Entropy Productions and Their Mathematical Representations: Clausius’ vs. Kelvin’s Views of the Second Law and Irreversibility

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Abstract

We provide a stochastic mathematical theory for the nonequilibrium steady-state dissipation in a finite, compact driven system in terms of the non-stationary irreversibility in its external drive. A surjective map is rigorously established through a lift when the state space is either a discrete graph or a continuous \( n \)-torus \( \mathbb{T}^n \). Our approach employs algebraic topological and graph theoretical methods. The lifted processes, with detailed balance, have no stationary distribution but a natural potential function and a corresponding Gibbs measure which is non-normalizable. We show that in the long-time limit the entropy production of the finite driven system precisely equals to the potential energy decrease in the lifted system. We argue that the two equivalent views of dissipations in our theory represent Clausius’ and Kelvin’s statements of the Second Law of Thermodynamics. Indeed, we have a modernized, combined Clausius-Kelvin statement: “A mesoscopic engine that works in completing irreversible internal cycles statistically has necessarily an external effect that lowering a weight accompanied with passing heat from a warmer to a colder body.”
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I. INTRODUCTION

There is a growing awareness toward a slow shifting in the foundation of the Second Law of Thermodynamics, from a macroscopic postulate concerning heat as a form of random mechanical motion [23] to a derivable mathematical discovery based on the stochastic dynamics of mesoscopic systems [16, 31]. The first significant attempt in this direction was carried out by L. Boltzmann through the equation that now bears his name and the H-theorem it derives. The theory is applicable to gas dynamics; a fundamental assumption underlying the classic work is a stosszahlansatz [7, 14]. Rigorous mathematical breakthrough on Boltzmann’s equation only became available very recently [34]. In 1950s, Bergmann and Lebowitz set up a general stochastic theory for closed as well as open mechanical systems that are consistent with Hamiltonian dynamics, and easily obtained an H-theorem like result [5]. It becomes increasingly clear in recent years that a stochastic description of the Nature is a very effective analytic tool from mathematics.

For dynamics that can be represented in terms of a Markov process, a rather coherent system of mesoscopic theory of entropy productions has emerged. See [8, 10, 26, 33, 36] and references cited within. More recently, when this theory is applied to general chemical reaction systems represented by stochastic kinetics of elementary reactions, a result that is consistent with and further generalizes Gibbsian macroscopic chemical thermodynamics has been obtained, as a mathematical limit by merely allowing the molecular numbers to be infinite [12, 13]. In particular it was able to show, rigorously for the first time, that for each and every elementary, reversible reaction with instantaneous forward and backward rates $R^+$ and $R^-$, the macroscopic entropy production rate is

$$\left( R^+ - R^- \right) \log \left( \frac{R^+}{R^-} \right) \quad [3, 18, 20, 29].$$

In a Markov description of a driven system, irreversible kinetic cycles have been identified as fundamental to entropy production [1, 15, 17, 27]. From the standpoint of an observer who simultaneously follows the system’s internal stochastic dynamics as well as the external driving mechanism, there is a dissipation associated with a “falling weight” [19], e.g., the work being done by an external agent as a spontaneous process. There are two different perspectives that fittingly echo the two fundamental statements of the Second Law of Thermodynamics, from Kelvin and
Planck and from Clausius respectively [24]:

“It is impossible to construct an engine which will work in a complete cycle, and produce no effect except the raising of a weight and the cooling of a heat-reservoir.”

“Heat can never pass from a colder to a warmer body without some other change, connected therewith, occurring at the same time.”

In the present paper, we shall show that in the setting of irreversible Markov processes, both with finite state space and on a continuous $n$-torus with local potential, counting kinetic cycles constitutes a lift of the Markov processes, respectively, into either an infinite-state Markov process or diffusion on $\mathbb{R}^n$. The lifted Markov process satisfies detailed balance; it has many different invariant measures. However, it has one natural potential function and thus a corresponding Gibbsian invariant measure. This “no-flux” Gibbs measure is non-normalizable; its unbounded potential function provides a rigorous notion of an “internal energy” function $\varphi_x$. This is a new feature of the present theory that is different from previous works that usually assume the existence of a unique stationary probability measure as $t \to \infty$.

We shall show that, in the limit of $t \to \infty$, the positive stationary entropy production rate in the original Markov process is precisely the change in mean internal energy, $E \equiv \mathbb{E}[\varphi]$, of the free energy dissipation $\dot{F} = \dot{E} - \dot{S}$ in the lifted system. The energetic part of the free energy grows linearly with $t$; the entropic part of the free energy dissipation vanishes as $t \to \infty$ in Cesàro’s sense $\dot{S} \equiv S(t)/t \to 0$. Surprisingly, in rigorous mathematics, we have not been able to show the stronger assertion that $dS(t)/dt \to 0$ in general except some very special cases.

Our mathematical theory, therefore, rigorously establishes an equivalence between the two famous statements concerning the Second Law of Thermodynamics: A cyclic view of dissipation and a non-stationary view of irreversibility. In fact, there is a continuous surjective map between the trajectories before and after the lifting: In the long-time behavior, the cycle completion and entropy production in the former is precisely represented by the potential change in the latter. Alternatively, dissipation in the former is due to indistinguishability of the locally equivalent states in the latter.

The paper is structured as follows: In Sec. II, we prove an embedding theorem that establishes a minimal lift of a continuous time, finite state Markov chain to a detailed balance process with a proper potential function. An equivalence between the path-dependent entropy production in the
former and the potential difference in the latter is provided. Then in Sec. [III] we prove the theorem that, in the limit of $t \to \infty$, equating the entropy production rate $\bar{\epsilon}_p(t)$ of the finite system with the Cesàro limit of $\epsilon_p(t)$ from the lifted system. For lifted, detailed balance systems, $\epsilon_p(t)$ can be expressed as $-dF/dt$ where free energy $F(t) = D_{KL}(p(t), \mu)$ is the relative entropy of $p(t)$ with respect to the Gibbs measure $\mu = e^{-\varphi}$. We show as $t \to \infty$, $F(t) = E(t) - S(t)$ has a linearly decreasing $E(t)$ and a sublinear $S(t)$ controlled by $\log t$. Therefore in the long time limit $\bar{\epsilon}_p$ equals to $-\dot{E}$.

Sec. [IV] is a mathematical generalization of Sec. [III] to diffusion processes on $n$-torus and their lifting to $\mathbb{R}^n$. The paper concludes with Sec. [V].

II. THE LIFTED MARKOV CHAIN AND ITS INFINITE STATE SPACE

In this section, we study the lifting of a continuous time, finite state Markov chain. First, we need some prerequisite in different fields.

A. Prerequisites

1. Graph Theory

Consider an undirected connected simple finite graph $(V, E)$, where $V$ is the vertices set, $E$ is the edges set. Simple means that there is at most one edge between two vertices, and there is no edge which connects a vertex to itself.

Definition. A cycle in graph $(V, E)$ is a sequence of distinct vertices $(x_0, x_1, \cdots, x_k)$, where there exists an edge connecting $x_i$ and $x_{i+1}$ ($i = 0, 1, \cdots, k$, regarding $x_{k+1}$ as $x_0$). Here we do not distinguish between a cycle with its inverse or shift, such as $(x_k, x_{k-1}, \cdots, x_0)$, $(x_1, x_2, \cdots, x_k, x_0)$.

Definition. A tree is a connected graph without cycle.

Definition. A subgraph of a graph $(V, E)$ is called a spanning tree if it is a tree, and contains all the vertices of $(V, E)$. Any undirected connected simple finite graph has at least one spanning tree.

Definition. The first Betti number of graph $(V, E)$ is $b(V, E) = |E| - |V| + 1$.

The following Lemma combines Theorem 1.5.1 and Theorem 1.5.3 in [6].
**Lemma 1.** $b(V, E) \geq 0$. $b(V, E) = 0$ if and only if $(V, E)$ is a tree. $b(V, E) = 1$ if and only if $(V, E)$ contains exactly one cycle.

**Lemma 2.** For graph $(V, E)$, we can find $b(V, E)$ cycles $c_1, c_2, \ldots, c_{b(V, E)}$, and each $c_i$ contains an edge $e_i^*$ which is not contained in any cycle $c_j$ with $j \neq i$.

**Proof.** Consider a spanning tree $(V, E')$ of $(V, E)$. By Lemma 1 we know that $|E| - |E'| = b(V, E)$. Consider an edge $e_i^*$ which is contained in $(V, E)$ but not $(V, E')$ (we have $b(V, E)$ of them). Adding each $e_i^*$ to $(V, E')$ will let this spanning tree have first Betti number 1, which means it forms exactly one cycle $c_i$. Now we get the desired $b(V, E)$ cycles. We call such edge $e_i^*$ as “special edge”.

