Microscopic reversibility and thermodynamic fluctuations

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Abstract

In this paper we show that certain properties of thermodynamic fluctuations which were derived long ago by Onsager and Onsager-Machlup as a consequence of microscopic reversibility , can actually hold also if the dynamics deviates from reversibility. This result is based on the explicit construction of models which can be analysed rigorously. What happens is that small scale

irreversibilities are washed out at the macroscopic level.

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I. 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 [?] and the second one by Onsager and Machlup [?] 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 equiliblrium and the problem can be discussed rigorously for arbitrary fluctuations.

The models we shall discuss belong to the category of interacting particle systems and have been analysed in detail in [?] and [?]. 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 II we describe the models and summarize the results of [?] needed for our purpose.

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

In section IV 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.

II. 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

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

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

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

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

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

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