Title: Theoretical description of unequilibrium energy transformation processes on the level of molecular structures

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Abstract:

The thesis is devoted to the thermodynamics of externally driven mesoscopic systems. These systems are so small that the thermodynamic limit ceases to hold and the probabilistic character of the second law cannot be ignored. Thermal forces becomes comparable to other forces acting on the system and they have to be incorporated in the underlying dynamical law, i.e., in the master equation for discrete systems, and in the Fokker-Planck equation for continuous ones. In the first part of the thesis we investigate dynamics and energetics of mesoscopic systems during non-equilibrium isothermal processes. Due to the stochastic nature of the dynamics, the work done on the system by the external forces must be treated as a random variable. We derive an exact analytical form of the work probability density for several model systems. In particular, the knowledge of the exact formula improves the analysis of experimental data using the recently discovered fluctuation theorems. In the second part of the thesis we study a non-equilibrium cyclic process which incorporates two isotherms with different temperatures. During the cycle, the system can produce a positive work on the environment. We analyze two specific models of such mesoscopic heat engines and we optimize their performance.

Keywords: stochastic thermodynamics, work probability density, stochastic heat engines, efficiency at maximum power, exact results