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MICROSCOPIC REVERSIBILITY AND THERMODYNAMIC FLUCTUATIONS

1. INTRODUCTION

Fundamental contributions to the theory of irreversible processes were the derivation of the reciprocal relations for transport coefficients in states deviating only slightly from equilibrium and the calculation of the most probable trajectory creating a fluctuation near equilibrium. The first result was obtained by Onsager in 1931 [1] and the second one by Onsager and Machlup [2] in 1953. The calculation of the most probable trajectory relies on the reciprocal relations which in turn are a consequence of microscopic reversibility. It turns out that the trajectory in question is just the time reversal of the most probable trajectory describing relaxation to equilibrium of a fluctuation. The latter is a solution to the hydrodynamical equations.

In this paper we discuss the following question: is microscopic reversibility a necessary condition for the validity of the above results? The answer to this question is far from obvious because in going from the microscopic to the macroscopic scale a lot of information is lost and irreversibilities at a small scale may be erased when taking macroscopic averages. We will show that this is in fact the case by exhibiting microscopically non reversible stochastic dynamics which nonetheless fluctuate following the same time- reversal rule of Onsager-Machlup. Actually our results are not restricted to situations near equilibrium and the problem can be discussed rigorously for arbitrary fluctuations.

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The models we shall discuss belong to the category of interacting particle systems and have been analysed in detail in [3] and [4]. In particular in the last reference we already made a connection with the Onsager-Machlup theory by showing that the regression to equilibrium of any fluctuation (even far from equilibrium) takes place with highest probability along a trajectory of the hydrodynamic equation. The models consist in a superposition of an accelerated symmetric Kawasaki process and a Glauber spin flip process.

The structure of the paper is as follows. In section 2 we describe the models and summarize the results of [4] needed for our purpose.

In section 3 we discuss under what conditions our dynamics becomes reversible with respect to the invariant measure, which will be a Bernoulli product measure.

In section 4 we give conditions sufficient to insure the validity of Onsager-Machlup time-reversal relation and show that they can be satisfied by irreversible dynamics. It also turns out that if the fluctuations are homogeneous in space any dynamics in the class considered satisfies Onsager-Machlup.

In the present paper we do not supply all the proofs which will be given in an more extended forthcoming publication.

2. Description of the models

The systems considered consist of particles moving on the sites of a lattice. There are two basic dynamical processes:

i) a particle can move to a neighbouring site if this is empty

ii) a particle can disappear or be created in a site according to whether this is occupied or empty.

The first process is clearly conservative while the second is not.

Mathematically we consider a family of Markov processes whose state space is $X_N = \{0,1\}^{Z_N}$, where N is an integer and Z_N denotes the set of integers modulo N. We shall denote with η a point in the state space, that is a configuration of the system. This is therefore given by a function $\eta(i)$ defined on each site and taking the values 0 or 1. For each N the dynamics is defined by the action of the generator L_N of the Markov process on functions $f(\eta)$

$$L_N f(\eta) = \frac{N^2}{2} \sum_{i \in Z_N} (f(\eta^{i,i+1}) - f(\eta)) + \sum_{i \in Z_N} c(i,\eta)(f(\eta^i) - f(\eta)) \tag{1}$$

where the addition in Z_N means addition modulo N

$$\eta^{i,k}(j) = \begin{cases} \eta(j) & \text{if} \quad j \neq i,k \\ \eta(k) & \text{if} \quad j = i \\ \eta(i) & \text{if} \quad j = k \end{cases} \tag{2}$$

(3) $$\eta^i(j) = \begin{cases} \eta(j) & \text{if} \quad j \neq i \\ 1 - \eta(i) & \text{if} \quad j = i \end{cases}$$

The coefficients $c(i, \eta)$ depend on the values of $\eta(j)$ with j within a fixed distance R from the site i. They are translation invariant that is $c(i, \eta) = c(\tau_i \eta)$ where $(\tau_k \eta)(j) = \eta(k + j)$. Let us consider now the unit interval $S = [0, 1)$ with periodic condition at the boundary and a function γ defined on S and taking values in $[0, 1]$. Let ν_γ^N the probability measure on the state space of the system obtained by assigning a Bernoulli distribution to each site, taking the product over all sites and defined by

