Fluctuations in Stationary non Equilibrium States

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In this paper we formulate a dynamical fluctuation theory for stationary non equilibrium states (SNS) which covers situations in a nonlinear hydrodynamic regime and is verified explicitly in stochastic models of interacting particles. In our theory a crucial role is played by the time reversed dynamics. Our results include the modification of the Onsager–Machlup theory in the SNS, a general Hamilton–Jacobi equation for the macroscopic entropy and a non equilibrium, non linear fluctuation dissipation relation valid for a wide class of systems.

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The Boltzmann–Einstein theory of equilibrium thermodynamic fluctuations, as described for example in Landau–Lifshitz [1], states that the probability for a fluctuation from equilibrium in a macroscopic region of volume $V$ is proportional to $\exp\{V\Delta S/k\}$ where $\Delta S$ is the variation of entropy density calculated along a reversible transformation creating the fluctuation and $k$ is the Boltzmann constant. This theory is well established and has received a rigorous mathematical formulation in classical equilibrium statistical mechanics via the so called large deviation theory [2]. The rigorous study of large deviations has been extended to hydrodynamic evolutions of stochastic interacting particle systems [3]. In a dynamical setting one may ask new questions, for example what is the most probable trajectory followed by the system in the spontaneous emergence of a fluctuation or in its relaxation to equilibrium. The Onsager–Machlup approach [4] answers precisely to this question: in the situation of a linear hydrodynamic equation, that is, close to equilibrium, the most probable emergence and relaxation trajectories are one the time reversal of the other. Developing the methods of [3], this theory has been extended to nonlinear regimes [5]. Onsager–Machlup assume the reversibility of the microscopic dynamics; however microscopically non reversible models were constructed where the above results still hold [6,7].

Emergence of large fluctuations, including Onsager–Machlup symmetry, has been observed in stochastically perturbed gradient type electronic devices [8]. In their work, these authors study also non gradient (i.e. non reversible) systems and observe violation of Onsager–Machlup symmetry.

In the present paper we formulate a general theory of large deviations for irreversible processes, i.e. when detailed balance condition does not hold. This question was previously addressed in [9]. Natural examples are boundary driven stationary non equilibrium states (SNS), e.g. a thermodynamic system in contact with two reservoirs, but our theory covers, as a special case, also the model systems considered in [10]. In our approach a crucial role is played by the time reversed dynamics with respect to the stationary non equilibrium ensemble.

Our results are:

1. The Onsager–Machlup relationship has to be modified: the emergence of a fluctuation takes place along a trajectory which is determined by the time reversed process.

2. We show that the macroscopic entropy solves a Hamilton–Jacobi equation generalizing to a thermodynamic context known results for finite dimensional Langevin equations [3] as those studied in [8]. The Hamilton–Jacobi equation can be solved perturbatively if we consider not too large fluctuations.

3. We test our theory in a stochastic model of interacting particles system, the boundary driven zero range process, in which we perform the computations explicitly. In particular it is possible to construct the microscopic time reversed process and to write the macroscopic entropy in a closed form.

4. For a large class of systems we obtain a non equilibrium non linear fluctuation dissipation relationship which links the macroscopic evolution of the system and of its time reversal to the thermodynamic force.

We are interested in many body system in the limit of infinitely many degrees of freedom. The basic assumptions of our theory are the following.

1) The microscopic evolution is given by a Markov process $X_t$ which represents the configuration of the system at time $t$. This hypothesis probably is not so restrictive because also the Hamiltonian case discussed in [1] in the end is reduced to the analysis of a Markov process. The stationary non equilibrium state (SNS) is described by a stationary, i.e. invariant with respect to time shifts, probability distribution $P_{st}$ over the trajectories of $X_t$. 
2) The macroscopic behavior of the system is described by diffusion type hydrodynamical equations of the form

$$\partial_t \rho = \sum_{i,j} \partial_{u_i} \{ D_{i,j}(\rho) \partial_{u_j} \rho \} = F(\rho)$$  \hspace{1cm} (1)

where $\rho = \rho_t(u)$ represents in general a vector of thermodynamic variables, e.g. the densities of different species of particles, and $D_{i,j}$ is a matrix acting on this vector. The interaction with the reservoirs appears as boundary condition to be imposed on solutions of (1). 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 $F(\bar{\rho}) = 0$.

