On some Derivations of Irreversible Thermodynamics from Dynamical Systems Theory

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Abstract

Recently proposed models of nonequilibrium systems use non interacting particle systems, hence cannot possess the property of Local Thermodynamic Equilibrium. The theories built around these models lead to the conclusion that the development of singular phase space distributions in chaotic dynamical systems constitute the fundamental mechanism at the origin of thermodynamic entropy production. We argue that this is not the case, and that the laws of Irreversible Thermodynamics only hold in the presence of Local Thermodynamic Equilibrium.

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I. Introduction

In this paper we analyze some conceptual features of microscopic theories of Irreversible Thermodynamics, proposed in the literature of the last decade. In particular, we analyze a theory which focusses on the idea of chaos, and of the consequent loss of information and singular phase space distributions. This way, we bring the discussion in Ref.[1] to a
more physical level. For brevity, we concentrate on the theory illustrated in Ref.[2], but similar approaches, although not identical to that of [2], can be found also in [3, 4].

In Ref.[2] (see also [3]), it is stated that irreversibility of macroscopic systems, as represented in the equations of Irreversible Thermodynamics by a strictly positive entropy production rate [5], is at its deepest level due to the singular character of the invariant measures (i.e. the states) of the corresponding microscopic dynamics, cf. [2, 6]. In [2] it is also asserted that the singular character of the steady states calls for a replacement of the Gibbs entropy as a dynamical definition of the physical entropy by a coarse-grained information entropy, which would save the operational interpretation of entropy as a measure of disorder. The reason for making these statements is that a proper coarse graining procedure can be used to study the nature of the singularities of the steady states of the relevant dynamical systems. No mention is made of the physical relevance of these models, and of the connection of the concept of information entropy, or disorder, with the physical entropy or heat.

It is important to observe that a consequence of this approach would be that the irreversible entropy production rate $\sigma$, in Irreversible Thermodynamics is nothing else than the loss of information about the system in the course of time, due to the chaotic microscopic dynamics.\footnote{Note, however, that the information entropy considered here is not the Kolmogorov-Sinai entropy.}

In this paper we will try to show that without interacting particles, the information interpretation of physical entropy and Irreversible Thermodynamics does not make physical sense, i.e. that heat needs physical particles not just loss of information, or singular phase space distributions. After a very brief outline of Irreversible Thermodynamics in section II, we give a critical account in sections III, and IV. of the theory developed in [2]. In section V, we consider a more general class of MB maps than those of [2]. The purpose of that section is to show that MB maps can be manipulated to obey laws formally similar to those of Irreversible Thermodynamics, like Fick’s law, simply because they are
be treated as random walks on a line. In section VI, we draw our conclusions.

II. Irreversible Thermodynamics

Here, we briefly summarize the fundamental notions of Irreversible Thermodynamics relevant to our discussion, following the standard book by de Groot and Mazur [5].

Irreversible Thermodynamics can be applied to systems which are sufficiently close to equilibrium that they can be described as being in first approximation locally in equilibrium, i.e. such that Local Thermodynamic Equilibrium (LTE) holds. Microscopically the existence of LTE is predicated for a given initial state of the system on a local exchange of energy and momentum between (interacting) particles, leading in a characteristic time to a local equilibrium state. If LTE holds, the specific (i.e., per unit mass) local entropy $s$ at a position $\vec{r}$ at time $t$ in the system is the same function of the local specific energy $u$, the local mass density $n$, and the local mass fractions $c = \{c_i\}_{i=1}^k$ of the $k$ constituents out of which the system consists, as in equilibrium. Thus, one can write:

$$s(\vec{r}, t) = s[u(\vec{r}, t), n(\vec{r}, t), c(\vec{r}, t)],$$  \hspace{1cm} (1)

where $s(\cdot, \cdot, \cdot)$ is the same function as in equilibrium. Local equilibrium also implies the validity of the Gibbs relation for a mass element followed along its center of mass motion, even if the total system is not in equilibrium, i.e.

$$T \frac{ds}{dt} = \frac{du}{dt} + p \frac{dv}{dt} - \sum_{i=1}^n \mu_i \frac{dc_i}{dt},$$  \hspace{1cm} (2)

holds, where

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \vec{v} \cdot \nabla$$  \hspace{1cm} (3)

is the co-moving (Lagrangian) time derivative, $p$ is the pressure, $v = 1/n$ is the specific volume, and $\mu_i$ is the chemical potential of component $i$.

Hydrodynamics is also based on LTE, on local conservation laws for $u$, $v$ and the $c_i$’s, and on local linear laws in which the gradients of macroscopic quantities play the role of
thermodynamic forces. In particular, we recall Fick’s law for tracer diffusion local flux:

\[ \mathbf{J}(\mathbf{r}, t) = -D \nabla n(\mathbf{r}, t) \]  
(4)

where, \( \mathbf{J} \) is the local mass flow due to the local density gradient \( \nabla n \), and \( D \) is the diffusion coefficient.