(4) $$\nu_\gamma^N\{\eta(k) = 1\} = \gamma\Big(\frac{k}{N}\Big).$$

The main object of our study is the empirical density μ_t^N:

(5) $$\mu_t^N(x) = \frac{1}{N} \sum_{k \in Z_N} \eta_t(k) \delta\Big(x - \frac{k}{N}\Big).$$

If we denote by Q_γ^N the distribution law of the trajectories $\mu_t^N(x)$ when the initial measure is concentrated on a configuration such that $\mu_0^N(x) \to \gamma(x)$ as $N \to \infty$, it is possible to show that Q_γ^N converges weakly as N goes to infinity to the measure concentrated on the path $\rho(t, x)$ that is the unique solution of

(6) $$\begin{cases} \partial_t \rho & = \frac{1}{2} \partial_x^2 \rho + B(\rho) - D(\rho) \\ \rho(0, \cdot) & = \gamma(\cdot) \end{cases}$$

with

(7) $$B(\rho) = E_{\nu_\rho}(c(\eta)(1 - \eta(0)))$$

(8) $$D(\rho) = E_{\nu_\rho}(c(\eta)\eta(0))$$

Where ν_ρ is the Bernoulli product distribution with $\gamma(x) \equiv \rho$. Typically $B(\rho)$ and $D(\rho)$ are polynomials in the variable ρ.

The equilibrium state corresponds to a density ρ_0 which is the solution of the equation $B(\rho) = D(\rho)$ that gives an absolute minimum of the potential $V(\rho) = \int^\rho [D(\rho') - B(\rho')] d\rho'$.

The above result is a law of large numbers that shows that the empirical density in the limit of large N behaves deterministically according to equation (6). We can now ask what is the probability that our system follows a trajectory different from the solution of (6) when N is large but not infinite. This probability is exponentially small in N and can be estimated using the methods of the theory of large deviations introduced for the systems of interest in [5] and developed in [3, 4]. The main idea consists in introducing a modified system for which the trajectory of interest (fluctuation) is typical being a solution of the corresponding hydrodynamic equation, and then comparing the two evolutions.

For this purpose we consider the Markov process defined by the generator

$$
\begin{aligned}
L^H_{N,t}f(\eta) = {} & \frac{N^2}{2} \sum_{|i-j|=1} \eta(i)(1-\eta(j))e^{H(t,\frac{j}{N})-H(t,\frac{i}{N})}[f(\eta^{i,j})-f(\eta)] \\
& + \sum_i c(i,\eta)[(1-\eta(i))e^{H(t,\frac{i}{N})} + \eta(i)e^{-H(t,\frac{i}{N})}][f(\eta^i)-f(\eta)]
\end{aligned} \tag{9}
$$

with c, $\eta^{k,j}$, η^i as previously defined and H can be interpreted as an external field.

The deterministic equation satisfied by the empirical density is now

$$
\begin{cases}
\partial_t \rho & = \frac{1}{2}\partial_x^2 \rho - \partial_x(\rho(1-\rho)\partial_x H) + B(\rho)e^H - D(\rho)e^{-H} \\
\rho(0,\cdot) & = \gamma(\cdot)
\end{cases} \tag{10}
$$

We remark that while equation (6) is of gradient type, equation (10) does not and this is due to the asymmetry of the exchange dynamics.

