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Macroscopic Fluctuation Theory 1: foundations and some applications

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Abstract

The macroscopic fluctuation theory is based on a single formula for the probability of joint fluctuations of thermodynamic variables and currents and its properties under time reversal. After giving an idea about its derivation we shall use it to introduce a natural generalization of the free energy and a new functional describing the thermodynamics of the time averaged currents. The singularities of these functionals are associated with phase transitions. An important consequence of the time reversal properties of the basic formula is that the hydrodynamic currents split into orthogonal parts having opposite time reversal behavior.

Why studying irreversible processes is so much more difficult than understanding equilibrium phenomena?

In equilibrium we have a well established phenomenological theory in terms of thermodynamic potentials which depend on few state variables.

In non equilibrium we do not know how to define meaningful analogs of, e.g. the entropy, the free energy,....: even in the simplest situations any relevant macroscopic quantity depends both on the system and the environment.

In equilibrium statistical mechanics we do not have to solve any equation of motion and the Gibbs distribution provides the basis for the calculation of macroscopic quantities and their fluctuations.

In non equilibrium we cannot bypass the dynamics even in the study of stationary states which we may consider as the simplest beyond equilibrium.

Over the last ten years a theory, now known as Macroscopic Fluctuation Theory (MFT), based on the study of rare fluctuations has been formulated.

This theory may be seen as an extension of Einstein equilibrium fluctuation theory to stationary nonequilibrium states combined with a dynamical point of view.

MFT is very powerful in studying concrete microscopic models but can be used also as a phenomenological theory. The input it requires are measurable transport coefficients. It leads to several new interesting predictions.

Einstein theory of equilibrium fluctuations

In Landau-Lifshitz book on statistical mechanics one finds the following formula for the probability of a fluctuation in a system in contact with an environment

$$P \simeq e^{-\frac{R_{min}}{T_0}} \tag{1}$$

where

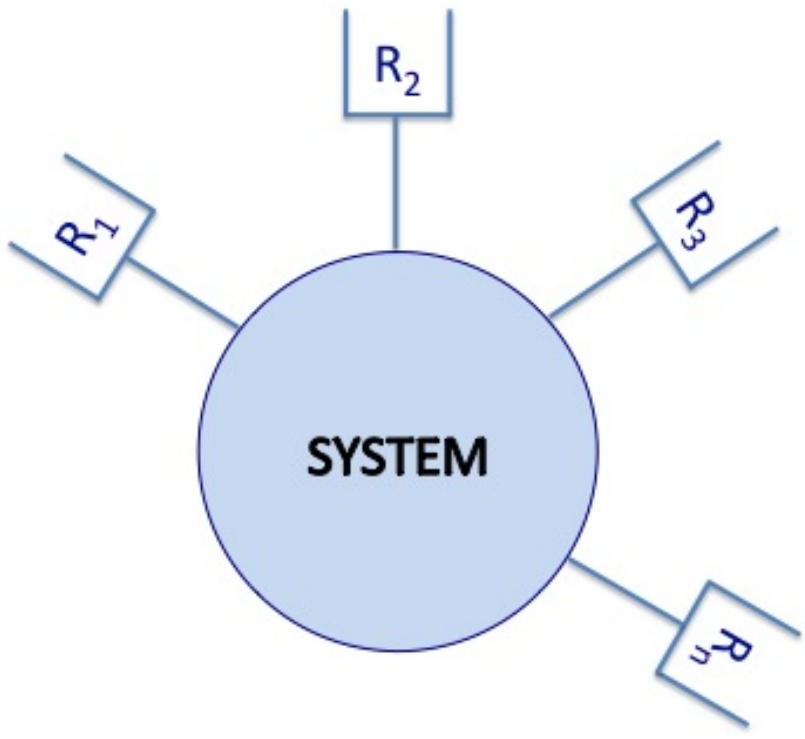
$$R_{min} = \Delta E - T_0 \Delta S + P_0 \Delta V \tag{2}$$

is the *minimal work* necessary to produce the fluctuation with a reversible transformation and $\Delta E, \Delta S, \Delta V$ are the corresponding variations of energy, entropy and volume. T_0, P_0 are the temperature and pressure of the environment.

The formula (1) is, I believe, the first example in physics of a large deviation estimate. A leading idea in recent research on nonequilibrium has been the extension of this type of estimates to fluctuations in stationary states with the aim of defining analogues of thermodynamic functionals. The notion of *minimal work* to create a fluctuation is meaningful also in stationary states. However we may expect a more complex entanglement of the variables describing the system and those related to the environment so that it is unlikely that quantities like U, S can be defined.

We consider a system connected to several reservoirs (the environment), possibly distributed continuously on the surface of the system, characterized by their chemical potentials. The reservoirs are assumed to be much larger than the system so that their state will be essentially constant in time. When the system is put in contact with the environment, after an initial stage we expect that a description in terms of diffusive processes may apply for a wide class of microscopic dynamics.

Typical nonequilibrium setting



Local equilibrium

Local equilibrium means that on macroscopic scale it is possible to define thermodynamic variables like density, temperature, ... which vary smoothly on the same scale. Microscopically, this implies that the system reaches a local equilibrium in a time which is short compared to the times typical of macroscopic evolution. So what characterizes situations in which this description applies is a separation of scales both in space and time. These assumptions are more or less explicit behind the theories dealing with non-equilibrium like Onsager near equilibrium theory.

Out of equilibrium dynamics plays a major role. In fact what distinguishes non-equilibrium is the presence of currents flowing through the system which have to be considered together with the usual thermodynamic variables. To make any progress we thus have to introduce dynamical equations for the macroscopic variables.

Hydrodynamic equations have been derived from models of microscopic dynamics. Ideally we should start from molecules interacting with realistic forces and evolving with Newtonian dynamics. This is beyond the reach of present day mathematical tools and much simpler models have to be adopted in the reasonable hope that some essential features are adequately captured.

Hydrodynamic equations

1. *The macroscopic state is completely described by the local density* $\rho = \rho(t, x)$ *and the associated current* $j = j(t, x)$.
2. *The macroscopic evolution is given by the continuity equation*

$$\partial_t \rho + \nabla \cdot j = 0 \tag{3}$$

together with the constitutive equation

$$j = J(t, \rho) = -D(\rho)\nabla\rho + \chi(\rho)\, E(t) \tag{4}$$

where the diffusion coefficient $D(\rho)$ *and the mobility* $\chi(\rho)$ *are* $d \times d$ *positive matrices. The transport coefficients* D *and* χ *satisfy the local Einstein relation*

$$D(\rho) = \chi(\rho)\, f_0''(\rho) \tag{5}$$

where f_0 *is the equilibrium specific free energy.*

The equations (3)–(4) *have to be supplemented by the appropriate boundary condition on* $\partial\Lambda$ *due to the interaction with the external reservoirs. If* $\lambda(t,x)$, $x \in \partial\Lambda$ *is the chemical potential of the external reservoirs, this boundary condition is*

$$f_0'\big(\rho(t,x)\big) = \lambda(t,x) \qquad\qquad x \in \partial\Lambda. \tag{6}$$

1. The large deviation formula for diffusive systems with a conserved quantity and some general consequences

Joint fluctuations of the density and the current

Consider a system in a stationary state characterized by a time independent solution $\bar{\rho}$ of the hydrodynamic equations and suppose that, due to a fluctuation, a value of the density ρ_0 is attained which is also the initial point of an arbitrary trajectory $\rho(t)$. Let in addition $j(t) - J(\rho(t))$ be a fluctuation of the current with respect to the value prescribed by the constitutive equation. The current j and the density ρ must always be connected by the continuity equation $\partial_t \rho(t) + \nabla \cdot j(t) = 0$.

