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Minimum Dissipation Principle in Stationary Non-Equilibrium States

L. Bertini,[1] A. De Sole,[2] D. Gabrielli,[3] G. Jona-Lasinio,[4] and C. Landim[5]

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We generalize to non equilibrium states Onsager's minimum dissipation principle. We also interpret this principle and some previous results in terms of optimal control theory. Entropy production plays the role of the cost necessary to drive the system to a prescribed macroscopic configuration.

KEY WORDS: Stationary non equilibrium states; lattice gases; minimum dissipation; optimal control.

1. INTRODUCTION

In his classic work on irreversible processes$^{(1,2)}$ Onsager introduced a quadratic functional of the thermodynamic fluxes (time derivatives of thermodynamic variables) and an associated variational principle, called the *minimum dissipation principle*, as a unifying macroscopic description of near equilibrium phenomena. The evolution of the thermodynamic fluxes is given by a system of linear equations which describes the relaxation to an equilibrium state. This system is the Euler equation associated to the minimum dissipation principle. Moreover the value of this functional along the solution of the relaxation equations is proportional to the entropy production. The Onsager reciprocity relationships are included in this

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[1] Dipartimento di Matematica, Università di Roma "La Sapienza," P.le A. Moro 2, 00185 Roma, Italy.

[2] Department of Mathematics, Harvard University, 1 Oxford Street, Cambridge, Massachusetts 02138.

[3] Dipartimento di Matematica, Università dell'Aquila, 67100 Coppito, L'Aquila, Italy.

[4] Dipartimento di Fisica and INFN, Università di Roma "La Sapienza," P.le A. Moro 2, 00185 Roma, Italy.

[5] IMPA, Estrada Dona Castorina 110, J. Botanico, 22460 Rio de Janeiro, Brazil and CNRS UMR 6085, Université de Rouen, 76128 Mont-Saint-Aignan Cedex, France.

principle which can be considered, as Onsager did, the dynamical analogue of the maximal entropy condition in equilibrium statistical mechanics.

Natural questions are how this theory can be extended to non equilibrium stationary states and how the restriction to small fluctuations can be relaxed. Typical examples of non equilibrium stationary states are systems in contact with reservoirs which maintain a constant flow of some physical quantity (heat, matter, electric charge,...). Other examples are provided by systems in weak external fields. The rigorous study of simple stochastic models of interacting particles(3–7) has provided insight on these issues. These models typically give rise to non linear hydrodynamic equations and, for equilibrium states, Onsager's theory is recovered as a first order approximation for small deviations.

In this paper we present a form of the minimum dissipation principle valid for a wide class of models which includes stationary non equilibrium states. For a detailed discussion of our general assumptions, which are satisfied for typical models of stochastic interacting particles, we refer to ref. 3. The basic points are a Markovian description of the microscopic dynamics, the existence of a macroscopic dynamics (hydrodynamics) and the validity of a dynamical large fluctuation principle which generalizes the well known Boltzmann–Einstein formula for the probability of thermodynamic fluctuations. The form of the hydrodynamic equations and the main consequence of the large fluctuation principle, i.e., a Hamilton–Jacobi equation for the entropy, will be introduced in the next section.

The minimum dissipation principle follows from the results obtained in the previous papers(3) and in particular from the decomposition of the hydrodynamic equation into two parts: a dissipative part proportional to the gradient of the entropy and a non dissipative term orthogonal to it. The two terms have opposite transformation properties under time reversal, the non dissipative part being in this respect akin to a magnetic term.

We emphasize that the minimum dissipation principle is of general validity. This has to be contrasted with the principle of minimal entropy production which is of limited validity.(8)

2. BASIC MACROSCOPIC EQUATIONS

We consider the macroscopic description of non equilibrium conservative systems, that is systems in which the number of particles is locally conserved. The analysis of microscopic models of stochastic lattice gases in contact with particles reservoirs and/or weak external fields suggests that the following scheme may characterize a wide class of physical systems.

