Stochastic thermodynamics of system with continuous space of states

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We analyze the stochastic thermodynamics of systems with continuous space of states. The evolution equation, the rate of entropy production, and other results are obtained by a continuous time limit of a discrete time formulation. We point out the role of time reversal and of the dissipation part of the probability current on the production of entropy. We show that the rate of entropy production is a bilinear form in the components of the dissipation probability current with coefficients being the components of the precision matrix related to the Gaussian noise. We have also analyzed a type of noise that makes the energy function to be strictly constant along the stochastic trajectory, being appropriate to describe an isolated system. This type of noise leads to nonzero entropy production and thus to an increase of entropy in the system. This result contrasts with the invariance of the entropy predicted by the Liouville equation, which also describes an isolated system.

I. INTRODUCTION

The microscopic theory of systems in thermodynamic equilibrium as advanced by Gibbs is based on the following assumptions. An energy function is defined on the phase space, which is the space of the positions and velocities of the elementary constituents of the system. A probability distribution is assigned to the phase space, which is the space of the positions and velocities of the elementary constituents of the system. A probability distribution is assigned to the phase space that depends on the positions and velocity only through the energy function. The entropy is directly related to the probability distribution and is a generalization of the Boltzmann entropy. As a consequence of these assumptions, the entropy becomes a function of the mean energy from which it is possible to define temperature by the Clausius relation, and derive the laws of equilibrium thermodynamics.

The Gibbs probability distribution does not properly characterize the thermodynamic equilibrium in a dynamic sense but is a necessary condition for equilibrium. The appropriate dynamic characterization of thermodynamic equilibrium is provided by the stochastic thermodynamics \[1,3\]. Within this approach, thermodynamic equilibrium occurs when the probability of occurrence of any trajectory equals the probability of occurrence of its time-reversal trajectory. This condition is also known as microscopic reversibility or detailed balance condition and is translated as the absence of entropy production. As a consequence, the net current of any type, such as heat current, will be absent, a property that provides meaning to thermodynamic equilibrium in a dynamic sense.

The distinguishing feature of the stochastic approach to thermodynamics is the microscopic definition of the rate of entropy production. Based on the macroscopic bilinear relation between entropy production and thermodynamic forces and affinities, Schnakenberg \[6\] proposed a microscopic expression for the entropy production of systems described by a master equation. The time variation of the entropy of these systems was shown to have two parts, one of them being the production of entropy, given by the Schnakenberg expression, and the other being the entropy flux \[\Phi \neq 0\]. The essential feature of the entropy production is its straight relationship with the irreversibility processes as expressed by the time-reversal symmetry \[11\]. The entropy production is also directly related to probability current so that in a nonequilibrium steady state these two quantities are nonvanishing \[12,13\]. The role of fluctuation theorems has also been addressed within the stochastic thermodynamics \[16,18\]. The entropy production was calculated for molecular motors \[19\], in chemical reaction networks \[16,20\], to determine the efficiency at maximum power \[21\], and in systems connected to multiple reservoirs \[2,5\]. It was also determined in irreversible interacting particle system where this quantity was shown to display a singular behavior at the transition point \[10,22,24\].

A formulation of stochastic thermodynamics for continuous system has also been developed, in which case the stochastic evolution equation is the Fokker-Planck equation. It is assumed, usually in an implicit form, that the time-reversal trajectory is identified as the reverse trajectory, which is also the case of systems described by a master equation examined above. This approach is appropriate for overdamped continuous systems \[25\]. For one particle, the expression for the rate of entropy production is proportional to the square of the probability current. However, the application to a system that reaches a non-equilibrium steady state, an extension of this expression is needed and in fact, it has been advanced \[26,27\].

For underdamped continuous systems, the reverse trajectory is no longer identified with the time-reversal trajectory and an adequate formulation should be employed \[25\]. For a system described by a Fokker-Planck-Kramers equation, which is the stochastic equation appropriate for particles with inertia, it has been found that the rate of entropy production is related to just one part of the probability current \[1,30,31\], called, for this reason, the dissipation probability current.

The present approach describes underdamped systems, that is, system consisting of particles with inertia, with continuous space of states. We focus on the production of entropy, understood as related to the probability of occurrence of a trajectory and its time reversal. When these two probabilities are equal we meet the condition
for the thermodynamic equilibrium. Defining the production of entropy as the logarithm of the ratio of these two probabilities, it vanishes in thermodynamic equilibrium.

We consider systems consisting of interacting particles evolving according to the laws of classical mechanics. In addition to the deterministic forces, the system is also subject to random forces so that the representative point in the space of states describes a continuous stochastic trajectory. The deterministic force is a sum of a time-reversal force and a force that lacks this property and is identified as the dissipative force. The evolution equation is a continuity equation for the probability density whose current is split into two parts. One of them is the ordinary current related to the time-reversal force. The other is the dissipative probability current related to the dissipative force and the noise.

The evolution equation in the continuous space of states and other properties are obtained by starting from a discrete time formulation and then taking the continuous time limit. In this sense the present method is distinct from the previous similar methods. Our main result is the expression for the rate of entropy production obtained from a discrete time expression of the production of entropy. The continuous time limit gives for the rate of entropy production a bilinear form in the components of the dissipative probability current which is positive definite. The vanishing of the dissipative probability current leads to no entropy production characterizing the thermodynamic equilibrium.

We analyze in detail two types of noises. One of them is the usual noise that describes the contact of a system with a heat reservoir. The other type makes the energy function to be strictly constant along a stochastic trajectory in phase space and thus describes an isolated system. There is no flux of entropy and the time variation of the entropy is entirely due to the generation of entropy inside the system. This result is distinct from that given by the Liouville equation which predicts an invariance of the entropy in time and no production of entropy, although this equation describes an isolated system.

It is convenient to regard the systems out of equilibrium as belonging in one of two classes. One of them includes the systems that are out of equilibrium because they have not yet relaxed to the equilibrium state. The other class includes those systems that are permanently out of equilibrium even when they have already relaxed to the stationary state. In this last case, entropy are permanently being produced by the system, a feature that characterizes an out of equilibrium state.

Differently from the energy, which is a conserved quantity, the entropy is not a conserved quantity but it cannot decrease, which is a brief statement of the second law of thermodynamics. Being a conserved quantity the increase of energy per unit time is given by

\[ \frac{dU}{dt} = \Phi_u, \]  

where \( \Phi_u \) is the rate at which energy is being introduced into the system. The entropy increase per unit time on the other hand is given by

\[ \frac{dS}{dt} = \Pi - \Phi, \]  

where \( \Phi \) is the rate at which entropy is being delivered to outside and \( \Pi \) is the entropy production and obeys the inequality \( \Pi \geq 0 \), a brief statement of the second law of thermodynamics.

The approach we use here starts with the discrete expression of the rate of the entropy production to reach the expression for continuous systems by taking the continuous time limit. Other approaches already consider the system to be continuous in time and start from the expression for the entropy flux defined as the heat flux divided by the temperature \( T \), or start by identifying the production of entropy as the relative entropy related to forward and backward processes.

