An equilibrium state with macroscopic correlations

Giada Basile

Dipartimento di Fisica, Università “La Sapienza”

Piazzale Aldo Moro 2, 00185 Roma, Italy

Giovanni Jona-Lasinio

Dipartimento di Fisica and INFN, Università “La Sapienza”

Piazzale Aldo Moro 2, 00185 Roma, Italy

Abstract

In this paper we show that the equilibrium macroscopic entropy of a generic non reversible
Kawasaki+Glauber dynamics is a non local functional of the density. This implies that equilibrium
correlations extend to macroscopic distances.

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I. INTRODUCTION

In the last two years considerable progress has been made in understanding stationary non equilibrium states (SNS). An important result, first established by Derrida, Lebowitz and Speer [3, 4] and then rederived in a simpler way from general principles in [2], is the non local character of the entropy in a boundary driven (i.e. interacting with reservoirs having different chemical potentials) simple exclusion system. The question naturally arises whether this is a general property of SNS. A different model, the boundary driven zero range, does not exhibit this property [1, 2] but one may suspect that this is related to the special character of the interaction. All these models are conservative in the sense that the number of particles is conserved.

In this note we present an example of an equilibrium state in which the entropy is a non local functional of the thermodynamic variables showing in this way that this is not an exclusive property of SNS. By an equilibrium state we mean a stationary state of an isolated system or of a system in contact with reservoirs characterized by the same chemical potential. Our conclusion is that non locality or macroscopic correlations is more likely to be a generic feature of non reversible dynamics. Indeed, in the model considered, the generator of the dynamics is not self-adjoint with respect to the equilibrium measure. This means that detailed balance does not hold for such an equilibrium ensemble.

The system considered evolves according to the so called Kawasaki+Glauber dynamics with generic transition rates for the Glauber process and will be described in the next section. Our analysis is based on a general Hamilton-Jacobi equation satisfied by the entropy in equilibrium or non equilibrium states and established in [1, 2]. The H-J equation for our model has a very complicated structure but for values of the thermodynamic variables near the stationary values can be solved by an iterative scheme of calculation. The entropy is non local already in the lowest approximation, i.e. at the level of gaussian fluctuations. One should mention that there are special choices of the transition probabilities which make the entropy of the model local in spite of a microscopic non reversible dynamics [3], however we are interested in properties with some degree of stability. A more detailed analysis of our example and of the non locality problem will be presented elsewhere.
II. THE MODEL

In this section we follow closely [5]. The model consists of particles on a lattice evolving according to 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, the rate depending on the nearby configuration.

The first process is 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 \( \eta \) 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 Markov generator \( L_N \) on functions \( f(\eta) \)

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

(1)

where the addition in \( Z_N \) means addition modulo \( N \)

\[
\eta^{i,k}(j) = \begin{cases} 
\eta(j) & j \neq i, k \\
\eta(k) & j = i \\
\eta(i) & j = k 
\end{cases}
\]

(2)

\[
\eta^i(j) = \begin{cases} 
\eta(j) & j \neq i \\
1 - \eta(i) & j = i 
\end{cases}
\]

(3)

The rates \( c(i,\eta) \) depend on the values of \( \eta(j) \) with \( j \) within a fixed distance \( R \) from the site \( i \). They are translation invariant, that is there exists a function \( c(\eta) \) such that \( c(i,\eta) = c(\tau_i \eta) \) where \( (\tau_k \eta)(j) = \eta(j - k) \). Let us consider now the unit interval \([0, 1)\) with periodic condition at the boundary and a function \( \gamma \) defined on \([0,1)\) and taking values in \([0, 1]\). Let \( \nu^N_\gamma \) 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

\[
\nu^N_\gamma \{\eta(k) = 1\} = \gamma\left(\frac{k}{N}\right)
\]

(4)
The main object of our study is the empirical density $\mu^N_t$:

$$
\mu^N_t(x) = \frac{1}{N} \sum_{k \in \mathbb{Z}} \eta_{N^2t}(k) \delta(x - \frac{k}{N})
$$

Let us denote by $Q^N_\gamma$ the distribution law of the trajectories $\mu^N_t(x)$ when the initial measure is the product measure $\nu^N_\gamma$. It is possible to show that $Q^N_\gamma$ converges weakly as $N$ goes to infinity to the measure concentrated on the path $\rho(t,x)$ that is the unique solution of

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

with

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

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

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

The equilibrium state corresponds to a density $\bar{\rho}$ 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 $\mu^N_t$ follows a trajectory different from a 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 [6] and developed in [5, 7]. The main idea consists in introducing a modified process for which the trajectory of interest (fluctuation) is 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

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

with $c, \eta^{k,j}, \eta^i$ as previously defined and $H(t,x)$ can be interpreted as an external potential.

