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Report on the PhD thesis of Yirui Zhang
„Theory and Computer Simulations of Systems
Driven Out-of-Equilibrium by
Local Energy Pumping”

Yirui Zhang's PhD Thesis is about a dream. A dream of finding a functional which is minimized in nonequilibrium steady states (NESS), which would allow one to construct NESS theory in a similar way that equilibrium thermodynamics is constructed based on entropy maximization. This is not an easy task and the way towards it, as in some medieval story, is littered with the corpses of those who have tried (and failed) to achieve that goal before, including the members of the Brussels school, with Prigogine and collaborators. Enormous literature on the subject has been generated over the last century, but the practical significance of these results is so far rather limited. But this does not mean, of course, that one should give up on any attempt at constructing such a theory, so let us look closer at how the Author attempts to undertake the task in this Thesis.

The Thesis is constructed a bit like a lab book or research diary, documenting successive attempts of the Author of finding a functional which is minimized in NESS. Some of these attempts fail, and then a new candidate function is tested. I like this approach, I find it much more engaging for the Reader than the theses which start with the end result in mind and then work their way backwards from there.

The structure of the Thesis is the following: Chapter 1 gives a short introduction to nonequilibrium thermodynamics, mentioning in particular the minimum entropy production principle and fluctuation theorems in stochastic thermodynamics. It is nicely written, but leaves a reader somewhat dissatisfied – given a long history of the problem I'd expect a more

in-depth presentation and critique of these concepts: do they work in general? If yes, why do we need to seek further? If not, then what is wrong with them? A longer exposition here will allow the reader to better comprehend the importance and depth of a problem at hand.

Next, in Section 2 the Author introduces a function \mathcal{T} , which is the ratio of the stored energy to the flux, $\mathcal{T} = (U - U_{eq})/J$ and tests whether it is minimized in NESS for a number of simple systems, involving heat conduction in 1d gas models. This is an interesting proposal, which, in my opinion, touches on several important properties of the nonequilibrium steady states: their energy storage capacity and the necessary presence of a flux, without which the NESS could not be maintained. \mathcal{T} itself has a dimension of time and can be interpreted as a relaxation time for the system to return to equilibrium, once the flux is stopped. Several systems are worked out in detail following this idea. They are characterized either by a bulk energy supply (i.e. the energy is supplied to every point in the system) or by the flux imposed by the boundary conditions. The first case might seem not too realistic for the heat flow problem, particularly in 3d, but there are other physical systems where it is a perfectly feasible scenario (i.e. groundwater table fed by the rain and drained by the rivers). Technically, the proofs that \mathcal{T} is minimized are based on introducing internal constraints into the system and showing that \mathcal{T} for the constrained systems is larger than the value of this function for an unconstrained system – in an analogy to similar proofs in classical equilibrium thermodynamics. In the thermal conduction system considered in the Thesis the constraints usually correspond to either an adiabatic wall or diathermal wall introduced into the system. In all of the examples worked out by the Author the function \mathcal{T} is found to be minimized in the steady state. However, a counterexample is then given at the end of Chapter 2, involving a large box with adiabatic walls connected to the system in one point. Such a box changes the total amount of energy stored in the system (and hence also \mathcal{T}), while not having impact on the final temperature profile. This shows that \mathcal{T} will not, in general, be connected to the NESS and the search for the appropriate functional need to be started anew.

A new attempt is thus made in Chapter 3, where an analog of the Helmholtz free energy for NESS is proposed, $U^* = U - \frac{\partial U}{\partial J} \cdot J$, which is the Legendre transform of U with respect to J .

The Author calls it an embedded energy, identifying it with the energy that must be present in the system to keep the NESS and hypothesizing that U^* is minimized in nonequilibrium steady

states. The first results are encouraging – the hypothesis is shown to work for the heat conduction system under the bulk energy supply and – even better – it works for the system with an external tank attached, for which the \mathcal{T} functional failed. However, then it is shown that the hypothesis does not hold for the system with an external energy flux imposed by the boundary conditions, and thus it needs to be rejected.

However, before proposing a new hypothesis, the Author makes a short detour and in Chapter 4 considers a movable wall problem. Again, we have a constraint in the form of an adiabatic wall, but this time the wall can move. For the simplest case where both parts have an equal number of particles, the system is shown to exhibit a second order nonequilibrium phase transition, with either a single stable steady state for small pumping rates (corresponding to symmetric position of the wall) or the three steady states (two asymmetric & stable and one symmetric and unstable). This is a very simple and yet physically insightful model, ideal for analysis of nonequilibrium steady states and various functionals that characterize them. The Author performs such an analysis here, finding in particular, that U^* correctly characterizes the nonequilibrium steady states in this model whereas \mathcal{T} - fails. Other functionals were also tested – in particular it was shown that entropy production does not provide a good characterization of NESS in this case.

In regard to this model, I would like to bring to the Author's attention the fact that it is far from clear that such an entity as "adiabatic movable wall" exists. The problem is that by moving and hitting the particles on both sides the piston transfers the energy from the hot side to the cold side [see e.g. J. L. Lebowitz, Stationary nonequilibrium Gibbsian ensembles, Phys. Rev. 114:1192–1202, 1959 or more recent works: Ch. Gruber and J. Piasecki, Stationary motion of the adiabatic piston, Phys. A 268:412–423 (1999), E. Kestemont, C. Van den Broeck, and M. Mansour, The "adiabatic" piston: And yet it moves, Europhys. Lett. 49:143–149 (2000) or Chernov, N., and J. L. Lebowitz. "Dynamics of a massive piston in an ideal gas: Oscillatory motion and approach to equilibrium." Journal of Statistical Physics 109:507–527 (2002)]. I wonder whether these effects could affect the results of the Thesis.

Coming back to the struggle of finding the proper function characterizing NESS the Author formulates yet another hypothesis in Chapter 5, introducing functional, B . The construction starts from the equilibrium free energy, adding to its differential an additional term $-Xd\lambda$, where λ is a parameter controlling the appearance of the steady state (with $\lambda=0$ corresponding

to equilibrium) and X – the state function conjugate to λ . For the latter, the following formula is proposed, $X \sim (U - U_{eq}) / \lambda$, linking it to the energy storage with the control parameter λ related to the flux supplied to the system. The function X is thus closely related to the time function \mathcal{T} introduced in Chapter 2. The functional B is then shown to correctly predict the nonequilibrium steady states in the movable adiabatic wall model. I am a bit surprised that it has not been checked on the model on which the functional U^* failed, i.e. the ideal gas under an external heat flow, but I guess it will be the subject of further investigation.

Even though the end goal (finding a functional which is minimized in NESS) has most likely not yet been achieved, the journey towards it still brought a lot of physical insights. The characterization of the phase transition in the movable piston system of Chapter 4 is one of them. Another set of interesting results is derived in Chapter 2.4, where 2d Ising-like systems under periodic energy supply are considered and it is shown that the energy storage depends sensitively on the mode of energy transfer into the system, with the systems storing more energy under large and rare energy delivery than small and frequent delivery.

Furthermore, a general idea of studying NESS by introducing constraints is, in my opinion, a very powerful one, and it will surely prove fruitful in future research.

To conclude, the reviewed thesis makes an important contribution to the thermodynamics of nonequilibrium steady states and fulfills all the statutory and customary requirements posed on theses aimed for obtaining the PhD degree and I recommend the admittance of MSc Yirui Zhang to the next stages of the doctoral process. On a personal side, I would like to add that I really enjoyed reading the Thesis!

P. Szymura