1. There exists an entropy functional $S(\{\rho_i\})$ which depends on a finite number of local thermodynamic variables ρ_i. The stationary state corresponds to a critical point of S so that it is a maximum of the entropy; here we stick to the physicists sign convention for S which is opposite to that of the previous papers. The relationship between S and the probability of a thermodynamic fluctuation is given by the Boltzmann–Einstein formula $P \approx \exp\{N^d \Delta S\}$ where N^d is the volume of the system.

2. The evolution of the fields $\rho_i = \rho_i(t, u)$, where u represents the macroscopic space coordinates and t the macroscopic time, is given by a divergence type hydrodynamical equations of the form (from now on we omit for simplicity the indices)

$$\partial_t \rho = \tfrac{1}{2} \nabla \cdot (D(\rho) \nabla \rho) - \nabla \cdot (\chi(\rho) E) = \mathscr{D}(\rho) \tag{1}$$

where D is the diffusion matrix, χ the Onsager matrix, and E the external field. Equation (1) is obtained in the diffusive scaling with a microscopic drift of order $1/N$. The interaction with the reservoirs appears as boundary conditions to be imposed on solutions of (1). We expect $D(\rho)$ and $\chi(\rho)$ to be local functions of the thermodynamic variables. We assume that there exists a unique stationary solution $\bar{\rho}$ of (1), i.e., a profile $\bar{\rho}(u)$, which satisfies the appropriate boundary conditions such that $\mathscr{D}(\bar{\rho}) = 0$. The entropy $S(\rho)$ attains its maximum for $\rho = \bar{\rho}$ and we normalize it so that $S(\bar{\rho}) = 0$.

3. The entropy S satisfies the following Hamilton–Jacobi functional derivative equation

$$\frac{1}{2} \left\langle \nabla \frac{\delta S}{\delta \rho}, \chi(\rho) \nabla \frac{\delta S}{\delta \rho} \right\rangle - \left\langle \frac{\delta S}{\delta \rho}, \mathscr{D}(\rho) \right\rangle = 0 \tag{2}$$

where $\langle \cdot, \cdot \rangle$ means integration with respect to the space variables.

It is not obvious that a relationship such as (2) connecting the macroscopic entropy with hydrodynamics and Onsager matrix should exist. In fact (2) can be interpreted as a far reaching generalization of the fluctuation-dissipation theorem since it allows to express even in non equilibrium states a stationary quantity like the entropy in terms of two dynamical macroscopic features of the system. This is one of the main results of ref. 3.

Another important result is the generalization to non equilibrium states of the Onsager–Machlup theory of dynamical fluctuations.[9] Suppose at time $t = -\infty$ the system is in the stationary state $\bar{\rho}$ and at time $t = 0$ we observe a profile ρ of the thermodynamic variable; we ask what is the trajectory along which this fluctuation has been created. In equilibrium the Onsager–Machlup theory tells us that this trajectory is most likely the time reversal of the relaxation path which solves the hydrodynamic equation (1) with initial condition ρ. In non equilibrium the characterization of such a trajectory requires the introduction of the adjoint hydrodynamics which is defined as the hydrodynamic equation associated to the time reversed microscopic dynamics. Indeed in ref. 3, to which we refer for more detail, we have shown that the exit path is the time reversed of the solution to the adjoint hydrodynamics with initial condition ρ.

In the present paper we shall also present a non probabilistic point of view in terms of optimal control theory. The dissipation function introduced in the next section is interpreted as a cost function when an external perturbation is used to produce a fluctuation. The Hamilton–Jacobi equation becomes the Bellman equation, see, e.g., ref. 10, of the associated control problem.