These equations are derived from the underlying microscopic dynamics through an appropriate scaling limit. The hydrodynamic equations represent laws of large numbers with respect to the probability measure $P_{st}$ conditioned on an initial state $X_0$. The initial conditions for (1) are determined by $X_0$. Of course many microscopic configurations give rise to the same value of $\rho_t(u)$. In general $\rho_t(u)$ is an approximate limit of a $\rho_N(X_t)$ as the number $N$ of degrees of freedom diverges.

3) The stationary measure $P_{st}$ admits a principle of large deviations describing the fluctuations of the thermodynamic variables appearing in the hydrodynamic equations. This means the following. The probability that in a macroscopic volume $V$ containing $N$ particles the evolution of the variable $\rho_N$ deviates from the solutions of the hydrodynamic equations and is close to some trajectory $\bar{\rho}$, is exponentially small and of the form

$$P_{st}(\rho_N(X_t) \approx \bar{\rho}_t(u), t \in [t_1, t_2]) \approx e^{-N S(\bar{\rho}_t)}$$

$$= e^{-N H(\bar{\rho})}$$  \hspace{1cm} (2)

where $H(\bar{\rho})$ is a functional which vanishes if $\bar{\rho}$ is a solution of (1) and $S(\bar{\rho}_t)$ is the entropy cost to produce the initial value $\rho_t$. We adopt the convention for the entropy sign opposite to the usual one, so that it takes the minimum value in the equilibrium state. We also normalize it so that $S(\bar{\rho}) = 0$. Therefore $H(\bar{\rho})$ represents the extra cost necessary in order that the system follow the trajectory $\bar{\rho}_t$. Finally $\rho_N(X_t) \approx \bar{\rho}_t(u)$ means closeness in some metric. This formula is a generalization of the Boltzmann–Einstein formula in which we set the Boltzmann constant $k = 1$.

4) Let us denote by $\Theta$ the time inversion operator defined by $\Theta X_t = X_{-t} = X^\ast_t$. The probability measure $P_{st}^\ast$ describing the evolution of the time reversed process $X^\ast_t$ is given by the composition of $P_{st}$ and $\Theta^{-1}$ that is

$$P_{st}^\ast(X^\ast_t = \phi_t, t \in [t_1, t_2]) = P_{st}(X_t = \phi_{-t}, t \in [-t_2, -t_1])$$  \hspace{1cm} (3)

We assume that the time reversed SNS also admits a hydrodynamic level of description.

Let $L$ be the generator of the microscopic dynamics. We remind that $L$ induces the evolution of functions of the process according to the equation $\partial_t E[f(X_t)] = E[(Lf)(X_t)]$, where $E$ stands for the expectation with respect to $P_t$, conditioned on the initial state $X_0$ \([2]\).

The time reversed dynamics is generated by the adjoint $L^\ast$ of $L$ with respect to the invariant measure $P_{in}$, that is

$$E_{P_{in}}[fLg] = E_{P_{in}}[(L^\ast f)g].$$

The measure $P_{in}$, which is the same for both processes, is a distribution over the configurations of the system and formally satisfies $L^\ast P_{in} = 0$. $E_{P_{in}}$ is the expectation with respect to $P_{in}$ and $f, g$ are functions of the configuration. We require that also the evolution generated by $L^\ast$ admits a hydrodynamic description, that we call the adjoint hydrodynamics, which, however, is not necessarily of the same form as (1). In fact the adjoint hydrodynamics can be non local in space.

In order to avoid confusion we emphasize that what it is usually called an equilibrium state, as distinguished from a SNS, corresponds to the special case $L^\ast = L$, i.e. the detailed balance principle holds. In such a case $P_{st}$ is invariant under time reversal and the two hydrodynamics coincide.

