Additivity Principle and stability of open systems : extension of Le Chatelier principle

Ohad Shpielberg and Eric Akkermans

Department of Physics, Technion, Israel Institute of Technology

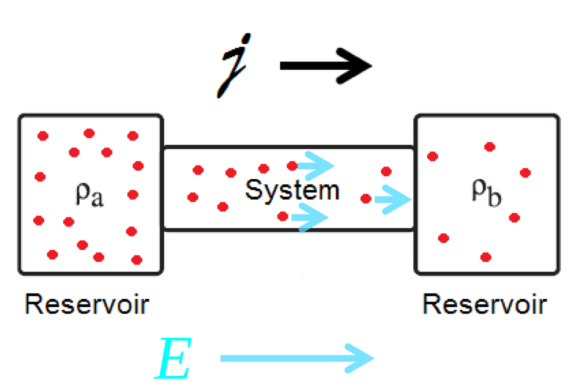
Introduction

The additivity principle (AP) is a useful tool to study out-of-equilibrium systems. However, the range of validity of the AP in open systems is still under discussion. Here, we study out-of-equilibrium systems within the macroscopic fluctuation theory (MFT). A condition for the stability of the AP solution is suggested by an extension of Le Chatelier principle (LCP) to out-of-equilibrium systems.

Overview

The macroscopic fluctuation theory provides a mathematical framework to understand the behavior of steady state out-of-equilibrium systems. However, obtaining an explicit expression for the probability distribution of e.g. the current [6], proves to be difficult. The AP [2] makes it easier to evaluate such a probability distribution.

Setup :

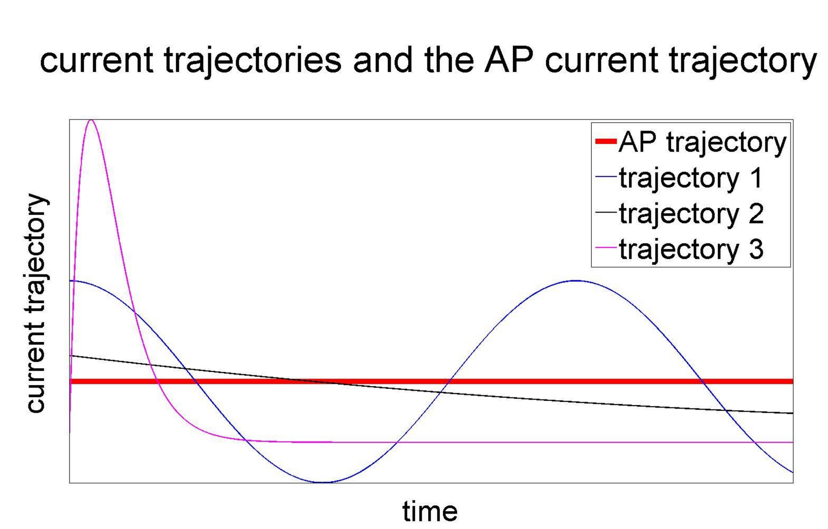


Unequal reservoir densities or a bulk field drive induce a diffusion current. We are interested in the probability that Q particles flow between the reservoirs during a long time interval.

Consider two reservoirs of particles, with fixed particle densities ρ_a, ρ_b, coupled through the system, where a bulk field may also drive the system. We are interested in $P_t(Q)$, the probability that Q particles flow between the reservoirs during a time t.

Macroscopic Fluctuation Theory and Additivity Principle

The MFT states that for $t \to \infty$, $P_t(Q) \sim \exp(-t\, I[J])$, where $J = Q/t$. The behavior of the large deviation function (LDF), $I[J]$, is governed by a "dominant trajectory" of the current which, in general, is hard to determine. The AP simplifies the problem by assuming that the dominant trajectory is the time independent one.



Among all possible current trajectories for the transfer of Q particles, the AP assumes that the time independent current dominates the LDF.

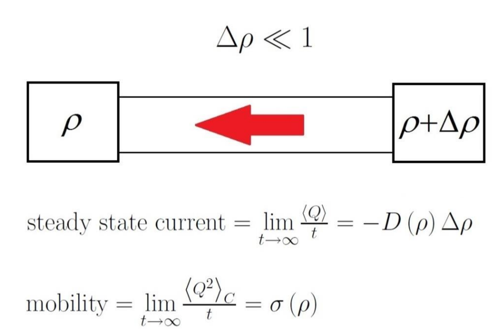
The additivity principle: diffusion and mobility

For $\rho_b - \rho_a \equiv \Delta\rho \ll 1$, the system is slightly out of equilibrium. Within the framework of the MFT, we define the macroscopic diffusion coefficient $D(\rho)$ and the mobility $\sigma(\rho)$ by

$$\lim_{t\to\infty} \langle Q \rangle / t = -D(\rho)\Delta\rho \qquad \lim_{t\to\infty} \langle Q^2 \rangle_C / t = \sigma(\rho) \qquad \langle Q \rangle \triangleq \int dQ\ P_t(Q) Q$$

Under the AP assumption, the LDF rewrites

$$\mathcal{L} = \inf_{\rho(x)} \int dx \frac{(J + D\partial_x \rho - \sigma E)^2}{2\sigma}$$



A small gradient leads to slightly out of equilibrium current and fluctuations characterized by the diffusion and mobility coefficients.

