Nonequilibrium Stationary States (Deterministic)

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Nonequilibrium stationary states (NESS) describe the state of a mechanical system driven and maintained out of equilibrium by external forces. The external forces can be mechanical or thermodynamical. Examples of mechanical forces are external non-Hamiltonian forces imposed on the system or boundary forcing for example in a shear flow. Thermodynamical forces occur when a system is coupled to several reservoirs which have different thermodynamical parameters such as temperatures, chemical potentials, or others potentials.

The main characteristic of a NESS is that it sustains sustain steady flows, for example energy flows (heat conduction), particles flow (like in heat or electrical conduction), momentum flows (like in shear flows). The occurence of these various flows in NESS can summarized by saying the NESS exhibits a positive *entropy production*.

To give a formal definition of a NESS, let M be the state space of the system and let $\Phi_t : M \to M$ be a group of invertible transformations which describe the dynamics of the system. We assume that a probability measure μ is given. The measure μ serves as a reference measure and is given *a-priori*. In applications it depends on the physical parameters of the system. We emphasize that, in general, μ is not an invariant measure for the dynamics ϕ_t.

Definition of NESS: A probability measure ν is a NESS for the dynamical system (M, Φ_t) with reference measure μ if

(i) The measure ν is Φ_t-invariant, i.e $\int f \circ \Phi_t d\nu = \int f d\nu$ for all t and all $f \in L^1(\nu)$.

(ii) The measure ν is ergodic, i.e. for ν-almost every $x \in M$, and for all $f \in L^1(\nu)$ $\lim_{t\to\infty} \frac{1}{t}\int_0^t f \circ \Phi_s(x)\, ds = \int f d\nu$.

(iii) The measure ν satisfies the SRB-property with respect to the reference measure μ, i.e., for any probability measure ρ which is absolutely continuous with respect to μ we have $\lim_{t\to\infty} \frac{1}{t}\int_0^t \left(\int f \circ \Phi_s d\rho\right) ds = \int f d\nu$ for a "sufficiently large class of functions".

The class of functions in (iii) is only vaguely defined since it may depend on the system considered and topological assumptions. As typical example one might assume that M is a Polish space, that Φ_t is continuous and in (iii) one chooses f to be bounded and continuous such that we have, in the weak topology, $\lim_{t\to\infty} \frac{1}{t} \int_0^t \left(\int \delta_{\Phi_s} d\rho\right) ds = \int f d\nu$.

Note also that the condition (iii) can be replaced by the condition that the ergodic average $\lim_{t\to\infty} \frac{1}{t} \int_0^t f \circ \Phi_s$ converge μ almost surely, i.e the NESS ν describes the statistics of almost every point with respect to the reference measure μ.

To illustrate this definition we consider two examples.

Example I: **Thermostats and "Microcanonical" approach to NESS.** In this example the system is driven out of equilibrium by an external Hamiltonian force. Let $x = (p, q) \in \mathbf{R}^n \times \mathbf{R}^n$ be the canonical coordinates of an Hamiltonian system with an Hamiltonian function $H(p, q)$ which we assume to be have compact level sets. The restriction μ_E of Lebesgue measure on $\mathbf{R}^{2n}$ to the compact energy surface $M_E = \{H = E\}$ is invariant under the flow $\Phi_t^{(0)}$ obtained by solving the Hamiltonian equation of motion $\dot{x} = J\nabla H$. Under generic non-degeneracy conditions on $H(p, q)$ the measures μ_E are absolutely continuous with respect to the Lebesgue measure on the energy surface and they will serve as our references measures.

The system is driven out of equilibrium by an external non-Hamiltonian force $F(p, q)$. In order to prevent the system form heating up one adds a thermostatting external force $\Theta(p, q)$ which constrains the system to stay on a fixed compact energy surface $\{H = E\}$. The equation of motion are then

$$\dot{x} \;=\; J\nabla H + F - \frac{\nabla H \cdot F}{\nabla H \cdot \nabla H} \nabla H \,, \tag{1}$$

and this defines a dynamical system (M_E, Φ_t) with reference measure M_E. By construction the flow Φ_t conserves energy but defines a dissipative dynamics. Therefore a NESS ν is expected to be singular with respect to μ_E.

Example II: **Heat reservoirs and Canonical approach to NESS.** In this example the system is driven out of equilibrium by thermodynamical forces. We consider a composite system consisting of a "small" system described by a Hamiltonian system with finitely many degrees of freedom H_S and M reservoirs which are Hamiltonian systems describing infinitely extended, spatially homogeneous systems of identical particles. Each reservoir is described by a Hamiltonian $H^{(i)}$, $i = 1, \cdots, M$ and the small system interacts with the i^{th} reservoir through a local interaction $V^{(i)}$. The total Hamiltonian for the system is $\sum_{i=1}^{M} H^{(i)} + H_S + \sum_{i=1}^{M} V^{(i)}$ and Φ^t is the corresponding Hamiltonian flow. In this example one drives the system out of equilibrium by assuming that initially each of the M reservoir is in equilibrium at some temperature T_i, i.e. it is described by a Gibbs measure $\mu^{(i)}_{T_i}$. In this case we take our reference measure to have the form $\mu = \mu^{(1)}_{T_i} \times \cdots \mu^{(M)}_{T_M} \times \mu_S$ where μ_S is an essentially arbitrary initial distribution for the small system.

We give next a formal definition of the entropy production.

Definition of the entropy production. Let μ_t be the image of the reference measure μ under the dynamics Φ_t. Under suitable regularity assumptions on the dynamics one writes the Radon-Nikodym derivative of μ_t with respect to μ as

$$\frac{d\mu_t}{d\mu} \,=\, e^{\int_0^t \sigma\circ\Phi_s \, ds}$$

for some function $\sigma(x)$ which one *defines* to be the entropy production. The entropy production does depend on the choice reference measure μ but two mutually absolutely continuous reference measures will lead to entropy productions which differ only by a (time-)boundary term.

In Example I, the entropy production is, up to boundary terms,

$$\sigma \,=\, \mathrm{div} F(x)$$

i.e. the entropy production is identified with *phase-space contraction rate* and can be also be interpreted as the work done on the system divided by "temperature" (identified in this case to the corresponding energy).

In Example II, the entropy production is, up to boundary terms,

$$\sigma \,=\, \sum_{i=1}^{M} \frac{F^{(i)}}{T_i}$$

where $F^{(i)}$ is the energy flow from the small system into the i^{th} reservoir.

If $H(\mu_1 \,|\, \mu_2)$ denote the relative entropy of μ_1 with respect to μ_2 then we have the identity

$$0 \leq H(\mu_t|\mu) = \int_0^t \int \sigma \circ \Phi^s \, d\mu \, ds \, .$$

and from the definition of the NESS we obtain that

$$\int \sigma d\nu \geq 0$$

i.e., the expectation of the entropy production in a NESS is nonnegative.

If the NESS ν is absolutely continuous with respect to the reference measure μ then the expectation of the entropy production vanishes. Thus a bona-fide NESS should be singular with respect to the reference measure and exhibit positive entropy production, i.e. $\int \sigma d\nu > 0$.

There a few examples where the existence of a NESS for deterministic systems as well as the positivity of entropy production as been established.

(i) Hyperbolic billiards under external forces: a particle moving through an array of convex obstacles is submitted to an external electric (and magnetic field) and a thermostat.

(ii) Open classical systems consisting of a collection of oscillators (harmonic or anharmonic) and the reservoirs are free phonons fields or infinite collection of harmonic oscillators.

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