Substituting the linear laws, such as (4), into the local conservation laws yields then the hydrodynamical equations, and with Eq.(2) one obtains a local entropy balance equation, which reads:

\[ n(\mathbf{r}, t) \frac{d\mathbf{s}}{dt}(\mathbf{r}, t) = -\nabla \cdot \mathbf{J}_s(\mathbf{r}, t) + \sigma_s(\mathbf{r}, t) \]  
(5)

Here the local entropy flow \( \mathbf{J}_s \) is the total entropy flow \( \mathbf{J}_{s,\text{tot}} \) minus a convective term \( n(\mathbf{r}, t)s(\mathbf{r}, t)\mathbf{v}(\mathbf{r}, t) \), \( \mathbf{v} \) being the local fluid velocity, and \( \sigma_s \geq 0 \) is the irreversible local entropy production, i.e. the local heat production. In particular, for tracer diffusion one has:

\[ \sigma_s(\mathbf{r}, t) = D \frac{[\nabla n(\mathbf{r}, t)]^2}{n(\mathbf{r}, t)}. \]  
(6)

III. Multibaker maps for Irreversible Thermodynamics

The dynamical theory of Irreversible Thermodynamics proposed in Ref.[2] is explicitly worked out on the so-called multibaker (MB) maps. In this section we recall the fundamental points of Gaspard’s theory, needed to understand its relation to Irreversible Thermodynamics. In the first place, MB maps consist of a one dimensional chain of baker maps, where the baker transformation moves geometric objects, like squares and rectangles from cut-up cells, in a way dictated by the baker dynamics \( \phi_L \), as illustrated in Fig.1 and defined as follows.

**Definition.** Let \( X = \bigcup_{i=-\infty}^{\infty} B_i \) be the union of the squares \( B_i = [0,1] \times [0,1], i \in \mathbb{Z} \). For
a positive integer $L$, let the transformation $\phi_L : X \rightarrow X$ be defined by

$$
\phi_L(i, x, y) = \begin{cases} 
(i - 1, 2x, \frac{y}{2}) & 0 \leq x < 1/2, 2 \leq i \leq L + 1 \\
(i + 1, 2x - 1, \frac{y + 1}{2}) & 1/2 \leq x \leq 1, 0 \leq i \leq L - 1 \\
(i - 1, x, y) & 0 \leq x < 1/2, i \leq 1, i \geq L + 2 \\
(i + 1, x, y) & 1/2 \leq x \leq 1, i \leq -1, i \geq L 
\end{cases}
$$

where $(i, x, y)$ represents a point $(x, y)$ in $B_i$. We say that $X$ is the MB space of the system $C = \cup_{i=1}^{L} B_i$ of length $L$, coupled to the two reservoirs $R_+ = \cup_{i=-\infty}^{0} B_i$ and $R_- = \cup_{i=L+1}^{\infty} B_i$.

The MB space is filled with "points", thought to represent noninteracting particles, according to a point-density, $n : X \rightarrow \mathbb{R}_+ \cup \{0\}$, which represents the number of points per unit volume in $X$. This point-density is supposed to make the connection between the MB map and physics, as explained in section IV. Because $\phi_L$ moves the points along the chain, the application of $\phi_L$ changes the point-density in $X$, making it into a "time" dependent distribution, $n_t$ say. For instance, begin with a distribution of points which is uniform on each $B_i$, and let the different densities on the different $B_i$'s be indicated by different shades, as in the top row of Fig.2. Then, the iterations of $\phi_L$ make horizontal strips of different point densities, originating from cells further and further away from any $B_i$ pile up with time in $B_i$, leading to a finer and finer layered structure of the point distribution (cf.fig.2).

As pointed out by Gaspard [2], real irreversible processes involve infinite particle reservoirs, for instance particle diffusion on a one-dimensional chain requires two reservoirs which are maintained indefinitely at different but fixed point-density values. By analogy, the point distribution on the MB space $X$ can be chosen in such a way that (cf. Eq.(25) below) the iterations of $\phi_L$ produce a point flow from the high density reservoir $R_+$, characterized by the point-density $n_+$, to the low density reservoir $R_-$, characterized by the point-density $n_-$. A density profile of this kind defines a time dependent measure $d\mu_t$ on $X$, with

$$
d\mu_t(i, x, y) = n_t(i, x, y) dx dy \quad \text{and} \quad \int_X d\mu_t = \infty \ ,
$$

$(7)$
which is not normalized because it represents the distribution of infinitely many points. This measure can be used to give a time dependent coarse grained description of the state of the system, defined by \( \{ \mu_t(B_i) \}_{i=-\infty}^{\infty} \), where \( \mu_t(B_i) = \int_{B_i} d\mu_t \) is the total “mass” in the square \( B_i \). A measure \( \mu \) which is invariant under the action of \( \phi_L \) is called a steady state.

Of the possible steady states for the MB map, the one considered in [2], \( \mu \) say, has a density profile made of two kinds of horizontal strips only: strips of constant point-density \( n_+ \), and strips of constant point-density \( n_- \). In the squares which are closer to the left reservoir the strips with density \( n_+ \) dominate, while those with point-density \( n_- \) dominate at the other end of the system. The corresponding coarse grained point distribution is linear in the squares label \( i \), for \( 1 \leq i \leq L \):

\[
\mu(B_i) = n_+ - \left( \frac{n_+ - n_-}{L+1} \right) i \quad \text{for any} \quad L \geq 1 ,
\]

and is associated with a steady flow of points \( J_\mu \), obeying the linear law

\[
J_\mu = -\tilde{D} \nabla n , \quad \text{with} \quad \nabla n \equiv \frac{n_+ - n_-}{L + 1} ,
\]

where \( \tilde{D} = 1/2 \) is a proportionality constant. This is so because at each time step the MB dynamics (7) moves half of each square \( B_i \) to the left (to \( B_{i-1} \)) and half to the right (to \( B_{i+1} \)), making the MB dynamics (7) equivalent to an unbiased random walk on a line (cf. Sect. V below). Formally, then, the MB chain verifies a linear relation which is reminiscent of Fick’s law (4). The next step one must take to derive relations similar to those of Irreversible Thermodynamics from MB dynamics is to associate this linear relation with some form of “entropy production”. To do this in the MB framework, one first observes that a non-normalized measure \( \mu \) cannot be used to characterize the state of the system through, e.g., its degree of “disorder”. However, thanks to the independence of the MB points, a probability distribution \( \chi \) can be constructed, considering the Poisson measure associated with \( \mu \),\(^2\) and taking as phase space \( \mathcal{M} \) of the whole system of infinitely

