DIPARTIMENTO DI FISICA

SAPIENZA
UNIVERSITÀ DI ROMA

INFN
Istituto Nazionale
di Fisica Nucleare

Dynamic and static large deviations in nonequilibrium statistical mechanics: an overview

Giovanni Jona-Lasinio

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Introduction

Success in proving the Fourier law from mechanics would represent a perfect realization of a reductionist program.

You can be less demanding and still obtain a reasonable understanding of a problem: we understood a lot on equilibrium, in particular on phase transitions and critical phenomena from the Ising model which is not a realistic system.

Stationary states are the simplest generalization of equilibrium states and we may ask whether we can develop a self-contained macroscopic description.

The hope is that stochastic particle models may play a role in non equilibrium similar to Ising in equilibrium.

Large deviations deal with fluctuations from a law of large numbers: in our case this is hydrodynamics.

Starting from the theory of large deviations in stochastic particle models, during the last ten years some progress has been achieved in understanding the macroscopic behavior in nonequilibrium. It has been a collective effort and many people have contributed to it.

Contents

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

Freidlin-Wentzell theory

Consider a stochastic differential equation

$$dx_t = b(x_t)dt + \epsilon\sigma dw_t, \tag{1}$$

where the vector field b is the drift and σ the diffusion matrix. One is interested in the limit $\epsilon \to 0$. Then the following holds: the probability that the solution stay close to a trajectory ϕ_t in a fixed time interval $[0, T]$ is

$$P(x_t \simeq \phi_t) \simeq \exp\left(-\frac{1}{\epsilon^2} I_T(\phi_t)\right), \tag{2}$$

where

$$I_T(\phi_t) = \frac{1}{2}\int_0^T dt(\dot{\phi} - b(\phi_t)\sigma^{-2}(\dot{\phi} - b(\phi_t)). \tag{3}$$

I_T is called the large deviation functional.

The estimate of the stationary distribution in the neighborhood of an equilibrium point follows

$$P(x) \simeq \exp\left(-\frac{1}{\epsilon^2} V(x)\right), \tag{4}$$

where $V(x) = I_\infty(\phi_t^*)$ with ϕ_t^* a trajectory connecting the equilibrium point to x and minimizing I_∞. If there are several equilibrium points or attractors the theory can be easily extended. $V(x)$ is called the quasi-potential.

Equation (4) reminds of the Einstein theory of equilibrium thermodynamic fluctuations which states that the probability of a fluctuation from equilibrium in a macroscopic region of volume $|\Lambda|$ is proportional to

$$\exp\{|\Lambda|\Delta S/k\},$$

where ΔS is the variation of entropy density calculated along a reversible transformation creating the fluctuation and k is the Boltzmann constant.

The lesson we learn is twofold:

1. *in the limit of small noise an estimate of the stationary distribution is reduced to the solution of a variational problem.*

2. *the quasi-potential is the analog of a thermodynamic function.*

Macroscopic systems out of equilibrium

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*

$$\partial_t \rho + \nabla \cdot j = 0 \tag{5}$$

together with the constitutive equation

$$j = J(\rho) = -D(\rho)\nabla\rho + \chi(\rho)E \tag{6}$$

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

$$D(\rho) = \chi(\rho)\, f_0''(\rho) \tag{7}$$

where f_0 is the equilibrium free energy of the homogeneous system.

The equations (5)–(6) have to be supplemented by the appropriate boundary conditions on $\partial\Lambda$ due to the interaction with the external reservoirs. Recalling that $\lambda_0(x)$, $x \in \partial\Lambda$, is the chemical potential of the external reservoirs, these boundary conditions are

$$f_0'\big(\rho(x)\big) = \lambda_0(x) \qquad\qquad x \in \partial\Lambda \tag{8}$$

We denote by $\bar\rho = \bar\rho(x)$, $x \in \Lambda$, the stationary solution, assumed to be unique, of (5), (6), and (8).

The basic dynamic large deviation formula for joint fluctuations of the empirical density and current

BDGJL

$$\mathbb{P}^N_{\mu^N}\left(\pi^N \approx \rho, \mathcal{J}^N \approx j \;\; t \in [0,T]\right) \sim \exp\{-N^d \mathcal{G}_{[0,T]}(\rho, j)\} \tag{9}$$

Here $\mathbb{P}^N_{\mu^N}$ is the stationary probability measure,

$$\mathcal{G}_{[0,T]}(\rho, j) = \begin{cases} V(\rho(0)) + \mathcal{I}_{[0,T]}(j) & \text{if } \partial_t \rho + \nabla \cdot j = 0 \\ +\infty & \text{otherwise} \end{cases} \tag{10}$$

$V(\rho)$ is the large deviation functional of the invariant measure and

$$\mathcal{I}_{[0,T]}(j) \;=\; \frac{1}{4}\int_0^T dt \left\langle [j - J(\rho)], \chi(\rho)^{-1}[j - J(\rho)] \right\rangle \tag{11}$$

in which we recall that

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

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

$$I_{[0,T]}(\rho) = \inf_{\substack{j\,: \\ \nabla\cdot j = -\partial_t \rho}} \mathcal{I}_{[0,T]}(j) \tag{12}$$

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

$$\partial_t \rho = \nabla \cdot \Big(D(\rho)\nabla\rho - \chi(\rho)\big[E + \nabla H\big]\Big) \tag{13}$$

which is a Poisson equation for H.