2. **Algebraic Graph Theory**

The definitions and notations in this part are from [25].

Now consider a directed connected simple finite graph $(V, E)$. The only difference is that now each edge $e$ is assigned an orientation. The inverse edge is denoted as $-e$. Define $\partial$ to be a $|V| \times |E|$ matrix which describes the relationship between $V$ and $E$. For $v \in V$, $e \in E$, $\partial_{ve}$ equals 1 if edge $e$ goes into vertex $v$, $-1$ if edge $e$ comes out of vertex $v$, and 0 otherwise.

**Definition.** An algebraic cycle $C$ is an element in the null space of $\partial$.

Consider the following graph:

![Graph Diagram]

The corresponding $\partial$ is

$$
\begin{bmatrix}
-1 & 0 & 0 & -1 & -1 \\
1 & 1 & 0 & 0 & 0 \\
0 & -1 & -1 & 0 & 1 \\
0 & 0 & 1 & 1 & 0
\end{bmatrix}
$$

The cycle $v_1, v_2, v_3, v_4 (e_1, -e_2, e_3, -e_4)$ corresponds to an algebraic cycle, $(1, -1, 1, -1, 0)$.

It is easy to see that each cycle corresponds to an algebraic cycle. In the following we do not distinguish between a cycle and its corresponding algebraic cycle.

**Lemma 3.** The $b(V, E)$ cycles in Lemma 2 constitute a basis of the algebraic cycle space.
Proof. From [25], we know that the dimension of algebraic cycle space is \( b(V, E) = |E| - |V| + 1 \). Furthermore, we can see that the \( b(V, E) \) cycles in Lemma 2 are linearly independent, since each of them has a unique “special edge”.

In the above example, consider this spanning tree:

```
  v1
 / \
\ /  \\
v2
 v3
 /   \
\ /    \\
v4
```

This means we can choose \( c_1 = (v_1, v_2, v_3) (1, -1, 0, 0, -1) \) (corresponds to edge \( e_2 \)) and \( c_2 = (v_1, v_3, v_4) (0, 0, 1, -1, 1) \) (corresponds to edge \( e_3 \)) as a basis. Then cycle \( c_3 = (v_1, v_2, v_3, v_4) (1, -1, 1, -1, 0) \) can be expressed as \( c_3 = c_1 + c_2 \).

In the following we only consider cycles (sometimes as algebraic cycles).

3. Potential of Markov chain

For a Markov chain, we define the potential gain of a trajectory \( i_1, \cdots, i_k \) as

\[
\sum_{j=1}^{k-1} \log \frac{q_{i_{j+1}i_j}}{q_{i_ji_{j+1}}}.
\]

If there exists a function on state space, \( f(i) \), such that the potential gain of a trajectory is the difference of this function on the two end states, then \( f(i) \) is a global potential of the Markov chain.

Global potential exists if and only if the potential gain of a closed trajectory is 0. In general, a finite Markov chain does not satisfy this condition.

A global potential is proper if different states have different potentials. (In this paper, potential is always calculated symbolically.)

4. Algebraic Topology

Definition. Let \( X \) be a topological space. A covering space of \( X \) is a topological space \( C \) together with a continuous surjective map \( p : C \to X \), such that for every \( x \in X \), there exists an open neighborhood \( U \) of \( x \), such that \( p^{-1}(U) \) is a union of disjoint open sets in \( C \), each of which is mapped homeomorphically onto \( U \) by \( p \). A path in \( X \) can be uniquely lifted to \( C \) with a given starting point.
Definition. A covering space is a universal covering space if it is simply connected. General space, such as connected graph or \( n \)-dimensional torus, has universal covering space. If exists, universal covering space is unique.

For a finite graph, its covering space is still a graph. Each vertex in the covering space has an image vertex in the original graph, and they have the same neighbors. We say that the covering space is locally isomorphic to the original graph.

B. Embedding a Markov chain into an \( n \)-torus

1. Motivation and Results

Consider a continuous time irreducible Markov chain with transition rate matrix \( Q = \{q_{ij}\} \). We require that \( q_{ij} > 0 \) if and only if \( q_{ji} > 0 \). Then we can define a graph \((V, E)\). Vertices are states of this Markov chain, and edges are possible transitions. We would like to study the reversibility of a trajectory. We define the potential gain of a trajectory \( i_1, \cdots, i_k \) as

\[
\sum_{j=1}^{k-1} \log \frac{q_{i_{j+1}i_j}}{q_{ij_i_{j+1}}}
\]

When a trajectory finishes a cycle, the potential gain is not zero in general, although it returns to its starting point. The aim is to find a new expression of the Markov chain, such that we can determine the potential gain of a trajectory by its starting point and ending point.

This means there exists a global potential, therefore potential gain is path-independent. The new expression should still be a Markov chain, and locally isomorphic to the original Markov chain.

A simple way is to expand all the cycles, such that there is no cycle in the new Markov chain. To be precise, this is the universal covering space of the original Markov chain. Covering space guarantees local isomorphism, and universal implies there is no cycle.

A problem of universal covering space is that different states may have the same potential, namely the potential is not proper. A natural idea is to glue states together if they have the same potential, but the result is difficult to study.

Now the goal is to find a new Markov chain, which is locally isomorphic to the original Markov chain, and has a proper global potential.
To illustrate our idea, consider a 3-state Markov chain, with one cycle $1 \rightarrow 2 \rightarrow 3 \rightarrow 1$. We can embed the corresponding graph into $S^1$, and then lift it to $\mathbb{R}$. Now it is $\cdots \rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow \cdots$. There exists a proper global potential. As long as we know the ends of a trajectory, we know the potential gain of this trajectory.

This problem implies relationship with the fundamental group of the original Markov chain. Notice that the potential gain of a trajectory is invariant if we exchange the order of cycles in the trajectory. Therefore we need the abelianization of the fundamental group. If the original Markov chain has first Betti number $n$, then the abelianization of its fundamental group is $\mathbb{Z}^n$. This is the fundamental group of $n$-dimensional torus $T^n$. Therefore we consider combining the Markov chain with $T^n$.

**Theorem 1** (torus version). For a Markov chain with $q_{ij} > 0 \iff q_{ji} > 0$, it can be embedded into $n$-torus $T^n$, such that any closed path has zero potential gain if and only if it is homotopy trivial, namely it could continuously transform into a single point. (For $n = 1$, only the cycle can be embedded.)

**Theorem 2** (lifted version). With the same condition above, one can find a Markov chain with a proper global potential, and it is locally isomorphic with the original Markov chain.

### 2. Proofs

We will prove the lifted version directly. We will use the example in Sec. IIA.

Regard $T^n$ as the unit hypercube $[0, 1]^n$ with opposite hypersurfaces glued together. For the original Markov chain with first Betti number $b(V, E) = n$, choose a spanning tree, and embed it into $T^n$. For each edge of the original Markov chain that is not in the spanning tree (we have $n$ of such special edges), assign a pair of opposite hypersurfaces to it. Draw this edge in $T^n$ while crossing the corresponding hypersurface once. Now we have embedded the original Markov chain into $T^n$.

Consider the universal covering space of $T^n$, $\mathbb{R}^n$. Correspondingly, the embedded Markov chain is lifted into $\mathbb{R}^n$. The lifted Markov chain is connected and locally isomorphic to the original Markov chain. A trajectory of the original Markov chain can be lifted into the new Markov chain. A trajectory of the lifted Markov chain can be folded back to the original Markov chain. We can assign an $n$-tuple coordinate to each unit hypercube. On the lifted Markov chain, moving along special edges is the only way to change the coordinate.
FIG. 1. In this example, the Markov chain (left) has first Betti number $b(V, E) = 2$, therefore we can choose a spanning tree (middle), which corresponds to two special edges $2 \rightarrow -3$ and $3 \rightarrow 4$. Embed the spanning tree into $\mathbb{T}^2$, which is a square in $\mathbb{R}^2$ with opposite boundaries glued. Assign special edge $2 \rightarrow -3$ to vertical boundaries, and $3 \rightarrow 4$ to horizontal boundaries. Then connect 2 and 3 across the vertical boundaries, connect 3 and 4 across the horizontal boundaries. Now we have embedded the Markov chain into $\mathbb{T}^2$ (right).

Consider a closed trajectory in the lifted Markov chain. The net number of each special edge appears in the trajectory equals the net number of corresponding hypersurface crossed, which is 0. Therefore, the net number of all special edges are 0. Fold this trajectory back to the original Markov chain, then it is an algebraic cycle. It is the linear combination of the cycles in the basis, where the basis is determined by the spanning tree. Now the coefficient of each cycle in the basis is the net number of corresponding special edge, which is 0. Therefore the folded trajectory as an algebraic cycle is all 0. Thus the closed trajectory in the lifted Markov chain has 0 potential gain.