Given a function $\rho(x,t)$ twice differentiable with respect to x and once with respect to t this equation determines uniquely the field H. The probability that the original system follows a trajectory different from a solution of (6) can now be expressed in terms of the field H and the polynomials B and D. We introduce the large deviation functional

$$
\begin{aligned}
I(\rho) = {} & \frac{1}{2}\int_0^{t_0}\int_0^1 dt\, dx \rho_t(1-\rho_t)(\partial_x H_t)^2 \\
& + \int_0^{t_0}\int_0^1 dt\, dx\, B(\rho_t)(1-e^{H_t}+H_t e^{H_t}) \\
& + \int_0^{t_0}\int_0^1 dt\, dx\, D(\rho_t)(1-e^{-H_t}-H_t e^{-H_t})
\end{aligned} \tag{11}
$$

Let G be a set of trajectories in the interval $[0,t_0]$. The large fluctuation estimate asserts that

$$
Q^N_\gamma(G) \simeq e^{-NI(G)} \tag{12}
$$

where

$$
I(G) = \inf_{\rho\in G} I(\rho) \tag{13}
$$

The symbol $\simeq$ has to be interpreted as asymptotic equality of the logarithms. From the equations (12), (13), one sees that to find the most probable trajectory that creates a certain state $\gamma(x)$ one has to find the $\rho(x,t)$ that minimizes $I(\rho)$ in the set G of all trajectories that connect the equilibrium state to $\gamma(x)$.

3. Reversibility

Reversibility means that a principle of detailed balance holds for the microscopic dynamics. Mathematically this is expressed by the self-adjointness of the generator of the process with respect to the scalar product defined by the measure.

A reversible measure for a process with generator of the form (1) exists only if we impose some restrictions on the functions c. The condition of reversibility is

$$(g, L_N f)_\mu = (L_N g, f)_\mu \tag{14}$$

for all functions f,g on X_N. In our case this condition reads

$$\begin{aligned} &\sum_\eta \Big[g(\eta)\Big(\frac{N^2}{2}\sum_i (f(\eta^{i,i+1}) - f(\eta)\Big) + \\ &\quad + \sum_i c(i,\eta)(f(\eta^i) - f(\eta))\Big]\mu(\eta) = \\ &= \sum_\eta \Big[\Big(\frac{N^2}{2}\sum_i (g(\eta^{i,i+1}) - g(\eta)\Big) + \\ &\quad + \sum_i c(i,\eta)(g(\eta^i) - g(\eta))f(\eta)\Big]\mu(\eta) \end{aligned} \tag{15}$$

that with some algebra, using the periodic boundary condition, can be trasformed into

$$\begin{aligned} &\sum_\eta \sum_i \frac{N^2}{2} g(\eta) f(\eta^{i,i+1})(\mu(\eta) - \mu(\eta^{i,i+1})) + \\ &\quad + \sum_\eta \sum_i g(\eta) f(\eta^i)(c(i,\eta)\mu(\eta) - c(i,\eta^i)\mu(\eta^i)) = 0 \end{aligned} \tag{16}$$

Since this equality must hold for every g and f, this condition is equivalent to

$$\begin{cases} \mu(\eta) - \mu(\eta^{i,i+1}) & = 0 \\ c(i,\eta)\mu(\eta) - c(i,\eta^i)\mu(\eta^i) & = 0 \end{cases} \tag{17}$$

for every η and i. The first condition imposes that the measure μ be of the form

$$\mu(\eta) = \mu\Big(\sum_{i=1}^{N} \eta(i)\Big) \tag{18}$$

that is to say μ must assign an equal weight to configurations with the same number of 1. The second condition, with a μ of this type, is a restriction for the functions c. The most general form of $c(i,\eta)$ that satisfies this condition is:

$$c(i,\eta) = c_1(1 - \eta(i))h(i,\eta) + c_2\eta(i)h(i,\eta) \tag{19}$$

with c_1 and c_2 arbitrary positive constant and $h(i,\eta)$ a function that does not depend on the variable $\eta(i)$ and such that $h(i,\eta) = h(\tau_i\eta)$. For processes of this type it is possible to compute explicitly the unique reversible measure that is a Bernoulli measure with parameter $p = \frac{c_1}{c_1+c_2}$. We emphasize that periodic boundary conditions are crucial for the validity of (19) with a nontrivial h.