The cost of this fluctuation will consist of two terms: the cost necessary to create the initial condition and the cost necessary to follow the trajectory $(j(t), \rho(t))$. We shall denote the first term by $V(\rho_0)$ and in non–equilibrium will represent the analog of $S_0 - S$. It turns out that the second term is proportional to the energy dissipated by the extra current $j(t) - J(\rho(t))$

$$\mathcal{I}_{[T_0,T_1]}(\rho, j) = \frac{1}{4} \int_{T_0}^{T_1} dt \int_{\Lambda} dx \, [j - J(\rho)] \cdot \chi(\rho)^{-1} [j - J(\rho)]. \quad (7)$$

For a simple interpretation of this formula think of an electric circuit. In this case χ^{-1} is the resistance and the double integral in (7) is the energy dissipated by $j(t) - J(\rho(t)$ according to Ohm's law. The factor $1/4$ is fixed by the Gaussian nature of the stochasticity responsible for the fluctuations and by the consistency with equilibrium.

The probability of joint fluctuations of density and current in a stationary state is

$$\begin{aligned} P\big((\rho_\epsilon(t), j_\epsilon(t)) \approx (\rho(t), j(t))\,,\, t \in [T_0, T_1]\,\big) \\ \asymp \exp\big\{ -\epsilon^{-d}\, \mathcal{R}_{[T_0,T_1]}(\rho, j)\big\}, \end{aligned} \tag{8}$$

where

$$\mathcal{R}_{[T_0,T_1]}(\rho, j) = V(\rho(T_0)) + \mathcal{I}_{[T_0,T_1]}(\rho, j). \tag{9}$$

Let us explain the meaning of the various symbols. The parameter ϵ is a dimensionless scaling factor, i.e. the ratio between the microscopic length scale (typical intermolecular distance) and the macroscopic one. The factor ϵ^{-d} is of the order of the number of particles in a macroscopic volume. The role of Avogadro's number in (1) is played here by ϵ^{-d}. With $\rho_\epsilon(t), j_\epsilon(t)$ we denote the empirical density and current corresponding to a coarse graining over a small macroscopic volume. Clearly these quantities depend on ϵ.

Large deviations of the density

It is not difficult to see that the functional $V(\rho)$ is related to $\mathcal{I}_{[T_0,T_1]}(\rho, j)$ by projection

$$V(\rho) = \inf_{\substack{\rho(t),j(t):\\ \nabla\cdot j=-\partial_t\rho\\ \rho(-\infty)=\bar{\rho},\rho(0)=\rho}} \mathcal{I}_{[-\infty,0]}(\rho, j), \tag{10}$$

where $\bar{\rho}$ is the stationary solution of the hydrodynamic equation.

Dynamic large deviation functional for the density

The large deviation functional for the density can be obtained by projection. We fix a path $\rho = \rho(t,u)$, $(t,u) \in [0,T] \times \Lambda$. There are many possible trajectories $j = j(t,u)$, differing by divergence free vector fields, such that the continuity equation is satisfied. By minimizing $\mathcal{I}_{[0,T]}(\rho, j)$ over all such paths j

$$I_{[0,T]}(\rho) = \inf_{\substack{j\,:\\ \nabla\cdot j = -\partial_t \rho}} \mathcal{I}_{[0,T]}(j) \tag{11}$$

Let F be the external field which generates the current j according to

$$j = -D(\rho)\nabla\rho + \chi(\rho)(E+F)\ .$$

and minimize with respect to F. We show that the infimum above is obtained when the external perturbation F is a gradient vector field whose potential H solves

$$\partial_t \rho = \nabla \cdot \Big(D(\rho)\nabla\rho - \chi(\rho)\big[E + \nabla H\big]\Big) \tag{12}$$

which is a Poisson equation for H.

Write

$$F = \nabla H + \widetilde{F} \tag{13}$$

We get

$$\mathcal{I}_{[0,T]}(j) = \frac{1}{4}\int_0^T dt \left\{ \langle \nabla H, \chi(\rho)\nabla H\rangle + \langle \widetilde{F}, \chi(\rho)\widetilde{F}\rangle \right\}$$

Therefore the infimum is obtained when $\widetilde{F} = 0$. Then $I_{[0,T]}(\rho)$ can be written

$$I_{[0,T]}(\rho) = \frac{1}{4}\int_0^T dt \left\langle \nabla H(t), \chi(\rho(t))\nabla H(t)\right\rangle \tag{14}$$

$$= \frac{1}{4}\int_{T_1}^{T_2} dt \left\langle \left[\partial_t \rho + \nabla\cdot J(\rho)\right] K(\rho)^{-1}\left[\partial_t\rho + \nabla\cdot J(\rho)\right]\right\rangle$$

where the positive operator $K(\hat\rho)$ is defined on functions $u : \Lambda \to R$ vanishing at the boundary $\partial\Lambda$ by $K(\hat\rho)u = -\nabla\cdot\big(\chi(\hat\rho)\nabla u\big)$.

Hamiltonian structure

We regard the functional (14) as an action function on the set of density paths. The corresponding Lagrangian is

$$L(\rho, \partial_t \rho) = \frac{1}{4} \int_\Lambda dx \left[\partial_t \rho + \nabla \cdot J(\rho)\right] K(\rho)^{-1} \left[\partial_t \rho + \nabla \cdot J(\rho)\right].$$

The associated Hamiltonian $\mathcal{H}(\rho, \pi)$ is obtained by the Legendre transform of $\mathcal{L}(\rho, \partial_t \rho)$:

$$\begin{aligned} \mathcal{H}(\rho, \pi) &= \sup_\xi \left\{ \int_\Lambda dx\, \xi\, \pi - \mathcal{L}(\rho, \xi) \right\} \\ &= \int_\Lambda dx \left\{ \nabla \pi \cdot \chi(\rho) \nabla \pi - \pi\, \nabla \cdot J(\rho) \right\}. \end{aligned} \tag{15}$$

The canonical equations associated to the Hamiltonian H are

$$\begin{cases} \partial_t \rho &= \nabla \cdot (D(\rho)\nabla\rho) - \nabla \cdot \chi(\rho)(E + 2\nabla\pi) \\ \partial_t \pi &= -\nabla\pi \cdot \chi'(\rho)(E + \nabla\pi) - \mathrm{Tr}\{D(\rho)\,\mathrm{Hess}(\pi)\} \end{cases} \tag{16}$$

where π vanishes at the boundary of Λ, and ρ satisfies (6). In this formula Hess(π) represents the Hessian of π, TrA the trace of a matrix A and χ' the matrix with entries $\chi'_{i,j}(\rho)$.
Observe that $(\rho(t), 0)$ is a solution of the canonical equations if $\rho(t)$ solves the hydrodynamic equation (3)-(6). In particular, $(\bar{\rho}, 0)$ is an equilibrium point of the canonical equations.

Time reversal and its consequences

To the time reversed process corresponds the adjoint generator with respect to the stationary ensemble. Let us define the operator inverting the time of a trajectory $[\theta f](t) = f(-t)$ for f scalar and $[\theta j](t) = -j(-t)$ for the current. The stationary adjoint process, that we denote by $\mathbb{P}^a$, is the time reversal of $\mathbb{P}$, i.e. we have $\mathbb{P}^a = \mathbb{P} \circ \vartheta^{-1}$. Then

$$\begin{aligned} &\mathbb{P}\Big(\rho,\ j\ \ t \in [-T,T]\Big) \\ &= \mathbb{P}^a\Big(\vartheta\rho,\ \vartheta j\ \ t \in [-T,T]\Big) \end{aligned} \tag{17}$$

At the level of large deviations this implies

$$\mathcal{R}_{[-T,T]}(\rho, j) = \mathcal{R}^a_{[-T,T]}(\vartheta\rho, \vartheta j) \tag{18}$$

where $\mathcal{R}^a_{[-T,T]}$ is the large deviation functional for the adjoint process.

More explicitely

$$V(\rho(T_0)) + \mathcal{I}_{[T_0,T_1]}(\rho, j) = V(\rho(T_1)) + \mathcal{I}^a_{[-T_1,-T_0]}(\theta\rho, \theta j). \quad (19)$$

We now assume that the adjoint dynamics admits a hydrodynamic description with a suitable external field. This assumption is very natural from the physical point of view. It expresses the fact that empirically by acting on a system with suitable external fields we can invert the evolution of a process. For example, we can arrange the action on the system in such a way that heat flows from a lower temperature to a higher temperature reservoir.

