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The large deviation approach to nonequilibrium diffusive systems: recent developments and an assessment

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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*

$$\partial_t \rho + \nabla \cdot j = 0 \qquad (1)$$

together with the constitutive equation

$$j = J(\rho) = -D(\rho)\nabla\rho + \chi(\rho)E \qquad (2)$$

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*

$$D(\rho) = \chi(\rho)\, f_0''(\rho) \qquad (3)$$

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

The equations (1)–(2) 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

$$f_0'\big(\rho(x)\big) = \lambda_0(x) \qquad\qquad x \in \partial\Lambda \tag{4}$$

We denote by $\bar\rho = \bar\rho(x)$, $x \in \Lambda$, the stationary solution, assumed to be unique, of (1), (2), and (4).

To state the third postulate, we need some preliminaries. Consider a time dependent variation $F = F(t, x)$ of the external field so that the total applied field is $E + F$. The local current then becomes $j = J^F(\rho) = J(\rho) + \chi(\rho)F$. Given a time interval $[T_1, T_2]$, we compute the energy necessary to create the extra current $J^F - J$ and drive the system along the corresponding trajectory:

$$L_{[T_1,T_2]}(F) = \int_{T_1}^{T_2} dt \left\langle \left[J^F(\rho^F) - J(\rho^F) \right] \cdot F \right\rangle = \int_{T_1}^{T_2} dt \left\langle F \cdot \chi(\rho^F) F \right\rangle \tag{5}$$

where $\cdot$ is the scalar product in $\mathbb{R}^d$, $\langle \cdot \rangle$ is the integration over Λ, and ρ^F is the solution of the continuity equation with current $j = J^F(\rho)$.

We define a *cost functional* on the set of space time trajectories as follows. Given a trajectory $\hat{\rho} = \hat{\rho}(t, x)$, $t \in [T_1, T_2], x \in \Lambda$, we set

$$I_{[T_1,T_2]}(\hat{\rho}) = \frac{1}{4} \inf_{F \,:\, \rho^F = \hat{\rho}} L_{[T_1,T_2]}(F) \tag{6}$$

namely we minimize over the variations F of the applied field which produce the trajectory $\hat{\rho}$. The introduction of this functional in the context of fluid dynamics equations appears to be new. The functional I (with the factor $1/4$) has a precise statistical interpretation within the context of stochastic lattice gases: it gives the asymptotics, as the number of degrees of freedom diverges, of the probability of observing a space time fluctuation of the empirical density.

The minimization in (6) can be performed explicitely

$$I_{[T_1,T_2]}(\hat\rho) = \frac{1}{4}\int_{T_1}^{T_2} dt \Big\langle \big[\partial_t\hat\rho + \nabla\cdot J(\hat\rho)\big]\, K(\hat\rho)^{-1} \big[\partial_t\hat\rho + \nabla\cdot J(\hat\rho)\big] \Big\rangle \quad (7)$$

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

Our third postulate then characterizes the free energy $\mathcal{F}(\rho)$ of the system with a density profile $\rho = \rho(x)$, $x \in \Lambda$, as the minimal cost to reach, starting from the stationary profile $\bar{\rho}$, the density profile ρ, in an infinitely long time interval.

3. *The nonequilibrium free energy of the system is*

$$\mathcal{F}(\rho) = \inf_{\substack{\hat{\rho}\,:\,\hat{\rho}(-\infty)=\bar{\rho} \\ \hat{\rho}(0)=\rho}} I_{[-\infty,0]}(\hat{\rho}) \tag{8}$$

By considering the functional in (7) as an action functional in variables $\hat{\rho}$ and $\partial_t \hat{\rho}$ and performing a Legendre transform, the associated Hamiltonian is

$$\mathcal{H}(\rho, \Pi) = \Big\langle \nabla\Pi \cdot \chi(\rho) \nabla\Pi \Big\rangle + \Big\langle \nabla\Pi \cdot J(\rho) \Big\rangle \tag{9}$$

where the *momentum* Π vanishes at the boundary of Λ. By noticing that the stationary solution of the hydrodynamic equation corresponds to the equilibrium point $(\bar{\rho}, 0)$ of the system with Hamiltonian $\mathcal{H}$ and $\mathcal{H}(\bar{\rho}, 0) = 0$, $\mathcal{F}$ must satisfy the Hamilton-Jacobi equation $\mathcal{H}\big(\rho, \delta\mathcal{F}/\delta\rho\big) = 0$.