\(^2\)The details can be found in [2, 7], but are not relevant for our discussion, because the Poisson measure is not used in the following calculations.
many independent points a part of the family $\mathcal{P}(X)$ of all subsets of $X$. Then, if $\chi$ is not singular with respect to the Lebesgue measure on $\mathcal{M}$, i.e. if one can write $d\chi(\Gamma) = f(\Gamma)d\Gamma$, for some density function $f$, a Gibbs-like “entropy” $S_G$ can be defined by:

$$S_G = -k_B \int_\mathcal{M} f(\Gamma) \log f(\Gamma) \, d\Gamma,$$

which can be interpreted as a measure of the disorder in the microscopic state of the system described by $\chi$, or as the amount of information available on that state. The derivation of expressions looking like those of Irreversible Thermodynamics, now proceeds as follows.

1. A particular partition of $X$ is introduced\(^3\) in order to define a coarse grained information entropy. This is done taking a partition $\mathcal{A}$ of $X$, evolving $\mathcal{A}$ with $\phi_L$ up to $k - 1$ times forward in time and up to $\ell$ times backwards, and then introducing the finer partition

$$\mathcal{A}_{\ell,k} = \phi_L^{-1}(\mathcal{A}) \vee \phi_L^{-(i-1)}(\mathcal{A}) \vee \ldots \vee \mathcal{A} \vee \ldots \phi_L^{(k-1)}(\mathcal{A}),$$

where the symbol $\vee$ indicates the intersection of all the sets of a given partition with those of another one. The partition $\mathcal{A}_{\ell,k}$ induces a partition on $\mathcal{M}$, $\{C_i^{(\ell,k)}\}$ say, introducing a graining of the phase space $\mathcal{M}$, out of which a (possibly time dependent) coarse grained information entropy can be defined. This is done by taking the (possibly time dependent) Poisson measure $\chi_i$ associated with a (possibly time dependent) measure $\mu_i$ on $X$, and writing:

$$S_{\mathcal{M}}^{(\ell,k)}(\chi_i) = - \sum_{\{C_i^{(\ell,k)}\}} \chi_i(C_i^{(\ell,k)}) \log \chi_i(C_i^{(\ell,k)}) .$$

This coarse grained entropy is introduced as a substitute of $S_G$, in order to have a quantity which is well defined even in the presence of singular phase space distributions, and allows the interpretation of “entropy” as a measure of disorder (cf. [2], p.370). In other words, this kind of entropy is invoked in order to deal with singular measures.

2. Unfortunately, $S_{\mathcal{M}}^{(\ell,k)}$ is difficult to handle, hence a limiting procedure is adopted in [2] in order to reduce $S_{\mathcal{M}}^{(\ell,k)}$ to a quantity which is easier to handle. This is done replacing

\(^3\)This partition was first correctly produced by Gilbert and Dorfman in Ref. [3].
\( S_{\mathcal{M}}^{(\ell,k)} \) with a new coarse grained information entropy defined on a class of subsets \( B \) of \( X \), as follows.

**Coarse grained information entropy:** Consider the subsets of \( X \) of the form \( B = \bigcup_i E_i \), with \( E_i \in \mathcal{A}_{\ell,k} \), and let \( \mu_t \) represent a time dependent distribution of points on \( X \). Correspondingly, the coarse-grained information entropy of \( B \) at time \( t \), \( S_{\ell,k}(B,t) \), is defined by

\[
S_{\ell,k}(B,t) = - \sum_{A \in \mathcal{A}_{\ell+1,k} \cap B} \mu_t(A) \log \mu_t(A) - 1 ,
\]

where the sum is carried out over all \( A \in \mathcal{A}_{\ell+1,k} \) whose union is \( B \).

Then, \( S_{\mathcal{M}}^{(\ell,k)}(\chi_t) \) is expressed by the sum \( S_{\ell,k}(X,t) + R_{\ell,k}(X,t) \), where \( R_{\ell,k}(X,t) \) represents a rest term which depends on the measures \( \mu_t(A) \) of the sets whose union is \( X \). According to Gaspard, \( R_{\ell,k}(X,t) \) becomes negligible with respect to \( S_{\ell,k}(X,t) \) in the limit of fine partitions, i.e. as the volumes of the sets \( A \) decrease towards zero, so that their measures also tend to zero, but becomes “important” if those measures grow much larger than 1 (cf. p.376 of [2]). There is a difficulty here: \( \chi_t \) is normalized and, for any partition \( \mathcal{A}_{\ell,k} \), \( S_{\mathcal{M}}^{(\ell,k)}(\chi_t) \) must be finite in order to fulfill its purpose, i.e. to be a meaningful measure of the disorder in the system. On the contrary, \( \mu_t \) is not a finite measure, and \( S_{\ell,k}(X,t) \), in general, cannot be finite either. Hence, the difference \( R_{\ell,k}(X,t) \) between the two coarse grained entropies is not finite, which makes unclear how \( S_{\mathcal{M}}^{(\ell,k)}(\chi_t) \) could be replaced by \( S_{\ell,k}(X,t) \). Gaspard overcomes this difficulty restricting the calculation of the coarse grained information entropy to sets \( B \) with \( \mu_t(B) < \infty \), presumably assuming that \( S_{\ell,k}(B,t) \) can still be taken as a measure of the “disorder” in \( B \) if the difference