Bertini *et al.* [1] have shown that convexity in the space of all possible current trajectories of the LDF implies the validity of the AP, and that

$$D\sigma'' \le D'\sigma' \qquad (1) \qquad D' \triangleq \frac{\partial}{\partial\rho} D(\rho)$$

for any ρ is a sufficient condition for the AP to be valid.

In the case of a non zero field, the condition becomes

$$D\sigma'' = D'\sigma' \qquad (2)$$

Hamiltonian point of view

To understand why the additivity principle is the generic solution , we propose the following picture. Consider the LDF, $I[J]$, as an action and $\mathcal{L}$ as a Lagrangian. Notice that the usual role of time is replaced here by the space coordinate. Since the Lagrangian does not explicitly depends on space, the corresponding Hamiltonian is space independent as well. This implies that the energy of the system equidistributes in space, which is the scenario we expect in equilibrium. This is the natural way to think of a thermodynamical system in equilibrium. Therefore, considering this mapping, a time independent current is to be expected in the generic case.

Le Chatelier principle revisited

For a system at equilibrium, the LCP states that a fluctuation will always bring back to the equilibrium state. This means that thermodynamic potentials are either convex or concave away from phase transitions.

The LDF may be considered an out-of-equilibrium version of an equilibrium thermodynamic potential. Therefore, it seems natural to extend the idea of LCP to non equilibrium. That is, the LDF is stable if it is convex with respect to current fluctuations.

Periodic vs. open systems

Implementing the previous idea to periodic systems leads to a stability criterion, $\sigma'' \le 0$ [3]. A direct use of LCP in open systems leads to a dead end. This is due to the fact that in periodic systems the density profile is constant whereas in open systems it is never so.

Cumulant Generating function formalism

Full knowledge of the current fluctuations can also be gained using the cumulant generating function (CGF). The CGF is defined as $\mu(\lambda) = \frac{1}{t}\ln\langle e^{\lambda Q}\rangle$, where the averaging is with respect to $P_t(Q)$. One can show that $\langle e^{\lambda Q}\rangle = \int d\, x d\tau S_E(x,\tau)$, where

$$S_E(x,\tau) = (D\partial_x\rho - E\sigma)\partial_x p - \frac{1}{2}\sigma(\partial_x p)^2 - (p - \lambda x)\partial_\tau \rho,$$

and ρ, p satisfy the equations of motion

$$\begin{cases} \partial_\tau \rho = \partial_x\big(D\partial_x\rho - \sigma(E + \partial_x p)\big) \\ \partial_\tau p = -D\partial_{xx} p - \frac{1}{2}\sigma[(\partial_x p)^2 + 2E\partial_x p], \end{cases}$$

and the boundary conditions $\begin{cases} \rho(0,t) = \rho_a & \rho(1,t) = \rho_b \\ p(0,t) = 0 & p(1,t) = -\lambda \end{cases}$

Results

Since the CGF is a Legendre transform of the LDF, the idea of convexity follows. The AP solution for the CGF is the time independent solution of the equations of motion. Considering only small perturbations $\delta\rho, \delta p$, the equations of motions can be linearized yielding (here $E = 0$)

$$\delta S^2 = \frac{1}{2}\sigma(\partial_x \delta p)^2 + \frac{1}{4}\frac{D'\sigma' - D\sigma''}{D}(\partial_x p)\delta\rho^2.$$

Clearly, if $\delta^2 S \ge 0$ the AP is satisfied. So, we recover (1), where now it is sufficient that $\sigma'' D \le D'\sigma'$ is satisfied only for ρ that corresponds to the AP solution. It is also clear why it is just a sufficient condition as the first term in $\delta^2 S$ is positive.