If a trajectory in the lifted Markov chain has 0 potential gain, then first its starting point and ending point should be of the same state. Otherwise the total number of edges containing the starting point state is odd, a contradiction. Also, if the starting point and ending point are different, then at least one component of their coordinates are different, which means the net number of the corresponding special edge is not 0. Thus the potential gain is not 0.

This finishes the proof of the lifted version. We prove that a path in the lifted Markov chain has
FIG. 2. Continued with Figure 1. $\mathbb{T}^2$ is lifted to its universal covering space $\mathbb{R}^2$. Accordingly the embedded Markov chain is lifted to a covering space (not universal), which is a larger Markov chain.

0 potential gain if and only if it is closed. Furthermore, a closed path in $\mathbb{T}^n$ is homotopy trivial if and only if its lifting in $\mathbb{R}^n$ is still closed (recall that the fundamental group of $\mathbb{T}^n$ is $\mathbb{Z}^n$). Therefore we also prove the torus version.
3. Properties

Consider a closed path in the original Markov chain. Using the notion of the “derived chain” \[17\], we can count all cycles completed in this path. Now decompose cycles with cycles in the basis, and count their net numbers. Then we know the net number of each cycle in the basis, which is the net number of the corresponding special edge. Also, the coordinate changes if and only if it passes the corresponding special edge.

This means that for the lifted path, the coordinate difference of its ends is just the net number of cycles completed (winding number). Two paths with the same ends have the same winding number.

When the path is not closed, the coordinate difference may not be exactly the winding number. For example, the trajectory \(1 \rightarrow 2 \rightarrow 3 \rightarrow 1 \rightarrow 3\) has one cycle completed, and \(1 \rightarrow 2 \rightarrow 3\) has no cycle completed. However, the absolute error for each cycle in the basis is at most 1. Therefore, counting cycles becomes counting the special edges, which is much simplified.

III. THERMODYNAMIC QUANTITIES OF MARKOV CHAINS

With a Markov process and its lift established, we now consider the entropy production of the corresponding Markov processes.

A. Stationary distributions and measures of finite-state Markov chain and its lifting

We consider a continuous-time finite-state Markov chain. The chain is irreducible, and for any states \(i, j\), the transition rates satisfy \(q_{ij} > 0 \iff q_{ji} > 0\).

We lift this Markov chain to be an \(n\)-dimensional Markov chain with infinite states, where \(n\) is the first Betti number of the former. State \(i\) is lifted to \(i_\alpha\), where \(\alpha \in \mathbb{Z}^n\). The lifted initial distribution is compatible with the original distribution: \(\bar{p}_i(0) = \sum_\alpha p_{i_\alpha}(0)\). Then we have \(\bar{p}_i(t) = \sum_\alpha p_{i_\alpha}(t)\).

The distribution of lifted Markov chain satisfies

\[
\frac{dp_{i_\alpha}}{dt} = \sum_{j_\beta \sim i_\alpha} \{ p_{j_\beta}q_{ji} - p_{i_\alpha}q_{ij} \}.
\]

We write \(j_\beta \sim i_\alpha\) if \(j_\beta\) and \(i_\alpha\) are adjacent.
For the finite Markov chain, starting from any initial distribution \( \bar{\pi}_i(0) \), it will converge to the unique stationary distribution \( \bar{\pi}_i \).

The lifted chain has an invariant measure

\[
\pi_{i_\alpha} = \bar{\pi}_i,
\]

where \( i_\alpha \) is a copy of state \( i \) in the original chain.

Since the lifted Markov chain has a global potential \( \varphi_{i_\alpha} \), one could construct a detailed balance stationary measure \( \mu_{i_\alpha} = \exp(-\varphi_{i_\alpha}) \), such that

\[
\mu_{i_\alpha} q_{ij} = \mu_{j_\beta} q_{ji}.
\]

To further study the stationary distributions and measures, we need to consider the relative entropy of \( p_i(t) \) with respect to any stationary measure \( \theta_{i_\alpha} \),

\[
D_{KL}(p, \theta) = \sum_i \sum_\alpha p_{i_\alpha}(t) \log \frac{p_{i_\alpha}(t)}{\theta_{i_\alpha}}.
\]

Remark of summation indices: In \( \sum_{j_\beta \sim i_\alpha} \), the adjacent pair \( (j_\beta, i_\alpha) \) is the same as \( (i_\alpha, j_\beta) \). In \( \sum_i \sum_\alpha \sum_{j_\beta \sim i_\alpha} \), \( (j_\beta, i_\alpha) \) and \( (i_\alpha, j_\beta) \) are counted separately. Thus

\[
\sum_{j_\beta \sim i_\alpha} f_{i_\alpha j_\beta} = \frac{1}{2} \sum_i \sum_\alpha \sum_{j_\beta \sim i_\alpha} f_{i_\alpha j_\beta}
\]

for any \( f_{i_\alpha j_\beta} \) with \( f_{i_\alpha j_\beta} = f_{j_\beta i_\alpha} \). \( \sum_i \sum_j \) is the same as \( \sum_i \sum \).

The following Lemma 4 can be found in many references [21, 32, 35].

**Lemma 4.** \( D_{KL}(p, \theta) \) is monotonically decreasing.

**Proof.**

\[
\frac{d}{dt} \sum_i \sum_\alpha p_{i_\alpha}(t) \log \frac{p_{i_\alpha}(t)}{\theta_{i_\alpha}} = \sum_i \sum_\alpha \frac{dp_{i_\alpha}(t)}{dt} \log \frac{p_{i_\alpha}(t)}{\theta_{i_\alpha}} + \sum_i \sum_\alpha \frac{dp_{i_\alpha}(t)}{dt}
\]

\[
= -\sum_i \sum_\alpha \sum_{j_\beta \sim i_\alpha} [p_{i_\alpha}(t)q_{ij} - p_{j_\beta}(t)q_{ji}] \log \frac{p_{i_\alpha}(t)}{\theta_{i_\alpha}}
\]

\[
= -\frac{1}{2} \sum_i \sum_\alpha \sum_{j_\beta \sim i_\alpha} [p_{i_\alpha}(t)q_{ij} - p_{j_\beta}(t)q_{ji}] \left[ \log \frac{p_{i_\alpha}(t)}{\theta_{i_\alpha}} - \log \frac{p_{j_\beta}(t)}{\theta_{j_\beta}} \right]
\]
\[
\sum_{i} \sum_{\alpha} \sum_{j, \sim i, \alpha} p_{i\alpha}(t) q_{ij} \log p_{i\alpha}(t) \frac{\theta_{j\beta}(t)}{p_{i\alpha}(t) \theta_{j\beta}} \leq - \sum_{i} \sum_{\alpha} \sum_{j, \sim i, \alpha} p_{i\alpha}(t) q_{ij} \left[ 1 - \frac{\theta_{i\alpha} p_{j\beta}(t)}{p_{i\alpha}(t) \theta_{j\beta}} \right]
\]

\[
= - \sum_{i, j} \bar{p}_i(t) q_{ij} + \sum_{j} \sum_{\beta} \sum_{i, \sim j, \beta} q_{ij} \frac{\theta_{i\alpha} p_{j\beta}(t)}{\theta_{j\beta}} = - \sum_{i, j} \bar{p}_i(t) q_{ij} + \sum_{j} \sum_{\beta} p_{j\beta}(t) \sum_{i} q_{ji} \theta_{j\beta}
\]

\[
= - \sum_{i, j} \bar{p}_i(t) q_{ij} + \sum_{j, i} \bar{p}_j(t) q_{ji} = 0.
\]

The inequality is from \(\log y \geq 1 - 1/y\). The equality holds if and only if \(p_{i\alpha}(t) = c \theta_{i\alpha}\) for a constant \(c\).

Then we can prove the following result:

**Proposition 1.** The lifted Markov chain has no stationary probability distribution.

**Proof.** Assume there exists a stationary probability distribution \(\eta_{i\alpha}\). Let \(p(t)\) be the stationary distribution, and \(\theta\) be \(\pi\), then \(D_{KL}(p, \pi)\) is a constant. This is true only if the equality holds in Lemma 4, which means \(\eta_{i\alpha} \pi_j = \eta_{j\beta} \pi_i\). Thus \(\eta\) and \(\pi\) only differ by a constant multiple. \(\pi\) is non-normalizable, so is \(\eta\).

**B. Instantaneous entropy production rate, free energy, and housekeeping heat**

For the finite Markov chain, one could define several thermodynamic quantities: entropy production rate, free energy, and housekeeping heat.

**Definition.** The instantaneous free energy of finite Markov chain \(\bar{F}(t)\) is defined as \(\bar{F}(t) = D_{KL}(\bar{p}, \bar{\pi})\).