In view of this assumption, the adjoint process satisfies a dynamical large deviations principle with $\mathbb{P}$ replaced by $\mathbb{P}^a$ and $\mathcal{I}$ replaced by $\mathcal{I}^a$ where

$$\mathcal{I}^a_{[T_0,T_1]}(\rho, j) = \frac{1}{4}\int_{T_0}^{T_1} dt \int_\Lambda dx\, [j - J^a(\rho)] \cdot \chi(\rho)^{-1}[j - J^a(\rho)] \quad (20)$$

in which $J^a(\rho)$ expresses the constitutive relationship of the adjoint hydrodynamics.

Relation (19) has far reaching consequences. By choosing $[T_0, T_1] = [-T, T]$, dividing both sides by $2T$, and taking the limit $T \to 0$, we find

$$\begin{aligned} \int_\Lambda dx\, \frac{\delta V}{\delta \rho} \nabla \cdot j = \frac{1}{2} \int_\Lambda dx\, [J(\rho) + J^*(\rho)] \cdot \chi(\rho)^{-1} j \\ - \frac{1}{4} \int_\Lambda dx\, [J(\rho) + J^a(\rho)] \cdot \chi(\rho)^{-1} [J(\rho) - J^a(\rho)], \end{aligned} \tag{21}$$

which has to be satisfied for any ρ and j. Integrating by parts the left hand side of (21) we obtain that

$$\begin{cases} J(\rho) + J^a(\rho) = -2\chi(\rho) \nabla \dfrac{\delta V}{\delta \rho} \\ \displaystyle\int_\Lambda dx\, J(\rho) \cdot \chi(\rho)^{-1} J(\rho) = \int_\Lambda dx\, J^a(\rho) \cdot \chi(\rho)^{-1} J^a(\rho). \end{cases} \tag{22}$$

These two equations are symmetric in J and J^a. The first equation may be considered as a fluctuation–dissipation relation for the currents.

We now define the *symmetric current* J_S by

$$J_S(\rho) = -\chi(\rho)\nabla\frac{\delta V}{\delta \rho}. \tag{23}$$

Since the stationary density $\bar{\rho}$ is a minimum for V, then $(\delta V/\delta\rho)(\bar{\rho}) = 0$. The symmetric current thus vanishes at the stationary profile,

$$J_S(\bar{\rho}) \;=\; 0. \tag{24}$$

We rewrite the hydrodynamic current as

$$J(\rho) = J_S(\rho) + J_A(\rho), \tag{25}$$

which defines the *antisymmetric current* J_A.

In view of these definitions, equations (22) become

$$\begin{cases} J^a(\rho) \;=\; J_S(\rho) - J_A(\rho)\;, \\ \displaystyle\int_\Lambda dx\, J_S(\rho)\cdot\chi(\rho)^{-1} J_A(\rho) = 0. \end{cases} \tag{26}$$

In this way we see that the splitting of the currents and the orthogonality property are a consequence of the existence of a time reversed dynamics admitting an hydrodynamic behavior. Moreover, inserting the first of the two equations (22) into the second we obtain the equation for V

$$\int_\Lambda dx\, \nabla\frac{\delta V}{\delta\rho}\cdot\chi(\rho)\nabla\frac{\delta V}{\delta\rho} - \int_\Lambda dx\,\frac{\delta V}{\delta\rho}\nabla\cdot J(\rho) = 0\,. \tag{27}$$

This will be interpreted as a Hamilton-Jacobi equation. V is the maximal positive solution to (27) which vanishes when $\rho = \bar\rho$. Since $J(\rho)$ and $J^a(\rho)$ play a symmetric role in (22), the Hamilton-Jacobi equation (27) holds replacing $J(\rho)$ with $J^a(\rho)$.

In view of the fluctuation-dissipation relation (22), we may write the hydrodynamic equation and the adjoint hydrodynamic equation as

$$\partial_t \rho = \nabla \cdot \left(\chi(\rho) \nabla \frac{\delta V}{\delta \rho} \right) - \nabla \cdot J_A(\rho),$$

$$\partial_t \rho = \nabla \cdot \left(\chi(\rho) \nabla \frac{\delta V}{\delta \rho} \right) + \nabla \cdot J_A(\rho)$$

respectively. Another way of writing the adjoint hydrodynamic equation is

$$\partial_t \rho = -\nabla \cdot D(\rho) \nabla \rho + \nabla \cdot \chi(\rho) \left(E + 2 \nabla \frac{\delta V}{\delta \rho} \right). \tag{28}$$

In spite of its appearance, the forward evolution of this equation is well posed. Indeed, the added external field $2\nabla(\delta V/\delta\rho)$ produces a second order term which makes the equation of parabolic type. In the case of equilibrium states the adjoint hydrodynamics coincides with the original one.

Identification of the optimal trajectory defining $V(\rho)$

Consider a trajectory connecting the density profiles ρ_{t_1} and ρ_{t_2} and its time reversal. Recalling (19) we have

$$V(\rho_{t_1}) + \mathcal{I}_{[t_1,t_2]}(\rho, j) = V(\rho_{t_2}) + \mathcal{I}^a_{[-t_2,-t_1]}(\theta\rho, \theta j)$$

By taking $\rho_{t_1} = \bar{\rho}$, which implies $V(\rho_{t_1}) = 0$, $\rho_{t_2} = \rho$, the $\inf$ over all possible trajectories and time intervals we obtain the variational expression of V (10)

$$V(\rho) = \inf_{\substack{\rho(t), j(t): \\ \nabla\cdot j = -\partial_t \rho \\ \rho(-\infty)=\bar{\rho}, \rho(0)=\rho}} \mathcal{I}_{[-\infty,0]}(\rho, j),$$

with the minimizer defined by

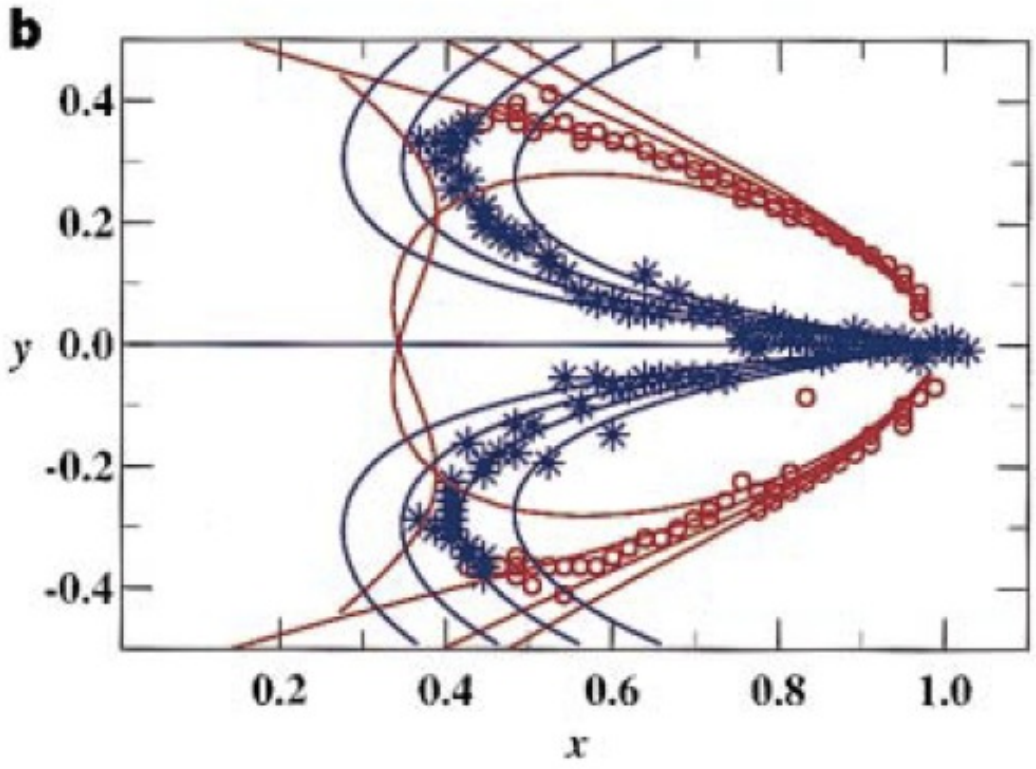
$$\mathcal{I}^a_{[-\infty,0]}(\theta\rho, \theta j) = 0 \tag{29}$$

that is $\theta\rho, \theta j$ must be a solution of the adjoint hydrodynamics.