II. EVOLUTION EQUATION

We consider a generic system whose state is defined as being the set of variables \( x_i \) understood as the components of a vector \( x \) belonging in a certain continuous space of states of a given dimension. As the system evolves in time, the point representing the vector \( x \) moves in the space of states, tracing a trajectory. Supposing that the system is in a certain state \( x \) at time \( t \), the question arises as to which trajectory the system will follow starting at \( x \). According to the stochastic assumption there is not just one trajectory starting from \( x \) but many possible trajectories, each one occurring with a certain probability.

To properly express the probability of occurrence of a certain trajectory during a given interval of time it is necessary to specify not only the initial and final points of the trajectory but also the intermediate points. These points are understood as a time sequence of random variables and the probability of the trajectory is a function of these variables. In addition, this probability could depend on previous states. However, according to the Markovian assumption adopted here, the probability of a trajectory will not depend conditionally on these other states. This assumption leads us to the conclusion that the probability of the whole trajectory can be set up by specifying the probabilities of small sections of the trajectory. The probability of these elementary trajectories dependent only on its initial and final points.

The probability of occurrence of an elementary trajectory that starts within the elementary volume of the space of states \( dx \) around the state \( x \) and ends within \( dx' \) around \( x' \), after a small interval of time \( \tau \), is written as

\[ P(x', x) dx' dx = K(x'|x) \rho(x) dx' dx, \]  

where \( \rho(x)dx \) is the probability of finding the system within \( dx \) around \( x \) at a given time \( t \) and \( K(x'|x)dx' \) is
the conditional probability of finding the system within
$dx'$ around $x'$ at time $t + \tau$, given the occurrence of state
$x$ at time $t$.

The main assumption of the present approach is that
$x'$ is obtained from $x$ by means of the following equation
valid for small values of $\tau$
\begin{equation}
    x'_i = x_i + F_i \tau + \xi_i \sqrt{\tau},
\end{equation}
where the forces $F_i(x)$ are given functions of $x$, and $\xi_i$ are
random variables with a Gaussian distribution $G(\xi|x)d\xi$,
understood as a conditional probability, where $\xi$, the
noise, denotes the vector with components $\xi_i$. The Gaus-
sian distribution is such that the random variables $\xi_i$ have
zero means and covariances $\langle \xi_i \xi_j \rangle = \Gamma_{ij}$. The conditional
probability distribution $K(x'|x)$ is obtained from $G(\xi|x)$
by performing the transformation $\xi \rightarrow x'$ dictated by (4).
That is, the conditional probability $K(x'|x)$ of $x$ at
time $t + \tau$ given $x$ at time $t$ is
\begin{equation}
    K(x'|x)dx' = G(\xi|x)d\xi,
\end{equation}
where the random variable $\xi$ is related to the random
variable $x'$ by (4).
To find the continuous time equation, we start by de-
noting by $\rho'(x')$ the probability distributions at time $t + \tau$,
and by $\rho(x)$ the probability distribution at $t$. They are re-
lated to the conditional probability $K$ through the equa-
tion
\begin{equation}
    \rho'(x') = \int K(x'|x)\rho(x)dx,
\end{equation}
understood as the evolution equation for the probability
distribution in a discretized form. To find the evolution
equation in the continuous form, one should take the limit
$\tau \rightarrow 0$, which is carried out as follows. We start by
multiplying both sides of equation (4) by an arbitrary
state function $F(x')$ and integrate in $x'$,
\begin{equation}
    \langle F \rangle' = \int F(x')K(x'|x)\rho(x)dxdx',
\end{equation}
where the average on the left-hand side is over the dis-
tribution $\rho'(x')$. Changing the integration from $x'$ to $\xi$ the result is
\begin{equation}
    \langle F \rangle' = \int F(x')G(\xi|x)\rho(x)dxd\xi,
\end{equation}
where here $x'$ is given by (4).
Next we need the expansion of $F(x')$ up to linear terms
in $\tau$. The expansion is obtained in two stages. First
we expand this function up to second powers of $\Delta x_i =
\Delta x_i = x_i' - x_i$,
\begin{equation}
    \Delta x_i = x_i' - x_i,
\end{equation}
where $\Delta x_i = F(x') - F(x)$. Replacing the expressions
(4) into this equation we reach the desired expansion
\begin{equation}
    \Delta F = \sum_i \frac{\partial F}{\partial x_i} F_i \tau + \xi_i \sqrt{\tau},
\end{equation}
valid up to terms of order $\tau$.
The expression (10) is replaced in equation (8) and the
integration in $\xi$ is carried out. Taking into account that
the average of $\xi_i$ vanishes, and that the average of $\xi_i \xi_j$
is $\Gamma_{ij}$, the term proportional do $\sqrt{\tau}$ disappears and the
whole right-hand side of the equation (8) turns out to be
proportional to $\tau$. After this procedure, we divide both
sides of the equation by $\tau$ to reach the result
\begin{equation}
    \frac{d}{dt} \langle F \rangle = \langle K^\dagger F \rangle,
\end{equation}
where we are considering that $\Delta \langle F \rangle/\tau \rightarrow \partial \langle F \rangle/\partial t$
when $\tau \rightarrow 0$, and $K^\dagger$ is the differential operator given by
\begin{equation}
    K^\dagger F = \sum_i F_i \frac{\partial F}{\partial x_i} + \frac{1}{2} \sum_{ij} \Gamma_{ij} \frac{\partial^2 F}{\partial x_i x_j},
\end{equation}
and is the adjoint of the differential operator $K$, defined by
\begin{equation}
    K \rho = - \sum_i \frac{\partial}{\partial x_i} (F_i \rho) + \frac{1}{2} \sum_{ij} \frac{\partial^2}{\partial x_i \partial x_j} (\Gamma_{ij} \rho).
\end{equation}
Writing equation (11) in the form
\begin{equation}
    \int F \frac{\partial \rho}{\partial t} dx = \int F \langle K^\dagger \rho \rangle dx,
\end{equation}
obtained by appropriate integrations by parts and by tak-
ing into account that $\rho$ vanishes rapidly in the limits of
integration, we conclude that
\begin{equation}
    \frac{\partial \rho}{\partial t} = K \rho,
\end{equation}
or in an explicit form,
\begin{equation}
    \frac{\partial \rho}{\partial t} = - \sum_i \frac{\partial}{\partial x_i} (F_i \rho) + \frac{1}{2} \sum_{ij} \frac{\partial^2}{\partial x_i \partial x_j} (\Gamma_{ij} \rho),
\end{equation}
which is the desired equation that gives the time evolu-
tion of the probability distribution $\rho(x,t)$ in a continuous
form, and is a Fokker-Planck equation [33–36].

III. PRODUCTION OF ENTROPY

A. Time reversal and entropy production

Irreversible processes are characterized by the lack of
time-reversal invariance which means that the probabil-
ity of the occurrence of a certain process is different from
the probability of its time reversal. In accordance with
thermodynamics, a measure of irreversibility is how much
entropy is being generated. Thus the production of en-
tropy is directly related to the lack of time reversibility.