One can generalize these results for $E \neq 0$. In this case, Bertini *et al.* have shown that a sufficient condition for the AP to be valid is for $D\sigma'' = D'\sigma'$. Applying the same method as before, we obtain

$$\delta S_E^2 = \frac{1}{2}\sigma(\partial_x \delta p)^2 + \frac{1}{4}\frac{D'\sigma' - D\sigma''}{D}\left((\partial_x p)^2 + 2E\partial_x p\right)\delta\rho^2.$$

Again, the origin of condition (2) of Bertini *et al.* is clear . However, solving the second equation of motion (with added field) for some arbitrary $\rho(x)$ yields that $(\partial_x \delta p)^2 + 2E\partial_x \delta p \ge 0$ for any E. Therefore, condition (1) is a sufficient condition for the validity of the AP even for a nonzero field.

Another useful generalization is in the case of non-conserving dynamics in the bulk. In that case, the MFT Lagrangian was generalized [4] to

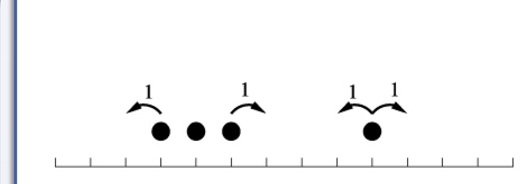
$$\frac{(J + D\partial_x\rho)^2}{2\sigma} + \Phi(k,\rho),$$

Where $\Phi(k,\rho)$ is a given function of the density and $k(x,\tau)$, the rate of matter created in the bulk. The same technique shows that the AP here is valid under the same conditions + a requirement on the convexity of Φ.

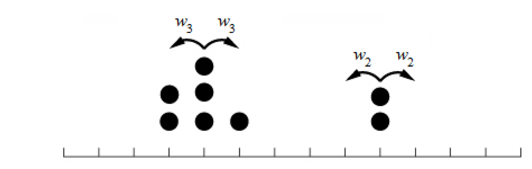
A class of stable processes for large currents

Consider the general class of energy transport models where $D = T^n$ and by Einstein relations $\sigma = 2T^{n+2}$. For high enough temperatures, many models should exhibit such power law behavior. Scaling arguments suggest that $T \sim J^{1/n+1}$ at high currents. One can infer the scaling of $\partial_x p$ from the equations of motion. Therefore, $\frac{D\sigma\prime - D\sigma\prime\prime}{D\sigma}(\partial_x p)^2 \sim J^{-4/n+1}$ and the positive term in δS^2 dominates. This implies that for this class of models, the AP is stable for high currents.

Stochastic processes



The symmetric exclusion process. Each particle hops to an empty neighbor with rate 1.



The zero range process. A particle hops to a near neighbor with rate w_n , where n denotes the number of onsite particles

Relevance to quantum models

The CGF of electron transport due to a voltage drop in mesoscopic disordered conductors is identical to the CGF of a classical process, the symmetric exclusion process, with densities 1,0 at the boundaries. In the symmetric exclusion process, particle hop between neighboring lattice sites, provided that the occupancy at each site is restricted to one. It is understood that the role of the Pauli exclusion is played by the exclusion of one particle per site, however, an exact mapping was never found.

Bernard and Doyon [5] required a 1d quantum heat transport process between two thermal baths to have conformal symmetry as well as Gallavoti-Cohen symmetry. They were able to show that this is a classical process, where each thermal bath injects "photons" in a Poisson process into the system. The "photons" are then absorbed in the other reservoir. The "photons" carry energy taken from the Boltzmann distribution of their respective thermal bath. The process is inherently ballistic, however, it can be generalized to be a diffusive process. It was shown microscopically by Kirone Mallick and macroscopically by the authors that the zero range process yields the same CGF in the large system size limit.

The two examples lead us to the idea that the CGF of quantum processes may be calculated using the macroscopic fluctuations theory and the AP.

Conclusions

- The additivity principle is a useful tool to obtain the steady state probability distribution of the current. However, a necessary and sufficient criterion for the validity of the AP using explicitly $D(\rho)$ and $\sigma(\rho)$ is still lacking.
- A generalization of the LCP to non equilibrium situations has been presented. It allows to understand results such as (1) within a more general framework.
- We have found a sufficient condition for the stability of the AP solution. This conditions generalizes previous results to accommodate more models.

This work was supported by the Israel Science Foundation Grant No.924/09.

References

[1] Bertini et al. *J. Stat. Phys.* **123**, 237 (2006) .
[2] Bodineau and Derrida, *PRL* **92**, 180601, (2004).
[3] Appert-Rolland et al. , *PRE* **78**, 021122, (2008).
[4] Bodineau, Lagouge, *J. Stat. Phys.* **139**, no. 2, 201 (2010).
[5] Bernard and Doyon, *J. Phys. A: Math. Theor.* **45** 362001 (2012).
[6] Akkermans, Bodineau, Derrida, Shpielberg, *EPL* **103**, 20001 (2013).
[7] Shpielberg and Akkermans, to be published.