**Definition.** The instantaneous entropy production rate of finite Markov chain \(\bar{e}_p(t)\) is defined as \[17\]

\[
\bar{e}_p(t) = \sum_{i \sim j} \left[ \bar{p}_i(t) q_{ij} - \bar{p}_j(t) q_{ji} \right] \log \frac{\bar{p}_i(t) q_{ij}}{\bar{p}_j(t) q_{ji}}.
\]

This definition is derived from the original idea of entropy production rate that it describes the difference between a process and its time inverse.

**Definition.** The instantaneous housekeeping heat of finite Markov chain \(\bar{Q}_{hk}(t)\) is defined as \(\bar{e}_p(t) + d\bar{F}(t)/dt\).  

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For the lifted Markov chain with probability distribution $p_{i\alpha}(t)$, since there is no stationary distribution, one could choose a stationary measure instead. In general stationary measure is not unique, therefore one could have different versions of free energy and housekeeping heat.

**Definition.** The instantaneous free energy with respect to stationary measure $\theta$, $F^\theta(t)$, is defined as $F^\theta(t) = D_{KL}(f, \theta)$. Its time derivative is

$$
\frac{dF^\theta(t)}{dt} = - \sum_{i\alpha\sim j\beta} [p_{i\alpha}(t)q_{ij} - p_{j\beta}(t)q_{ji}] \log \frac{p_{i\alpha}(t)\theta_{ji}}{p_{j\beta}(t)\theta_{ij}}.
$$

**Definition.** The instantaneous entropy production rate $e_p(t)$ is defined as

$$
e_p(t) = \sum_{i\alpha\sim j\beta} [p_{i\alpha}(t)q_{ij} - p_{j\beta}(t)q_{ji}] \log \frac{p_{i\alpha}(t)q_{ij}}{p_{j\beta}(t)q_{ji}}.
$$

**Definition.** The instantaneous housekeeping heat with respect to stationary measure $\theta$, $Q^\theta_{hk}(t)$, is defined as

$$Q^\theta_{hk}(t) = e_p(t) + \frac{dF^\theta(t)}{dt} = \sum_{i\alpha\sim j\beta} [p_{i\alpha}(t)q_{ij} - p_{j\beta}(t)q_{ji}] \log \frac{\theta_{ij}q_{ij}}{\theta_{ji}q_{ji}}.
$$

From Lemma 4, $\frac{dF^\theta(t)}{dt} \leq 0$. From the definition of instantaneous entropy production rate, $e_p(t) \geq 0$. For $Q^\theta_{hk}(t)$, we have the same result.

**Proposition 2.** $Q^\theta_{hk}(t) \geq 0$.

**Proof.**

$$Q^\theta_{hk}(t) = \sum_i \sum_{\alpha} \sum_{j\beta \sim i\alpha} p_{i\alpha}(t)q_{ij} \log \frac{\theta_{ij}q_{ij}}{\theta_{ji}q_{ji}} \geq \sum_i \sum_{\alpha} \sum_{j\beta \sim i\alpha} p_{i\alpha}(t)q_{ij} \left[1 - \frac{\theta_{ij}q_{ij}}{\theta_{ji}q_{ji}}\right]$$

$$= \sum_{i,j} \bar{p}_{i}(t)q_{ij} - \sum_i \sum_{\alpha} p_{i\alpha}(t) \sum_{j\beta \sim i\alpha} q_{ji} \theta_{ji} = \sum_{i,j} \bar{p}_{i}(t)q_{ij} - \sum_i \sum_{\alpha} p_{i\alpha}(t) \sum_j q_{ij} \theta_{i\alpha}$$

$$= \sum_{i,j} \bar{p}_{i}(t)q_{ij} - \sum_{i,j} \bar{p}_{i}(t)q_{ij} = 0.
$$

The inequality is from $\log y \geq 1 - 1/y$. 

Thus we have the decomposition

$$e_p(t) = Q^\theta_{hk}(t) + [-dF^\theta(t)/dt],$$

where each term is non-negative. This is also valid for the finite Markov chain version.
C. Time limits of thermodynamic quantities

Since $\bar{p}(t)$ converges to $\bar{\pi}$, $\bar{F}(t)$ and $d\bar{F}(t)/dt$ converge to 0, $\bar{e}_p(t)$ and $\bar{Q}_{hk}(t)$ converge to the stationary entropy production rate

$$\bar{e}_p = \sum_{i \sim j} [\bar{\pi}_i q_{ij} - \bar{\pi}_j q_{ji}] \log \frac{\bar{\pi}_i q_{ij}}{\bar{\pi}_j q_{ji}}.$$ 

For the lifted Markov chain, $p(t)$ does not converge to a stationary distribution, therefore we do not have the stationary version of these quantities. However, we can still study their behavior as $t \to \infty$.

If we set $\theta$ to be the periodic stationary measure $\pi$, then $Q_{h\kappa}^\theta(t)$ converges to

$$\sum_{i \sim j} [\bar{\pi}_i q_{ij} - \bar{\pi}_j q_{ji}] \log \frac{\bar{\pi}_i q_{ij}}{\bar{\pi}_j q_{ji}},$$

which is just $\bar{e}_p$.

If we set $\theta$ to be the detailed balance stationary measure $\mu$, then $Q_{h\kappa}^\mu(t) \equiv 0$ since $\mu_{i\alpha} q_{ij} = \mu_{j\beta} q_{ji}$.

For the time limit of $e_p(t)$, we have the following theorem. The proof is in the next part.

**Theorem 3.** Assume the initial distribution $p_{i\alpha}(0)$ has finite covariance matrix. Then $e_p(t)$ converges to $\bar{e}_p$ in Cesàro’s sense that $\lim_{T \to \infty} \frac{1}{T} \int_0^T e_p(t) dt = \bar{e}_p$.

In summary, $e_p = Q_{h\kappa}^\theta + (-dF^\theta / dt)$, where $e_p$, $Q_{h\kappa}^\theta$ and $-dF^\theta / dt$ are non-negative.

$e_p \to \bar{e}_p$ in Cesàro’s sense, $dF^\mu / dt = -e_p \to -\bar{e}_p$ in Cesàro’s sense, $Q_{h\kappa}^\mu \equiv 0$, $dF^\pi / dt \to 0$ in Cesàro’s sense, $Q_{h\kappa}^\pi \to \bar{e}_p$ in general sense.

Therefore, the periodic stationary measure $\pi$ and the detailed balance stationary measure $\mu$ reach the maximum and minimum of $Q_{h\kappa}^\theta$, $\bar{e}_p$ and 0, as $t \to \infty$.

For the two special stationary measures $\theta$ and $\mu$, the expectation of their Radon-Nikodym derivative is

$$\sum_{i\alpha} p_{i\alpha}(t) \frac{\mu_{i\alpha}}{\pi_{i\alpha}}.$$ 

Since

$$dF^\pi(t)/dt - dF^\mu(t)/dt = \sum_{i\alpha \sim j\beta} [p_{i\alpha}(t) q_{ij} - p_{j\beta}(t) q_{ji}] \log \frac{\mu_{i\alpha} \pi_{j\beta}}{\mu_{j\beta} \pi_{i\alpha}} = Q_{h\kappa}^\rho(t) - Q_{h\kappa}^\mu(t),$$

we have

$$\frac{d}{dt} \sum_{i\alpha} p_{i\alpha}(t) \frac{\mu_{i\alpha}}{\pi_{i\alpha}} = dF^\pi(t)/dt - dF^\mu(t)/dt = Q_{h\kappa}^\pi(t) - Q_{h\kappa}^\mu(t) \to \bar{e}_p.$$
D. Proof of Theorem 3

The proof consists of the following Lemmas 5-8. The key idea is that we have

\[ e_p(t) - \bar{e}_p(t) = \frac{dF(t)}{dt} - \frac{dF^\pi(t)}{dt}. \]  

(1)

We have \( \frac{d\bar{F}(t)}{dt} \to 0 \) and \( \bar{e}_p(t) \to \bar{e}_p \). For \( F^\pi(t) \), we prove \( \frac{dF^\pi(t)}{dt} < 0 \), and \( F^\pi(t) > -C \log t \) for large \( t \). Thus

\[ \lim_{T \to \infty} \frac{1}{T} \int_0^T \frac{dF^\pi(t)}{dt} \, dt = 0, \]

therefore we have

\[ \lim_{T \to \infty} \frac{1}{T} \int_0^T e_p(t) \, dt = \bar{e}_p. \]

These results are not enough, however, for proving \( \frac{dF^\pi(t)}{dt} \to 0 \). Thus we do not have \( e_p(t) \to \bar{e}_p \).

