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Summary

Thesis: Theory and computer simulations of systems driven out-of-equilibrium by local energy pumping

In this thesis, we have studied nonequilibrium physics from the point of view of nonequilibrium thermodynamics. In particular, we search for a variational principle for nonequilibrium steady states (NESS) in closed systems subjected to the heat or matter flow. As an alternative to the disputed maximum/minimum entropy production principles, it should be simple and based on measurable quantities.

The main part of this thesis is devoted to studying three hypotheses, or more precisely, three propositions of nonequilibrium potentials that are hypothesized to be minimized in NESS. The examination methodology is as follows: for a general test model, we measure the potential of the system under an internal constraint and compare with its value without the constraint; for systems with competing steady states, we measure the potential in each steady state and compare. A minimization hypothesis predicts that the potential of the constrained system would be greater than that of the unconstrained one; the potential of the stable state would be the smallest among all steady states. (For a maximization hypothesis, the predictions would be reversed.)

Our first hypothesis is over a quantity $\mathcal{T}$ inspired by dimensional analysis and defined as the ratio of energy storage (with respect to the equilibrium energy) to the total heat flow J_U. This quantity has the interpretation of the (initial) characteristic time of energy dissipation for the system to return to equilibrium. This hypothesis is tested extensively, with an ideal gas model under five modes of energy supplies; an ideal gas driven by a temperature gradient; a Hagen-Poiseuille flow; an Ising model under periodic (in time) and spatially inhomogeneous (local) energy supplies. In addition, simulation results of the Lennard-Jones fluid and a Rayleigh-Bédard system are recounted (reproduced from [1][1]). All the above models support this hypothesis. Unfortunately, this promising variational principle fails to account for situations where, in the thought experiment, the system is locally connected to a heat tank.

To account for such situations, we have based the second hypothesis on a quantity, which we called the embedded energy U^*, since it is the energy U minus the outflow of energy in the characteristic time $\tau = \partial U / \partial J_U$. It is defined as the Legendre transform

[1] [1] R. Hołyst et. al., Phys. Rev. E **99**, 042118 (2019)

of the steady state energy with respect to the total heat flow. This definition is motivated by the Helmholtz free energy, which can be viewed as the Legendre transform of the energetic fundamental relation with respect to entropy. Two models have been used to study this hypothesis: an ideal gas surrounded by a thermostat and subjected to a homogeneous bulk energy supply, and an ideal gas between two thermostats of different temperatures. Calculations of the latter system have shown that the hypothesis is not satisfied over certain parameter ranges defining the internal constraints. This could be related to the fact that in these parameter ranges, other variables characterizing the system have to be taken into account.

This reflection has lead to the last hypothesis, which concerns a Helmholtz-like potential B. The form of the potential is introduced through a series of postulates. The motivation is the correspondence principle, and its form closely mimics that of the Helmholtz free energy, with an additional term to account for the contribution from nonequilibrium. This additional term is proportional to $\mathcal{T}$. Using the ideal gas model under a homogeneous bulk energy supply, we have obtained the explicit form of this potential and of other state functions. Consistency checks of the scheme show that: first, these expressions of the state functions also follow the correspondence principle; second, the Maxwell relations are satisfied. Next, for the movable wall model – a model exhibiting multiple steady states, B correctly predicts the steady state condition and the stable steady state.

The second message of the thesis concerns energy storage. Using the Ising model with local periodic energy supplies, we have found that the energy storage is sensitive to the details of the supply method. Specifically, more energy is stored under large and rare delivery than small and frequent delivery; more energy is stored when the delivery area is larger.

The last important message of the thesis is the proposition of the movable wall model. This is an ideal gas under a homogeneous bulk energy supply, with an adiabatic movable wall as the internal constraint. Although the model is relatively simple and analytical, it has extremely interesting behavior. First, the model exhibits nonequilibrium phase transition. The order parameter of this transition is the stable steady state position of the movable wall. Second, beyond the critical point, the system exhibits multiple steady states. The system is stable when the subsystems are not symmetric (that is, the wall is not in the center) and stores more energy in the stable state.