Work, dissipation, and fluctuations in nonequilibrium physics

Foreword

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Abstract

We introduce and present the proceedings of the conference “Work, dissipation, and fluctuations in nonequilibrium physics” held in Brussels, 22–25 March 2006 under the auspices of the International Solvay Institutes for Physics and Chemistry and organized by the Center for Nonlinear Phenomena and Complex Systems of the Université Libre de Bruxelles. To cite this article: B. Derrida et al., C. R. Physique 8 (2007).

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Résumé


Mots-clés : Fluctuations de non-équilibre ; Théorème de fluctuations ; Travail hors d’équilibre ; État stationnaire hors d’équilibre

Since its foundations by Boltzmann, Einstein, Gibbs, Maxwell, and others, statistical mechanics has become, over the 20th century, a very mature part of physics. Among its first successes, a microscopic statistical interpretation was given to the entropy, which was a purely thermodynamic quantity based on the second law of thermodynamics before Boltzmann. Furthermore, a conceptually simple framework was established through statistical ensembles to understand and predict the macroscopic properties of physical systems at thermal equilibrium. Already with the work of Einstein, Smoluchowski, and Perrin, the importance of thermal fluctuations was understood for systems at equilibrium. This allowed the determination of molecular sizes and the Avogadro number, and definitively confirmed the reality of atoms in 1908. Until the 1950s, relationships between fluctuation and dissipation were obtained in nonequilibrium systems close to equilibrium. These relationships are known under the names of \textit{Onsager} reciprocity relations, \textit{Green–Kubo} formulas, and the \textit{fluctuation–dissipation theorem}, which all concern the regime of linear response of a

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system slightly perturbed out of its equilibrium state. However, the realm of nonequilibrium phenomena extends from close to far from equilibrium and includes nucleations, phase separations, domain growths, aging processes, pattern formations, dissipative structures, oscillations and turbulence, as well as collective behaviors in biological and social systems. The field of statistical physics has thus known considerable developments away from equilibrium.

Since the mid 1980s and under the impulse of dynamical systems theory, the fluctuations have been studied in regimes away from equilibrium, especially in systems maintained in nonequilibrium steady states or driven by time-dependent external forcing. Remarkable new relationships have been recently discovered in the large-deviation properties of nonequilibrium fluctuations. The large deviations go beyond the small deviations around the statistical averages. If the small deviations obey central limit theorems or their Levy generalizations, the large deviations are ruled by functions depending on the amplitude of the deviations and characterizing the decay rate of the probability of such deviations. The newly discovered relationships include the so-called fluctuation theorem and the nonequilibrium work relation, which have been shown to hold both close and far from equilibrium. They concern nonequilibrium fluctuating quantities such as the currents of energy or particles crossing the system, the work performed by some external forcing, or the heat dissipated by the system to its environment.

For instance, according to the second law of thermodynamics, a current $J$ crossing an electric circuit at temperature $T$ and in a field $E$ induces an increase of entropy at the average rate $E\langle J \rangle/(k_B T)$, in units of Boltzmann’s constant $k_B$. However, the current $J$ fluctuates on small scales, which is a problem for macroscopic thermodynamics as first mentioned by Maxwell during the 19th century. Today, the second law has been refined thanks to the newly discovered fluctuation theorem. This latter states that, over a long time interval $t$, the probability $\text{Pro}(X)$ of observing a fluctuation $X = EJt/(k_B T)$ satisfies

\[
\frac{\text{Pro}(X)}{\text{Pro}(-X)} \sim \exp(X)
\]  

(1)

This shows that the negative fluctuations are less and less probable as the time interval $t$ increases while the most likely fluctuations obey the second law with the average value $\langle X \rangle$ increasing linearly with time $t$. In practice, the negative fluctuations can only be observed in very small systems and on rather short times since they are exponentially suppressed according to Eq. (1).

Similarly, one knows from the second law that one has to provide a positive work $W$ to bring back a system initially at equilibrium to its initial state after an arbitrary transformation, when the system is in contact with a single heat bath at a fixed temperature $T$. What the nonequilibrium work relation says is that, due to fluctuations, the work $W$ has a probability distribution which satisfies

\[
\langle \exp\left(-\frac{W}{k_B T}\right) \rangle = 1
\]  

(2)

where $\langle \cdot \rangle$ denotes an average over all the initial conditions (and on all the realizations of the thermal noise in the case of stochastic dynamics). For Eq. (2) to be satisfied, events with negative $W$ should exist. Their probability is, however, very small as soon as $W$ exceeds a few $k_B T$. Clausius’ inequality $\langle W \rangle \geq 0$ follows from the nonequilibrium work relation (2) combined with Jensen’s inequality $\langle \exp(x) \rangle \geq \exp(\langle x \rangle)$.

By their ability to deal with fluctuation quantities, these new relationships extend nonequilibrium thermodynamics from macroscopic to small systems, which are affected by fluctuations due to their discrete molecular structure. They are thus fundamental for the future development of the statistical physics of molecular motors and other nonequilibrium nanosystems. Moreover, they allow us to understand how the second law of thermodynamics holds for statistical ensembles in spite of the fluctuations at the level of the individual trajectories. Besides, all these new results shed a new light on irreversibility and on the origin of the thermodynamic time asymmetry and open new perspectives on the implications of the second law.

The state of the art on these advances has been established during the conference “Work, dissipation, and fluctuations in nonequilibrium physics” held in Brussels, 22–25 March 2006 under the auspices of the International Solvay Institutes for Physics and Chemistry and organized by the Center for Nonlinear Phenomena and Complex Systems of the Université Libre de Bruxelles. The conference gathered 80 participants including many prominent contributors to the topic. The present special issue contains the proceedings of the conference. The volume is organized into the following categories:
• Fundamentals of the fluctuation theorems and nonequilibrium work relations (G. Gallavotti; C. Jarzynski; E.G.D. Cohen and R. van Zon);
• Experiments on the fluctuation theorems and nonequilibrium work relations (S. Joubaud, N.B. Garnier, F. Douarche, A. Petrosyan, and S. Ciliberto; F. Ritort);
• Theoretical studies of the fluctuation theorems and nonequilibrium work relations (T. Bodineau and B. Derrida; A. Imparato and L. Peliti; B. Cleuren, C. Van den Broeck, and R. Kawai; D. Andrieux and P. Gaspard);
• Novel aspects of entropy production (C. Maes and K. Netočný; P. Gaspard; V. Lecomte, C. Appert-Rolland, and F. van Wijland);
• Dynamical systems approaches and properties (S.R. Williams, D.J. Evans, and E. Mittag; T. Taniguchi and G.P. Morriss; R. van Zon, S.S. Ashwin, and E.G.D. Cohen; P. Visco, A. Puglisi, A. Barrat, E. Trizac, and F. van Wijland);
• Molecular motors and cyclic processes (F. Ritort; K. Sekimoto; T. Monnai, A. Sugita, and K. Nakamura);
• Quantum systems (W. De Roeck; D. Alonso, I. de Vega, and E. Hernandez-Concepcion);
• Relativistic systems (A. Fingerle).

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