For the lifted Markov chain, the entropy of distribution \( p_{i\alpha}(t) \) is

\[ h[p(t)] = \sum_{i\alpha} -p_{i\alpha}(t) \log p_{i\alpha}(t). \]

**Lemma 5.** Assume the initial distribution \( p(0) \) has finite entropy. Then \( \lim_{T \to \infty} \frac{1}{T} \int_0^T e_p(t) \, dt \) for \( F^\pi(0) - F^\pi(T) + \bar{F}(T) - \bar{F}(0) \).

Proof. We have

\[ \frac{dF^\pi(t)}{dt} + e_p(t) = \frac{1}{2} \sum_{i,j} [\bar{p}_i(t)q_{ij} - \bar{p}_j(t)q_{ji}] \log \frac{\bar{\pi}_i q_{ij}}{\bar{\pi}_j q_{ji}} = \frac{d\bar{F}(t)}{dt} + \bar{e}_p(t). \]

Therefore

\[ \frac{1}{T} \int_0^T e_p(t) \, dt - \frac{1}{T} \int_0^T \bar{e}_p(t) \, dt = \frac{1}{T} [F^\pi(0) - F^\pi(T) + \bar{F}(T) - \bar{F}(0)]. \]

Since \( \bar{p}(t) \) converges to \( \bar{\pi} \), \( \bar{F}(t) \) converges to 0, therefore \( \bar{F}(T) \) is bounded.

\[ F^\pi(0) - \bar{F}(0) = h[\bar{p}(0)] - h[p(0)], \text{ which is finite.} \]

\[ F^\pi(T) + h[p(T)] = - \sum_i \bar{p}_i(T) \log \bar{\pi}_i, \text{ which is bounded. Thus } \lim_{T \to \infty} F^\pi(T)/T = - \lim_{T \to \infty} h[p(T)]/T. \]

We also have \( \lim_{T \to \infty} \frac{1}{T} \int_0^T e_{\bar{p}}(t) \, dt = \bar{e}_p \).

Therefore \( \lim_{T \to \infty} \frac{1}{T} \int_0^T e_p(t) \, dt - \bar{e}_p = - \lim_{T \to \infty} h[p(T)]/T. \)

\[ \square \]
We have a famous result that the maximal entropy under fixed variance is achieved by normal distributions [30]:

**Lemma 6.** For a continuous probability density function \( p \) on \( \mathbb{R}^n \) with fixed covariance matrix \( \Sigma \), its entropy \( h[p] \) satisfies

\[
h[p] \leq \frac{1}{2} \left[ n + \log \left( 2^n \pi^n \det \Sigma \right) \right].
\]

The equality holds if and only if \( p \) is an \( n \)-dimensional normal distribution with covariance matrix \( \Sigma \).

The last step is using variance to bound entropy. But variance does not naturally exist for all Markov chains. Also, the distribution is discrete. We can utilize the embedding of Markov chain into \( n \)-torus, then expand it. Now the lifted Markov chain is embedded into \( \mathbb{R}^n \). Since we only embed finite states into a torus, we can put hypercubes centered at each state, such that these hypercubes do not intersect. Denote the length of these hypercubes by \( l \). Then we construct a Markov process with finite density function.

The initial density is 0 outside all hypercubes, and equals \( p_{i\alpha}(0)/l^n \) in the hypercube centered at state \( i\alpha \). For a point inside the hypercube centered at state \( i\alpha \), it has transition rate \( q_{ij} \) to jump to an adjacent hypercube centered at state \( j\beta \). The destination is uniformly distributed in this hypercube. Therefore, the density of this new Markov process at time \( t \) is 0 outside all hypercubes, and equals \( p_{i\alpha}(t)/l^n \) in the hypercube centered at state \( i\alpha \). At any time, the entropies of the Markov chain distribution and this Markov process distribution only differ by a constant \( n \log l \). Now the process is in \( \mathbb{R}^n \), and the distribution is continuous.

**Lemma 7.** Consider the Markov process \( X(t) \) on \( \mathbb{R}^n \) defined above with initial distribution \( p(x, 0) \). Assume the initial distribution has finite covariance matrix. Then there exist constants \( C, T_0 \) such that for any \( T > T_0, i, j = 1, \ldots, n, |\text{Cov}[X(T)]_{ij}| \leq CT^2 \).

**Proof.** For any jump, the step length at each coordinate direction has an upper bound \( L \). Then starting from any initial distribution, for \( i = 1, \ldots, n, \Delta t > 0 \) and any \( 0 \leq \Delta t' \leq \Delta t \),

\[
\text{Var}[X_i(t + \Delta t') - X_i(t)] \leq \left[ X_i(t + \Delta t') - X_i(t) \right]^2 \leq \mathbb{E}N^2(t, t + \Delta t') \leq \mathbb{E}N^2(t, t + \Delta t),
\]

where \( N(t, t + \Delta t) \) is the number of jumps in time interval \( [t, t + \Delta t] \).
Now set \( q = \max q_{ij} \), and define a new process with transition rates \( q'_{ij} = q \). Denote the number of jumps in time interval \([t, t + \Delta t]\) by \( N_0(t, t + \Delta t) \), then we have \( N(t, t + \Delta t) \leq N_0(t, t + \Delta t) \). \( N_0(t, t + \Delta t) \) is a Poisson variable with parameter \( q\Delta t \), therefore \( \mathbb{E}N_0^2(t, t + \Delta t) = q\Delta t + (q\Delta t)^2 < \infty \).

Then we can choose a constant \( G \) and a small enough \( \Delta t \) such that for any \( 0 \leq \Delta t' \leq \Delta t \),

\[
\text{Var}\left[X_i(t + \Delta') - X_i(t)\right] \leq G\Delta t,
\]

regardless of the value of \( X(t) \).

Denote \( D = \max_i \text{Var}[X_i(0)] \).

For a fixed \( T > 0 \), set \( m = \lceil T/\Delta t \rceil \). Then

\[
\text{Cov}[X(T)] = \text{Cov}\{X(0) + [X(\Delta t) - X(0)] + \cdots + [X(T) - X((m-1)\Delta t)]\}.
\]

For two random variables \( Y, Z \), we have \( |\text{Cov}(Y, Z)| \leq \sqrt{\text{Var}[Y]\text{Var}[Z]} \).

Applying this inequality to \( \text{Cov}[X(T)] \), we have

\[
|\text{Cov}[X(T)]_{ij}| \leq D + 2m\sqrt{2DG\Delta t} + 2m^2G\Delta t
\]

When \( T \) is large enough, \( |\text{Cov}[X(T)]_{ij}| \leq 3(T/\Delta t)^2G\Delta t. \)

When \( |\text{Cov}[X(T)]_{ij}| \leq CT^2 \), \( \det \text{Cov}[X(T)] \leq n!C^2nT^{2n} \). Combining the above two lemmas, we have

**Lemma 8.** For the lifted Markov process \( X(t) \) on \( \mathbb{R}^n \), assume the initial distribution \( p(x, 0) \) has finite covariance matrix. Then its entropy at time \( T \), \( h(T) \), is controlled by \( C'' \leq h(T) \leq C' \log T \) for \( T \) large enough, where \( C' \) and \( C'' \) are constants. Therefore \( \lim_{T \to \infty} h(T)/T = 0 \).

This finishes the proof of Theorem 3.

### E. Entropy production as energy dissipation

Consider the free energy with detailed balance stationary measure \( \mu = \exp(-\varphi) \)

\[
F^\mu(t) = \sum_{i\alpha} p_{i\alpha}(t) \log \frac{p_{i\alpha}(t)}{\mu_{i\alpha}} = \sum_{i\alpha} p_{i\alpha}(t) \log p_{i\alpha}(t) + \sum_{i\alpha} p_{i\alpha}(t)\varphi_{i\alpha}.
\]

Here \( S(t) = -\sum_{i\alpha} p_{i\alpha}(t) \log p_{i\alpha}(t) \) is the entropy, and \( E(t) = \sum_{i\alpha} p_{i\alpha}(t)\varphi_{i\alpha} \) is the mean potential energy. Thus \( F^\mu(t) = E(t) - S(t) \).

For \( E(t) \), we have the following result:
**Proposition 3.** The time derivative of $E(t)$ converges to the negative stationary entropy production rate,
\[
\frac{dE(t)}{dt} \to -\bar{e}_p.
\]

**Proof.**
\[
\frac{dE(t)}{dt} + \bar{e}_p(t) = \sum_{i_\alpha \sim j_\beta} [p_{i_\alpha}(t)q_{ij} - p_{j_\beta}(t)q_{ji}] \log \frac{\mu_{i_\alpha} \bar{p}_i(t)q_{ij}}{\mu_{j_\beta} \bar{p}_j(t)q_{ji}} \to \frac{1}{2} \sum_{i,j} (\bar{\pi}_i q_{ij} - \bar{\pi}_j q_{ji}) \log \frac{\bar{\pi}_i}{\bar{\pi}_j}.
\]

The last term is the time derivative of $\sum_i \bar{p}_i(t) \log \bar{p}_i(t)$ when $\bar{p}_i(t) = \bar{\pi}_i$, which is 0. 