Write

$$F = \nabla H + \widetilde{F} \tag{14}$$

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

$$I_{[0,T]}(\rho) = \frac{1}{4}\int_0^T dt \left\langle \nabla H(t), \chi(\rho(t))\nabla H(t)\right\rangle \tag{15}$$

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

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

Time reversal

To the time reversed process corresponds the adjoint generator with respect to the invariant measure. 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 $\mathbb{P}^{N,a}_{\mu^N}$, is the time reversal of $\mathbb{P}^{N}_{\mu^N}$, i.e. we have $\mathbb{P}^{N,a}_{\mu^N} = \mathbb{P}^{N}_{\mu^N} \circ \vartheta^{-1}$. Then

$$\begin{aligned} &\mathbb{P}^{N}_{\mu^N}\Big(\pi^N \approx \rho,\ \mathcal{J}^N \approx j\ \ t \in [-T,T]\Big) \\ &= \mathbb{P}^{N,a}_{\mu^N}\Big(\pi^N \approx \vartheta\rho,\ \mathcal{J}^N \approx \vartheta j\ \ t \in [-T,T]\Big) \end{aligned} \tag{16}$$

At the level of large deviations this implies

$$\mathcal{G}_{[-T,T]}(\rho, j) = \mathcal{G}^a_{[-T,T]}(\vartheta\rho, \vartheta j) \tag{17}$$

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

The previous relationship has far reaching consequences. By dividing both sides by $2T$ and taking the limit $T \to 0$ we find

$$
\begin{aligned}
-\Big\langle \frac{\delta V}{\delta\rho}, \nabla \cdot j \Big\rangle &= -\big\langle J(\rho) + J^a(\rho), \chi(\rho)^{-1} j \big\rangle \\
&\quad + \frac{1}{2}\big\langle J(\rho) + J^a(\rho), \chi(\rho)^{-1}[J(\rho) - J^a(\rho)] \big\rangle \qquad (18)
\end{aligned}
$$

which has to be satisfied for any ρ and j. Integrating by parts the left hand side

$$
J(\rho) + J^a(\rho) = -2\chi(\rho)\nabla \frac{\delta V}{\delta\rho} \qquad (19)
$$

$$
\big\langle J(\rho), \chi(\rho)^{-1} J(\rho) \big\rangle = \big\langle J^a(\rho), \chi(\rho)^{-1} J^a(\rho) \big\rangle \qquad (20)
$$

Inserting finally the first of these two equations into the second we obtain the equation for V

$$\left\langle \nabla \frac{\delta V}{\delta \rho}, \chi(\rho) \nabla \frac{\delta V}{\delta \rho} \right\rangle - \left\langle \frac{\delta V}{\delta \rho}, \nabla \cdot J(\rho) \right\rangle = 0 \tag{21}$$

This is the Hamilton-Jacobi equation associated to the variational characterization of V

$$V(\rho) = \inf_{\substack{\rho\,:\,\rho(-\infty)=\bar{\rho} \\ \rho(0)=\rho}} I_{[-\infty,0]}(\rho) \tag{22}$$

This interpretation follows by considering the functional I as an action functional in the variables ρ and $\partial_t \rho$ and performing a Legendre transform. The associated Hamiltonian is

$$\mathcal{H}(\rho,\pi) = \Big\langle \nabla\pi \cdot \chi(\rho) \nabla\pi \Big\rangle + \Big\langle \nabla\pi \cdot J(\rho) \Big\rangle \tag{23}$$

where π is the conjugate momentum.

The quasi-potential and the identification of the minimizing trajectory

The variational characterization of V follows again by a time reversal argument which allows also to identify the minimizing trajectory. Consider a trajectory connecting the density profiles ρ_{t_1} and ρ_{t_2}. From time reversal we have

$$V(\rho_{t_1}) + I_{[t_1,t_2]}(\rho) = V(\rho_{t_2}) + I^a_{[-t_2,-t_1]}(\theta\rho) \qquad (24)$$

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 with the minimizer defined by

$$I^a_{[-\infty,0]}(\theta\rho) = 0 \qquad (25)$$

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

The adjoint hydrodynamics

The adjoint hydrodynamics follows immediately recalling the relationship between J and J^a

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

We have

$$\partial_t\rho + \nabla J^a = \partial_t\rho + \nabla\{D(\rho)\nabla\rho - \chi(\rho)(E + 2\nabla\frac{\delta V}{\delta\rho})\} = 0 \quad (26)$$

The minimizer is therefore the time reversal of the relaxation solution of this equation connecting ρ to $\bar{\rho}$. The optimal field to create the fluctuation is $F = 2\nabla\frac{\delta V}{\delta\rho}$, that is minus twice the dissipative thermodynamic force.

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^*.