more explicitely the functional $\mathcal{F}$ is the maximal solution of the infinite dimensional Hamilton-Jacobi equation

$$\left\langle \nabla \frac{\delta \mathcal{F}}{\delta \rho} \cdot \chi(\rho) \nabla \frac{\delta \mathcal{F}}{\delta \rho} \right\rangle - \left\langle \frac{\delta \mathcal{F}}{\delta \rho} \nabla \cdot J(\rho) \right\rangle = 0 \qquad (10)$$

where, for ρ that satisfies (4), $\delta \mathcal{F} / \delta \rho$ vanishes at the boundary of Λ. By maximal solution we mean that any solution to (10) (satisfying $F(\bar{\rho}) = 0$) is a lower bound for $\mathcal{F}$, as defined in (8).

The optimal trajectory ρ^* for the variational problem (8) is characterized as follows. Let

$$J^*(\rho) = -2\chi(\rho)\nabla\frac{\delta\mathcal{F}}{\delta\rho} - J(\rho) \tag{11}$$

then ρ^* is the time reversal of the solution to

$$\partial_t\rho+\nabla\cdot J^*(\rho) = \partial_t\rho+\nabla\cdot\Big\{D(\rho)\nabla\rho-\chi(\rho)\Big[E+2\,\nabla\frac{\delta\mathcal{F}}{\delta\rho}\Big]\Big\} = 0 \tag{12}$$

with the boundary condition (4).

The classical thermodynamic setting considers only spatially homogeneous systems in which ρ does not depend on x. In this case the variation of the free energy between $\bar{\rho}$ and ρ is the minimal work required to drive the system from $\bar{\rho}$ to ρ, which is realized by a *quasi static* transformation through equilibrium states.

The previous analysis however shows that, starting from an equilibrium or a stationary nonequilibrium state $\bar{\rho}$, optimal time dependent trajectories exist which over an an infinite interval of time and through nonequilibrium states, take the system from $\bar{\rho}$ and ρ. In the first case it is easy to show that the same free energy difference is obtained as in the classical thermodynamic setting. In nonequilibrium our definition of free energy is based on the notion of optimal trajectory and for the moment we have no other definition to compare with.

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

$$f(\rho, x) = \int_{\bar{\rho}(x)}^{\rho} dr \int_{\bar{\rho}(x)}^{r} dr' \, f_0''(r') = f_0(\rho) - f_0(\bar{\rho}(x)) - f_0'(\bar{\rho}(x)) \left[\rho - \bar{\rho}(x)\right] \tag{13}$$

the maximal solution of H-J is

$$\mathcal{F}(\rho) = \int_{\Lambda} dx \, f(\rho(x), x) \tag{14}$$

Define *macroscopic reversibility*

$$J^*(\rho) = -2\chi(\rho)\nabla\frac{\delta\mathcal{F}}{\delta\rho} - J(\rho) = J(\rho) \tag{15}$$

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

$$J(\rho) = -\chi(\rho)\nabla\frac{\delta\mathcal{F}}{\delta\rho}(\rho) \tag{16}$$

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

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 free energy $\mathcal{F}$

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

By Legendre duality we have the change of variable formulae $h = \frac{\delta \mathcal{F}}{\delta \rho}$, $\rho = \frac{\delta \mathcal{G}}{\delta h}$, so that the Hamilton-Jacobi equation (10) can then be rewritten in terms of $\mathcal{G}$ as

$$\Big\langle \nabla h \cdot \chi\Big(\frac{\delta \mathcal{G}}{\delta h}\Big) \nabla h \Big\rangle - \Big\langle \nabla h \cdot D\Big(\frac{\delta \mathcal{G}}{\delta h}\Big) \nabla \frac{\delta \mathcal{G}}{\delta h} - \chi\Big(\frac{\delta \mathcal{G}}{\delta h}\Big) E \Big\rangle = 0 \quad (17)$$