3. MINIMUM DISSIPATION IN NON EQUILIBRIUM STATES

The extension of the minimum dissipation principle to non equilibrium states follows from a structural property of the hydrodynamics in non equilibrium states established in ref. 3. By using the Hamilton–Jacobi equation (2), we showed that we can decompose the right hand side of (1) as the sum of a gradient of the entropy $S(\rho)$ and a vector field $\mathscr{A}$ orthogonal to it in the metric induced by the operator K^{-1} where $Kf = -\nabla\cdot(\chi(\rho)\,\nabla f)$, namely

$$\mathscr{D}(\rho) = -\frac{1}{2}\nabla\cdot\left(\chi(\rho)\,\nabla\frac{\delta S}{\delta\rho}\right) + \mathscr{A}(\rho) \tag{3}$$

with

$$\left\langle K\frac{\delta S}{\delta\rho}, K^{-1}\mathscr{A}(\rho)\right\rangle = \left\langle\frac{\delta S}{\delta\rho}, \mathscr{A}(\rho)\right\rangle = 0 \tag{4}$$

Since $\mathscr{A}$ is orthogonal to $\delta S/\delta\rho$, it does not contribute to the entropy production.

Both terms of the decomposition vanish in the stationary state that is when $\rho = \bar{\rho}$. Whereas in equilibrium the hydrodynamic is the gradient flow of the entropy S, the term $\mathscr{A}(\rho)$ is characteristic of non equilibrium states. Note that, for small fluctuations $\rho \approx \bar{\rho}$, small differences in the chemical potentials at the boundaries, small external fields E, $\mathscr{A}(\rho)$ becomes a second order quantity and Onsager theory is a consistent approximation.

Equation (3) is interesting because it separates out the dissipative part of the hydrodynamic evolution associated to the thermodynamic force $\frac{\delta S}{\delta \rho}$ and provides therefore an important physical information. Notice that the thermodynamic force $\frac{\delta S}{\delta \rho}$ appears linearly in the hydrodynamic equation even when this is non linear in the macroscopic variables.

In general, the two terms of the decomposition (3) are non local in space even if $\mathscr{D}$ is a local function of ρ. This is the case for the simple exclusion process discussed in refs. 3 and 4. Furthermore while the form of the hydrodynamic equation does not depend explicitly on the chemical potentials, $\frac{\delta S}{\delta \rho}$ and $\mathscr{A}$ do.

The adjoint hydrodynamics mentioned in Section 2 is easily obtained from the decomposition (3). In fact in ref. 3 it is shown that it has the form

$$\partial_t \rho = \mathscr{D}^*(\rho) = -\frac{1}{2} \nabla \cdot \left(\chi(\rho) \, \nabla \frac{\delta S}{\delta \rho} \right) - \mathscr{A}(\rho) \tag{5}$$

that is $\mathscr{A}$ is odd under time reversal.

To understand how the decomposition (3) arises microscopically let us consider a stochastic lattice gas. Let L be its Markov generator; we can write it as follows

$$L = \tfrac{1}{2}\,(L + L^+) + \tfrac{1}{2}\,(L - L^+) \tag{6}$$

where L^+ is the adjoint of L with respect to the invariant measure, namely the generator of the time reversed microscopic dynamics. The term $L - L^+$ behaves like a Liouville operator, i.e., is antihermitian and, in the scaling limit, produces the term $\mathscr{A}$ in the hydrodynamic equation. This can be verified explicitly in the boundary driven zero–range model discussed in ref. 3. In the appendix we briefly discuss this model under more general conditions including a weak external field. For this model the decomposition (3) can be obtained in two ways: macroscopically from $\mathscr{D}(\rho)$ and $S(\rho)$, microscopically deriving the hydrodynamics from the above decomposition of the generator.

Since the adjoint generator can be written as $L^+ = (L + L^+)/2 - (L - L^+)/2$, the adjoint hydrodynamics must be of the form (5). In particular if the microscopic generator is self–adjoint, we get $\mathscr{A} = 0$ and thus $\mathscr{D}(\rho) = \mathscr{D}^*(\rho)$. On the other hand, it may happen that microscopic non reversible processes, namely those for which $L \neq L^+$, can produce macroscopic reversible hydrodynamics if $L - L^+$ does not contribute to the hydrodynamic limit. This happens in the examples discussed in ref. 11.