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

The hydrodynamic equations in terms of V

$$
\begin{aligned}
\partial_t \rho &= \nabla \cdot \Big(\chi(\rho) \nabla \frac{\delta V}{\delta \rho} \Big) + \mathcal{A}(\rho) \\
\partial_t \rho &= \nabla \cdot \Big(\chi(\rho) \nabla \frac{\delta V}{\delta \rho} \Big) - \mathcal{A}(\rho)
\end{aligned}
$$

The second equation is the hydrodynamics corresponding to the time reversed system. The Hamilton–Jacobi equation implies the orthogonality condition

$$
\Big\langle \frac{\delta V}{\delta \rho} \, , \, \mathcal{A}(\rho) \Big\rangle = 0
$$

The above decompositions remind of the electrical conduction in presence of a magnetic field.

Consider the motion of electrons in a conductor: a simple model is given by the effective equation,

$$\dot{\mathbf{p}} = -e\Big(\mathbf{E} + \frac{1}{mc}\mathbf{p} \wedge \mathbf{H}\Big) - \frac{1}{\tau}\mathbf{p} \qquad (27)$$

where $\mathbf{p}$ is the momentum, e the electron charge, $\mathbf{E}$ the electric field, $\mathbf{H}$ the magnetic field, m the mass, c the velocity of the light, and τ the relaxation time. The dissipative term $\mathbf{p}/\tau$ is orthogonal to the Lorenz force $\mathbf{p} \wedge \mathbf{H}$. We define time reversal as the transformation $\mathbf{p} \mapsto -\mathbf{p}$, $\mathbf{H} \mapsto -\mathbf{H}$. The time reversed evolution is given by

$$\dot{\mathbf{p}} = e\Big(\mathbf{E} + \frac{1}{mc}\mathbf{p} \wedge \mathbf{H}\Big) - \frac{1}{\tau}\mathbf{p} \qquad (28)$$

Let us consider in particular the Hall effect where we have conduction along a rectangular plate immersed in a perpendicular magnetic field H with a potential difference across the long side. The magnetic field determines a potential difference across the short side of the plate. In our setting on the contrary it is the difference in chemical potentials at the boundaries that introduces in the equations a *magnetic–like* term.

A control theory point of view

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

$$\partial_t \rho = -\nabla J(\rho) - \nabla(\chi(\rho) F) \tag{29}$$

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

$$\frac{1}{4} \int_{t_1}^{t_2} ds \, \langle F(s), \chi(\rho^F(s)) F(s) \rangle \tag{30}$$

where $\rho^F(s)$ is the solution of (29). 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 (30). This is a standard problem in control theory.

Let

$$\mathcal{V}(\rho) = \inf \frac{1}{4}\int_{t_1}^{t_2} ds\, \langle F(s), \chi(\rho^F(s))F(s)\rangle \tag{31}$$

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

$$\min_F \left\{ \frac{1}{4}\big\langle F, \chi(\rho)F \big\rangle + \left\langle \nabla(J(\rho) + \chi(\rho)F), \frac{\delta \mathcal{V}}{\delta \rho} \right\rangle \right\} = 0 \tag{32}$$

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

$$F = 2\nabla \frac{\delta \mathcal{V}}{\delta \rho} \tag{33}$$

By substituting in (32) 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

$$f(\rho, x) = \int_{\bar{\rho}(x)}^{\rho} dr \int_{\bar{\rho}(x)}^{r} dr' \, f_0''(r') = f_0(\rho) - f_0(\bar{\rho}(x)) - f_0'\big(\bar{\rho}(x)\big)\big[\rho - \bar{\rho}(x)\big] \qquad (34)$$

the maximal solution of H-J is

$$V(\rho) = \int_{\Lambda} dx \, f\big(\rho(x), x\big) \qquad (35)$$

Define *macroscopic reversibility*

$$J^*(\rho) = -2\chi(\rho)\nabla\frac{\delta V}{\delta\rho} - J(\rho) = J(\rho) \tag{36}$$

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

$$J(\rho) = -\chi(\rho)\nabla\frac{\delta V}{\delta\rho}(\rho) \tag{37}$$

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

2. Applications

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

$$\left\langle \nabla h \cdot \chi\left(\frac{\delta G}{\delta h}\right) \nabla h \right\rangle - \left\langle \nabla h \cdot D\left(\frac{\delta G}{\delta h}\right) \nabla \frac{\delta G}{\delta h} - \chi\left(\frac{\delta G}{\delta h}\right) E \right\rangle = 0 \quad (38)$$

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

We define

$$C_n(x_1, \ldots, x_n) = \frac{\delta^n G}{\delta h(x_1) \cdots \delta h(x_n)} \Big|_{h=0} \tag{39}$$

By expanding (38) around the stationary state we obtain after non trivial manipulations and combinatorics the following recursive equations for the correlation functions

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

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

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

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

For the pair correlations write

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

where

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

We then obtain the following equation for B

$$\mathcal{L}^\dagger B(x,y) = \alpha(x)\delta(x-y) \tag{40}$$

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,

$$L_x = D_{ij}(\bar\rho(x))\partial_{x_i}\partial_{x_j} + \chi'_{ij}(\bar\rho(x))E_j(x)\partial_{x_i} \tag{41}$$

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.