\[
R_{\ell,k}(B,t) = - \sum_i \chi_t(C^{(\ell,k)}_i) \log \chi_t(C^{(\ell,k)}_i) - S_{\ell,k}(B,t) ,
\]

where the sum is over the sets \( C^{(\ell,k)}_i \) concerning \( B \) only, is small compared to \( S_{\ell,k}(B,t) \).

**3.** The total rate of information entropy change in one time step is now defined by:

\[
\Delta_{t+1} S_{\ell,k}(B,t) = S_{\ell,k}(B,t+1) - S_{\ell,k}(B,t) .
\]
This rate of change is then broken into a sum of two terms:
\[ \Delta_{\text{el}} S_{\ell,k} = \Delta_{\epsilon} S_{\ell,k} + \Delta_{i} S_{\ell,k}, \]  
(17)
where \( \Delta_{\epsilon} S_{\ell,k}(B,t) \) is called the change in information entropy due to the flow between \( B \) and its environment, and \( \Delta_{i} S_{\ell,k}(B,t) \) that due to irreversible information entropy production. In particular, the information entropy change due to flow is defined as:
\[ \Delta_{\epsilon} S_{\ell,k}(B,t) = S_{\ell,k}(\phi^{-1} B, t) - S_{\ell,k}(B, t), \]  
(18)
while the information entropy production is defined by:
\[ \Delta_{i} S_{\ell,k}(B,t) = S_{\ell,k}(B, t + 1) - S_{\ell,k}(\phi^{-1} B, t). \]  
(19)

4. Finally, in section 8.6.6 of [2], it is stated that the stationary linear density profile (9) leads to the desired relation, formally looking like a relation of Irreversible Thermodynamics, after the following sequence of limits is taken:
\[ \lim_{\varepsilon \to 0} \lim_{(\nabla n/n) \to 0} \lim_{L \to \infty} \frac{n}{(\nabla n)^2} \Delta_{i} S_{0,1} = D_G. \]  
(20)
Here \( \varepsilon \) is the size of the cells of \( A_{0,1} \), and \( D_G \) should be the MB diffusion coefficient 1/2. In page 384 of [2], it is then stated that the origin of the result represented by Eq.(20) is: “the singular character of the underlying microscopic steady-state”, and that the information entropy production: “would indeed vanish if the limiting steady state measure was absolutely continuous with respect to the Liouville measure”. In other words, non singular distributions would yield no information entropy production, hence would yield \( D_G = 0 \) instead of 1/2.

Steps 1 – 4 lead Gaspard to the conclusion that the singularity of the steady states constitutes the “fundamental mechanism at the origin of the thermodynamic entropy production” [6].

This, however, raises a question. If the MB points represent noninteracting particles, the MB system does not have the property of LTE and, as discussed more in detail in the
next sections, $\nabla n$ cannot be considered as a thermodynamic force. It is striking, then, that results reminiscent of those of Irreversible Thermodynamics could be derived in this framework. A more careful analysis of the steps 1–4 seems necessary.

This analysis reveals a number of problems with the approach of [2]. In the first place the sequence of limits given in (20) is incompatible with the claim made in step 2 that $R_{\ell,k}$ can be neglected, it makes all subsequent calculations inconsistent, and does not yield $D_G = 1/2$. In fact, letting $L$ grow without letting $\nabla n$ decrease correspondingly rapidly,\(^4\) produces larger and larger point densities in most of the system. Then, if the sets of the partition have a fixed volume $\varepsilon > 0$, their measures will grow much larger than $1$ in most of the system, and the term $R_{\ell,k}$ will become correspondingly “important”.

The sequence of limits that must be taken (and which is actually taken in section 8.6.5 of [2]) to make $R_{\ell,k}$ negligible, to exploit the singular character of the steady state $\mu$, and to obtain the value $1/2$, is the following:

$$\lim_{\varepsilon_u \to 0} \lim_{(\nabla n/n) \to 0} \lim_{L \to \infty} \lim_{\varepsilon_s \to 0} \frac{n}{(\nabla n)^2} \Lambda_i S_{0,1} = \frac{1}{2}. \quad (21)$$

Here, $\varepsilon_u$ is the (largest) size of the cells of $A_{0,1}$ along the unstable direction, while $\varepsilon_s$ is the (largest) size of the cells along the stable direction. In Eq. (21), the volume of the cells of the partition goes to zero with fixed finite density, as $\varepsilon_u \to 0$, while $L$ remains finite. Therefore, the measure of each partition cell tends to zero, as required by step 2 above. The subsequent two limits change the initial finite system of length $L$, with a regular distribution of points, into an infinite system, with a singular distribution of points so that, when the last limit ($\varepsilon_s \to 0$) is taken, a finite quantity is obtained. Unfortunately, $S_{\ell,k}$ [$S_{0,1}$, in particular] diverges, losing the meaning of “measure of disorder”, when the first limit is taken. Moreover, the sequence of limits of Eq. (21) has no physical meaning, because there is no phase space over which the limit of fine graining, needed to separate the microscopic from the macroscopic scales, is taken. Indeed, the first half of this limit is taken in the space of a finite system, while the second half is taken in the space of an

\(^4\)In Gaspard’s calculations $\nabla n$ is fixed and equals 1 (cf. [2], section 8.6.5).
infinite extended system.