Given a trajectory in the space of states, the time-
reversal trajectory may not be, generally speaking, its
reverse, as illustrated in figure 1. If a trajectory starts at the point \( x \) and ends at \( x' \), the reverse starts at \( x' \) and ends at \( x \), and may not coincide with the time-reversal trajectory which is understood as follows. Let \( x \rightarrow \bar{x} \) be a mapping that associates to each state \( x \) a time-reversal state \( \bar{x} \). If \( x \) and \( x' \) are the initial and final states of a trajectory then the initial and final states of the time-reversal trajectory are, respectively, \( \bar{x}' \) and \( \bar{x} \). That is, the final state of the original trajectory maps onto the initial state of the time-reversal trajectory and vice-versa.

The type of time-reversal mapping that we consider is such that \( x_i \) either changes its sign or keep its sign in the transformation \( x \rightarrow \bar{x} \). It is thus convenient to classify the variables \( x_i \) into two categories. If \( x_i \) keeps its sign it belongs in the first category or is of the even type. If \( x_i \) changes sign, it belongs in the second category or is of the odd type. It is worth mentioning that if \( \bar{x}_i \bar{x}_j = x_i x_j \), then \( x_i \) and \( x_j \) belong in the same category, otherwise they belong in distinct categories.

The time reversal of a vector state function such as the force \( F \) is defined in terms of its components. The time reversal of \( F_i \) is denoted \( \bar{F}_i \) and equals \( F_i \) or \( -F_i \) according to whether \( x_i \) is of the even or odd type, respectively.

In general, the probability of occurrence of a certain trajectory \( x \rightarrow x' \), during a small interval of time \( \tau \), which is

\[
P(x', x) = K(x'|x)\rho(x),
\]

is different from the probability of occurrence of the time-reversal trajectory \( \bar{x}' \rightarrow \bar{x} \), which is

\[
P(\bar{x}, \bar{x}') = K(\bar{x}|\bar{x}')\rho(\bar{x}').
\]

A very special situation occurs when the probability of a trajectory and its time reversal is equal. Thermodynamic equilibrium corresponds to the case when this equality occurs for all trajectories. A measure of the departure from equilibrium may be given by the logarithm of the ratio of these two probabilities,

\[
\ln \frac{P(x', x)}{P(\bar{x}, \bar{x}')}.
\]

a quantity that vanishes when the two probabilities are equal. We must integrate over all possible trajectories occurring during the interval of time \( \tau \), leading us to the following expression for the production of entropy during the interval of time \( \tau \),

\[
\int P(x', x) \ln \frac{P(x', x)}{P(\bar{x}, \bar{x}')} dx dx'.
\]

The rate of production of entropy \( \Pi \) is defined by dividing (20) by \( \tau \) and by multiplying by the Boltzmann constant \( k \),

\[
\Pi = \frac{k}{\tau} \int P(x', x) \ln \frac{P(x', x)}{P(\bar{x}, \bar{x}')} dx dx',
\]

and it is understood that we should take the limit \( \tau \rightarrow 0 \). Writing this equation in the equivalent form

\[
\Pi = \frac{k}{2\tau} \int \{P(x', x) - P(\bar{x}, \bar{x}')\} \ln \frac{P(x', x)}{P(\bar{x}, \bar{x}')} dx dx',
\]

it becomes clear that \( \Pi \geq 0 \) because the integrand is never negative. In terms of the conditional probability, the rate of entropy production reads

\[
\Pi = \frac{k}{2\tau} \int \{K(x'|x)\rho(x) - K(\bar{x}|\bar{x}')\rho(\bar{x}')\} \times
\]

\[
\times \ln \frac{K(x'|x)\rho(x)}{K(\bar{x}|\bar{x}')\rho(\bar{x}')} dx dx'.
\]

For the discrete space of states, the integral is replaced by a summation, in which case this expression becomes the expression proposed by Schnakenberg for the production of entropy related to a master equation.

The expression (20) is not the entropy \( S \) of the system, which is defined by

\[
S = -k \int \rho(x) \ln \rho(x) dx,
\]
and, in general, it is not either the variation of the entropy with time $dS/dt$, which is
\[
dS/dt = \frac{k}{2\tau} \int \{ K(x'|x)\rho(x) - K(\bar{x}|\bar{x}')\rho(\bar{x}') \} \ln \frac{\rho(x)}{\rho(\bar{x}')} \, dx' \, dx,
\]
where we assumed that $\rho(\bar{x}) = \rho(x)$. The difference $\Phi = \Pi - dS/dt$ is given by
\[
\Phi = \frac{k}{2\tau} \int \{ K(x'|x)\rho(x) - K(\bar{x}|\bar{x}')\rho(\bar{x}') \} \ln \frac{K(x'|x)}{K(\bar{x}|\bar{x}')},
\]
and is interpreted as the flux of entropy per unit time from the system to the outside.

**B. Rate of entropy production**

Next we wish to determine the rate of entropy production in the limit $\tau \to 0$. We recall that the conditional probability $K(x'|x)$ is related to the noise probability distribution by relation (3), where $G(\xi|x)$ is the probability distribution of the noise $\xi$, related to $x'$ by
\[
\xi_i = \frac{1}{\sqrt{\tau}} (x'_i - x_i - F_i(x)\tau),
\]
where $F_i$ are functions of $x$.

We assume that the noises $\xi_i$ are distributed according to the Gaussian distribution $G(\xi|x)$ in several variables, with zero means and covariances $\langle \xi_i \xi_j \rangle = \Gamma_{ij}$ that may depend on $x$. Given the covariances, the Gaussian distribution is uniquely determined and is given by
\[
G(\xi|x) = \frac{1}{Z} \exp\left\{-\frac{1}{2} \sum_{ij} \xi_i B_{ij} \xi_j \right\},
\]
where
\[
Z = \int \exp\left\{-\frac{1}{2} \sum_{ij} \xi_i B_{ij} \xi_j \right\} d\xi,
\]
and $B$, the matrix with elements $B_{ij}$, is the inverse of the covariance matrix $\Gamma$, and may depend on $x$. As $G(\xi|x)$ describes a probability distribution, the eigenvalues of the precision matrix $B$ and of the covariant matrix $\Gamma$ are greater or equal to zero.