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

$$V_m(\rho) = \int_\Lambda du\, f_m(\rho(u)) \tag{42}$$

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
BDGJL

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

$$\mathcal{I}_{[0,T]}(j) \;=\; \frac{1}{4}\int_0^T dt \left\langle [j - J(\rho)], \chi(\rho)^{-1}[j - J(\rho)] \right\rangle \qquad (43)$$

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.

$$J(x) = \frac{1}{T}\int_0^T j(x,t)dt \tag{44}$$

and define

$$\Phi(J) = \lim_{T\to\infty} \inf_j \frac{1}{T}\,\mathcal{I}_{[0,T]}(j)\;, \tag{45}$$

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

$$\Phi(J) - \Phi(-J) = \Phi(J) - \Phi^a(J) = -2\langle J, E\rangle + \int_{\partial\Lambda} d\Sigma\,\lambda_0\,J\cdot\hat{n} \tag{46}$$

Note that the right hand side of (46) is the power produced by the external field and the boundary reservoirs. Entropy production can be simply derived from $\Phi(J)$).

Universality in current fluctuations

Appert-Rolland, Derrida, Lecomte, van Wijland

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

$$\psi_J(s) = \lim_{t\to\infty} \frac{\ln\langle \exp -sQ\rangle}{t} = \Phi^*(s) \qquad (47)$$

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

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

from which they obtain

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

Current fluctuations with a step initial density profile

Derrida, Gerschenfeld

By direct calculation they proved that the generating function of the moments of the integrated current $Q_t = \int_0^t j(t')dt'$ for exclusion processes takes the asymptotic form for large t

$$\left\langle e^{\lambda Q_t} \right\rangle \asymp e^{\sqrt{t}\mu(\lambda,\rho_a,\rho_b)}\,, \qquad (48)$$

with $\mu(\lambda, \rho_a, \rho_b)$ given by

$$\mu(\lambda, \rho_a, \rho_b) = \frac{1}{\pi} \int_{-\infty}^{\infty} dk \log \left[1 + \omega e^{-k^2} \right]\,, \qquad (49)$$

and where ω is a function of ρ_a, ρ_b and λ

$$\omega = \rho_a(e^{\lambda} - 1) + \rho_b(e^{-\lambda} - 1) + \rho_a\rho_b(e^{\lambda} - 1)(e^{-\lambda} - 1)\,. \qquad (50)$$

Furthermore $\mu(\lambda, \rho_a, \rho_b)$ satisfies a symmetry very reminiscent of the fluctuation theorem

$$\mu\Big(\lambda, \rho_a, \rho_b\Big) = \mu\left(-\lambda + \log\frac{\rho_b}{1-\rho_b} - \log\frac{\rho_a}{1-\rho_a}, \rho_a, \rho_b\right) \qquad (51)$$

They then showed that these results can be understood and extended using the macroscopic fluctuation theory. They considered two cases

- *the annealed case* where one averages $e^{\lambda Q_t}$ both on the history and on the initial condition

$$\mu_{\text{annnealed}}(\lambda) = \lim_{t\to\infty} \frac{1}{\sqrt{t}} \log \left[\left\langle e^{\lambda Q_t} \right\rangle_{\text{history, initial condition}} \right]; \tag{52}$$

- *the quenched case*, where one averages $e^{\lambda Q_t}$ only on the history for a typical initial condition

$$\mu_{\text{quenched}}(\lambda) = \lim_{t\to\infty} \frac{1}{\sqrt{t}} \left\langle \log \left[\left\langle e^{\lambda Q_t} \right\rangle_{\text{history}} \right] \right\rangle_{\text{initial condition}} . \tag{53}$$

In the annealed case the result for SSEP can be used to obtain the distribution of Q_t for several other models. This has generically the non-gaussian decay $\exp[-q^3/t]$.

A model with two conservation laws

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Stationary nonequilibrium properties for a heat conduction model

Cédric Bernardin*
Université de Lyon, CNRS (UMPA), and Ecole Normale Supérieure de Lyon, 46, allée d'Italie, 69364 Lyon Cedex 07 France
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We consider a stochastic heat conduction model for solids composed of N interacting atoms. The system is in contact with two heat baths at different temperatures T_ℓ and T_r. The bulk dynamics conserves two quantities: the energy and the deformation between atoms. If $T_\ell \neq T_r$, a heat flux occurs in the system. For large N, the system adopts a linear temperature profile between T_ℓ and T_r. We establish the hydrodynamic limit for the two conserved quantities. We introduce the fluctuation field of the energy and of the deformation in the nonequilibrium steady state. As N goes to infinity, we show that this field converges to a Gaussian field and we compute the limiting covariance matrix. The main contribution of the paper is the study of large deviations for the temperature profile in the nonequilibrium stationary state. A variational formula for the rate function is derived following the recent macroscopic fluctuation theory of Bertini *et al.* [J. Stat. Phys. **107**, 635 (2002); Math. Phys., Anal. Geom. **6**, 231 (2003); J. Stat. Phys. **121**, 843 (2005)].

The ABC model

We here consider - both from a microscopic and macroscopic point of view - a model with two conservation laws. Given an integer $N \geq 1$ let $Z_N = \{1, \dots, N\}$ be the discrete ring with N sites so that $N + 1 \equiv 1$. The microscopic space state is given by $\Omega_N = \{A, B, C\}^{Z_N}$ so that at each site $x \in Z_N$ the occupation variable, denoted by η_x, take values in the set $\{A, B, C\}$; one may think that A, B stand for two different species of particles and C for an empty site. Note that this state space takes into account an exclusion condition: at each site there is at most one species of particles.