An example

D. G. Luchinsky, P. V. E. McClintock, Nature **389**, *463 (1997)*

$$d\mathbf{x}_t = \mathbf{f}(\mathbf{x}_t)dt + \epsilon d\mathbf{w}_t, \quad \mathbf{f}(\mathbf{x}) = (x - x^3 - axy^2, -(1 + x^2)y)$$



Interpretation of the quasi-potential

It is easy to see that $V(\rho)$ is equal to the energy dissipated by the thermodynamic force $-\nabla\frac{\delta V}{\delta \rho}$ along the optimal trajectory denoted ρ^*.

$$
\begin{aligned}
V(\rho) &= \int_{-\infty}^{0} dt \left\langle \frac{\delta V}{\delta \rho}, \partial_t \rho^* \right\rangle \\
&= \int_{-\infty}^{0} dt \left\langle \frac{\delta V}{\delta \rho}, \nabla \cdot J^a(\rho^*) \right\rangle = \int_{-\infty}^{0} dt \left\langle (-J^a(\rho^*)) \cdot \nabla \frac{\delta V}{\delta \rho} \right\rangle
\end{aligned}
$$

Charged particle in a magnetic field

As a simple illustration let us consider a charged particle in a viscous medium subjected to a magnetic field,

$$\dot{p} = \frac{e}{mc}\, p \wedge H - \frac{1}{\tau} p \,, \tag{30}$$

where p is the momentum, e the charge, H the magnetic field, m the mass, c the velocity of the light, and τ the relaxation time. The dissipative term p/τ is orthogonal to the Lorenz force $p \wedge H$.

We define time reversal as the transformation $p \mapsto -p$, $H \mapsto -H$. In this case the adjoint equation coincides with the time reversed dynamics, which is given by

$$\dot{p} = -\frac{e}{mc}\, p \wedge H - \frac{1}{\tau} p \tag{31}$$

In this example, $J_S(p) = p/\tau$ and $J_A(p) = -(e/mc)p \wedge H$.

Gas of independent particles

Another simple example is the case of a system of independent particles, the corrisponding transport coefficients are $D(\rho) = I$ and $\chi(\rho) = \rho I$ where D_0, χ_0 are scalar and I denotes the identity matrix.

In the one dimensional case, with $\Lambda = (0, L)$, $\lambda(0) = \lambda_0$, $\lambda(L) = \lambda_1$ the stationary density profile is $\bar{\rho}(x) = \rho_0(1 - x/L) + \rho_1 x/L$ where ρ_0 and ρ_1 are the densities associated to λ_0 and λ_1. In this case

$$J_{\mathrm{S}}(\rho) = -\nabla\rho + \frac{\rho_1 - \rho_0}{L}\,\frac{\rho}{\bar{\rho}}$$

$$J_{\mathrm{A}}(\rho) = -\frac{\rho_1 - \rho_0}{L}\,\frac{\rho}{\bar{\rho}}$$

Circulation of a fluid in a ring

A more interesting example is provided by the circulation of a fluid in a ring. In absence of an external field we have an equilibrium state with constant density $\bar{\rho}$ and $J(\bar{\rho}) = 0$. If we switch on a constant weak driving field E tangent to the ring the system moves rigidly with a current $J(\bar{\rho}) = \chi(\bar{\rho})E$ and $V(\rho)$ is the same as in equilibrium. Time reversal corresponds to inverting the current, that is to changing E with $-E$. In this case $J_A(\rho) = \chi(\rho)E$.

A simple calculation shows that J_S and J_A are orthogonal.

A general principle

Given the hydrodynamic equation, that is the transport coefficients $D(\rho)$ and $\chi(\rho)$, the orthogonal splitting of the current induced by the quasi-potential $V(\rho)$ characterizes completely the macroscopic behavior of diffusive systems in stationary states.

A control theory point of view

We consider the system in presence of an extra field F so that the hydrodynamic equation is

$$\partial_t \rho = -\nabla J(\rho) - \nabla(\chi(\rho)F) \tag{32}$$

We want to choose F to drive the system from its stationary state $\bar{\rho}$ to an arbitrary state ρ with minimal cost. We define the cost function as before

$$\frac{1}{4}\int_{t_1}^{t_2} ds\, \langle F(s), \chi(\rho^F(s))F(s)\rangle \tag{33}$$

where $\rho^F(s)$ is the solution of (32). More precisely, given $\rho(t_1) = \bar{\rho}$ we want to drive the system to $\rho(t_2) = \rho$ by an external field F which minimizes (33). This is a standard problem in control theory.

Let

$$\mathcal{V}(\rho) = \inf \frac{1}{4} \int_{t_1}^{t_2} ds \, \langle F(s), \chi(\rho^F(s)) F(s) \rangle \tag{34}$$

where the infimum is taken with respect to all fields F which drive the system to ρ in an arbitrary time interval $[t_1, t_2]$. The optimal field F can be obtained by solving the Bellman equation which reads

$$\min_F \left\{ \frac{1}{4} \langle F, \chi(\rho) F \rangle + \left\langle \nabla(J(\rho) + \chi(\rho) F), \frac{\delta \mathcal{V}}{\delta \rho} \right\rangle \right\} = 0 \tag{35}$$

It is easy to express the optimal F in terms of $\mathcal{V}$; we get

$$F = 2 \nabla \frac{\delta \mathcal{V}}{\delta \rho} \tag{36}$$

By substituting in (35) this reduces to the Hamilton-Jacobi equation.

Characterization of equilibrium states

We define the system to be in *equilibrium* if and only if the current in the stationary profile $\bar{\rho}$ vanishes, i.e. $J(\bar{\rho}) = 0$. In this case, even in presence of external fields (e.g. gravitational or centrifugal fields), the Hamilton-Jacobi equation can be solved. Let

$$f(\rho, x) = \int_{\bar{\rho}(x)}^{\rho} dr \int_{\bar{\rho}(x)}^{r} dr' \; f_0''(r') = f_0(\rho) - f_0(\bar{\rho}(x)) \\ - f_0'\big(\bar{\rho}(x)\big)\big[\rho - \bar{\rho}(x)\big] \tag{37}$$

the maximal solution of H-J is

$$V(\rho) = \int_{\Lambda} dx \; f\big(\rho(x), x\big) \tag{38}$$

Define *macroscopic reversibility*

$$J^a(\rho) = -2\chi(\rho)\nabla\frac{\delta V}{\delta\rho} - J(\rho) = J(\rho) \tag{39}$$

We have the following theorem
$J(\bar{\rho}) = 0$ *is equivalent to macroscopic reversibility.*
In the case of macroscopic reversibility the Hamilton-Jacobi equation reduces to

$$J(\rho) = -\chi(\rho)\nabla\frac{\delta V}{\delta\rho}(\rho) \tag{40}$$

We remark that, even if the free energy V is a non local functional, the equality $J(\rho) = J^a(\rho)$ implies that the thermodynamic force $\nabla\delta V/\delta\rho$ is local.

A heuristic derivation of the fundamental formula for a lattice gas

The basic microscopic model is given by a stochastic lattice gas with a weak external field and particle reservoirs at the boundary. More precisely, let $\Lambda \subset R^d$ be a smooth domain and set $\Lambda_N = N\Lambda \cap Z^d$; we consider a Markov process on the state space X^{Λ_N}, where X is a subset of N, e.g. $X = \{0, 1\}$ when an exclusion principle is imposed. The number of particles at the site $i \in \Lambda_N$ is denoted by $\eta_i \in X$ and the whole configuration by $\eta \in X^{\Lambda_N}$. The dynamical evolution is given by a continuous time Markov process on the state space X^{Λ_N}.