In the decomposition of free energy $F^\mu(t) = E(t) - S(t)$, the first term is asymptotically linear with $t$, and the second term is sub-linear with $t$ (controlled by $C \log t$).

The entropy production of the finite Markov chain, which cannot be described by system status quantities directly, is reflected by the free energy/potential energy dissipation of the lifted Markov chain.

**IV. LIFTING AND THERMODYNAMIC QUANTITIES OF MULTIDIMENSIONAL DIFFUSION PROCESSES**

**A. Diffusion processes on Euclidean space and torus**

Consider a time-homogeneous diffusion process $X(t)$ on $\mathbb{R}^n$:
\[
dX(t) = \Gamma(X)dB(t) + b(X)dt,
\]
where $B(t)$ is an $n$-dimensional standard Brownian motion. The drift parameter $b(x)$ is $\mathbb{R}^n \to \mathbb{R}^n$, $C^\infty$, with period 1 for each component. The diffusion parameter $\Gamma(x)$ is $\mathbb{R}^n \to \mathbb{R}^{n \times n}$, non-degenerate for each $x$, $C^\infty$, and 1-periodic for each component. We shall also denote $D(x) = \frac{1}{2} \Gamma(x) \Gamma^T(x)$. It is positive definite for each $x$. All vectors are $n \times 1$.

The transition probability density function $f(x, t | x_0)$ of the diffusion process $X(t)$ is the fundamental solution to the linear, Kolmogorov forward equation:
\[
\frac{\partial f(x, t)}{\partial t} = -\nabla \cdot \left[ b(x)f(x, t) \right] + \nabla \cdot \nabla \cdot \left[ D(x)f(x, t) \right].
\] (2)

For an $n \times n$ matrix $M$ with $i$-th row $M_i$, $\nabla \cdot M$ is defined as $n \times 1$ vector $(\nabla \cdot M_1, \cdots, \nabla \cdot M_n)^T$. 

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In parallel, consider a time-homogeneous diffusion process $X(t)$ on $\mathbb{T}^n$, where $\mathbb{T}^n$ is defined as $[0, 1)^n$:

$$d\bar{X}(t) = \bar{\Gamma}(\bar{X})dB(t) + \bar{b}(\bar{X})dt.$$ 

Here $\bar{B}(t)$ is an $n$-dimensional standard Brownian motion on $\mathbb{T}^n$. $\bar{\Gamma}(\cdot)$ and $\bar{b}(\cdot)$ are the restrictions of $\Gamma(\cdot)$ and $b(\cdot)$ on $\mathbb{T}^n$. Similarly, the transition probability density function for $\bar{X}(t)$, $\bar{f}(\bar{x}, t|\bar{x}_0)$ satisfies the Kolmogorov forward equation:

$$\frac{\partial \bar{f}(\bar{x}, t)}{\partial t} = -\nabla \cdot [\bar{b}(\bar{x})\bar{f}(\bar{x}, t)] + \nabla \cdot \nabla \cdot [\bar{D}(\bar{x})\bar{f}(\bar{x}, t)],$$

(3)

in which $\bar{D}(\cdot)$ and $\bar{b}(\cdot)$ are the restrictions of $D(\cdot)$ and $b(\cdot)$ on $\mathbb{T}^n$.

For the above diffusion process $X(t)$ on $\mathbb{R}^n$ with periodic diffusion and drift, we can “fold” the trajectories to $\mathbb{T}^n$ by

$$\bar{X}(t) = X(t) \mod 1,$$

where $\mod 1$ is for every component. Since $b(\cdot)$ and $\Gamma(\cdot)$ are 1-periodic, the folded process on $\mathbb{T}^n$ is exactly the above diffusion process $\bar{X}(t)$ on $\mathbb{T}^n$. Therefore, the corresponding density function on $\mathbb{T}^n$ is

$$\bar{f}(\bar{x}, t) = \sum_{i_1=-\infty}^{+\infty} \cdots \sum_{i_n=-\infty}^{+\infty} f(\bar{x} + i_1e_1 + \cdots + i_ne_n, t),$$

(4)

where $e_k$ is an elementary $n$-vector, with 1 as its $k$-th component and 0 for other components. Eq. (4) can be directly verified based on the linearity of Kolmogorov forward equation.

For the diffusion process $\bar{X}(t)$ on $\mathbb{T}^n$, we can also lift it to a diffusion process $X(t)$ on $\mathbb{R}^n$, and the above relationship between $f(\bar{x}, t)$ and $\bar{f}(\bar{x}, t)$ is still valid.

**B. Stationary distributions and measures**

The diffusion process $\bar{X}(t)$ on $\mathbb{T}^n$ has a stationary distribution $\bar{\rho}(\bar{x})$. Its 1-periodic continuation to $\mathbb{R}^n$,

$$\rho(x) = \bar{\rho}(x \mod 1),$$

is a stationary measure of the diffusion process $X(t)$ on $\mathbb{R}^n$.

To further study the stationary distributions and measures, we need to consider the relative entropy of $f(\bar{x}, t)$ with respect to any stationary measure $\nu(\bar{x})$

$$\mathcal{D}_{KL}[f(t), \nu] = \int_{\mathbb{R}^n} f(\bar{x}, t) \log \frac{f(\bar{x}, t)}{\nu(\bar{x})} d\bar{x}.$$
Lemma 9. $D_{KL}[f(t), \nu]$ is monotonically decreasing with $t$.

Proof. 

$$D_{KL}[f(t), \nu] = \frac{d}{dt} \int_{\mathbb{R}^n} f \log \frac{f}{\nu} \, dx = \int_{\mathbb{R}^n} \frac{\partial f}{\partial t} \log \frac{f}{\nu} \, dx + \int_{\mathbb{R}^n} \frac{\partial f}{\partial t} \, dx$$

$$= \int_{\mathbb{R}^n} [-\nabla \cdot (b_f) + \nabla \cdot (D_f)] \log \frac{f}{\nu} \, dx$$

$$= \int_{\partial \mathbb{R}^n} \nabla \cdot \left[ -b_f \log \frac{f}{\nu} + \nabla \cdot (D_f) \log \frac{f}{\nu} \right] \, dS - \int_{\mathbb{R}^n} [-b_f + \nabla \cdot (D_f)] \cdot \nabla \left( \log \frac{f}{\nu} \right) \, dx$$

$$= -\int_{\mathbb{R}^n} [-bf + f \nabla \cdot D + D \nabla f] \cdot \left( \frac{\nu}{f} \nabla f \right) \, dx$$

$$= -\int_{\mathbb{R}^n} \left[ -bf + f \nabla \cdot D + D \frac{\nu}{f} \nabla f \right] \cdot \nabla \left( \frac{f}{\nu} \right) \, dx$$

$$= -\int_{\partial \mathbb{R}^n} \nabla \cdot \left[ -bf + f \nabla \cdot (D_f) - D \nabla f + D \frac{\nu}{f} \nabla f \right] \cdot \nabla \left( \frac{f}{\nu} \right) \, dx$$

$$= \int_{\partial \mathbb{R}^n} \nabla \cdot \left( D \left( \frac{\nu}{f} \nabla f - \nabla \nu \right) \right) \cdot \nabla \left( \frac{f}{\nu} \right) \, dx$$

$$= \int_{\partial \mathbb{R}^n} \nabla \cdot \left( \frac{f}{\nu} D f \nabla \nu \right) \, dS + \int_{\mathbb{R}^n} \frac{f}{\nu} \nabla \cdot \left[ D \left( \frac{\nu}{f} \nabla f - \nabla \nu \right) \right] \, dx$$

$$= \int_{\partial \mathbb{R}^n} \nabla \cdot \left( \frac{f}{\nu} D f \nabla \nu \right) \, dS + \int_{\mathbb{R}^n} \left( D f \nabla \frac{\nu}{f} \right) \cdot \nabla \frac{f}{\nu} \, dx$$

$$= -\int_{\mathbb{R}^n} \left( f \nabla \nu - \nu \nabla f \right)^T \frac{D}{f \nu^2} (f \nabla \nu - \nu \nabla f) \, dx,$$

which is non-positive. It is 0 if and only if $f \nabla \nu = \nu \nabla f$, namely $\nabla \log f = \nabla \log \nu$, thus $f = c\nu$ for a constant $c$.