To determine the rate of entropy production, we write (25) in terms of the Gaussian distribution by the use of (5) and by employing the conditional probability $K(\bar{x}|\bar{x}')$ related to the time-reversal trajectory,
\[
K(\bar{x}|\bar{x}')d\bar{x} = G(\xi'|x')d\xi',
\]
where $\xi'$ is given by
\[
\xi'_i = \frac{1}{\sqrt{\tau}} (\bar{x}_i - \bar{x}'_i - F_i(\bar{x}')\tau).
\]
Notice that the right-hand side of (31) is not the time reversal of the right-hand side of (27). For this reason, we are using the notation $\xi^*_i$ and not $\bar{\xi}_i$. In terms of the Gaussian distribution, the rate of entropy production reads
\[
\Pi = \frac{k}{2\tau} \int \left\{ G(\xi|x)\rho(x) - G(\xi^*|\bar{x}')\rho(\bar{x}') \right\} \times
\]
\[
\times \ln \frac{G(\xi|x)\rho(x)}{G(\xi^*|\bar{x}')\rho(\bar{x}')},
\]
which is obtained by a change of variables from $x'$ to $\xi$, given by (27) and we remark that $\xi^*_i$ is related to both $x'$ and $x$ by (31) so that all terms in the integrand involve only the variables $\xi$ and $x$.

Before we start the calculation, we assume two properties of the covariances, the denial of which would lead to an artificial production of entropy. The first property is
\[
\Gamma_{ij}(\bar{x}) = \Gamma_{ij}(x),
\]
and is valid also for $B_{ij}(x)$, $Z(x)$ and $\rho(x)$. The second property is that $\Gamma_{ij}(x)$ vanishes whenever $x_i$ and $x_j$ belong in distinct categories, that is, if one is even and the other is odd, and is also valid for $B_{ij}(x)$. This property is conveniently written as
\[
\Gamma_{ij}(x_i x_j) = \Gamma_{ij}(x_i x_j).
\]

**C. Additive noise**

We consider here the case in which the covariance matrix $\Gamma$ does not depend on $x$, and the same is valid for the precision matrix $B$. We start by expanding the expression
\[
\ln \frac{G(\xi|x)\rho(x)}{G(\xi^*|\bar{x}')\rho(\bar{x}')} = \frac{1}{2} \sum_{ij} B_{ij}(\xi^*_i \xi^*_j - \xi_i \xi_j) - \ln \frac{\rho(x')}{\rho(x)}.
\]
where
\[ D_i(x) = \frac{1}{2} [F_i(x) + F_i(x)]. \] (40)
The first term of (36), up to terms of order \( \sqrt{\tau} \), becomes
\[ \sum_{ij} B_{ij} [\xi_i D_j(x) + \xi_j D_i(x)] \sqrt{\tau}. \] (41)

Considering that up to terms of order \( \sqrt{\tau} \), \( x'_j = x_i + \xi_i \sqrt{\tau} \), and using the property (33) for \( \rho \), the second term of (36) becomes
\[ -\sum_k \frac{\partial \ln \rho}{\partial x_k} \xi_k \sqrt{\tau}. \] (42)

Collecting these results, we may write
\[ \ln \frac{G(\xi|x)\rho(x)}{G(\xi'|x)|\rho(x')} = A(\xi, x) \sqrt{\tau}, \] (43)
where
\[ A = \sum_i A_i \xi_i, \] (44)
and
\[ A_i = 2 \sum_j B_{ij} D_j - \frac{\partial \ln \rho}{\partial x_i}. \] (45)

In a similar fashion we find
\[ G(\xi|x)\rho(x) - G(\xi'|x')\rho(x') = G(\xi|x)\rho(x)A(\xi, x) \sqrt{\tau}, \] (46)
and the rate of entropy production becomes
\[ \Pi = \frac{k}{2} \int G(\xi|x)\rho(x)[A(\xi, x)]^2 d\xi dx. \] (47)
Replacing the result (44) for \( A \) in the expression (47), performing the integral in \( \xi \), and bearing in mind that \( \langle \xi_i \xi_j \rangle = \Gamma_{ij} \), we reach the following desired result for the rate of entropy production,
\[ \Pi = \frac{k}{2} \sum_{ij} A_i \Gamma_{ij} A_j \rho dx, \] (48)
which is clearly nonnegative because the eigenvalues of \( \Gamma_{ij} \) are nonnegative.

Comparing equations (26) and (28), we observe that they differ from the last factor in the integrand of both equations. An expression for \( dS/dt \) can thus be obtained by using the same reasoning that led us from (28) to (48). The result is
\[ dS \frac{dt}{dt} = -\frac{k}{2} \sum_{ij} A_i \Gamma_{ij} \frac{\partial \rho}{\partial x_j} dx. \] (49)
To find an expression for the flux of entropy \( \Phi \), we recall that \( \Phi = \Pi - dS/dt \). Subtracting the expressions (48) and (49), we get
\[ \Phi = k \sum_i A_i D_i \rho dx, \] (50)
where we used the relation \( B \Gamma = I \).

IV. PROBABILITY CURRENT

A. Dissipation probability current

The evolution equation (16) can be written in the following form
\[ \frac{\partial \rho}{\partial t} = -\sum_i \frac{\partial J_i^c}{\partial x_i}, \] (51)
where
\[ J_i^c = F_i \rho - \frac{1}{2} \sum_j \frac{\partial}{\partial x_j} (\Gamma_{ij} \rho). \] (52)

In this form, the evolution equation is a continuity equation and \( J_i^c \) is the probability current. Next, we wish to split the probability currents into two parts, one of them being invariant under time reversal. To this end, we consider first the splitting of the force \( F_i \).

Any force \( F_i(x) \) can always be split into two parts, one of them being
\[ D_i(x) = \frac{1}{2} [F_i(x) + \bar{F}(\bar{x})], \] (53)
and the other being
\[ F'_i(x) = \frac{1}{2} [F_i(x) - \bar{F}(\bar{x})]. \] (54)
That is,
\[ F_i(x) = F'_i(x) + D_i(x). \] (55)

The first part \( F'_i \) is invariant under time reversal, holding the time-reversal property
\[ \bar{F}_i(\bar{x}) = -F'_i(\bar{x}). \] (56)

In an explicit form, if \( F'_i \) is an odd type of force, which is identified as an ordinary force, the time-reversal property reads \( F'_i(x) = F'_i(\bar{x}) \). If \( F_i \) is an even type of force, the time-reversal property reads \( F'_i(x) = -F'_i(\bar{x}) \). From (56), it follows that \( A_i = \partial F'_i / \partial x_i \) holds the property
\[ A_i(\bar{x}) = -A_i(x). \] (57)
The second part \( D_i \) is the dissipative part, which holds the property
\[ \bar{D}_i(\bar{x}) = D_i(x). \] (58)
If \( D_i \) is an odd type of force, this property reads \( D_i(x) = -D_i(\bar{x}) \), and \( D_i \) is identified with a dissipative force, an example of which is the ordinary dissipation proportional to the velocity. If \( D_i \) is an even type of force, this property reads \( D_i(x) = D_i(\bar{x}) \). Only the second part, \( D_i \), that lacks the time-reversal property, contributes to the production of entropy as can be observed by looking at equations (45) and (47).
In an analogous manner, the probability current is split into two parts
\[ J_i^e = J_i^r + J_i, \] (59)
where the first part is the reversible probability current,
\[ J_i^r = F_i^r \rho \] (60)
which is invariant under time reversal, holding the property (58) because \( \rho(x) = \rho(x) \), and the second part is the irreversible probability current,
\[ J_i = D_i \rho - \frac{1}{2} \sum_j \frac{\partial \rho \Gamma_{ij}}{\partial x_j}, \] (61)
which holds the property (58) because \( \Gamma_{ij}(\bar{x}) = \Gamma_{ij}(x) \).