The deterministic equation satisfied by the empirical density is now

$$
\begin{cases}
\partial_t \rho & = \frac{1}{2} \partial_x^2 \rho - \partial_x(\rho(1 - \rho)\partial_x H) + B(\rho)e^H - D(\rho)e^{-H} \\
\rho(0,\cdot) & = \gamma(\cdot)
\end{cases}
$$
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 $\mu^N_t$ in the unperturbed system follows a trajectory different from a solution of (6) can now be expressed in terms of $H$ and the polynomials $B$ and $D$. We introduce the large deviation functional

$$I(\rho_t) = \frac{1}{2} \int_0^t \int_0^1 dt dx \rho_t(1 - \rho_t)(\partial_x H_t)^2 + \int_0^t \int_0^1 dt dx B(\rho_t)(1 - e^{H_t} + H_t e^{H_t}) + \int_0^t \int_0^1 dt dx D(\rho_t)(1 - e^{-H_t} - H_t e^{-H_t})$$

(11)

Let $\rho_t$ be a trajectory in the interval of time $[0, t_0]$ with initial profile $\gamma$; assume that the initial configuration of the process $\eta_0$ is fixed and such that $\mu_0^N(x) \to \gamma(x)$ as $N \to \infty$. The large fluctuation estimate asserts that

$$P_{\eta_0}^N(\mu_t^N \sim \rho_t, t \in [0, t_0]) \simeq e^{-NI(\rho_t)}$$

(12)

where $P_{\eta_0}^N$ is the probability distribution of the unperturbed process $\eta_t$ starting in $\eta_0$. The sign $\simeq$ has to be interpreted as asymptotic equality of the logarithms. Equation (12) is a dynamical generalization of Einstein formula for thermodynamic fluctuations. From this equation one sees that the trajectory that creates a certain profile $\rho(x)$ with highest probability is the one that minimizes $I(\rho_t)$ in the set $G$ of all trajectories that connect the equilibrium state $\bar{\rho}$ to $\rho(x)$.

Let us introduce the quantity

$$S(\rho) = \inf_{\rho_t \in G} I(\rho_t)$$

(13)

that we shall call the entropy associated to the profile $\rho$. One can show, from the large deviation estimate (12), that in equilibrium

$$P_{eq}^N(\mu^N \sim \rho) \simeq e^{-NS(\rho)}$$

(14)

In this way we recover dynamically the usual Einstein formula. Note that the sign of the entropy is the opposite of that used in the physical literature.
III. THE HAMILTON-JACOBI EQUATION AND ITS CONSEQUENCES

The functional $I(\rho)$ has the form of an action integral associated to the Lagrangian

$$\mathcal{L}(\rho, \dot{\rho}) = \frac{1}{2} \int_0^1 dx \rho (1 - \rho_t) \left( \partial_x H_t \right)^2 + \int_0^1 dx B(\rho_t)(1 - e^{H_t} + H_t e^{H_t}) + \int_0^1 dx D(\rho_t)(1 - e^{-H_t} - H_t e^{-H_t})$$ (15)

where $H(\rho, \dot{\rho})$ is determined by (10). By Legendre transform we can define the Hamiltonian

$$\mathcal{H}(\rho, H) = \int_0^1 dx \left( \frac{1}{2} H \partial_x^2 \rho + \frac{1}{2} (\partial_x H)^2 \rho (1 - \rho) - B(\rho)(1 - \exp H) - D(\rho)(1 - \exp -H) \right)$$ (16)

The entropy $S(\rho)$ then satisfies the Hamilton-Jacobi equation

$$\mathcal{H}(\rho, \frac{\delta S}{\delta \rho}) = 0$$ (17)