IV. The Lorentz channel

The reason for considering MB maps in Refs.[2] is that they are believed to be simplified models for the much closer to physics two dimensional Lorentz gas, where a single particle moves freely, i.e.

\[
\begin{align*}
\dot{q} &= \frac{p}{m} \\
\dot{p} &= 0 \\
\text{with } & m = 1,
\end{align*}
\]

through a periodic arrangement of fixed hard disks, from which it scatters elastically. More precisely, the MB of Section III above is taken in [2] to be a “caricature of the Birkhoff map of the Lorentz channel” (cf. [2], p. 251). The Lorentz channel [2] is a kind of Lorentz gas in which the \( y \) coordinate is bounded, e.g. \( 0 \leq y \leq Y \) with \( Y > 0 \), and the region covered by the scatterers is finite also in the \( x \) direction, as depicted in Fig. 3. The corresponding Birkhoff map is a two-dimensional representation of its dynamics where, usually, one variable represents the point of impact of the moving particle, at each collision, and the other variable represents the direction of the velocity after a collision. If one complements the Lorentz channel with one reservoir of particles to the left and one to the right of the region occupied by the scatterers, and one accepts the analogy of the MB dynamics with the Birkhoff map of the Lorentz channel, one may conclude that the analysis performed explicitly for the MB map could be repeated, at least in principle, for the Lorentz channel.

Consider then a finite set of scatterers, like in Fig. 3, and treat the regions to the left and to the right of the scatterers as two particle reservoirs, each containing independently moving particles, with one reservoir having more particles per unit volume \( n_+ \) than the other \( n_- \). Except for the details of the dynamics, the Lorentz channel now looks similar to the MB map, and one could imagine that a similar kind of transport takes place in the two systems. In that case one could write the global linear law

\[
J_x = -\bar{D}_L \nabla n, \quad \text{with } \nabla n = \frac{n_+ - n_-}{L},
\]
similar to Eq.(10), where $\bar{D}_L$ is a proportionality constant. In the case of the Lorentz channel, we would then have a particle current from the high particle density to the low particle density reservoir. But similarly to the points of the MB map, the Lorentz particles move independently of each other. Hence, the Lorentz channel is effectively an ensemble of 1-particle systems, where the motion of each particle takes place in a different member of the ensemble. Then, studying the simultaneous motion of many independently moving particles, one obtains the average behavior of an ensemble of 1-particle Lorentz systems. In this case, a non vanishing average current $J_x$ can be established only if the averaging ensemble is not uniform in phase space, i.e. if it is biased as in the case that $n_+ > n_-$. 

After the derivation of Eq.(23), one would like to repeat steps 1–4 of section III, in order to obtain the corresponding expression for the information entropy production of the Lorentz channel. Unfortunately, this is not possible in practice, but there is a claim implicit in the supposed analogy between MB maps and Lorentz gas systems, which is explicitly made in even more general terms at, e.g., the end of section 8.6.6 of [2]. This claim can be stated as follows. Assume that Eq.(23) is valid for the independently moving particles of the Lorentz channel, and use the information entropy of section III.\(^5\) Then, taking the same sequence of limits mentioned in point 4 of section III, one would obtain $\bar{D}_L$, thus proving the existence of a steady state with a positive information entropy production rate. This, could then be interpreted as a measure of the production of heat in the system, due to the dissipative diffusion process described by Fick’s law.

We note that Gaspard and other authors appear to consider the restriction to noninteracting particles as a mild (merely technical) condition, only needed to perform explicit calculations (cf. Ref.[6], and see Ref.[3] for other authors’ similar views). However, even neglecting the problems associated with the steps 1–4, evidenced in Section III, there is a difficulty. This system does not possess the property of LTE. For instance, all particles have the same speed, instead of having a local Maxwell velocity distribution. One then

\(^5\) It is assumed in [2] that the information entropy could be computed, at least in principle, for the Lorentz channel.
realizes that the net flow obtained by averaging over the ensemble of Lorentz channels described here, is not due to the interactions among the particles, or the particles and their environment, which would effectively constitute a thermodynamic (driving) force. The flow is merely due to “counting”, i.e. to the choice of a biased ensemble—the reservoirs with different densities—which has more members whose single particle travels from the left to the right than vice versa. Therefore, in the Lorentz channel there cannot possibly be any dissipation or any irreversible entropy production, and the definition of information entropy production (19) reveals its unphysical nature. This point will be further discussed in Section VI.

V. Multibaker maps revisited

The main advantage of MB maps is that they can be analyzed in full detail explicitly: it is easy to prove a number of results about them. It is convenient to do this in a slightly more general context than that of [2], since this requires no extra effort, and allows us to demonstrate that: a) the only property of MB maps needed to derive the linear law (10), is the similarity of the MB dynamics with a random walk on the line; b) that this random walk must be unbiased.

As a consequence, singular phase space distributions appear to be unnecessary to derive laws which formally look like those of Irreversible Thermodynamics, despite the great importance attributed to such distributions in Ref.[2].