4. The minima of $I(\rho)$

Let us consider a fluctuation that can be connected to the equilibrium density by a trajectory solution of the hydrodynamical equation (6). Then from the form of $I(\rho)$ it is obvious that such a fluctuation relaxes most likely following this trajectory. In fact the corresponding H is zero which implies $I = 0$. We want to investigate now the trajectory that creates the non-equilibrium state $\gamma(x)$ with highest probability, that is to say the trajectory $\rho(x,t)$ with the boundary conditions

$$\lim_{t\to-\infty} \rho(x,t) = \rho_0 \tag{20}$$

$$\rho(x,0) = \gamma(x) \tag{21}$$

that minimizes the functional I, with ρ_0 the equilibrium state.

We consider polynomials B and D of the form

$$B(\rho) = c_1 A(\rho)(1-\rho) \tag{22}$$

$$D(\rho) = c_2 A(\rho)\rho \tag{23}$$

with c_1 and c_2 arbitrary positive constant and $A(\rho)$ a generic strictly positive polynomial. Note that the potential that generates the polynomial part of the hydrodynamic equation with B and D of this type is always a single well potential with only one stable equilibrium point.

In this case it is possible to prove (see Appendix) that the unique solution of our variational problem is the function $\rho^*(x,t)$ defined by

$$\rho^*(x,t) = \rho(x,-t) \tag{24}$$

where $\rho(x,t)$ is the solution of the hydrodynamic equation which relaxes to equilibrium. $\rho^*(x,t)$ is therefore a solution of the hydrodynamic equation with inverted drift

$$\partial_t \rho = -\frac{1}{2}\partial_x^2\rho + D(\rho) - B(\rho) \tag{25}$$

Equation (24) is the Onsager-Machlup time-reversal relation.

All reversible processes generate hydrodynamic equations with coefficient $B(\rho)$ and $D(\rho)$ of the form (22) and (23), so for all these systems (24) holds. It is most interesting that (24) can hold for irreversible models too; namely if we consider processes with functions c of the form

$$c(i,\eta) = c_1(1-\eta(i))h_1(i,\eta) + c_2\eta(i)h_2(i,\eta) \tag{26}$$

with h_2 different from h_1, we obtain a irreversible process, but if we choose h_2 in such a way that

$$E_{\nu_\rho}(h_2(\eta)) = E_{\nu_\rho}(h_1(\eta)) \tag{27}$$

the polynomials B and D that we obtain are of the requested form for the validity of (24). An illuminating example is:

$$c(i,\eta) = c_1(1-\eta(i))\eta(i+1)\eta(i-1) + c_2\eta(i)\eta(i+1)\eta(i+2)\,. \tag{28}$$

The microscopic irreversibility of this model is evident, but the polynomials B and D are of the wanted form (22), (23):

$$B(\rho) = c_1(1-\rho)\rho^2 \tag{29}$$

$$D(\rho) = c_2\rho^3\,. \tag{30}$$

If we consider only spatially homogeneous fluctuations we can solve explicity the equation (10) for the field H

$$H = \log\frac{\dot\rho + \sqrt{\dot\rho^2 + 4B(\rho)D(\rho)}}{2B(\rho)} \tag{31}$$

and we obtain an expression of the functional I in terms of the trajectories ρ only:

$$\begin{aligned} I(\rho) = \int \Bigg(& B(\rho) + D(\rho) - \sqrt{\dot\rho^2 + 4B(\rho)D(\rho)} + \\ & + \dot\rho\log\frac{\dot\rho + \sqrt{\dot\rho^2 + 4B(\rho)D(\rho)}}{2B(\rho)}\Bigg)dt\,. \end{aligned} \tag{32}$$

One can show quite generally that for a fluctuation which can be connected to equilibrium by a solution of (6) the minimizing trajectory satisfies (24) (ρ depends now only on t) for all polynomials B and D. Therefore in this case any dynamics reversible or irreversible satisfies the time-reversal relation of Onsager-Machlup. A similar argument applies also to the case in which the fluctuation cannot be directly connected to equilibrium by a solution of (6). This can happen for example if the potential has local minima.