We first consider a weakly asymmetric dynamics that fits in the framework discussed so far that is defined by choosing the following transition rates. If the occupation variables across the bond $\{x, x+1\}$ are (ξ, ζ), they are exchanged to (ζ, ξ) with rate $c^E_{x,x+1} = \exp\{(E_\xi - E_\zeta)/(2N)\}$ for fixed constant external fields E_A, E_B, E_C.

The hydrodynamic equations for the densities of A and B particles are given by

$$\partial_t \begin{pmatrix} \rho_A \\ \rho_B \end{pmatrix} = \Delta \begin{pmatrix} \rho_A \\ \rho_B \end{pmatrix} - \nabla \cdot \begin{pmatrix} \rho_A(1-\rho_A) & -\rho_A\rho_B \\ -\rho_A\rho_B & \rho_B(1-\rho_B) \end{pmatrix} \times \begin{pmatrix} E_A - E_C \\ E_B - E_C \end{pmatrix}$$

of course the density of C particles is then $\rho_C = 1 - \rho_A - \rho_B$.

The functional $I_{[T_1,T_2]}$ with $D=1$ and mobility

$$\chi(\rho_A,\rho_B) = \begin{pmatrix} \rho_A(1-\rho_A) & -\rho_A\rho_B \\ -\rho_A\rho_B & \rho_B(1-\rho_B) \end{pmatrix} \tag{54}$$

is the dynamical large deviation functional associated to this model. The free energy is the maximal solution of the Hamilton-Jacobi equation which can be easily computed. Namely,

$$\begin{aligned} V^0_{m_A,m_B}(\rho_A,\rho_B) = \int dx\, \Big[\rho_A \log\frac{\rho_A}{m_A} + \rho_B \log\frac{\rho_B}{m_B} \\ + (1-\rho_A-\rho_B)\log\frac{1-\rho_A-\rho_B}{1-m_A-m_B}\Big] \end{aligned}$$

where $\int dx\, \rho_A = m_A$ and $\int dx\, \rho_B = m_B$. If E_A, E_B and E_C are not all equal, this model is a nonequilibrium model nevertheless, in view of the periodic boundary conditions, its free energy is independent of the external field.

We next discuss a different choice of the weakly asymmetric perturbation which, as we shall see, does not fit in the scheme discussed so far. This choice is the one referred to in the literature as the ABC *model*. The transition rates are the following. If the occupation variables across the bond $\{x, x+1\}$ are (ξ, ζ), they are exchanged to (ζ, ξ) with rate $\exp\{V(\xi, \eta)/N\}$ where $V(A, B) = V(B, C) = V(C, A) = -\beta/2$ and $V(B, A) = V(C, B) = V(A, C) = \beta/2$ for some $\beta > 0$. Therefore the A-particles prefer to jump to the left of the B-particles but to the right of the C-particles while the B-particles prefer to jump to the the left of the C-particles, i.e. the preferred sequence is ABC and its cyclic permutations. These rates do not satisfy the local detailed balance.

The hydrodynamic equations are

$$\partial_t \begin{pmatrix} \rho_A \\ \rho_B \end{pmatrix} + \nabla \cdot \begin{pmatrix} J_A(\rho_A, \rho_B) \\ J_B(\rho_A, \rho_B) \end{pmatrix} = 0$$

where

$$J(\rho_A, \rho_B) = \begin{pmatrix} J_A(\rho_A, \rho_B) \\ J_B(\rho_A, \rho_B) \end{pmatrix} = \begin{pmatrix} -\nabla \rho_A + \beta \rho_A (1 - 2\rho_B - \rho_A) \\ -\nabla \rho_B + \beta \rho_B (2\rho_A + \rho_B - 1) \end{pmatrix}$$

The asymmetric term in the present hydrodynamic equations is not of the form $\nabla \cdot \big(\chi(\rho) E\big)$ as in (5)–(7). Hence the the theorem requiring the free energy to be local does not apply.

The appropriate cost functional is however still given by the solution of Hamilton-Jacobi. In the case of equal densities $\int dx\, \rho_A = \int dx\, \rho_B = 1/3$, a straightforward computation shows that for any positive β the solution is given by

$$
\begin{aligned}
V^{\beta}_{\frac{1}{3},\frac{1}{3}}(\rho_A, \rho_B) &= V^{0}_{\frac{1}{3},\frac{1}{3}}(\rho_A, \rho_B) \\
&+\beta \int_0^1 dx \int_0^1 dy\, y \Big\{ \rho_A(x)\rho_B(x+y) + \rho_B(x)[1-\rho_A(x+y) \\
&\qquad - \rho_B(x+y)] + [1-\rho_A(x) - \rho_B(x)]\rho_A(x+y) \Big\} + \varkappa
\end{aligned}
$$

where $V^{0}_{\frac{1}{3},\frac{1}{3}}$ is the functional in (55) with $m_A = m_B = 1/3$ and $\varkappa$ is the appropriate normalization constant. This result has been already obtained by direct computations from the invariant measure. Indeed, in this case, the ABC model is *microscopically* reversible and the invariant measure can be computed explicitly. The macroscopic reversibility of the model is expressed as the identity, which holds in the case of equal densities, $J(\rho) = J^*(\rho)$.