B. Time variation of the entropy

The variation of the entropy
\[ S = -k \int \rho \ln \rho dx, \] (62)
with time is
\[ \frac{dS}{dt} = -k \int \frac{\partial \rho}{\partial t} \ln \rho dx. \] (63)
Using the evolution equation in the form (51), it can be written as
\[ \frac{dS}{dt} = k \sum_i \int \frac{\partial J_i^e}{\partial x_i} \ln \rho dx, \] (64)
Replacing \( J_i^e \) by \( J_i^r + J_i \), the right-hand side will be a sum of two terms, one of which involves the integral
\[ \sum_i \int \frac{\partial J_i^e}{\partial x_i} \ln \rho dx = \sum_i \int \frac{\partial F_i^r}{\partial x_i} \rho dx, \] (65)
where the equality was obtained by two integrations by parts. But this expression vanishes in view of the property (67) and we are left only with the second part,
\[ \frac{dS}{dt} = -k \sum_i \int J_i \frac{\partial \ln \rho}{\partial x_i} dx, \] (66)
where an integration by parts has been performed.

If we define \( F_i^{ir} = J_i / \rho \), we may write, after an integration by parts,
\[ \frac{dS}{dt} = k \sum_i \int \frac{\partial F_i^{ir}}{\partial x_i} \rho dx, \] (67)
In this form we see that the time variation of the entropy is related to the change in the volume of phase space, measured by the divergence of \( F^{ir} \).

C. Rate of entropy production

The comparison of equations (68) and (49) indicates that \( J_i \) is related to \( A_i \) by
\[ J_i = \frac{\rho}{2} \sum_j A_j \Gamma_{ij}, \] (68)
Inverting this relation, we find
\[ A_i = \frac{2}{\rho} \sum_j B_{ij} J_j, \] (69)
where we used \( B \Gamma = I \), which leads us to the following expression
\[ A_i = 2 \sum_j B_{ij} D_j - \frac{\partial \ln \rho}{\partial x_i} - \sum_{jk} B_{ij} \frac{\partial \Gamma_{jk}}{\partial x_k}, \] (70)
obtained by using (71), where again we used \( B \Gamma = I \).

We have seen above that the rate of entropy production is given by expression (48), which was demonstrated to be the rate of entropy for the case in which \( \Gamma_{ij} \) does not depend on \( x \), in which case the expression (70) for \( A_i \) does not have the last term on the right-hand. Although we did not show that the expression (48) is also valid for the case in which \( \Gamma_{ij} \) depends on \( x \), we assume that it expresses the rate of entropy production in this case, with \( A_i \) given by (70).

Using the relation between \( A_i \) and \( J_i \), the rate of entropy production can be written in terms of the dissipation probability current as
\[ \Pi = k \sum_i \int J_i A_i dx, \] (71)
or as
\[ \Pi = 2k \sum_{ij} \int \frac{1}{\rho} J_i B_{ij} J_j dx. \] (72)
This expression is clearly nonnegative because the eigenvalues of \( B \) are nonnegative and we notice that it is related only to the dissipation part of the probability current. When \( B \) is diagonal, this formula was considered by Tomé and de Oliveira [31] and derived by Spinney and Ford [31] by a method which has similarities with the present approach. The expression (72) was derived by Chetrite and Gawedzki [30] by identifying the production of entropy as a relative entropy related to forward and backward processes.

The flux of entropy \( \Phi \) is obtained by recalling that \( \Phi = \Pi - dS/dt \). Subtracting the expressions (72) and (64), we get
\[ \Phi = 2k \sum_{ij} \int J_i B_{ij} L_j dx, \] (73)
where
\[ L_j = D_j - \frac{1}{2} \sum_k \frac{\partial \Gamma_{jk}}{\partial x_k} \]  
(74)

which can also be written as
\[ \Phi = k \sum_i \int A_i L_i \rho \, dx. \]  
(75)

V. ENERGY, HEAT AND WORK

From now on, we wish to describe a system that may be acted by internal as well as by external forces. The internal forces are considered to be conservative forces in the sense that they are derived from an energy function \( E(x) \) associated to the system. Let \( x_i \) and \( x_j \) be a pair of even and odd variables, respectively. Then the even conservative force \( F^c_i \) and the odd conservative force \( F^e_i \) are obtained from the energy function \( E(x) \) by
\[ F^c_i = \frac{\partial E}{\partial x_j}, \quad F^e_j = \frac{\partial E}{\partial x_i}. \]  
(76)
The energy function holds the time-reversal property, \( E(\bar{x}) = E(x) \), guaranteeing the time-reversal property of the conservative forces.

In addition to the internal forces \( F^c_i \), the system, if it is not isolated, may be acted by external forces \( F^e_i \) which are also considered to be time reversal. The force \( F^e_i \) becomes a sum of these two forces
\[ F^e_i = F^c_i + F^e_i, \]  
(77)
and the evolution equation (16) becomes
\[ \frac{\partial \rho}{\partial t} = - \sum_i \frac{\partial F^c_i \rho}{\partial x_i} - \sum_i \frac{\partial F^e_i \rho}{\partial x_i} - \sum_i \frac{\partial J_i}{\partial x_i}. \]  
(78)

From the property (70), it follows at once the following result
\[ \sum_i \frac{\partial F^c_i}{\partial x_i} = 0. \]  
(79)
Using this property, we find
\[ \sum_i \frac{\partial F^c_i \rho}{\partial x_i} = \sum_i F^c_i \frac{\partial \rho}{\partial x_i}. \]  
(80)
which can be written as
\[ - \sum_i F^c_i \frac{\partial \rho}{\partial x_i} = \sum_{(ij)} \left( \frac{\partial E}{\partial x_i} \frac{\partial \rho}{\partial x_j} - \frac{\partial E}{\partial x_j} \frac{\partial \rho}{\partial x_i} \right) = \{ E, \rho \}, \]  
(81)
where the summation extends over all pairs \((i, j)\) such that \( x_i \) and \( x_j \) consist of a pair of conjugate variables such that the \( x_j \) is even and \( x_i \) is odd, and this summation is recognized as the Poisson brackets between \( E \) and \( \rho \).