We now derive a fundamental consequence of our assumptions, that is the relationship between the action functionals $I$ and $I^\ast$ associated to the dynamics $L$ and $L^\ast$. From equation (1) and our assumptions it follows that also $P_{st}^\ast$ admits a large deviation principle with functional $I^\ast$ given by

$$I^\ast_{[t_1, t_2]}(\bar{\rho}) = I_{[-t_2, -t_1]}(\bar{\rho})$$  \hspace{1cm} (4)

with obvious notations. More explicitly this equation reads

$$S(\bar{\rho}_t) + J^\ast_{[t_1, t_2]}(\bar{\rho}) = S(\bar{\rho}_t) + J_{[-t_2, -t_1]}(\bar{\rho})$$  \hspace{1cm} (5)

where $\bar{\rho}_t, \bar{\rho}_t$ are the initial and final points of the trajectory and $S(\bar{\rho}_t)$ the entropy associated with the creation of the fluctuations $\bar{\rho}_t$ starting from the SNS. The functional $J^\ast$ vanishes on the solutions of the adjoint hydrodynamics. To compute $J^\ast$ it is necessary to know the macroscopic entropy $S$, which is determined by the microscopic invariant measure $P_{in}$. We shall see that $S$ can be also obtained as the solution of a Hamilton–Jacobi equation involving only macroscopic quantities. From (5) we can already obtain the generalization of Onsager-Machlup relationship for SNS.

The physical situation we are considering is the following. The system is macroscopically in the stationary state $\bar{\rho}$ at $t = -\infty$ but at $t = 0$ we find it in the state $\rho_0$. We want to determine the most probable trajectory followed in the spontaneous creation of this fluctuation. According to (2) this trajectory is the one that minimizes $J$ among all trajectories connecting $\bar{\rho}$ to $\rho_0$ in the time interval $[-\infty, 0]$. From (5) we have

$$J_{[-\infty, 0]}(\bar{\rho}) = J^\ast_{[0, \infty]}(\bar{\rho}) + S(\rho_0)$$  \hspace{1cm} (6)

The right hand side is minimal if $J^\ast_{[0, \infty]}(\bar{\rho}) = 0$ that is $\bar{\rho}$ is a solution of the adjoint hydrodynamics. The existence of such a relaxation solution is due to the fact that the stationary solution $\bar{\rho}$ is attractive also for the
adjoint hydrodynamics. We have therefore the following generalization of Onsager-Machlup to SNS

“In a SNS the spontaneous emergence of a macroscopic fluctuation takes place most likely following a trajectory which is the time reversal of the relaxation path according to the adjoint hydrodynamics”

Let us assume $J$ of the form

$$J_{[t_1,t_2]}(\rho) = \frac{1}{2} \int_{t_1}^{t_2} dt \langle W, K(\rho) W \rangle$$  \hspace{1cm} (7)

where $W = \partial_\rho - F(\rho)$, $F(\rho)$ has been defined in (3). $\langle \cdot , \cdot \rangle$ denotes integration in the space variable and $K(\rho)$ is an appropriate positive kernel which we assume to be known and reflects, at the macroscopic level, the stochasticity of the system. This form of $J$ is typical for diffusion processes described by finite dimensional Langevin equations \[2\] and is what we expect if the hydrodynamic equations are of the diffusion type \[3\]. This is also what we find for the model discussed later.

From (3) or (2) we have that the entropy is related to $J$ by

$$S(\rho) = \inf_{\rho} J_{[\infty,0]}(\rho)$$  \hspace{1cm} (8)

where the infimum is taken over all trajectories connecting $\rho$ to $\rho_0$. Therefore $S$ must satisfy the Hamilton-Jacobi equation associated to the action functional $J$. A simple calculation gives

$$\frac{1}{2} \left( \delta S \right)_{\rho} K^{-1}(\rho) \left( \delta S \right)_{\rho} + \left( \delta S \right)_{\rho} F = 0$$  \hspace{1cm} (9)

One can try to solve this functional derivative equation by successive approximations. Let $\rho(u)$ be the stationary profile in the SNS. If we expand $S$ as a Volterra functional series in the argument $\rho - \rho_0$, equation (3) reduces to a system of equations for the kernels of the expansion which can be solved by iteration. Applications of (3) to various models will be discussed in (4).