Consider the same MB space \( X = R_+ \cup C \cup R_- \) of section III, and let the MB dynamics be more generally defined by:

\[
\phi_L(i, x, y) = \begin{cases} 
(i - 1, x/p, py) & 0 \leq x < p \\
(i + 1, (x - p)/(1 - p), (1 - p)y + p) & p \leq x \leq 1 \\
(i - 1, x, y) & 0 \leq x < p \\
(i + 1, x, y) & p \leq x \leq 1 \\
\end{cases} \quad \text{for} \quad 0 \leq i \leq L + 1
\]

with \( p \in (0, 1) \). This map reduces to the MB map of section III if \( p = 1/2 \). Like in section III, let the points of \( X \) be loaded with a “density” \( n \) which defines a given measure on \( X \).
For instance, let the initial point-density equal the constant $n_0 \geq 0$ in $C$, and let the reservoirs $R_{\pm}$ feed points into $C$ at the fixed densities $n_{\pm}$. Similarly to section III, the iterations of $\phi_L$ gradually replace the density $n_0$ in $C$ by a structure made of alternating horizontal layers of point-density $n_+$ and $n_-$. This layered structure keeps changing forever, becoming finer and finer as the number $t$ of iterations of $\phi_L$ increases. However, on the coarse grained level in $C$, defined by the set of the measures of the full squares $\{\mu_t(B_i)\}_{i=1}^L$, the evolution of the distribution may reach a steady state $\mu$ in a finite time. This is possible because many different local distributions yield the same coarse grained distribution. For example, let $p = 1/2$ and take the following initial density in $C$:

$$
n(i, x, y) = \left\{ \begin{array}{ll}
L + 1, & 0 \leq y < \frac{L+1-i}{L+1} \\
0, & \frac{L+1-i}{L+1} \leq y \leq 1
\end{array} \right. \quad (25)
$$

with $n_+ = L + 1$ and $n_- = 0$. This density $n$ is not invariant under the iterations of $\phi_L$, but the corresponding coarse grained distribution in $C$, $\{\mu_t(B_l)\}_{l=1}^L$, is invariant. In fact, if we have

$$
\mu_t(B_i) = L + 1 - i \quad \text{for } 1 \leq i \leq L, \quad (26)
$$

one iteration yields:

$$
\mu_{t+1}(B_i) = \frac{1}{2} [\mu_t(B_{i-1}) + \mu_t(B_{i+1})] \quad (27)
$$

$$
\mu_{t+1}(B_i) = \frac{1}{2} [L + 1 - (i - 1) + L + 1 - (i + 1)] = L + 1 - i \quad (28)
$$

which is $\mu_t(B_i)$. On the level of the coarse grained densities, the evolution implied by the MB map with $p = 1/2$, Eq.(27), is that of an unbiased random walk on the line, where the MB parameter $p$ is identified with the transition probability of the random walk.

In this discrete setting, $\mu_t(B_i)$ is the coarse grained density of $B_i$ at time $t$, since the area of $B_i$ is 1, and one can call “linear” a coarse grained density profile with a constant “gradient” defined by $\nabla_i \mu_t = \mu_t(B_i) - \mu_t(B_{i-1})$. Thus, the distribution defined by Eq.(26) is a linear coarse grained density profile, with the following property.

**THM 1.** Let $\phi_L$ be the MB map defined on $X$ by Eqs. (24), and let $n_+ > n_- \geq 0$. Then, the linear coarse grained density profile in $C$ is invariant under the MB dynamics if and
only if \( p = 1/2 \) (i.e., if and only if the MB dynamics is equivalent, on the coarse grained level, to an unbiased random walk on the line).

**Proof.** Any linear density profile has the form

\[
\mu(B_i) = \mu(B_0) + \frac{i}{L+1}(\mu(B_{L+1}) - \mu(B_0)).
\]

One iteration of \( \phi_L \) transforms this into

\[
\mu_1(B_i) = p\mu(B_{i+1}) + (1-p)\mu(B_{i-1}) = \mu(B_0) + \frac{2p + i - 1}{L+1}(\mu(B_{L+1}) - \mu(B_0))
\]

which equals \( \mu(B_i) \) if and only if \( p = 1/2 \). \( \Box \)

The coarse grained steady state is also unique. In fact, one has the following.

**Thm 2.** For given \( p \in (0,1) \) and given \( n_+ > n_- \geq 0 \), the invariant coarse grained distribution on \( C \) is unique and takes the form

\[
\mu(B_i) = \frac{1}{D_L} \left[ n_+ (1-p)^i D_{L-i} + n_- p^{L-i+1} D_{i-1} \right], \quad (29)
\]

where

\[
D_j = \frac{(1-p)^{j+1} - p^{j+1}}{1-2p} \quad \text{for} \quad p \neq 1/2 \quad (30)
\]

\[
D_j = \frac{j+1}{2^j} \quad \text{for} \quad p = 1/2 . \quad (31)
\]

**Proof.** The system of equations defining the steady state is:

\[
\begin{align*}
\mu(B_1) &= (1-p)n_+ + p\mu(B_2) \\
\mu(B_2) &= (1-p)\mu(B_1) + p\mu(B_3) \\
\vdots \\
\mu(B_i) &= (1-p)\mu(B_{i-1}) + p\mu(B_{i+1}) \\
\vdots \\
\mu(B_L) &= (1-p)\mu(B_{L-1}) + pn_-
\end{align*}
\]