The evolution equation (78) then becomes
\[ \frac{\partial \rho}{\partial t} = \{ E, \rho \} - \sum_i \frac{\partial F^c_i \rho}{\partial x_i} - \sum_i \frac{\partial J_i}{\partial x_i}. \]  
(82)
The time evolution of the average of the energy \( \langle E(x) \rangle \), understood as the thermodynamic internal energy \( U \) of the system, is obtained by multiplying (52) by \( E(x) \) and integrating in \( x \). The result is
\[ \frac{dU}{dt} = \sum_i \int J_i \frac{\partial E}{\partial x_i} \, dx + \sum_i \int F^c_i \frac{\partial E}{\partial x_i} \, dx, \]  
(83)
obtained after appropriate integrations by parts. The first summation on the right hand-side is identified as the total heat flux introduced into the system,
\[ \Phi_q = \sum_i \int J_i \frac{\partial E}{\partial x_i} \, dx, \]  
(84)
and the second as minus the work performed by the system per unit time, or power generated by the system,
\[ \Phi_w = - \sum_i \int F^c_i \frac{\partial E}{\partial x_i} \, dx. \]  
(85)
The equation (83) acquires the form
\[ \frac{dU}{dt} = \Phi_q - \Phi_w, \]  
(86)
which is understood as the global conservation of energy, and \( \Phi_u \) in equation (11) is \( \Phi_u = \Phi_q - \Phi_w \).

VI. A SPECIAL TYPE OF NOISE

The noise, which is represented by the covariances matrix \( \Gamma \) is not yet fully specified. Some of their essential properties have already been presented in equations (33) and (34), and are: \( \Gamma_{ij}(\bar{x}) = \Gamma_{ij}(x) \); and \( \Gamma_{ij}(x) \) vanishes whenever \( x_i \) and \( x_j \) consists of a pair of even and odd types. There are many choices of noise depending on the physical situation one wants to describe. Here we take a look at the type of noise that leaves a certain quantity \( E(x) \) invariant along the trajectory determined by this noise. The quantity \( E \) is strictly constant in every possible stochastic trajectory, and not only on the average. If two states \( x \) and \( x' \) are related by
\[ x'_i = x_i + F_i \tau + \xi_i \sqrt{\tau}, \]  
(87)
then the expansion of \( E(x') - E(x) \) up to terms of order \( \tau \) is
\[ E(x') - E(x) = \sum_i \frac{\partial E}{\partial x_i} (F_i \tau + \xi_i \sqrt{\tau}) + \frac{1}{2} \sum_{ij} \frac{\partial^2 E}{\partial x_i \partial x_j} \Gamma_{ij} \tau, \]  
(88)
where as before \( \Gamma_{ij} \) denotes the covariance of the random variables \( \xi_i \).
If $E(x’) = E(x)$ along the trajectory then the following constraint should be obeyed
\[ \sum_j \xi_j f_j = 0, \quad (89) \]
where
\[ f_j = \frac{\partial E}{\partial x_j}, \quad (90) \]
and
\[ \sum_i f_i F_i + \frac{1}{2} \sum_{ij} \Gamma_{ij} \frac{\partial f_i}{\partial x_j} = 0. \quad (91) \]
The first condition means that the random variables are not independent variables but are connected by (89). Multiplying (89) by $\xi_i$ and taking the average over the random variable $\xi$, we find
\[ \sum_j \Gamma_{ij} f_j = 0, \quad (92) \]
which relates the covariances and $f_i$. Owing to the relation (92), the condition (91) is equivalently expressed by
\[ F_i = \frac{1}{2} \sum_j \frac{\partial \Gamma_{ij}}{\partial x_j}. \quad (93) \]
If a certain quantity remains constant along a stochastic trajectory, the random variables $\xi_i$ should be connected by (89), and $F_i$ should be related to the covariances by (93).

Replacing the condition (89) in equation (74), we see that the quantity $L_i$ vanishes and so does the flux of entropy, given by (73). In other terms, the flux of entropy vanishes for the conservative noise that we are considering here and one concludes from this property that the variation of the entropy of the system $dS/dt$ equals the rate of the entropy production $\Pi$.

A noise that meet the condition (89) is set up as follows. For $i \neq j$, let $\xi_{ij}$ be random variables with zero means, each one with variance $\lambda_{ij} = \lambda_{ji} \geq 0$, that is, $\langle \xi_{ij}^2 \rangle = \lambda_{ij}$. These are independent random variables, except $\xi_{ij}$ and $\xi_{ji}$ which are related by $\xi_{ji} = -\xi_{ij}$. (94)

The random variable $\xi_i$ is defined in terms of these new random variables by
\[ \xi_i = \sum_{j(\neq i)} \xi_{ij} f_j. \quad (95) \]
Using property (94), the condition (91) follows immediately. We recall that $f_i = \partial E/\partial x_i$ and may depend on $x$, where $E(x)$ is the conserved quantity.

From (95) we may determine the covariances $\Gamma_{ij} = \langle \xi_i \xi_j \rangle$. Using the property (94) we find
\[ \Gamma_{ij} = -\lambda_{ij} f_i f_j, \quad (96) \]
for $i \neq j$, and
\[ \Gamma_{ii} = \sum_{j(\neq i)} \lambda_{ij} f_j^2. \quad (97) \]
From these results, we see that (92) is verified.

VII. THERMODYNAMIC EQUILIBRIUM

A. Noise-dissipation relation

From now on we consider only the situations such that the external forces are not present, in which case the evolution equation is
\[ \frac{\partial \rho}{\partial t} = \{ E, \rho \} - \sum_i \frac{\partial J_i}{\partial x_i}. \quad (98) \]
It remains to choose which type of noise to use. The choice of noise, represented by the covariances $\Gamma_{ij}$, and of the dissipative forces $D_i$ is guided by the type of situation one wants to describe. If we wish to describe an equilibrium situation, the noise represented by the covariances $\Gamma_{ij}$ and the dissipation represented by $D_i$ cannot be arbitrary but must hold a relationship between them, a noise-dissipation relation.

For long times, the density $\rho$ will reach a stationary density $\rho_e$, which makes the right-hand side of equation (98) to vanish. If $J_i(\rho_e)$ is nonzero for some $i$, then $\Pi$ is nonzero and the stationary state will be a state in which entropy is continuously been produced, and this is not an equilibrium state. The thermodynamic equilibrium is characterized by the vanishing of the entropy production which implies that $J_i$ should vanish for all $i$. Denoting by $\rho_e$ the equilibrium probability distribution then the condition for thermodynamic equilibrium is
\[ J_i(\rho_e) = 0, \quad (99) \]
for all $i$. Recalling the definition of $J_i$, given by (61), this condition is equivalent to
\[ D_j - \frac{1}{2} \sum_k \frac{\partial \Gamma_{jk}}{\partial x_k} = \frac{1}{2} \sum_k \Gamma_{jk} \frac{\partial \ln \rho_e}{\partial x_k}, \quad (100) \]
for all $i$.

Let us analyze the types of covariances $\Gamma_{ij}$ and the dissipative force $D_i$ that may lead the system to the thermodynamic equilibrium. As the quantity $J_i(\rho_e)$ vanishes for each $i$, the second summation on the right-hand side of equation (98) disappears and the first summation must vanish as well, that is,
\[ \{ E, \rho \} = 0. \quad (101) \]
This equation is fulfilled if \( \rho_c \) is a function of \( E \), that is if \( \rho_c(x) = \rho(E(x)) \) depends on \( x \) through the energy function \( E(x) \). In other words, in the thermodynamic equilibrium, the probability density is a function of the energy function, which is the main property of the equilibrium Gibbs distributions. The general condition for thermodynamic equilibrium is reduced to the condition represented by equation (100) where \( \rho_c \) is understood as a function of the energy function \( E(x) \). With this understanding, the equation (100) is the noise-dissipation relation.