The markov process is specified by transition rates $c_{i,j}(\eta)$ describing the jump of a particle from a site i to its nearest neighbor j and rates $c_i^{\pm}(\eta)$ describing the appearance or loss of a particle at the boundary site i.
The reservoirs are characterized by a chemical potential λ. We assume that the rates satisfy a local detailed balance condition with respect to a Gibbs measure associated to some Hamiltonian H. Typically, for a non equilibrium model, we can consider Λ the cube of side one and the system under a constant force E/N. Moreover we choose the chemical potential λ so that $\lambda(j/N) = \lambda_0$ if the first coordinate of j is 0, $\lambda(j/N) = \lambda_1$ if the first coordinate of j is N, and impose periodic boundary conditions in the other directions.

Deatailed balance in the bulk

$$c_{i,j}(\eta) \;=\; \exp\big\{ -\big[H(\sigma^{i,j}\eta) - H(\eta)\big]\big\}\, c_{j,i}(\sigma^{i,j}\eta)\,, \quad i,j \in \Lambda_N \tag{41}$$

where for $i, j \in \Lambda_N$, $\sigma^{i,j}\eta$ is the configuration obtained from η by moving a particle from i to j.

Detailed balance at the boundary

$$c_{i,j}(\eta) \;=\; \exp\big\{-\big[H(\sigma^{i,j}\eta)-H(\eta)\big]-\lambda_j\big\}\, c_{j,i}(\sigma^{i,j}\eta)\,, \quad i \in \Lambda_N,\, j \notin \Lambda_N \tag{42}$$

To define the current denote by $N_t^{i,j}$ the number of particles that jumped from i to j in the macroscopic time interval $[0,t]$. At the boundary we adopt the convention that $N_t^{i,j}$ represents the number of particles created at j due to the reservoir at i if $i \notin \Lambda_N$, $j \in \Lambda_N$ and that $N_t^{i,j}$ represents the number of particles that left the system at i by jumping to j if $i \in \Lambda_N$, $j \notin \Lambda_N$. The difference $J_t^{i,j} = N_t^{i,j} - N_t^{j,i}$ is the net number of particles flown across the bond $\{i,j\}$ in the time interval $[0,t]$. In other words, given a path $\eta(s)$, $0 \le s \le t$, the instantaneous current $dJ_t^{i,j}/dt$ is a sum of δ–functions localized at the jump times across the bond $\{i,j\}$ with weight $+1$, respectively -1, if a particle jumps from i to j, respectively from j to i.

We now define the empirical current density

$$j^N(t,x) = \frac{1}{N^{d+1}} \sum_{\{i-j\}} (i-j)\delta(x - i/N) \frac{dJ_t}{dt}^{i,j} \tag{43}$$

where the sum is over unoriented bonds such that $|i-j| = \frac{1}{N}$ Fix a current profile $j(t,x)$ and an initial configuration η^N; in order to make $j(t,x)$ typical, we introduce an external field F. Let ρ be the solution of

$$\begin{cases} \partial_t \rho + \nabla \cdot j = 0 \\ \rho(0,x) = \rho_0(x) \end{cases} \tag{44}$$

and $F : [0,T] \times \Lambda \to R^d$ be the vector field such that

$$\begin{aligned} j &= J(\rho) + \chi(\rho)F \\ &= -\frac{1}{2} D(\rho)\nabla\rho + \chi(\rho)\{\nabla H + F\} \end{aligned}$$

We introduce a perturbed measure $P^{N,F}_{\eta^N}$ which is obtained by modifying the rates as follows

$$c^F_{i,j}(\eta) \;=\; c_{i,j}(\eta)\, e^{N^{-1}F(t,i/N)\cdot(j-i)}$$

One can show by a direct calculation that

$$\begin{aligned}\frac{dP^N_{\eta^N}}{dP^{N,F}_{\eta^N}} \;&\sim\; \exp\Big\{ - N^d \frac{1}{2}\int_0^T dt\, \langle F, \chi(\rho) F\rangle \Big\} \\ &=\; \exp\Big\{ - N^d I_{[0,T]}(j)\Big\}\end{aligned}$$

Moreover, under $P^{N,F}_{\eta^N}$, as $N\to\infty$, $j^N(t,x)$ converges to $j(t,x)$. Therefore,

$$\begin{aligned}&P^N_{\eta^N}\Big(j^N(t,x)\approx j(t,x),\;\; (t,u)\in[0,T]\times\Lambda\Big) \\ &\quad = E^{N,F}_{\eta^N}\Big(\frac{dP^N_{\eta^N}}{dP^{N,F}_{\eta^N}}\;{\scriptstyle\{j^N\approx j\}}\Big) \sim e^{-N^d I_{[0,T]}(j)}\end{aligned}$$

where $E^{N,F}_{\eta^N}$ denotes expectation with respect to the perturbed probability measure $P^{N,F}_{\eta^N}$.

Introducing now the empirical density

$$\pi^N(u) = \frac{1}{N^d} \sum_{x \in \Lambda_N} \delta(u - x/N)\eta_x$$

we can write the fundamental formula in the form

$$\mathbb{P}\big(\pi^N \approx \rho(t,u), j^N \approx j(t,u), \;\; t \in [0,T]\big) \sim \exp\{-N^d \beta \mathcal{R}_{[0,T]}(\rho, j)\} \tag{45}$$

We emphasize that we need to allow general non–gradient external fields F. On the other hand for the large deviation principle of the density it is sufficient to consider gradient external fields.

2. Applications

An example of calculation of $V(\rho)$: the boundary driven simple exclusion process

We consider the variational problem defining $V(\rho)$ for the one-dimensional simple exclusion process and show that the associated Hamilton-Jacobi equation

$$\int_\Lambda \left(\nabla \frac{\delta V}{\delta \rho} \rho(1-\rho) \nabla \frac{\delta V}{\delta \rho} + \frac{\delta V}{\delta \rho} \Delta \rho \right) dx = 0 \tag{46}$$

can be reduced to the a non-linear ordinary differential equation.. We look for a solution of the Hamilton-Jacobi equation (46) by performing the change of variable

$$\frac{\delta V}{\delta \rho(x)} = \log \frac{\rho(x)}{1-\rho(x)} - \phi(x;\rho) \tag{47}$$

for some functional $\phi(x;\rho)$ to be determined satisfying the boundary conditions $\phi(\pm 1) = \log \rho(\pm 1)/[1-\rho(\pm 1)]$.

Inserting (47) into (46), we get that

$$
\begin{aligned}
0 &= -\int_\Lambda dx\, \nabla\Big(\log\frac{\rho}{1-\rho} - \varphi\Big)\rho(1-\rho)\nabla\varphi \\
&= -\int_\Lambda dx\, \Big[\nabla\rho\nabla\phi - \rho(1-\rho)(\nabla\varphi)^2\Big].
\end{aligned}
$$

Adding and subtracting $e^{\varphi}/(1+e^{\varphi})$, we may rewrite the previous integral as

$$
\begin{aligned}
&-\int_{\Lambda} dx\, \nabla\Big(\rho - \frac{e^{\varphi}}{1+e^{\varphi}}\Big)\nabla\varphi \\
&\quad -\int_{\Lambda} dx\, \Big(\rho - \frac{e^{\varphi}}{1+e^{\varphi}}\Big)\Big(\rho - \frac{1}{1+e^{\varphi}}\Big)(\nabla\varphi)^2.
\end{aligned}
$$

Since $\rho - e^{\phi}/(1+e^{\phi})$ vanishes at the boundary, an integration by parts yields

$$
0 = \int_{\Lambda} dx\, \Big(\rho - \frac{e^{\varphi}}{1+e^{\varphi}}\Big)\Big(\Delta\varphi + \frac{(\nabla\varphi)^2}{1+e^{\varphi}} - \rho(\nabla\varphi)^2\Big). \tag{48}
$$

We thus obtain a solution of the Hamilton-Jacobi if we solve the following ordinary differential equation which relates the functional $\phi(x) = \phi(x; \rho)$ to ρ

$$\begin{cases} \dfrac{\Delta\phi(x)}{[\nabla\phi(x)]^2} + \dfrac{1}{1+e^{\phi(x)}} = \rho(x) \quad x \in (-1,1)\,, \\ \\ \phi(\pm 1) = \log \rho(\pm 1)/[1-\rho(\pm 1)]\,. \end{cases} \tag{49}$$

This equation admits a unique monotone solution which is the relevant one for the quasi-potential. computation shows that the derivative of the functional

$$V(\rho) = F(\rho) + \int_\Lambda dx \left\{ (1-\rho)\phi + \log\left[\frac{\nabla\phi}{\nabla\bar{\rho}\,(1+e^{\phi})} \right] \right\} \tag{50}$$

is given by (47) when $\phi(x; \rho)$ solves (49).

