007) P02006.
- D. Andrieux, P. Gaspard, T. Monnai, and S. Tasaki, The fluctuation theorem for currents in open quantum systems, New J. Phys. 11 (2009) 043014.