The hydrodynamic equations can be written in terms V

$$\partial_t \rho = \nabla(\chi(\rho)\nabla \frac{\delta V}{\delta \rho})$$

where $\rho = (\rho_A, \rho_B)$.

3. Phase transitions

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

$$\mathcal{H}(\rho,\pi) = \Big\langle \nabla\pi \cdot \chi(\rho)\nabla\pi \Big\rangle + \Big\langle \nabla\pi \cdot J(\rho) \Big\rangle \tag{56}$$

are

$$\rho_t + \nabla\cdot\chi(\rho)E \;=\; \nabla\cdot D(\rho)\nabla\rho \;-\; 2\nabla\cdot\chi(\rho)\nabla\pi \tag{57}$$
$$\pi_t + E\cdot\chi'(\rho)\nabla\pi \;=\; -\nabla\pi\cdot\chi'(\rho)\nabla\pi - D(\rho)\nabla\nabla\pi \tag{58}$$

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 $\mathscr{M}_{\mathsf{s}}$ associated to the equilibrium position $(\bar{\rho}, 0)$. The unstable manifold $\mathscr{M}_{\mathsf{u}}$ 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, $\mathscr{M}_{\mathsf{u}}$ 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 M_{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 $W : \mathscr{M}_{\mathsf{u}} \to R$ by

$$W(\rho, \pi) \, = \, \int_\gamma \hat{\pi} \, d\hat{\rho} \ \ , \qquad (59)$$

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

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

$$V(\rho) \;=\; \inf\left\{W(\rho,\pi)\,,\; \pi\,:\,(\rho,\pi)\in\mathscr{M}_{\mathsf{u}}\right\}. \tag{60}$$

Indeed, fix ρ and consider π such that (ρ, π) belongs to M_{u}. Let $(\hat{\rho}(t), \hat{\pi}(t))$ be the solution of the Hamilton equation starting from (ρ, π) at $t = 0$. Since $(\rho, \pi) \in \mathscr{M}_{\mathsf{u}}$, $(\hat{\rho}(t), \hat{\pi}(t))$ 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 for (22). Since $\mathcal{L}(\hat{\rho}, \hat{\rho}_t) = \langle \hat{\pi}\, \hat{\rho}_t \rangle - \mathcal{H}(\hat{\rho}, \hat{\pi})$ and $\mathcal{H}(\hat{\rho}(t), \hat{\pi}(t)) = 0$, the action of such path $\hat{\rho}(t)$ is given by $I_{(-\infty,0]}(\hat{\rho}) = W(\rho, \pi)$. The right hand side selects among all such paths the one with minimal action.

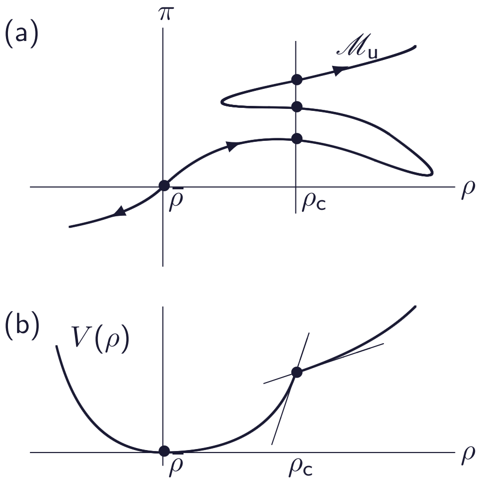

Figure: (a) Picture of the unstable manifold. (b) Graph of the quasi-potential. ρ_c is a caustic point.

In a neighborhood of the fixed point $(\bar{\rho}, 0)$, the unstable manifold $\mathscr{M}_{\mathsf{u}}$ can be written as a graph, namely it has the form $\mathscr{M}_{\mathsf{u}} = \{(\rho, \pi) : \pi = m_{\mathsf{u}}(\rho)\}$ for some map m_{u}. In this case, the infimum is trivial and $V(\rho) = W(\rho, m_{\mathsf{u}}(\rho))$. 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 $\mathcal{G}_E$

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

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 $(\varphi,\rho) \in \mathscr{M}_{\mathsf{u}}$. Therefore,

$$V_E(\rho) = \inf\big\{\mathcal{G}_E(\rho,\varphi)\,,\, \varphi\ :\ (\varphi,\rho)\in\mathscr{M}_{\mathsf{u}}\big\} - \mathcal{G}_E(\bar\rho_E, s'(\bar\rho_E))\ . \quad (61)$$

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.

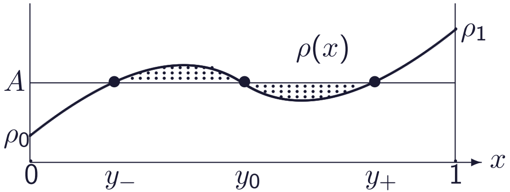

Figure: Graph of a caustic density profile for $E = \infty$. The shaded regions have equal area.