The above lemma is also valid for diffusion on torus, thus $D_{KL}[\tilde{f}(t), \tilde{\rho}]$ is monotonically decreasing for any $\tilde{f}$. If the diffusion on torus has another stationary distribution $\tilde{\theta}$, then $D_{KL}[\tilde{\theta}, \tilde{\rho}]$ is a constant. However it should decrease unless $\tilde{\rho} = c\tilde{\theta}$, which means $\tilde{\theta} = \tilde{\rho}$. Therefore, the diffusion on torus has unique stationary distribution, and any initial distribution will converge to it.

The lifted diffusion on $\mathbb{R}^n$ has no stationary distribution. An intuition is that $\mathbb{R}^n$ is not compact, and the density function $f(x, t)$ will converge to 0 at each $x$ as $t \to \infty$. 

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Proposition 4. The lifted diffusion process has no stationary probability distribution.

Proof. Assume there exists a stationary probability distribution $p$. Let $f(t) = p$, then $D_{KL}(p, \rho)$ is a constant. This is true only if the equality holds in Lemma[9] which means $p$ and $\rho$ only differ by a constant multiple. However $\rho$ is non-normalizable, so is $f$. \hfill \Box

Notice that
\[
\sum_{i_1 = -\infty}^{+\infty} \ldots \sum_{i_n = -\infty}^{+\infty} f(\bar{x} + i_1 e_1 + \cdots + i_n e_n, t) = \bar{f}(\bar{x}, t)
\]
will converge to $\bar{\rho}(\bar{x})$.

Different from lifted Markov chain, the detailed balance measure does not always exist for lifted diffusion.

If the detailed balance measure exists, then the probability flux satisfies
\[
J = \nabla \cdot (Df) - bf = 0.
\]

This is equivalent with
\[
-D^{-1}(\nabla \cdot D - b) = \nabla \log f.
\]

In general, this is impossible, since $D^{-1}(\nabla \cdot D - b)$ may not be curl-free (conservative).

The idea of lifting is that, the process has asymmetric cycles. For Markov chain, since cycle number is finite, we can expand all of them, such that in the lifted Markov chain, there is no asymmetric cycle. For diffusion process on $T^n$, there are $n$ non-trivial basic cycles, which might be asymmetric. We expand these cycles and lift the process into $\mathbb{R}^n$. However, there are still infinite many local cycles in the lifted process, which are homotopic to a single point. In such local cycles, the curl is not always 0, therefore these cycles might be asymmetric, and we cannot expand all of them [28].

Assume that $-D^{-1}(\nabla \cdot D - b) = \nabla g(\bar{x})$ is curl-free in $\mathbb{R}^n$. Then there exists a detailed balance stationary measure, $\mu(\bar{x}) = ce^{g(\bar{x})}$, where $c$ is any positive number. Then $J = \nabla \cdot (D\mu) - b\mu = 0$.

C. Instantaneous entropy production rate, free energy, and housekeeping heat

For the diffusion process $\bar{X}(t)$ on $T^n$, one could define several thermodynamics quantities: entropy production rate, free energy and housekeeping heat.

Definition. The instantaneous free energy on torus $\bar{F}(t)$ is defined as $\bar{F}(t) = D_{KL}(\bar{f}, \bar{\rho})$. 

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Definition. The instantaneous entropy production rate on torus $\mathcal{E}_p(t)$ is defined as \([17]\)

$$
\mathcal{E}_p(t) = \int_{\mathbb{T}^n} \frac{1}{f} [-b f + f \nabla \cdot D + D \nabla f] D^{-1} [-b f + f \nabla \cdot D + D \nabla f] d\mathbf{x}.
$$

This definition is derived from the original idea of entropy production rate that it describes the difference between a process and its time inverse.

Definition. The instantaneous housekeeping heat on torus $\mathcal{Q}_{hk}(t)$ is defined as $\mathcal{E}_p(t) + d\mathcal{F}(t)/dt$.

For the lifted diffusion process $X(t)$ on $\mathbb{R}^n$ with probability density function is $f(x, t)$, since there is no stationary distribution, one could choose a stationary measure instead. In general stationary measure is not unique, therefore one could have different versions of free energy and housekeeping heat.

Definition. The instantaneous free energy with respect to stationary measure $\nu$, $F^\nu(t)$, is defined as

$$
F^\nu(t) = \int_{\mathbb{R}^n} \left[ -b f + f \nabla \cdot D + D \nabla f \right] \cdot \left[ \frac{\nabla f}{f} + D^{-1} \nabla \cdot D - D^{-1} b \right] d\mathbf{x}.
$$

Definition. The instantaneous entropy production rate $e_p(t)$ is defined as \([17]\)

$$
e_p(t) = \int_{\mathbb{R}^n} (-b f + f \nabla \cdot D + D \nabla f)^T f^{-1} D^{-1} (-b f + f \nabla \cdot D + D \nabla f) d\mathbf{x}
$$

$$
= \int_{\mathbb{R}^n} \left[ -b f + f \nabla \cdot D + D \nabla f \right] \cdot \left[ \frac{\nabla f}{f} + D^{-1} \nabla \cdot D - D^{-1} b \right] d\mathbf{x}.
$$

Definition. The instantaneous housekeeping heat with respect to stationary measure $\nu$, $Q^\nu_{hk}(t)$, is defined as

$$
Q^\nu_{hk}(t) = e_p(t) + dF^\nu(t)/dt = \int_{\mathbb{R}^n} \left[ -b f + f \nabla \cdot D + D \nabla f \right] \cdot \left[ \frac{\nabla f}{f} + D^{-1} \nabla \cdot D - D^{-1} b \right] d\mathbf{x}.
$$

From Lemma 9, $dF^\nu(t)/dt \leq 0$. Since $D$ is positive definite, $e_p(t) \geq 0$. For $Q^\nu_{hk}(t)$, we have the same result.

**Proposition 5.** $Q^\nu_{hk}(t) \geq 0$.

**Proof.**

$$
Q^\nu_{hk}(t) = \int_{\mathbb{R}^n} \left[ -b f + f \nabla \cdot D + D \nabla f \right] \cdot \left[ \frac{\nabla f}{f} + D^{-1} \nabla \cdot D - D^{-1} b \right] d\mathbf{x}
$$
\[
\int_{\mathbb{R}^n} f \left[ \frac{\nabla \nu}{\nu} + D^{-1} \nabla \cdot D - D^{-1} b \right]^T D \left[ -D^{-1} b + D^{-1} \nabla \cdot D + \frac{\nabla f}{f} \right] \, dx
\]
\[
= \int_{\mathbb{R}^n} f \left[ \frac{\nabla \nu}{\nu} + D^{-1} \nabla \cdot D - D^{-1} b \right]^T D \left[ -D^{-1} b + D^{-1} \nabla \cdot D + \frac{\nabla \nu}{\nu} \right] \, dx
\]
\[
+ \int_{\mathbb{R}^n} f \left[ \frac{\nabla \nu}{\nu} + D^{-1} \nabla \cdot D - D^{-1} b \right]^T D \left[ -\frac{\nabla \nu}{\nu} + \frac{\nabla f}{f} \right] \, dx.
\]

Since \( D \) is positive definite, the first term is non-negative. The second term equals
\[
\int_{\mathbb{R}^n} [D \nabla \nu + \nu \nabla \cdot D - b \nu]^T f \left[ -\frac{\nabla \nu}{\nu} + \frac{\nabla f}{f} \right] \, dx
\]
\[
= \int_{\mathbb{R}^n} [D \nabla \nu + \nu \nabla \cdot D - b \nu]^T \nabla \left( \frac{f}{\nu} \right) \, dx
\]
\[
= -\int_{\mathbb{R}^n} \frac{f}{\nu} \nabla \cdot [D \nabla \nu + \nu \nabla \cdot D - b \nu] \, dx = 0,
\]
since \( \nu \) is a stationary measure, \( \nabla \cdot \nabla \cdot (D \nu) - \nabla \cdot (b \nu) = 0 \).

Thus we have the decomposition
\[
e_p(t) = Q_{hh}^\nu(t) + [-dF^\nu(t)/dt],
\]
where each term is non-negative. This is also valid for the torus version.

**D. Time limits of thermodynamic quantities**

Since \( \bar{f}(t) \) converges to \( \bar{\rho} \), \( F(t) \) and \( dF(t)/dt \) converge to 0, \( e_p(t) \) and \( Q_{hh}(t) \) converge to the stationary entropy production rate
\[
e_p = \int_{\mathbb{T}^n} \frac{1}{\bar{\rho}} [-b \bar{\rho} + \bar{\rho} \nabla \cdot D + D \nabla \bar{\rho}]^T D^{-1} [-b \bar{\rho} + \bar{\rho} \nabla \cdot D + D \nabla \bar{\rho}] \, d\bar{x}.
\]

For the lifted diffusion process, \( f(t) \) does not converge to a stationary distribution, therefore we do not have the stationary version of these quantities. However, we can still study their behavior as \( t \to \infty \).