To formulate the minimum dissipation principle, we construct a functional of the variables ρ and $\dot{\rho}$ such that the Euler equation associated to the vanishing of the first variation under arbitrary changes of $\dot{\rho}$ is the hydrodynamic equation (1). We define the *dissipation function*

$$F(\rho, \dot{\rho}) = \langle(\dot{\rho} - \mathscr{A}(\rho)), K^{-1}(\dot{\rho} - \mathscr{A}(\rho))\rangle \tag{7}$$

and the functional

$$\Phi(\rho, \dot{\rho}) = -\dot{S}(\rho) + F(\rho, \dot{\rho}) = -\left\langle \frac{\delta S}{\delta \rho}, \dot{\rho} \right\rangle + \langle(\dot{\rho} - \mathscr{A}(\rho)), K^{-1}(\dot{\rho} - \mathscr{A}(\rho))\rangle \tag{8}$$

which generalize the corresponding definitions in refs. 1 and 2.

It is easy to verify that

$$\delta_{\dot{\rho}} \Phi = 0 \tag{9}$$

is equivalent to the hydrodynamic equation (1). Furthermore, a simple calculation gives

$$F|_{\dot{\rho} = \mathscr{D}(\rho)} = \frac{1}{4} \left\langle \nabla \frac{\delta S}{\delta \rho}, \chi(\rho) \nabla \frac{\delta S}{\delta \rho} \right\rangle \tag{10}$$

that is $2F$ on the hydrodynamic trajectories equals the entropy production rate as in Onsager's near equilibrium approximation.

The dissipation function for the adjoint hydrodynamics is obtained by changing the sign of $\mathscr{A}$ in (7).

The decompositions (3) and (5) remind 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, see, for example,(12)

$$\dot{\mathbf{p}} = -e \left(\mathbf{E} + \frac{1}{mc} \mathbf{p} \wedge \mathbf{H} \right) - \frac{1}{\tau} \mathbf{p} \tag{11}$$

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 adjoint evolution is given by

$$\dot{\mathbf{p}} = e \left(\mathbf{E} + \frac{1}{mc} \mathbf{p} \wedge \mathbf{H} \right) - \frac{1}{\tau} \mathbf{p} \tag{12}$$

where the signs of the dissipation and the electromagnetic force transform in analogy to (3) and (5).

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.

4. FLUCTUATION, DISSIPATION, AND OPTIMAL CONTROL

The spontaneous motion of the systems considered follows the hydrodynamic equation (1). We introduce an external perturbation v acting on the system in such a way that the hydrodynamical equation becomes

$$\partial_t \rho = \tfrac{1}{2} \nabla \cdot (D(\rho) \nabla \rho) - \nabla \cdot (\chi(\rho) E) + v = \mathscr{D}(\rho) + v \tag{13}$$

We want to choose v to drive the system from its stationary state $\bar{\rho}$ to an arbitrary state ρ with minimal cost. A simple cost function is

$$\tfrac{1}{2} \int_{t_1}^{t_2} ds \ \langle v(s), K^{-1}(\rho(s))\, v(s) \rangle \tag{14}$$

where $\rho(s)$ is the solution of (13) and we recall that $K(\rho) f = -\nabla \cdot (\chi(\rho) \nabla f)$. More precisely, given $\rho(t_1) = \bar{\rho}$ we want to drive the system to $\rho(t_2) = \rho$ by an external field v which minimizes (14). This is a standard problem in control theory, see ref. 10. Let

$$\mathscr{V}(\rho) = \inf \tfrac{1}{2} \int_{t_1}^{t_2} ds \langle v(s), K^{-1}(\rho(s))\, v(s) \rangle \tag{15}$$

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

$$\min_v \left\{ \frac{1}{2} \langle v, K^{-1}(\rho)\, v \rangle - \left\langle \mathscr{D}(\rho) + v, \frac{\delta \mathscr{V}}{\delta \rho} \right\rangle \right\} = 0 \tag{16}$$