We consider now the so called zero-range process which models a nonlinear diffusion of a lattice gas, see e.g. (3). The model is described by a positive integer variable $\eta(x)$ representing the number of particles at site $x$ and time $\tau$ of a finite lattice which for simplicity we assume one-dimensional. The particles jump with rates $g(\eta(x))$ to one of the nearest-neighbor sites $x+1$ or $x-1$ with probability 1/2. The function $g(k)$ is non decreasing and $g(0) = 0$. We assume that our system interacts with two reservoirs of particles in positions $N$ and $-N$ with rates $p_+$ and $p_-$ respectively. The microscopic dynamics is then defined by the generator \[4\]

$$L_{\eta} f(\eta) = \frac{1}{2} \sum_{x=-N}^{N} \left( g(\eta(x)) \nabla_{\eta} \eta(x) + \nabla_{\eta} \eta(x) f(\eta(x)) \right) + \frac{1}{2} p_+ [f(\eta^x) - f(\eta)] + \frac{1}{2} p_- [f(\eta^{-x}) - f(\eta)]$$  \hspace{1cm} (10)

where $\nabla_{\eta} = \eta^{x+1} - \eta^x$ and $\nabla_{\eta} = \eta^{x-1} - \eta^x$.

with the condition $\eta^0 = 0$, and $\eta^\pm x$ is the configuration obtained from $\eta$ when a particle jumps from $x$ to $y$. Similarly $\eta^{N,N+1}(\eta) = \eta(\eta^0 - 1)$, $\eta^{-N,N-1}(\eta) = \eta(\eta^0 - 1)$ and $\eta^{N,N-1}(\eta)$ is the configuration $\eta$ after addition of a particle at the point $N(-N)$.

It is remarkable that the invariant measure for this process can be constructed explicitly \[4\]. It is the grand-canonical measure obtained by the product of the marginal distributions

$$P_N(\eta(x) = k) = \frac{\lambda^N(x)}{\sum_{k=1}^N \lambda^N(x)} Z_N^{-1}(x)$$  \hspace{1cm} (11)

where

$$\lambda_N(x) = \frac{p_+ + p_- - 2}{2(N+1)} x + \frac{p_+ + p_-}{2}$$  \hspace{1cm} (12)

and

$$Z_N(x) = 1 + \sum_{k=1}^N \frac{\lambda^N(x)}{\sum_{k=1}^N \lambda^N(x)}$$  \hspace{1cm} (13)

We emphasize that, if $p_- \neq p_+$, the generator $L_N$ is not self-adjoint with respect to the invariant measure so that the process is different from its time reversal and detailed balance does not hold.

Let us introduce now the macroscopic time $t = \tau / N^2$ and space $u = x / N$ and the empirical density

$$\rho_N(t, u) = \frac{1}{N} \sum_{x=-N}^{N} \eta_{N}(x) \delta(u - x/N)$$  \hspace{1cm} (14)

Then one can prove that in the limit $N \to \infty$ the empirical density \[4\] tends in probability to a continuous function $\rho_\infty(x)$ which satisfies the following hydrodynamic equation

$$\partial_t \rho = \frac{1}{2} \partial_u \left( D(\rho) \partial_u \rho \right) = \frac{1}{2} \partial^2 \phi(\rho) = F(\rho)$$  \hspace{1cm} (15)

where $\phi(\rho)$ is the inverse function of

$$\rho(\phi) = \frac{1}{Z(\phi)} \sum_{k=0}^{\infty} \frac{\phi^k}{g(1) \cdots g(k)}$$  \hspace{1cm} (16)