The equations (99) and (101) are the two conditions that give the equilibrium probability distribution. The first condition represents the detailed balance condition or microscopic reversibility and the second is related to the conservation of energy. These two conditions are the ones used implicitly by Maxwell in his second derivation of the velocity distribution that bears his name [37].

### B. Canonical setting

Let us consider two relevant cases. The first is the one in which \( \rho_c \) is proportional to \( e^{-\beta E} \), which corresponds to the Gibbs canonical distribution. In this case equation (100) reduces to

\[
D_j - \frac{1}{2} \sum_{k} \frac{\partial \Gamma_{jk}}{\partial x_k} = -\frac{\beta}{2} \sum_{k} \Gamma_{jk} \frac{\partial E}{\partial x_k},
\]

which is the noise-dissipation relation for the present case.

Using relation (100), the flux of entropy (73) reduces to the following simple form

\[
\Phi = k \sum_i \int J_i \frac{\partial \ln \rho_c}{\partial x_i} dx = -\frac{1}{T} \sum_i \int J_i \frac{\partial E}{\partial x_i} dx.
\]

The comparison of the expressions (103) and (84) gives the relation

\[
\Phi = -\frac{\Phi_q}{T},
\]

which connects the flux of entropy and the heat flux. Since \( dU/dt = \Phi_q \) and \( dS/dt = \Pi - \Phi \), we reach the relation

\[
\frac{dS}{dt} = \Pi + \frac{1}{T} \frac{dU}{dt}.
\]

Near equilibrium, the rate of entropy production vanishes and we are left with the relation \( dU = TdS \), which confirms that the noises and dissipation satisfying the noise-dissipation relation (102) describe a system in contact with a reservoir at a temperature \( T \).

If the temperature is kept constant, then the variation with time of the free energy \( F = U - TS \) is related to the entropy production by \( dF/dt = -\Pi T \), which follows from (105). Since \( \Pi \geq 0 \), then \( dF/dt \leq 0 \) and the free energy decreases monotonically in time towards its equilibrium value. It is satisfying to realize that this inequality can be regarded as the H theorem of Boltzmann. Indeed, if we define the H function of Boltzmann by

\[
H = \int \rho \ln \frac{\rho}{\rho_c} dx,
\]

and recalling that \( \rho_c \) is proportional do the exponent of \(-\beta E\), we see that \( H \) equals \(-\beta F\), except for an additive constant, a relation giving the result

\[
\frac{dH}{dt} = -\beta \frac{dF}{dt} = k\Pi \geq 0,
\]

which is understood as the H theorem of Boltzmann.

### C. Microcanonical setting

The second relevant case is the one in which \( \rho_c \) vanishes unless \( E(x) = E_0 \), which corresponds to the Gibbs microcanonical distribution. This condition is met if the left and right hand sides of the equation (100) vanish, which give the conditions

\[
D_i = \frac{1}{2} \sum_j \frac{\partial \Gamma_{ij}}{\partial x_j},
\]

and

\[
\sum_j \Gamma_{ij} \frac{\partial E}{\partial x_j} = 0.
\]

The covariances obeying this relation is obtained from the special type of noise that we have analyzed above.

Replacing result (108) into the expression (74), we see that \( L_i \) vanishes identically and so does the flux of entropy, given by (50). The heat flux also vanishes. To see this, it suffices to observe that the covariances and dissipative forces, characterized by equations (108) and (109), yields

\[
J_i = -\frac{1}{2} \sum_j \Gamma_{ij} \frac{\partial \rho}{\partial x_j},
\]

which replaced in the expression (83) and making use of relation (109) gives the vanishing of \( \Phi_q \). Thus not only the flux of entropy is absent but also the heat flux, confirming that the noise characterized by (108) and (109) describe an isolated system.

The insertion of the expression (110) into the equation (83) gives the evolution in the form

\[
\frac{\partial \rho}{\partial t} = \{E, \rho\} + \frac{1}{2} \sum_{ij} \frac{\partial}{\partial x_i} \Gamma_{ij} \frac{\partial \rho}{\partial x_j},
\]

and describes an isolated system as we have demonstrated. In this sense it is similar to the Liouville equation

\[
\frac{\partial \rho}{\partial t} = \{E, \rho\},
\]
that describes a isolated system. However, in the case of the Liouville equation, the entropy is strictly constant in time, and there is no entropy production. This is in contrast with thermodynamic law of the increase of entropy in isolated systems, but in agreement with the equation \((111)\), which will generate entropy. The variation of the entropy, which equals the rate of entropy production \(\Pi\), is given by

\[
\frac{dS}{dt} = \frac{k}{2} \sum_{ij} \int \frac{\Gamma_{ij}}{\rho} \frac{\partial \rho}{\partial x_j} \frac{\partial \rho}{\partial x_i} dx,
\]

which is clear nonnegative because \(\Gamma_{ij}\) has nonnegative eigenvalues, and we conclude that \(dS/dt \geq 0\).

VIII. MECHANICAL SYSTEM

A. General equations

Here we apply the results obtained previously to a mechanical system composed by a certain number of interacting particles with equal masses. The positions of the particles are denoted by \(x_i\), understood as even variables, and the momenta of the particles by \(p_i\), understood as odd variables. The discrete time equations of motion are

\[
x_i' = x_i + \frac{p}{m} \tau, \quad (114)
\]

\[
p_i' = p_i + F_i \tau + D_i \tau + \xi_i \sqrt{\tau}, \quad (115)
\]

where \(F_i(x)\) is a conservative force that depends only on \(x\), that is, \(F_i = -dV/dx\), and \(D_i\) is the dissipative force. The conservative force \(F_i\) and \(p_i/m\) hold the property \((108)\), as desired, and the dissipative force is assumed to hold the property \((108)\), which reads \(D_i(x, -p) = -D_i(x, p)\).

The equation \((108)\) that gives the time evolution of the probability density \(\rho(x, p)\) reads

\[
\frac{\partial \rho}{\partial t} = \{\mathcal{H}, \rho\} - \sum_i \frac{\partial J_i}{\partial p_i}, \quad (116)
\]

where \(\mathcal{H}\) is the energy function

\[
\mathcal{H} = \sum_i \frac{p_i^2}{2m} + V(x). \quad (117)
\]

and we recall that \(F_i = -\partial \mathcal{H}/\partial x_i\) and \(p_i/m = \partial \mathcal{H}/\partial p_i\).