(32)
where the array \((\mu(B_1), \ldots, \mu(B_L))\) can easily be computed by means of Cramer’s rule, because the determinant of the matrix of coefficients

\[
D_L = \det \begin{pmatrix}
1 & -p & 0 & 0 & \cdots & 0 \\
-(1-p) & 1 & -p & 0 & \cdots & 0 \\
0 & -(1-p) & 1 & -p & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & \cdots & 1
\end{pmatrix}
\] (33)

never vanishes. This can be seen as follows. The structure of matrix (33) yields:

\[
D_L = D_{L-1} - AD_{L-2} \quad \text{with} \quad A = p(1-p)
\] (34)

hence \(D_L\) is an element of a Fibonacci sequence, with \(D_0 = D_1 = 1\), which yields:

\[
D_L = c_1 \omega_1^L + c_2 \omega_2^L,
\] (35)

with \(\omega_{1,2}\) solutions of \(\omega^2 - \omega + A = 0\). Then, the conditions for \(L = 0, 1\) lead to

\[
D_L = \frac{(1 + \sqrt{1 - 4A})^{L+1} - (1 - \sqrt{1 - 4A})^{L+1}}{2^{L+1} \sqrt{1 - 4A}}
\] (36)

i.e. to Eq.(30), while the limit of Eq.(30) as \(p \to 1/2\) leads to Eq.(31). Therefore, \(D_L \neq 0\) and the system (32) has a unique solution. Now, it suffices to verify that Eq.(29) is a solution of the system (32). One finds that (29) is a solution of (32) if the conditions:

\[
D_{L-i} = D_{L-i-1} - AD_{L-i-2}
\]

\[
D_i = D_{i-1} - AD_{i-2}
\]

hold. But these conditions hold because (34) holds.

Clearly, any linear profile verifies a linear law like (10), if the local flow of MB points is defined by

\[
J_i = (1 - p)\mu(B_i) - p\mu(B_{i+1}),
\] (37)

---

\(^6\)For similar calculations of \(D_L\) see, e.g., chapter 5 of Ref.[8].
(the difference between what flows to the right and what flows to the left, at the interface between \( B_i \) and \( B_{i+1} \)). Indeed, for a linear density profile, i.e., for a steady state \( \mu \) of the map with \( p = 1/2 \), one can write

\[
J_i = -\bar{D} \nabla_i \mu ,
\]

with \( \bar{D} = 1/2 \) and \( \nabla_i \mu = \text{const} = (n_+ - n_-)/(L+1) \). This shows that all that is needed to derive a linear law like (38) for a MB map, is its equivalence to an \textit{unbiased} random walk. It is also interesting to note that for \( p \) larger than a critical value \( p_c \), the flow goes in the direction opposite to that of the gradient. This is a consequence of the following property of \( \phi_L \).

\textbf{THM 3.} The steady state flow of the MB map defined by Eq. (24) vanishes if and only if

\[
p = p_c = \frac{1}{1 + (n_+ / n_-)^{1/(L+1)}} .
\]

\textbf{Proof.} If the local flow vanishes everywhere, one has a steady state because what is lost by each square in one iteration is exactly replaced by what comes in from the square’s two nearest neighbors (cf. the definition of flow Eq. (37).):

\[
(1 - p)\mu(B_{i-1}) + p\mu(B_{i+1}) = p\mu(B_i) + (1 - p)\mu(B_i) = \mu(B_i) .
\]

Moreover, \( J_i = 0 \) means:

\[
0 = (1 - p)\mu(B_i) - p\mu(B_{i+1}) \quad \text{i.e.} \quad \mu(B_{i+1}) = \frac{1 - p}{p} \mu(B_i)
\]

whence \( \mu(B_i) = [(1 - p)/p]^{i+1} \mu(B_1) \), \( \mu(B_i) = (1 - p)/pn_+ \), and \( n_- = [(1 - p)/p]^{L+1} n_+ \). This yields Eq. (39). At the same time, if \( p = p_c \), the uniqueness of the coarse grained steady state proved in THM 2 implies that the local flow vanishes.

In conclusion, the only property of the MB dynamics which is needed to derive Eq. (38) is its equivalence, on the coarse grained level, to an unbiased random walk. As a matter
of fact, Eq.(38) holds also for the following transformation in \( C \) (cf. Fig.4):

\[
\phi_L(i, x, y) = \begin{cases} 
(i - 1, 2x, y/2) & x \leq 0.5 \quad y \leq i/L + 1 \\
(i - 1, 2x, (y+1)/2) & x \leq 0.5 \quad y > i/L + 1 \\
(i + 1, 2x - 1, (y + i/(L + 1))/2) & x > 0.5 \quad 0 \leq y \leq 1 
\end{cases}
\]  

(41)

whose coarse grained dynamics is given by Eq.(27), and is compatible with a steady state which is not singular with respect to the Lebesgue measure. Although this map is not time reversal invariant, hence does not belong to the class of maps considered in [2],\(^7\) it illustrates that singular steady states are not necessary to obtain the linear law (38) from deterministic dynamics.

VI. Discussion

1. The singularities of a steady state for the MB map (7), are held responsible in [2] for the positive information entropy production rate \( \sigma \) in these systems, and the corresponding linear density profile is there interpreted as one instance of Fick’s law. It is then stated in [2] that the same holds for general nonequilibrium systems (including, perhaps, quantum mechanical ones), and that, therefore, the fundamental mechanism at the origin of thermodynamic entropy production has been understood in terms of chaotic dynamics, and singular phase space distributions. In this framework, entropy or heat production are both just a loss of information.