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

We define

$$C_n(x_1, \ldots, x_n) = \frac{\delta^n \mathcal{G}}{\delta h(x_1) \cdots \delta h(x_n)} \Big|_{h=0} \tag{18}$$

By expanding (17) around the stationary state we obtain after non trivial manipulations and combinatorics the following recursive equations for the correlation functions

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

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

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

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

$\mathcal{L}_{n+1}^{\dagger}$ is the formal adjoint of the operator $\mathcal{L}_{n+1} = \sum_{k=1}^{n+1} L_{x_k}$, where L_x is defined

$$L_x = D_{ij}(\bar{\rho}(x))\partial_{x_i}\partial_{x_j} + \chi'_{ij}(\bar{\rho}(x))E_j(x)\partial_{x_i} \tag{20}$$

For $n = 1$, that is for the density-density correlation function the general equation reduces to

$$\mathcal{L}^{\dagger} B(x, y) = \alpha(x)\delta(x - y) \tag{21}$$

where $B(x, y)$ is defined by

$$C(x, y) = C_{\mathsf{eq}}(x)\delta(x - y) + B(x, y) \tag{22}$$

and

$$\alpha(x) = \partial_{x_i}\left[\chi'_{ij}\left(\bar{\rho}(x)\right) D_{jk}^{-1}\left(\bar{\rho}(x)\right) \bar{J}_k(x)\right] \tag{23}$$

Thermodynamics of currents

Currents involve time in their definition so it is natural to consider space-time thermodynamics. We define a *cost functional* to produce a current trajectory $j(t,x)$ by rewriting (5) in terms of $j(t,x)$ instead of $\rho(t,x)$

$$\mathcal{I}_{[0,T]}(j) \; = \; \frac{1}{4}\int_0^T dt\, \langle [j - J(\rho)], \chi(\rho)^{-1}[j - J(\rho)] \rangle \qquad (24)$$

in which we recall that

$$J(\rho) = -\frac{1}{2}D(\rho)\nabla\rho + \chi(\rho)E \; .$$

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 and define

$$\Phi(J) = \lim_{T\to\infty} \inf_{j} \frac{1}{T}\, \mathcal{I}_{[0,T]}(j)\ , \tag{25}$$

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

$$\Phi(J) - \Phi(-J) = \Phi(J) - \Phi^{a}(J) = -2\langle J, E\rangle + \int_{\partial\Lambda} d\Sigma\, \lambda_0\, J\cdot\hat{n} \tag{26}$$

Note that the right hand side of (26) is the power produced by the external field and the boundary reservoirs (recall E is the external field and λ_0 the chemical potential of the boundary reservoirs).
Entropy production can be simply derived from $\Phi(J)$).

Dynamical phase transitions

Let us denote by U the functional obtained by restricting the infimum in (25) to divergence free current paths j, i.e.

$$U(J) = \inf_{\rho} \frac{1}{2} \langle [J - J(\rho)], \chi(\rho)^{-1} [J - J(\rho)] \rangle \qquad (27)$$

where the infimum is carried out over all the density profiles $\rho = \rho(u)$ satisfying the appropriate boundary conditions. From (25) and (27) 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 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 us) these transitions exist.

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

$$\psi_J(s) = \lim_{t\to\infty} \frac{\ln\langle \exp -sQ\rangle}{t} = \Phi^*(s) \tag{28}$$

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

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

from which they obtain

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

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Stationary nonequilibrium properties for a heat conduction model

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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)].

Summary

We have developed a phenomenological theory for the description of stationary nonequilibrium states of diffusive systems requiring as input the transport coefficients which are measurable quantities. In particular

1. we have introduced a variational principle leading to a natural definition of the free energy for nonequilibrium states.
2. this principle implies that macroscopic long range correlations are a generic property of stationary nonequilibrium as experimentally observed.
3. we have introduced a new thermodynamic functional $\Phi(J)$ of time averaged currents. Its singularities are associated to the existence of dynamical phase transitions which spontaneously break time translational invariance.