Dynamical phase transitions: singularities of $\Phi(J)$

Let us denote by U the functional obtained by restricting the infimum in (45) to divergence free current paths j, i.e.

$$U(J) = \inf_{\rho} \frac{1}{4} \langle [J - J(\rho)], \chi(\rho)^{-1} [J - J(\rho)] \rangle \tag{62}$$

where the infimum is carried out over all the density profiles $\rho = \rho(u)$ satisfying the appropriate boundary conditions. This functional was introduced by Bodineau and Derrida to describe the fluctuations of the time averaged current e.g. in SSEP. From the definition it follows that $\Phi \leq U$. There are two possibilities, $\Phi = U$ or the strict inequality $\Phi < U$. They correspond to different dynamical states. The transition from one regime to the other is a dynamical phase transition.

Consider as an example a ring in which an average current J is flowing in presence of an external field E. Depending on J, E, $D(\rho)$, $\chi(\rho)$ and their derivatives, a constant density profile or a traveling wave is the optimal choice. It has been shown that in the weakly asymmetric exclusion model (by Bodineau and Derrida) and in the Kipnis-Marchioro-Presutti model (by BDGJL) these transitions exist.

A sufficient condition for $\Phi = U$

We consider the case when the matrices $D(\rho)$ and $\chi(\rho)$ are multiple of the identity, i.e., there are strictly positive scalar functions still denoted by $D(\rho)$, $\chi(\rho)$, so that $D(\rho)_{i,j} = D(\rho)\delta_{i,j}$, $\chi(\rho)_{i,j} = \chi(\rho)\delta_{i,j}$, $i, j = 1, \ldots, d$. We denote derivatives with a superscript. Let us first consider the case with no external field, i.e. $E = 0$. If

$$D(\rho)\chi''(\rho) \leq D'(\rho)\chi'(\rho) \quad \text{for any } \rho \tag{63}$$

then $\Phi = U$. In this case U is necessarily convex.
Moreover if

$$D(\rho)\chi''(\rho) = D'(\rho)\chi'(\rho) \quad \text{for any } \rho \tag{64}$$

then we have $\Phi = U$ for any external field E.

Condition (63) is satisfied e.g. for the symmetric simple exclusion process, where $D = 1$ and $\chi(\rho) = \rho(1 - \rho)$, $\rho \in [0, 1]$. Condition (64) is satisfied either if D is proportional to χ' or χ is constant and D arbitrary. Examples are the zero range model, where $D(\rho) = \Psi'(\rho)$ and $\chi(\rho) = \Psi(\rho)$ for some strictly increasing function $\Psi : R_+ \to R_+$, and the non interacting Ginzburg–Landau model, where $D(\rho)$, $\rho \in R$, is an arbitrary strictly positive function and $\chi(\rho)$ is constant.

4. Large deviations for reaction-diffusion systems

Glauber+Kawasaki dynamics: the dynamical functional

J-L, Landim, Vares

Unlike the models discussed so far, the so-called *Glauber + Kawasaki* process is not a lattice gas in the sense that the number of particles is not locally conserved. A reaction term allowing creation/annihilation of particles is added in the bulk. The hydrodynamics is

$$\partial_t \rho = \Delta\rho + b(\rho) - d(\rho) = \Delta\rho + v \tag{65}$$

where the reaction terms b and d are polynomials in ρ. The associated large deviation functional for the density is

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

$$\left. + \Big\langle b(\rho), \big(1 - e^H + He^H\big)\Big\rangle + \Big\langle d(\rho), \big(1 - e^{-H} - He^{-H}\big)\Big\rangle \right\} \tag{66}$$

where the external potential H is connected to the fluctuation ρ by

$$\partial_t \rho = \Delta\rho - \nabla\cdot\big(\rho(1-\hat\rho)\nabla H\big) + b(\rho)e^H - d(\rho)e^{-H} \tag{67}$$

G+K dynamics: density-current-source fluctuations

Bodineau, Lagouche

The hydrodynamic equation has a local source term v and we are interested in the joint fluctuations of ρ, $J(\rho) = -\nabla\rho$, $v = b(\rho) - d(\rho)$. The large deviation functional is given by

$$\mathcal{I}_0(\rho, j, v) = \int_0^T dt \Big\langle \left\{ \frac{1}{4} \frac{\big(j - J(\rho)\big)^2}{\chi(\rho)} + \Phi\Big(\rho, v\Big) \right\} \Big\rangle, \tag{68}$$

with

$$\Phi(\rho, v) = b(\rho) + d(\rho) - \sqrt{v^2 + 4d(\rho)b(\rho)} + v \log\left(\frac{\sqrt{v^2 + 4d(\rho)b(\rho)} + v}{2b(\rho)}\right) \tag{69}$$

where ρ, j and v are connected by the equation

$$\partial_t \rho = -\nabla j + v \tag{70}$$

Quadratic approximation of the quasi-potential

Basile, J-L

The Hamiltonian associated to the large deviation functional for this model is not quadratic

$$\mathcal{H}(\rho,\pi) = \int du \Big\{ \frac{1}{2}\pi\Delta\rho + \frac{1}{2}(\nabla\pi)^2\rho(1-\rho) \\ -b(\rho)(1-\exp\pi) - d(\rho)(1-\exp-\pi) \Big\} \tag{71}$$

where π is the conjugate momentum. The Hamilton-Jacobi equation

$$\mathcal{H}(\rho, \frac{\delta V}{\delta\rho}) = 0 \tag{72}$$

is therefore very complicated but can be solved by successive approximations using as an expansion parameter $\rho - \bar{\rho}$ where $\bar{\rho}$ is a solution of $B(\rho) = D(\rho)$ that is a stationary solution of hydrodynamics.