Missing, however, is the physical interpretation of \( \sigma \) as an irreversible heat production. For instance, the particles of the Lorentz channel, the closest physical analogs of the points of the MB maps, move independently of each other, thus no local equilibrium can possibly be established. In fact, the speed distribution of the Lorentz channel is locally and globally a delta function rather than locally Maxwellian, and the density profile is not locally smooth, but alternates between the values \( n_+ \) and \( n_- \) over arbitrarily small scales. This is not the case of a state characterized by LTE; the diffusion approximation cannot

\(^7\)We owe this observation to an anonymous referee.
be applied to this case, and $\sigma$ cannot be considered an irreversible heat production.\footnote{Similar considerations hold for the Lorentz channel studied by \cite{9}, where the temperature consists of a complicated layered structure fluctuating between the two boundary values $T_+$ and $T_-$. In this case, it is the validity of Fourier’s law that cannot be established.}

2. One can further observe that since the Lorentz particles do not interact with each other, the particle concentration surrounding each particle is irrelevant for the motion of this particle, since it is “unaware” of the presence of any other particles. There is therefore no thermodynamic driving force here as in Fick’s law, and no irreversible entropy production either. Confusion here may be caused by the fact that the Lorentz gas is often considered to be an example of a dilute gas. But this is not so; here is what Tolman says about these gases (\cite{10} Chapter X, section 86, page362): In the present chapter we shall study the equilibrium conditions for such systems, when the molecules or other elements composing the system can be taken as interacting only weakly with each other, so that the energy of the system as a whole can be regarded as practically equal to the sum of the energies of the individual elements treated as independent of one another. As a typical example of such systems we may take a dilute gas, the degree of dilution being great enough so that the constituent molecules can be regarded FOR THE MOST PART [our capitals] as free rather than engaged in the process of collision. Here, the capital letters stress the fact that a dilute gas is weakly interacting, but that yet interactions are needed for LTE to be established. Clearly, the weaker the interactions, the longer the time needed for LTE to be established, if not initially present. This can be interpreted by saying that the definition of an ideal gas involves two limits: a large time limit and a limit of decreasing frequency of interactions, and that the first limit must be taken first. This way one obtains a sequence of systems verifying LTE, whose interactions are however less and less frequent, or whose interaction energy is smaller and smaller compared their total energy. This is not what happens with the Lorentz gas, in which one can say that the frequency of moving particles interactions, or the interaction energy, is set to zero before LTE can be established.

That noninteracting particle systems, although chaotic, most often do not obey the
standard laws of thermodynamics is known; see, for instance, how this has been clearly pointed out in Ref.[11]. In particular, the model described in Fig.4 of [11] shows that a density gradient in an isolated system of noninteracting particles does not necessarily lead to a flow allowing the system to relax to a state without gradients. This is not a violation of any principle of thermodynamics: the gradient is not a thermodynamic force in this case, hence particles can remain trapped for arbitrarily long times in a “high density” region without knowing how crowded that region is, and how empty other regions are.

We conclude that noninteracting particle systems are unsuitable to study the laws of Irreversible Thermodynamics, for which LTE is essential, and that the definition of entropy production (19) is unsuitable to the purpose of Irreversible Thermodynamics.

3. The question remains: which kind of microscopic dynamics is responsible for the macroscopic laws of Irreversible Thermodynamics? It is now clear that chaoticity by itself is not enough. Our analysis implies that interactions which allow the system to reach LTE are necessary, and that not all kinds of randomization have to do with heat, although heat production is certainly the result of some kind of randomization. In this context, the recent interesting work by Mejia-Monasterio, Larralde and Leyvraz [14] has the merit of showing how local Maxwellian distributions can be obtained when the interactions among particles are indirect, i.e. are mediated by the host environment.10

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9 Indeed, it may not even be necessary if the conclusions of, e.g., [12] for a nonequilibrium system and of [13] for an equilibrium system, could be extended to more realistic systems. In fact, the models considered in [12, 13] are nonchaotic billiards, but have properties similar to those of chaotic billiards.

10 This work is based on a Lorentz model with rotating scatterers and stochastic boundaries.
References


Figure 1: An infinite chain of squares $B_i$, for $-\infty < i < \infty$, constitutes the phase space of the MB map. The top row of squares is transformed into the bottom row of squares by $\phi_L$. The action of $\phi_L$ moves half squares along the chain as indicated by the arrows: the half squares labelled by the un-primed letters are transformed into the half squares labelled by the primed letters.

Figure 2: Initially each square $B_i$ is endowed with a uniform density represented by one of the shades, as in the top row of the figure. The consecutive applications of $\phi_L$ change the initial point-density distribution, creating a layered structure whose complexity increases with the number of iterations. In this process, the initial density distribution in the system ($1 \leq i \leq L$) is gradually replaced by the densities of the reservoirs $n_\pm$ represented by no shade.
Figure 3: A finite array of elastic scatterers is placed inside an infinite (in the horizontal direction) slab, delimited in the vertical direction by elastically reflecting walls. Particles are fed into the region covered by the scatterers by two reservoirs, characterized by two different particle densities $n_+$ and $n_-$. 

Figure 4: A kind of MB map whose dynamics in the system are described by the arrows. If the initial phase space distribution is properly chosen, the dynamics does not produce a singular distribution, but a distribution with a unique discontinuity in each $B_m$, separating a region with constant point-density $n_+$ from a region with constant point-density $n_-$. In $B_m$ (central square in the top row) this discontinuity is placed at $y_d = m/(L+1)$, and is represented by the horizontal line separating the two different shades.