Correlation functions

We are concerned only with *macroscopic correlations* which are a generic feature of nonequilibrium models. Microscopic correlations which decay as a summable power law disappear at the macroscopic level.
We introduce the *pressure* functional as the Legendre transform of the quasi-potential V

$$G(h) = \sup_{\rho} \left\{ \langle h\rho \rangle - V(\rho) \right\}$$

By Legendre duality we have the change of variable formulae $h = \frac{\delta V}{\delta \rho}$, $\rho = \frac{\delta G}{\delta h}$, so that the Hamilton-Jacobi equation can then be rewritten in terms of G as

$$\left\langle \nabla h \cdot \chi\Big(\frac{\delta G}{\delta h}\Big) \nabla h \right\rangle - \left\langle \nabla h \cdot D\Big(\frac{\delta G}{\delta h}\Big) \nabla \frac{\delta G}{\delta h} - \chi\Big(\frac{\delta G}{\delta h}\Big) E \right\rangle = 0 \quad (51)$$

where h vanishes at the boundary of Λ. As for equilibrium systems, G is the generating functional of the correlation functions.

We define

$$C_n(x_1,\ldots,x_n)=\frac{\delta^n G}{\delta h(x_1)\cdots\delta h(x_n)}\Big|_{h=0} \tag{52}$$

By expanding (51) around the stationary state we obtain after non trivial manipulations and combinatorics the following recursive equations for the correlation functions

$$\frac{1}{(n+1)!}\mathcal{L}^{\dagger}_{n+1}C_{n+1}(x_1,x_2,\ldots,x_{n+1})$$

$$=\Bigg\{\sum_{N(\vec{\imath})=n-1}^{\vec{\imath}}\frac{1}{K(\vec{\imath})}\nabla_{x_1}\cdot\Big(\chi^{(\Sigma(\vec{\imath}))}(\bar{\rho}(x_1))C_{\vec{\imath}}(x_1,\ldots,x_n)\nabla_{x_1}\delta(x_1-x_{n+1})\Big)$$

$$-\sum_{N(\vec{\imath})=n,i_n=0}^{\vec{\imath}}\frac{1}{K(\vec{\imath})}\nabla_{x_1}\cdot\nabla_{x_1}\Big(D^{(\Sigma(\vec{\imath})-1)}(\bar{\rho}(x_1))C_{\vec{\imath}}(x_1,\ldots,x_{n+1})\Big)$$

$$+\sum_{N(\vec{\imath})=n,i_n=0}^{\vec{\imath}}\frac{1}{K(\vec{\imath})}\nabla_{x_1}\cdot$$

$$\Big(\chi^{(\Sigma(\vec{\imath}))}(\bar{\rho}(x_1))C_{\vec{\imath}}(x_1,\ldots,x_{n+1})E(x_1)\Big)\Bigg\}^{sym}$$

For the pair correlations write

$$C(x,y) = C_{\rm eq}(x)\delta(x-y) + B(x,y)$$

where

$$C_{\rm eq}(x) = D^{-1}(\bar\rho(x))\chi(\bar\rho(x))$$

We then obtain the following equation for B

$$\mathcal{L}^\dagger B(x,y) = \alpha(x)\delta(x-y) \tag{53}$$

where $\mathcal{L}^\dagger$ is the formal adjoint of the elliptic operator $\mathcal{L} = L_x + L_y$ given by, using the usual convention that repeated indices are summed,

$$L_x = D_{ij}(\bar\rho(x))\partial_{x_i}\partial_{x_j} + \chi'_{ij}(\bar\rho(x))E_j(x)\partial_{x_i} \tag{54}$$

and

$$\alpha(x) = \partial_{x_i}\left[\chi'_{ij}\left(\bar\rho(x)\right) D^{-1}_{jk}\left(\bar\rho(x)\right)\bar J_k(x)\right]$$

where $\bar J = J(\bar\rho) = -D(\bar\rho(x))\nabla\bar\rho(x) + \chi(\bar\rho(x))E(x)$ is the macroscopic current in the stationary profile.

Sample of experimental results

W. B. Li, P. N. Segre, J. V. Sengers, R. W. Gammon, J. Phys.: Condensed Matter **23A** , *A119 (1994)*

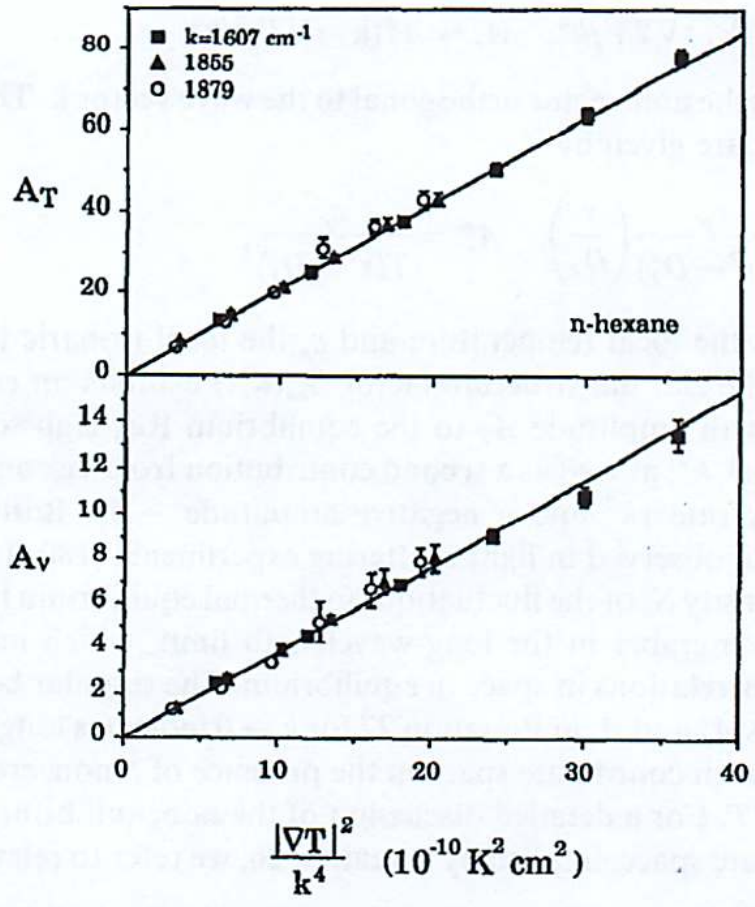


Figure 7 Amplitudes A_T and A_v of the nonequilibrium fluctuations in liquid *n*-hexane at an average temperature of 25°C as a function of $(\nabla T^2)/k^4$. The symbols indicate experimental values obtained by Li et al (186). The solid lines represent the values predicted from Equations 27 and 28. Adapted from Ref. 186.

Diffusive systems with periodic boundary conditions

We consider a system on a ring satisfying the Einstein relation $D(\rho) = \chi(\rho) f_0^{"}(\rho)$. In the case of constant field E the stationary solution is simply the constant function $\bar{\rho}(u) = m$. We define

$$f_m(\rho) = \int_m^\rho dr \int_m^r dr' f_0^{"}(r')$$

We claim that the quasi-potential is

$$V_m(\rho) = \int_\Lambda du \, f_m(\rho(u)) \tag{55}$$

for any value of the external field E.
If $E = 0$, by using the Einstein relation it is easy to check that V_m solves the Hamilton-Jacobi equation. If E is a constant, since the boundary conditions are periodic, we have that

$$\left\langle \frac{\delta V_m}{\delta \rho}, \nabla \cdot \chi(\rho) E \right\rangle = 0$$

hence V_m solves the Hamilton-Jacobi equation for any (constant) external field E.