This is a very complicated functional derivative equation which however can be solved by successive approximations using as an expansion parameter $\rho - \bar{\rho}$ where $\bar{\rho}$ is a solution of $B(\rho) = D(\rho)$ that is a stationary solution of hydrodynamics. For $\rho = \bar{\rho}$ we have $\frac{\delta S}{\delta \rho} = 0$. We are looking for an approximate solution of (17) of the form

$$S(\rho) = \frac{1}{2} \int_0^1 dx \int_0^1 dy (\rho(x) - \bar{\rho}) k(x, y) (\rho(y) - \bar{\rho}) + o(\rho - \bar{\rho})^2$$ (18)

The kernel $k(x, y)$ is the inverse of the density correlation function. It is more convenient, as in [2], to work directly with the correlation function using the Legendre transform of the entropy $G(h)$, which is the pressure corresponding to the chemical potential profile $h$

$$G(h) = \sup_{\rho} \{ \langle h, \rho \rangle - S(\rho) \}$$ (19)

$G(h)$ satisfies the dual Hamilton-Jacobi equation

$$\mathcal{H} \left( \frac{\delta G}{\delta h}, h \right) = 0$$ (20)

We are looking for an approximate solution of (20) of the form

$$G(h) = \int_0^1 dx h(x) \bar{\rho} + \frac{1}{2} \int_0^1 dx \int_0^1 dy h(x) c(x, y) h(y) + o(h^2)$$ (21)

where $c(x, y)$ is related to $k(x, y)$ by the following relation

$$\int c(x, y) k(y, z) dy = \delta(x - z)$$ (22)
By inserting (21) in (20) we obtain the following equation for \( c(x, y) \)

\[
\frac{1}{2} \partial_x^2 c(x, y) - (d_1 - b_1) c(x, y) - \frac{1}{2} \bar{\rho} (1 - \bar{\rho}) \partial_x^2 \delta(x - y) + b_0 \delta(x - y) = 0
\]  

(23)

where

\[
b_1 = B'(\bar{\rho})|_{\rho = \bar{\rho}}, \quad d_1 = D'(\bar{\rho})|_{\rho = \bar{\rho}}
\]

and

\[
b_0 = B(\bar{\rho}) = D(\bar{\rho}) = d_0
\]

(24)

It is now easy to find the equation for \( k(x, y) \) by combining (23) with (22)

\[
\frac{1}{2} \bar{\rho} (1 - \bar{\rho}) \partial_x^2 k(x, y) - b_0 k(x, y) - \frac{1}{2} \partial_x^2 \delta(x - y) + (d_1 - b_1) \delta(x - y) = 0
\]

(25)

If the entropy is a local functional of the density, \( k(x, y) \) has the form \( k(x, y) = f(\bar{\rho}) \delta(x - y) \)
which inserted in (25) gives

\[
f(\bar{\rho}) = [\bar{\rho} (1 - \bar{\rho})]^{-1}
\]

(26)

and

\[
b_0 [\bar{\rho} (1 - \bar{\rho})]^{-1} - (d_1 - b_1) = 0
\]

(27)

Therefore if \( b_0, b_1, d_1 \) do not satisfy this equation the entropy cannot be a local functional of the density.

The equation for \( c(x, y) \) simplifies by writing

\[
c(x, y) = \bar{\rho} (1 - \bar{\rho}) \delta(x - y) + b(x, y)
\]

(28)

obtaining the following equation for \( b(x, y) \)

\[
- \frac{1}{2} \partial_x^2 b(x, y) + (d_1 - b_1) b(x, y) = (\bar{\rho} (1 - \bar{\rho})(b_1 - d_1) + b_0) \delta(x - y)
\]

(29)

Remark that \( d_1 - b_1 \), being the second derivative of the potential calculated in a minimum, is positive and the solution of equation (29) is exponentially decreasing. The macroscopic correlations in the equilibrium states of our system are therefore of short range when compared to the stationary non equilibrium correlations of the simple exclusion process considered in [2].

In [9] the gaussian process describing, in the same model, central limit type fluctuations was studied. When the \( t \to \infty \) limit is taken one finds that the stationary correlations of such a process agree, as one could expect, with the macroscopic correlations we have calculated in the gaussian approximation.
IV. CONCLUSIONS

The calculation presented in this paper supports the conjecture that macroscopic correlations are a generic feature of equilibrium states of non reversible lattice gases. It shows in addition that the Hamilton-Jacobi equation provides an effective approach to the study of the macroscopic entropy in cases which are more complex than the conservative lattice gases considered in [2].

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