We are looking for an approximate solution of (72) of the form

$$V(\rho) = \frac{1}{2}\int du \int dv(\rho(u)-\bar{\rho})k(u,v)(\rho(v)-\bar{\rho}) + o(\rho-\bar{\rho})^2 \quad (73)$$

The kernel $k(u,v)$ is the inverse of the density correlation function $c(u,v)$.

$$\int c(u,y)k(y,v)dy = \delta(u-v) \quad (74)$$

By inserting (73) in (72) one can show that $k(u,v)$ satisfies the following equation

$$\frac{1}{2}\bar{\rho}(1-\bar{\rho})\Delta_u k(u,v) - b_0 k(u,v) - \frac{1}{2}\Delta_u\delta(u-v) + (d_1-b_1)\delta(u-v) = 0 \quad (75)$$

where

$$b_1 = b'(\rho)\big|_{\rho=\bar{\rho}}, \quad d_1 = d'(\rho)\big|_{\rho=\bar{\rho}}$$

and

$$b_0 = b(\bar{\rho}) = d(\bar{\rho}) = d_0 \quad (76)$$

If V is a local functional of the density, $k(u,v)$ must be of the form $k(u,v) = f(\bar{\rho})\delta(u-v)$ which inserted in (75) gives

$$f(\bar{\rho}) = [\bar{\rho}(1-\bar{\rho})]^{-1} \tag{77}$$

and

$$b_0[\bar{\rho}(1-\bar{\rho})]^{-1} - (d_1 - b_1) = 0. \tag{78}$$

Therefore if b_0, b_1, d_1 do not satisfy the last equation the entropy cannot be a local functional of the density. It can be shown that in this case time reversal invariance is violated and the adjoint hydrodynamics is different from (65). This calculation supports the conjecture that macroscopic correlations are a generic feature of equilibrium states of non reversible lattice gases.

5. Large deviations in the hyperbolic case

Hydrodynamics of ASEP

The hydrodynamic equation has the form of a hyperbolic conservation law

$$\rho_t + (f(\rho))_x = 0 \tag{79}$$

where $f(\rho) = \rho(1-\rho)$. This equation has to be understood in a weak sense. Existence and uniqueness hold if an additional entropy condition is imposed on the solution. Introduce a pair of functions h, g such that $g' = f'h'$ define

$$K_{h,\rho}(\Phi) = -\int_0^T \int_0^1 \partial_t \Phi h(\rho) + \partial_x \Phi g(\rho) dx dt \tag{80}$$

Φ is a test function. A solution ρ satisfies the entropy condition if

$$K_{h,\rho}(\Phi) \leq 0 \tag{81}$$

for all bounded convex functions h.

The quasi-potential for the asymmetric exclusion process
Derrida, Lebowitz, Speer

1. The case $\rho_a \geq \rho_b$

$$V(\{\rho\};\rho_a,\rho_b) = -(b-a)K(\rho_a,\rho_b) + \sup_{F(x)} \int_a^b dx\,\rho(x)\log\left[\rho(x)(1-F(x))\right] + (1-\rho(x))\log\left[(1-\rho(x))F(x)\right], \tag{82}$$

where the supremum is over all *monotone nonincreasing* functions $F(x)$ which for $a \leq x < y \leq b$ satisfy

$$\rho_a = F(a) \geq F(x) \geq F(y) \geq F(b) = \rho_b. \tag{83}$$

where

$$K(\rho_a,\rho_b) = \sup_{\rho_b \leq \rho \leq \rho_a} \log[\rho(1-\rho)], \tag{84}$$

2. The case $\rho_a \leq \rho_b$

$$V(\{\rho\};\rho_a,\rho_b)) = -(b-a)K(\rho_a,\rho_b) + \tag{85}$$
$$\inf_{a\leq y\leq b}\left\{\int_a^y dx\,\rho(x)\,\mathsf{log}\left[\rho(x)(1-\rho_a)\right] + (1-\rho(x))\,\mathsf{log}\left[(1-\rho(x))\rho_a\right]\right.$$
$$\left. + \int_y^b dx\,\rho(x)\,\mathsf{log}\left[\rho(x)(1-\rho_b)\right] + (1-\rho(x))\,\mathsf{log}\left[(1-\rho(x))\rho_b\right]\right\}.$$

where

$$K(\rho_a,\rho_b) = \min\left[\log\rho_a(1-\rho_a), \log\rho_b(1-\rho_b)\right], \tag{86}$$

6. Conclusions

Large deviation theory has produced a phenomenological description of stationary nonequilibrium states of diffusive systems requiring as input the transport coefficients which are measurable quantities. In particular

1. we have a variational principle leading to a natural definition of the free energy for nonequilibrium states whose singularities are interpreted as phase transitions.
2. this principle implies that macroscopic long range correlations are a generic property of stationary nonequilibrium as experimentally observed.
3. we have a variational principle associated with the observation of time averaged currents: this implies the existence of dynamical phase transitions which spontaneously break time translational invariance.

4. In the theory developed so far the boundary conditions are kept fixed: the study under boundary conditions (chemical potentials, volume...) which slowly change on the macroscopic time scale is a next natural step.