Thermodynamics of currents: the $\Phi(J)$ functional

Currents involve time in their definition so it is natural to consider space-time thermodynamics. The *cost functional* to produce a current trajectory $j(t,x)$ is

$$\mathcal{I}_{[0,T]}(j) \;=\; \frac{1}{4}\int_0^T dt\,\big\langle [j-J(\rho)], \chi(\rho)^{-1}[j-J(\rho)]\big\rangle \qquad (56)$$

in which we recall that

$$J(\rho) = -D(\rho)\nabla\rho + \chi(\rho)E\;.$$

where $\rho = \rho(t,u)$ is obtained by solving the continuity equation $\partial_t\rho + \nabla\cdot j = 0$.

Let $J(x)$ be the time average of $j(t,x)$ that we assume divergence free, i.e.

$$J(x) = \frac{1}{T}\int_0^T j(x,t)dt \tag{57}$$

and define

$$\Phi(J) = \lim_{T\to\infty} \inf_j \frac{1}{T}\,\mathcal{I}_{[0,T]}(j)\;, \tag{58}$$

where the infimum is carried over all paths $j = j(t,u)$ having time average J.
This functional is convex and satisfies a Gallavotti-Cohen type relationship

$$\Phi(J) - \Phi(-J) = \Phi(J) - \Phi^a(J) = -\langle J, E\rangle + \int_{\partial\Lambda} d\Sigma\,\lambda_0\, J\cdot\hat{n} \tag{59}$$

Note that the right hand side of (59) is the power produced by the external field and the boundary reservoirs. Entropy production can be simply derived from $\Phi(J)$).

Lagrangian phase transitions: singularities of $V(\rho)$

BDGJL

We want to show that the quasi-potential $V(\rho)$ of the weakly asymmetric simple exclusion process is non-differentiable for large values of the external field if $\rho_0 < \rho_1$. For this we switch to a Hamiltonian picture. The canonical equations associated to the Hamiltonian

$$\mathcal{H}(\rho,\pi) = \Big\langle \nabla\pi \cdot \chi(\rho)\nabla\pi \Big\rangle + \Big\langle \nabla\pi \cdot J(\rho) \Big\rangle \tag{60}$$

are

$$\rho_t + \nabla \cdot \chi(\rho)E \;=\; \nabla \cdot D(\rho)\nabla\rho \;-\; 2\nabla \cdot \chi(\rho)\nabla\pi \tag{61}$$

$$\pi_t + E \cdot \chi'(\rho)\nabla\pi \;=\; -\nabla\pi \cdot \chi'(\rho)\nabla\pi - D(\rho)\nabla\nabla\pi \tag{62}$$

in this formula, $D(\rho)\nabla\nabla\pi = \sum_{i,j} D_{i,j}(\rho)\partial^2_{x_i,x_j}\pi$.

Since $\bar{\rho}$ is a stationary solution of the hydrodynamic equation the Hamiltonian dynamics admits the equilibrium position $(\bar{\rho}, 0)$. Consider the solution of the canonical equations with initial condition $(\rho, 0)$. Due to $\bar{\rho}$ being globally attractive for the hydrodynamics, such a solution of the canonical equations converges to the equilibrium position $(\bar{\rho}, 0)$ as $t \to +\infty$. The set of points $\{(\rho, \pi) \,:\, \pi = 0\}$ is therefore the stable manifold $\mathscr{M}_{\mathrm{s}}$ associated to the equilibrium position $(\bar{\rho}, 0)$. The unstable manifold $\mathscr{M}_{\mathrm{u}}$ is defined as the set of points (ρ, π) such that the solution of the canonical equations starting from (ρ, π) converges to $(\bar{\rho}, 0)$ as $t \to -\infty$. By the conservation of the energy, $\mathscr{M}_{\mathrm{u}}$ is a subset of the manifold $\{(\rho, \pi) \,:\, \mathcal{H}(\rho, \pi) = \mathcal{H}(\bar{\rho}, 0) = 0\}$.

A basic result in Hamiltonian dynamics is the following . Given a closed curve $\gamma = \{(\rho(\alpha), \pi(\alpha))\,,\ \alpha \in [0,1]\}$, the integral $\oint_\gamma \pi\, d\rho \ = \int_0^1 \langle \pi(\alpha)\, \rho_\alpha(\alpha) \rangle\, d\alpha$ is invariant under the Hamiltonian evolution. This means that, by denoting with $\gamma(t)$ the evolution of γ under the Hamiltonian flow, $\oint_{\gamma(t)} \pi\, d\rho \ = \oint_\gamma \pi\, d\rho$. In view of this result, if γ is a closed curve contained in the unstable manifold $\mathscr{M}_{\rm u}$ then $\oint_\gamma \pi\, d\rho \ = \lim_{t \to -\infty} \oint_{\gamma(t)} \pi\, d\rho \ = 0$. We can therefore define the pre-potential $W : \mathscr{M}_{\rm u} \to R$ by

$$\mathcal{G}(\rho, \pi) \ = \ \int_\gamma \hat{\pi}\, d\hat{\rho} \ , \tag{63}$$

where the integral is carried over a path $\gamma = (\hat{\rho}, \hat{\pi})$ in $\mathscr{M}_{\rm u}$ which connects $(\bar{\rho}, 0)$ to (ρ, π). The possibility of defining such potential is usually referred to by saying that $\mathscr{M}_{\rm u}$ is a Lagrangian manifold.

The relationship between the quasi-potential and the pre-potential is given by

$$V(\rho) \;=\; \inf\left\{\mathcal{G}(\rho,\pi)\,,\; \pi \;:\; (\rho,\pi)\in \mathscr{M}_{\mathrm{u}}\right\}\,. \tag{64}$$

Indeed, fix ρ and consider π such that (ρ,π) belongs to $\mathscr{M}_{\mathrm{u}}$. Let $(\hat\rho(t),\hat\pi(t))$ be the solution of the Hamilton equation starting from (ρ,π) at $t=0$. Since $(\rho,\pi)\in\mathscr{M}_{\mathrm{u}}$, $(\hat\rho(t),\hat\pi(t))$ converges to $(\bar\rho,0)$ as $t\to-\infty$. Therefore, the path $\hat\rho(t)$ is a solution of the Euler-Lagrange equations for the action $I_{(-\infty,0]}$, which means that it is a critical path.