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

$$v = K(\rho) \frac{\delta \mathscr{V}}{\delta \rho} \tag{17}$$

Hence (16) now becomes

$$\frac{1}{2}\left\langle \frac{\delta \mathscr{V}}{\delta \rho}, K(\rho)\frac{\delta \mathscr{V}}{\delta \rho}\right\rangle + \left\langle \mathscr{D}(\rho), \frac{\delta \mathscr{V}}{\delta \rho}\right\rangle = 0 \tag{18}$$

By identifying the cost functional $\mathscr{V}(\rho)$ with $-S(\rho)$, Eq. (18) coincides with the Hamilton–Jacobi equation (2).

By inserting the optimal v (17) in (13) and identifying $\mathscr{V}$ with $-S$, we get that the optimal trajectory $\rho(t)$ solves the time reversed adjoint hydrodynamics, namely

$$\partial_t \rho = -\mathscr{D}^*(\rho) \tag{19}$$

where $\mathscr{D}^*(\rho)$ is given in (5). The optimal field v does not depend on the non dissipative part $\mathscr{A}$ of the hydrodynamics.

The generalized Onsager–Machlup relationship(3) states that a spontaneous fluctuation is created most likely by following the solution of (19). By choosing the "right" cost function (14), this coincides with the best trajectory for the control problem.

APPENDIX A: ZERO RANGE PROCESS WITH BOUNDARY CONDITIONS AND WEAK EXTERNAL FIELD

Consider the zero range process which models a nonlinear diffusion of a lattice gas, see, e.g., ref. 13. The model is described by a positive integer variable $\eta_x(\tau)$ representing the number of particles at site x and time τ of a finite subset Λ_N of the d-dimensional lattice, $\Lambda_N = \mathbf{Z}^d \cap N\Lambda$ where Λ is a bounded open subset of $\mathbf{R}^d$. The particles jump with rates $g(\eta_x)$ to one of the nearest-neighbor sites. The function $g(k)$ is increasing and $g(0)=0$. We assume that our system interacts with particle reservoirs at the boundary of Λ_N whose activity at site x is given by $\psi(x/N)$ for some given smooth strictly positive function $\psi(u)$. We consider the process also in a (space dependent) external potential $H(u)$ which modifies the rates by a local drift.

The dynamics is specified by the generator $L_N^H = L_{N,\,\text{bulk}}^H + L_{N,\,\text{bound.}}^H$ where

$$\begin{aligned} L_{N,\,\text{bulk}}^H f(\eta) &= \tfrac{1}{2} \sum_{\substack{x,\,y \in \Lambda_N \\ |x-y|=1}} g(\eta_x)\, e^{H(y/N)-H(x/N)} [f(\eta^{x,\,y}) - f(\eta)] \\ L_{N,\,\text{bound.}}^H f(\eta) &= \tfrac{1}{2} \sum_{\substack{x \in \Lambda_N,\, y \notin \Lambda_N \\ |x-y|=1}} \{ g(\eta_x)\, e^{H(y/N)-H(x/N)} [f(\eta^{x,\,-}) - f(\eta)] \\ &\qquad + \psi(y/N)\, e^{H(x/N)-H(y/N)} [f(\eta^{x,\,+}) - f(\eta)] \} \end{aligned} \tag{A1}$$

in which $\eta^{x,y}$ is the configuration obtained from η when a particle jumps from x to y, and $\eta^{x,\pm}$ is the configuration where we added (resp. subtracted) one particle at x. With respect to the boundary driven zero range process considered in ref. 3, we simply introduced in the macroscopic scale a small space dependent drift $N^{-1}\nabla H(u)$ in the motion of the particles. The invariant measure μ_N of this model is a product measure of the same form of the one discussed in ref. 3 in the case $H=0$.