where $Z(\phi)$ is the normalization constant as in (3). The function $\phi$ is well defined because the right hand side of (16) is strictly increasing in $\phi \geq 0$. Then $\rho(\phi)$ is the equilibrium density corresponding to the activity $\phi$. The boundary conditions for (16) are $\phi(\rho(\pm 1)) = p_\pm$. 
From the knowledge of the invariant measure one can calculate the adjoint generator \( L_N^* \) given by
\[
(L_N^* f)(\eta) = \frac{1}{2} \sum_{x=1}^{N} g(\eta(x)) \frac{\lambda_N(x+1)}{\lambda_N(x)} \nabla_{x,x+1} f + \frac{1}{2} \sum_{x=1}^{N} g(\eta(x)) \frac{\lambda_N(x-1)}{\lambda_N(x)} \nabla_{x,x-1} f + \frac{1}{2} \lambda_N(N) f(\eta^N) - f(\eta) + \frac{1}{2} \lambda_N(-N) f(\eta^{-N}) - f(\eta) .
\]

Notice that the form of (17) is the same as (10) with the rates modified in such a way to invert the particle flux. From (17) one can derive the adjoint hydrodynamics
\[
\partial_t \rho = \frac{1}{2} \delta^2 \phi(\rho) - \alpha \partial_u \left( \frac{\phi(\rho)}{\lambda(u)} \right) = F^*(\rho)
\]
with \( \lambda(u) = \frac{\partial}{\partial u} \rho(u) + \frac{\partial}{\partial u} \rho^2(u) \) and \( \alpha = \frac{\partial}{\partial u} \rho(u) - \frac{\partial}{\partial u} \rho^2(u) \). The boundary condition for (18) are the same as for (15). For the detailed computations we refer the reader to [19].

The second term on the right hand side of (18) is produced by the new rates in (17). As expected, it is proportional to the difference of the chemical potentials.

In this model one can compute the action functionals \( J(\rho) \) and \( J^*(\rho) \). The result is
\[
J_{[t_1,t_2]}(\rho) = \frac{1}{2} \int_{t_1}^{t_2} dt \left\langle \nabla_u W, \frac{1}{\phi(\rho)} \nabla_u W \right\rangle \quad (19)
\]
\[
J^*_{[t_1,t_2]}(\rho) = \frac{1}{2} \int_{t_1}^{t_2} dt \left\langle W^*, \frac{1}{\phi(\rho)} \nabla_u W^* \right\rangle \quad (20)
\]
where, \( W^* = \partial_t \rho - F^*(\rho) \). Moreover \( J \) and \( J^* \) are defined to be infinite if \( \rho \) does not satisfy the boundary conditions stated above.

The entropy \( S(\rho) \) can be easily computed from the expression (11) for the invariant measure
\[
S(\rho) = \int du \left[ \rho(u) \log \frac{\phi(\rho(u))}{\lambda(u)} - \log \frac{\rho(u)}{\lambda(u)} \right] \quad (21)
\]

From equations (19), (20) and (21), one can verify explicitly equation (13) and the generalized Onsager-Machlup relationship.

We deduce now a twofold generalization of the celebrated fluctuation–dissipation relationship: it is valid in non equilibrium states and in non linear regimes. Such a relationship will hold provided the rate function \( J^*_{[t_1,t_2]} \) of the time reversed process is of the form (11) with the same metric \( K(\rho) \) but a different vector field \( F^* \) describing the hydrodynamics of the adjoint process, namely
\[
J^*_{[t_1,t_2]}(\rho) = \frac{1}{2} \int_{t_1}^{t_2} dt \left\langle W^*, K(\rho) W^* \right\rangle \quad (22)
\]

By taking the variation of the equation (15), a simple computation gives
\[
F(\rho) + F^*(\rho) = -K(\rho)^{-1} \frac{\delta S}{\delta \rho} \quad (23)
\]

This relation holds for the non-equilibrium zero-range model discussed before. We also note that it holds for the equilibrium reversible models for which the large deviation principle has been rigorously proven such as the simple exclusion process (12) and the Landau–Ginzburg model (19) and its non-gradient version (20). It is also easy to check that the linearization of (24) around the stationary profile \( \bar{\rho} \) yields a fluctuation–dissipation relationship which in equilibrium reduces to the usual one.

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