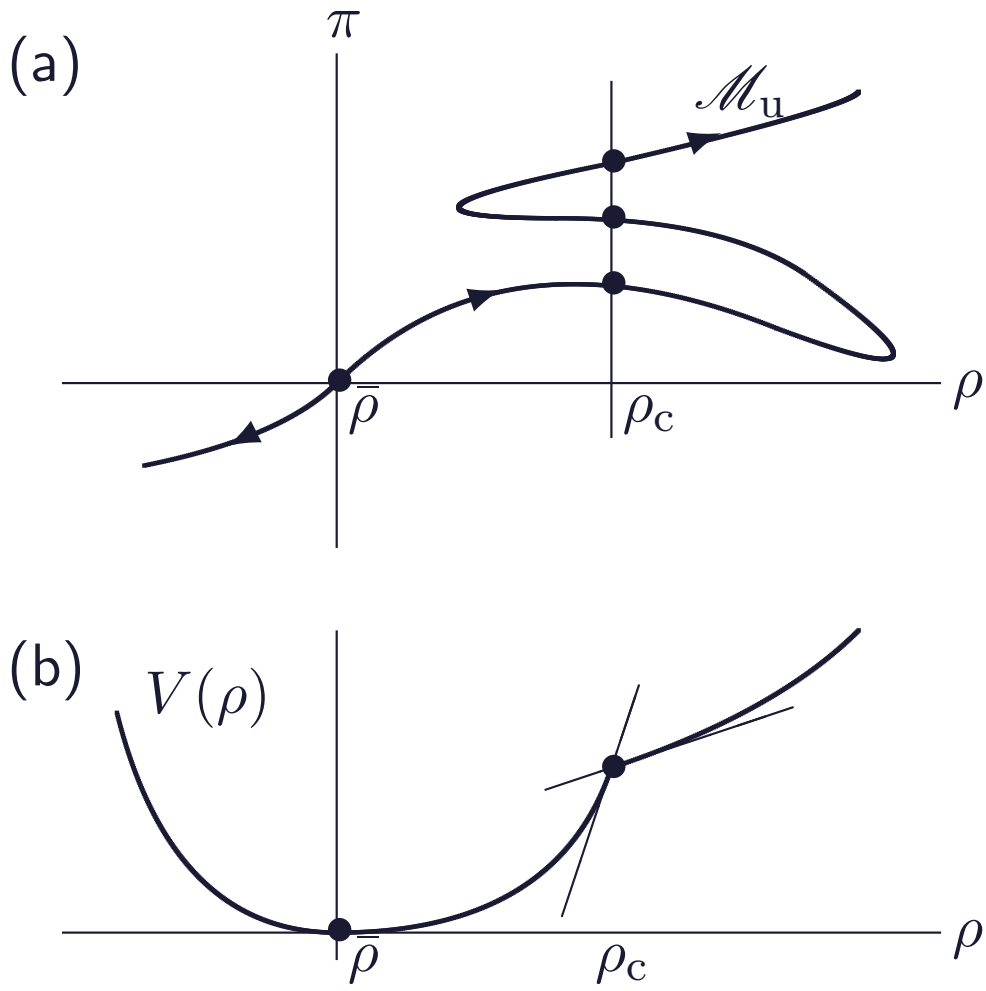


Figure: (a) Picture of the unstable manifold. (b) Graph of the quasi-potential. ρ_{c} is a caustic point, e.g., $\mathcal{G}(\rho_{\mathrm{c}}, \pi_1) = \mathcal{G}(\rho_{\mathrm{c}}, \pi_3)$.

In a neighborhood of the fixed point $(\bar{\rho}, 0)$, the unstable manifold $\mathscr{M}_{\mathrm{u}}$ can be written as a graph, namely it has the form $\mathscr{M}_{\mathrm{u}} = \{(\rho, \pi) : \pi = m_{\mathrm{u}}(\rho)\}$ for some map m_{u}. In this case, the infimum is trivial and $V(\rho) = \mathcal{G}(\rho, m_{\mathrm{u}}(\rho))$. In general this is not true globally and it may happen, for special ρ, that the variational problem admits more than a single minimizer (Figure 1.a). The set of profiles ρ for which the minimizer is not unique is called the caustic. In general, it is a codimension one submanifold of the configuration space. We call the occurrence of this situation a Lagrangian phase transition. In this case, profiles arbitrarily close to each other but lying on opposite sides of the caustic are reached by optimal paths which are not close to each other. This implies that on the caustics the first derivative of the quasi-potential is discontinuous (Figure 1.b).

Consider the case of the weakly asymmetric exclusion with $D = 1$, $\rho(1-\rho)$ and E constant. Introducing the functional $\mathcal{G}_E$

$$\mathcal{G}_E(\rho,\varphi) = \int_0^1 \Big[s(\rho) + s(\varphi_x/E) + (1-\rho)\varphi - \log\left(1+e^{\varphi}\right)\Big]\, dx \ ,$$

with $s(\rho) = \rho\log\rho + (1-\rho)\log(1-\rho)$ it can be shown that

$$\int_\Gamma \langle \pi, d\rho\rangle \ = \ \mathcal{G}_E\big(\rho(1),\phi(1)\big) \ - \ \mathcal{G}_E\big(\rho(0),\phi(0)\big) \ .$$

Hence $W_E(\rho,\pi) = \mathcal{G}_E(\rho,\varphi) - \mathcal{G}_E(\bar\rho_E, s'(\bar\rho_E))$, where $(\varphi,\rho)\in\mathscr{M}_{\rm u}$. Therefore,

$$V_E(\rho) = \inf\left\{\mathcal{G}_E(\rho,\varphi)\,,\varphi\,:(\varphi,\rho)\in\mathscr{M}_{\rm u}\right\} - \mathcal{G}_E(\bar\rho_E, s'(\bar\rho_E)) \ . \quad (65)$$

It is not difficult to show that in the limit $E = \infty$, if the density profile ρ is suitably chosen, the variational principle admits two minimizers. Then by a continuity argument one shows that this persists when the external field E is large.

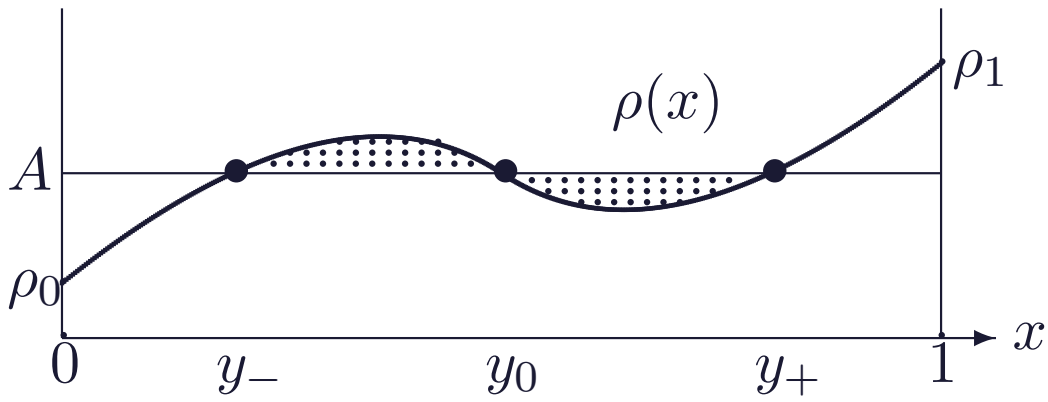


Figure: Graph of a caustic density profile for $E = \infty$. The shaded regions have equal area.

Dynamical phase transitions

There is a model of heat conduction introduced by Kipnis, Marchioro and Presutti characterized macroscopically by $D = 1$ and $\chi = \rho^2$. One can show that in equilibrium with periodic boundary conditions and for small J

$$\Phi(J) = \frac{1}{2}\frac{J^2}{\bar{\rho}^2} \tag{66}$$

where $\bar{\rho}$ is the flat equilibrium profile. For $J > J_c, \quad \Phi(J) < \frac{1}{2}\frac{J^2}{\bar{\rho}^2}$ for a time dependent density profile which is a traveling wave of the form $\rho_0(x - vt)$. Translation invariance in time is spontaneously broken.

Universality in current fluctuations

C. Appert-Rolland, B. Derrida, V. Lecomte, F. van Wijland, Phys.Rev. E **78**, *021122 (2008)*

Let $Q(t) = \int_0^t j(t')dt'$ the total integrated current during the time interval $(0, t)$. Define the generating function of the cumulants of Q

$$\psi_J(s) = \lim_{t\to\infty} \frac{\ln\langle \exp -sQ\rangle}{t} = \Phi^*(s) \tag{67}$$

where the brackets denote an average over the time evolution during $(0, t)$. $\Phi^*(s)$ is the Legendre transform of $\Phi(J)$. The authors estimate $\Phi(J)$ from the large deviation formula

$$\mathbb{P}(\{\rho(x,t), j(x,t)\}) \simeq \exp -\frac{L}{4}\int_0^T dt \left\langle [j - J(\rho)], \chi(\rho)^{-1}[j - J(\rho)]\right\rangle$$

from which they obtain

$$\lim_{t\to\infty} \frac{\langle Q^{2n}\rangle}{t} = B_{2n-2}\frac{2n!}{n!(n-1)!}D(\frac{-\chi\chi''}{8D^2})^n L^{2n-2}$$