Let

$$Z(\varphi)=1+\sum_{k=1}^{\infty}\frac{\varphi^k}{g(1)\cdots g(k)} \tag{A2}$$

set $R(\varphi)=\varphi\,\frac{Z'(\varphi)}{Z(\varphi)}$, and denote by $\phi(\rho)$ the inverse function of $\varphi\mapsto R(\varphi)$. By the computations given in ref. 3, we get that the hydrodynamic equation is

$$\begin{cases}\partial_t\rho(t,u)=\frac{1}{2}\,\Delta\phi(\rho(t,u))-\nabla\cdot(\phi(\rho(t,u))\,\nabla H(u)) & u\in\Lambda\\ \phi(\rho(t,u))=\psi(u) \qquad u\in\partial\Lambda\end{cases} \tag{A3}$$

which is of the form (1) with $D(\rho)=\phi'(\rho)\,\mathbb{1}$, $\chi(\rho)=\phi(\rho)\,\mathbb{1}$, and $E=\nabla H$.

Let us denote by $\bar\rho(u)$ the stationary solution of (A3), the associated activity $\lambda(u)=\phi(\bar\rho(u))$ solves

$$\begin{cases}\frac{1}{2}\,\Delta\lambda(u)-\nabla\cdot(\lambda(u)\,\nabla H(u))=0 & u\in\Lambda\\ \lambda(u)=\psi(u) \qquad u\in\partial\Lambda\end{cases} \tag{A4}$$

It is not difficult to show that the entropy $S(\rho)$ is given by

$$S(\rho)=-\int_\Lambda du\left[\rho(u)\log\frac{\phi(\rho(u))}{\lambda(u)}-\log\frac{Z(\phi(\rho(u)))}{Z(\lambda(u))}\right] \tag{A5}$$

where Z has been defined in (A2).

The decomposition (3) of the hydrodynamics (A3) is

$$-\frac{1}{2}\nabla\cdot\left(\phi(\rho)\,\nabla\frac{\delta S}{\delta\rho}\right)=\frac{1}{2}\,\Delta\phi(\rho)-\frac{1}{2}\nabla\cdot\left(\frac{\phi(\rho)}{\lambda}\,\nabla\lambda\right)$$

$$\mathscr{A}(\rho)=-\nabla\cdot(\phi(\rho)\,\nabla H(u))+\frac{1}{2}\nabla\cdot\left(\frac{\phi(\rho)}{\lambda}\,\nabla\lambda\right) \tag{A6}$$

and it is not difficult to check that the orthogonality condition

$$\left\langle\frac{\delta S}{\delta\rho},\mathscr{A}(\rho)\right\rangle=0 \tag{A7}$$

holds.

Recalling that μ_N is the invariant measure let us consider the process with initial condition ν, where ν is a product measure with density profile $\rho_0(u)$, namely

$$\frac{d\nu}{d\mu_N}(\eta) = \prod_{x \in \Lambda_N} \left(\frac{\phi(\rho_0(x/N))}{\lambda(x/N)} \right)^{\eta(x)} \frac{Z(\lambda(x/N))}{Z(\phi(\rho_0(x/N)))}$$

Let now ν_τ be the distribution at time τ and $\mathscr{H}(\nu_\tau \mid \mu_N) = -\int d\mu_N \frac{d\nu_\tau}{d\mu_N} \log \frac{d\nu_\tau}{d\mu_N}$ the relative entropy of ν_τ with respect the μ_N. By local equilibrium it is possible to show that, as $N \to \infty$

$$\frac{d}{dt} \mathscr{H}(\nu_{N^2 t} \mid \mu_N) \to \frac{1}{2} \left\langle \nabla \frac{\delta S}{\delta \rho}(\rho(t)), \phi(\rho(t)) \nabla \frac{\delta S}{\delta \rho}(\rho(t)) \right\rangle \tag{A8}$$

where $\rho(t)$ is the solution of the hydrodynamic equation (A3) with initial condition ρ_0. We see therefore that in the scaling limit we obtain the dissipation in (10) from the microscopic entropy production.

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