We analyze initially the ordinary case in which the dissipative force is proportional to the momentum, \(D_i = -\gamma p_i\), and the covariances are diagonal and do not depend on \(x\) nor on \(p\), and are given by \(\Gamma_{ii} = 2m\gamma\beta_i\). In this case the quantity \(J_i\) is

\[
J_i = -\gamma \left( p_i \rho + \frac{m}{\beta_i} \frac{\partial \rho}{\partial p_i} \right). \quad (118)
\]

Replacing in equation \((116)\), the evolution equation reads

\[
\frac{\partial \rho}{\partial t} = \{\mathcal{H}, \rho\} + \gamma \sum_i \frac{\partial \rho}{\partial p_i} + \gamma m \sum_i \frac{1}{\beta_i^2} \frac{\partial^2 \rho}{\partial p_i^2}, \quad (119)
\]

which we recognize as the Fokker-Planck-Kramers equation for many particles.

If \(\beta_i = \beta\) is the same for all \(i\), the noise-dissipation relation is obeyed for the Gibbs probability density \(\rho_e\) proportional to \(e^{-\beta \mathcal{H}}\) and the equation \((119)\) describes a system in contact with a reservoir at a temperature \(T = 1/k\beta\). For long times the system relax to the equilibrium state. If \(\beta_i\) are distinct, then for long times the system reaches a nonequilibrium stationary state because \(J_i\) cannot be zero for all \(i\) and \(\Pi \neq 0\). In this case the equation can be understood as describing a system in contact with several heat reservoirs at temperatures \(T_i = k\beta_i\).

Another situation is the one in which \(\rho_e\) vanishes unless \(\mathcal{H}(x, p) = E_0\), which we have discussed above, and understood as describing an isolated system. In equilibrium, it leads to the Gibbs microcanonical distribution. In the present case where the equation of motion is given by \((113)\) and \((115)\), the covariances are related only to the momentum variable, so that the relation \((109)\) gives

\[
\sum_j \Gamma_{ij} p_j = 0. \quad (120)
\]

The solution for \(\Gamma_{ij}\) is

\[
\Gamma_{ij} = -\lambda_{ij} p_i p_j, \quad i \neq j, \quad (121)
\]

\[
\Gamma_{ii} = \sum_{j \neq i} \lambda_{ij} p_j^2, \quad (122)
\]

where \(\lambda_{ij} = \lambda_{ji} \geq 0\), which replaced into \((108)\) gives again the usual form of the dissipative force

\[
D_i = -\gamma_i p_i, \quad \gamma_i = \frac{1}{2} \sum_{j(i)} \lambda_{ij}. \quad (123)
\]

The explicit form of \(J_i\) is

\[
J_i = \frac{1}{2} \sum_{j(i) \neq i} \lambda_{ij} p_j \left( p_i \frac{\partial \rho}{\partial p_j} - p_j \frac{\partial \rho}{\partial p_i} \right). \quad (124)
\]

The flux of entropy \(\Phi\) vanishes identically and the time variation of entropy \(dS/dt\) equals the rate of entropy \(\Pi\). Using expression \((113)\), we find

\[
\frac{dS}{dt} = \frac{k}{2} \sum_{i < j} \lambda_{ij} \int \frac{1}{\rho} \left( p_i \frac{\partial \rho}{\partial p_i} - p_j \frac{\partial \rho}{\partial p_j} \right)^2 dx, \quad (125)
\]

and we may conclude that \(dS/dt \geq 0\).
B. Weakly interacting particles

As an example of a system that evolves with strictly constant energy, we consider a system of weakly interacting particles in which case the energy function can be taken as being just the kinetic energy,

\[ \mathcal{H} = \sum_i p_i^2 / 2m. \]  

(126)

The evolution equation is

\[
\frac{\partial \rho}{\partial t} = \{ \mathcal{H}, \rho \} + \frac{1}{2} \sum_{ij} \frac{\partial}{\partial p_i} \Gamma_{ij} \frac{\partial \rho}{\partial p_j},
\]

(127)

where the covariances depend on \( p_i \) according to \([121]\) and \([122]\).

As the energy function is strictly constant in time, the equilibrium probability density is \( \rho_c(p) \) is proportional to \( \delta(\mathcal{H}(p) - E_0) \), as we have already seen. To solve equation \([127]\), we assume a probability distribution of the following form \( \rho(p) = g(p) \delta(\mathcal{H}(p) - E_0) \), which we expect to be valid near equilibrium, where

\[
g = \frac{1}{\zeta} \exp\left\{ -\frac{1}{2} \sum_{i \neq j} b_{ij} p_i p_j \right\},
\]

(128)

and the quantities \( b_{ij} \) are time dependent. Replacing this form in the evolution equation we find the following equation for \( b_{ij} \), for \( i \neq j \),

\[
\frac{db_{ij}}{dt} = -\alpha_{ij} b_{ij},
\]

(129)

where

\[
\alpha_{ij} = \lambda_{ij} + \frac{1}{2} \sum_{k(\neq i)} \lambda_{ik} + \frac{1}{2} \sum_{k(\neq j)} \lambda_{jk}.
\]

(130)

The solution for \( b_{ij} \) is

\[
b_{ij} = c_{ij} e^{-\alpha_{ij} t},
\]

(131)

and we see that for long times the probability distribution decays exponentially with time to the equilibrium distribution.

Let us determined the variation of entropy \( dS/dt \), which for the present case equals the rate of entropy production. Using equation \([113]\), we find

\[
\frac{dS}{dt} = \frac{k}{2} \sum_{i \neq j} b_{ij}^2 \{ \langle p_i^2 \rangle - \langle p_i \rangle^2 \} + \sum_{k(\neq i)} \lambda_{ik} \langle p_k^2 \rangle \langle p_j^2 \rangle,
\]

(132)

where the averages are determined by using the equilibrium probability distribution. We see that \( dS/dt \) is positive and decays exponentially to zero.

I the probability density is only a function of the momenta, we see that the Poisson brackets in \([127]\) vanishes but that is not the case of last term on the right-hand side of \([127]\). The vanishing of the Poisson brackets means that the Liouville equation gives \( \rho \) constant in time and thus do not relax to the equilibrium solution, if it was out of equilibrium at the beginning. This is in contrast with the solution of equation \([127]\) which predicts a relaxation to equilibrium and a nonzero production of entropy, and \( dS/dt > 0 \) out of equilibrium.

IX. CONCLUSION

We have developed an approach to stochastic thermodynamics of systems with continuous space of states. The results were obtained by continuous time limit of a discrete time formulation, which includes the evolution equation and the rate of entropy production. We have emphasized the role of the time reversal and of the dissipation probability current in the properties related to irreversible processes. When this part of the probability current vanishes, the rate of entropy production vanishes, and the equilibrium sets in. The rate of entropy production was shown to be a bilinear form in the components of the dissipation probability current and is positive definite.

We have also analyzed a type of noise that makes the energy function to be strictly constant along a stochastic trajectory and thus describing an isolated system. The increase in entropy is entirely due to the generation of entropy inside the system. This theoretical result is in agreement with thermodynamics in the sense that the entropy of an isolated system, in general, increases. This result contrasts with the prediction given by the Liouville equation that the entropy is constant in time, and there is not generation of entropy, although this equation describes an isolated system as the energy is strictly constant in time.

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