5. Concluding remarks

The models we have considered are rather special and the periodic boundary conditions play a crucial role for the validity of our argument. It is necessary to study to what extent the result can be generalized. However an important principle has been demonstrated: microscopic reversibility is not a necessary condition for the validity of certain macroscopic reversibility properties.

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Appendix: Minimization of $I(\rho)$

The basic point is that for polynomials of the form (22), (23), it is possible to write explicitely the field H that generates the solutions of equation (25):

$$H = \log \frac{c_2 \rho^*}{c_1(1-\rho^*)} \,. \tag{A1}$$

For this reason it is possible to obtain on the solutions of (25) an expression of the functional I in terms of the trajectory $\rho(x,t)$ only. Using (25), integrating by parts and remembering the periodic boundary condition, we obtain the expression:

$$I(\rho^*) = \int_{-\infty}^{0} \int_{0}^{1} \partial_t \rho^* \log\Big(\frac{c_2\rho^*}{c_1(1-\rho *)}\Big) dt\, dx \,. \tag{A2}$$

The value of this functional can be immediatly calculated and depends only on the values of $\rho^*(x,t)$ at $t=0$ and $t=-\infty$:

$$\begin{aligned} I(\rho) = \Big\{ \int_0^1 \rho^*(x,t) \log(\frac{c_1}{c_2}) dx + \int_0^1 \rho^*(x,t) \log \rho^*(x,t) dx + \\ + \int_0^1 (1-\rho^*(x,t)) \log(1-\rho^*(x,t)) dx \Big\} \Big|_{t=-\infty}^{t=0} \,. \end{aligned} \tag{A3}$$

We now compare the value of the functional on a generic trajectory that connects the equilibrium state to the state $\gamma(x)$ with the value of the functional on the solution of (25) connecting the same states. Define

$$I(\rho) - I(\rho^*) = \Delta(\rho) \tag{A4}$$

we have

$$\Delta(\rho) = \int_{-\infty}^{0}\int_{0}^{1}\Big(\frac{1}{2}\rho(1-\rho)(\partial_x H)^2 + c_1(1-\rho)A(\rho)(1-e^{H}+He^{H}) + \\ + c_2\rho A(\rho)(1-e^{-H}-He^{-H}) - \partial_t\rho\, log\Big(\frac{c_2\rho}{c_1(1-\rho)}\Big)\Big)\,dt\,dx\,. \tag{A5}$$

To obtain this expression we have used (A3). Using equation (10) and integrating by parts we obtain finally the expression

$$\Delta(\rho) = \int_{-\infty}^{0}\int_{0}^{1}\Big(\frac{1}{2}\rho(1-\rho)\Big(\partial_x H - \frac{\partial_x\rho}{\rho(1-\rho)}\Big)^2 + \\ + c_1(1-\rho)A(\rho)\Big(1-e^{H}+He^{H}-e^{H}\log\frac{c_2\rho}{c_1(1-\rho)}\Big) + \\ + c_2\rho A(\rho)\Big(1-e^{-H}-He^{-H}+e^{-H}\log\frac{c_2\rho}{c_1(1-\rho)}\Big)\Big)\,dx\,dt\,. \tag{A6}$$

The final step consists in introducing a new field F

$$F = \log\Big(\frac{c_2\rho}{c_1(1-\rho)}\Big) - H\,. \tag{A7}$$

This field is constructed in such a way that the value $F=0$ generates a $\rho(x,t)$ solution of (25). The functional $\Delta(\rho)$ in terms of F becomes

$$\Delta(\rho) = \frac{1}{2}\int_{-\infty}^{0}\int_{0}^{1} dt\,dx\,\rho(1-\rho)(\partial_x F)^2 + \\ + \int_{-\infty}^{0}\int_{0}^{1} dt\,dx\,c_1(1-\rho)A(\rho)(1-e^{F}+Fe^{F}) + \\ + \int_{-\infty}^{0}\int_{0}^{1} dt\,dx\,c_2\,\rho A(\rho)(1-e^{-F}-Fe^{-F}) \tag{A8}$$

This functional is obviously positive and zero only if F is zero.

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