If we set \( \nu \) to be the periodic stationary measure \( \rho \), then \( Q_{hh}^\rho(t) \) converges to
\[
\int_{\mathbb{T}^n} [-b \bar{\rho} + \bar{\rho} \nabla \cdot D + D \nabla \bar{\rho}] \cdot \left[ \frac{\nabla \bar{\rho}}{\bar{\rho}} + D^{-1} \nabla \cdot D - D^{-1} b \right] \, d\bar{x},
\]
which is just \( e_p \).

If we set \( \nu \) to be the detailed balance stationary measure \( \mu \) (if exists), then \( Q_{hh}^\mu(t) \equiv 0 \) since \( \nabla \cdot (D \mu) - b \mu = 0 \).

For the time limit of \( e_p(t) \), we have the following theorem. The proof is in the next part.
Theorem 4. For any initial distribution \( f(x, 0) \) that has a finite covariance matrix, the entropy production rate of diffusion process \( X(t) \) on \( \mathbb{R}^n \), \( e_p(t) \), also converges to \( \bar{e}_p \) in Cesàro’s sense that

\[
\lim_{T \to \infty} \frac{1}{T} \int_0^T e_p(t) \, dt = \bar{e}_p.
\]

In summary, \( e_p = Q^\nu_{hk} + (-dF^\nu / dt) \), where \( e_p \), \( Q^\nu_{hk} \) and \( -dF^\nu / dt \) are non-negative.

\( e_p \to \bar{e}_p \) in Cesàro’s sense, \( dF^\mu / dt = -e_p \to -\bar{e}_p \) in Cesàro’s sense, \( Q^\mu_{hk} \equiv 0 \), \( dF^\rho / dt \to 0 \) in Cesàro’s sense, \( Q^\rho_{hk} \to \bar{e}_p \) in general sense.

Therefore, the periodic stationary measure \( \rho \) and the detailed balance stationary measure \( \mu \) reach the maximum and minimum of \( Q^\nu_{hk} \), \( \bar{e}_p \) and \( 0 \), as \( t \to \infty \).

When \( -D^{-1}(\nabla \cdot D - b) \) is not curl-free, \( \mu \) does not exist, and the minimum of \( Q^\nu_{hk} \) is larger than 0.

For the two special stationary measures \( \rho \) and \( \mu \), the expectation of their Radon-Nikodym derivative is

\[
\int_{\mathbb{R}^n} f(t) \frac{\mu}{\rho} \, dx.
\]

Since

\[
dF^\rho(t)/dt - dF^\mu(t)/dt = \int_{\mathbb{R}^n} \left[ -bf + f\nabla \cdot D + D\nabla f \right] \cdot \left[ \frac{\nabla \rho}{\rho} - \frac{\nabla \mu}{\mu} \right] \, dx = Q^\rho_{hk}(t) - Q^\mu_{hk}(t),
\]

we have

\[
\frac{d}{dt} \int_{\mathbb{R}^n} f(t) \frac{\mu}{\rho} \, dx = dF^\rho(t)/dt - dF^\mu(t)/dt = Q^\rho_{hk}(t) - Q^\mu_{hk}(t) \to \bar{e}_p.
\]

E. Proof of Theorem

The proof consists of the following lemmas. The key idea is that we have

\[
e_p(t) - \bar{e}_p(t) = \frac{dF(t)}{dt} - \frac{dF^\rho(t)}{dt}.
\]

Also \( \bar{e}_p(t) \to \bar{e}_p \), \( d\bar{F}(t)/dt \to 0 \).

For \( F^\rho(t) \), we prove \( dF^\rho(t)/dt \leq 0 \), and \( F^\rho(t) > -C \log t \) for large \( t \). Thus

\[
\lim_{T \to \infty} \frac{1}{T} \int_0^T \frac{dF^\rho(t)}{dt} \, dt = 0,
\]

therefore we have

\[
\lim_{T \to \infty} \frac{1}{T} \int_0^T e_p(t) \, dt = \bar{e}_p.
\]
But these are not enough for $dF^p(t)/dt \to 0$, therefore we do not have $e_p(t) \to \bar{e}_p$.

For a distribution $q(x)$, its entropy is defined as

$$h[q] = \int_{\mathbb{R}^n} -q(x) \log q(x) dx.$$  

**Lemma 10.** Assume the initial distribution $f(x, 0)$ has finite covariance matrix for any $x$. Then $\lim_{T \to \infty} \frac{1}{T} \int_0^T e_p(t) dt - \bar{e}_p = 0$ is equivalent with $\lim_{T \to \infty} F^\rho(T)/T = 0$.

**Proof.** We have

$$e_p(t) - \bar{e}_p(t) = \int_{\mathbb{R}^n} \frac{1}{f} (\nabla f)^T Df \nabla f dx - \int_{\mathbb{R}^n} \frac{1}{\bar{f}} (\nabla \bar{f})^T D\bar{f} \nabla \bar{f} dx = -\frac{dF^\rho(t)}{dt} + \frac{d\bar{F}(t)}{dt}.$$  

Thus

$$\frac{1}{T} \int_0^T e_p(t) dt - \frac{1}{T} \int_0^T \bar{e}_p(t) dt = \frac{1}{T} [F^\rho(0) - F^\rho(t) + \bar{F}(T) - \bar{F}(0)].$$

Since $f(x, t)$ converges to $\rho(x)$, $\bar{F}(t)$ converges to 0, therefore $\bar{T}$ is bounded.

$F^\rho(0) - \bar{F}(0) = h[\bar{f}(0)] - h[f(0)]$. Since $f(x, 0)$ has finite covariance matrix, Lemma 6 shows that $h[f(0)]$ is finite, so as $h[\bar{f}(0)]$.

We also have $\lim_{T \to \infty} \frac{1}{T} \int_0^T \bar{e}_p(t) dt = \bar{e}_p$.

Therefore $\lim_{T \to \infty} \frac{1}{T} \int_0^T e_p(t) dt - \bar{e}_p = \lim_{T \to \infty} F^\rho(T)/T$.  

\[\square\]

The next step is to control $F^\rho(T)$ for large $T$. Since $F^\rho(T) = -h[f(T)] - \int_{\mathbb{R}^n} f(x, T) \log \rho dx$, and $\int_{\mathbb{R}^n} f(x, T) \log \rho dx$ converges to $\int_{\mathbb{R}^n} \rho(x) \log \rho(x) dx$, which is finite, we only need to show $h[f(T)]/T \to 0$.

Since $f(x, t) \leq \bar{f}(x, t)$, $\bar{f}(x, t)$ converges to $\rho(x)$, $f(x, t)$ has a uniform upper bound for large $t$. Therefore $h[p(t)]$ has a finite lower bound for large $t$. We only need to control $h[f(t)]$ from above. From Lemma 6 we need to control the covariance matrix of the diffusion process.

**Lemma 11.** Consider the diffusion process $X(t)$ on $\mathbb{R}^n$ with initial distribution $f(x, 0)$. Assume the initial distribution $f(x, t)$ has finite covariance matrix. Then there exist constants $C, T_0$ such that for any $T > T_0$, $i, j = 1, \cdots, n$, $|\text{Cov}[X(T)]_{ij}| \leq CT^2$.

**Proof.** For the diffusion process $X(t)$ on $\mathbb{R}^n$, we have the infinitesimal mean

$$\mathbb{E}[X(t + \Delta t) - X(t) \mid X(t) = x_0] = b(x_0) \Delta t + O(\Delta t^2).$$  

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We also have the infinitesimal variance

\[ \mathbb{E}\{[X(t + \Delta t) - X(t)][X(t + \Delta t) - X(t)]^T \mid X(t) = x_0\} = \Gamma(x_0)\Gamma(x_0)^T \Delta t + O(\Delta t^2). \]

Therefore the covariance matrix satisfies

\[ \text{Cov}[X(t + \Delta t) \mid X(t) = x_0] = \Gamma(x_0)\Gamma(x_0)^T \Delta t + O(\Delta t^2). \]

Set \( G = \max_{x,i} [\Gamma(x)\Gamma(x)^T]_{ii} \). Then we can choose a small enough \( \Delta t \) such that for any \( 0 \leq \Delta t' \leq \Delta t \),

\[ \text{Var}[X_i(t + \Delta t') - X_i(t)] \leq 2G \Delta t, \]

regardless of the value of \( X(t) \).

Denote \( D = \max_i \text{Var}[X_i(0)] \).

For a fixed \( T > 0 \), set \( m = \lceil T/\Delta t \rceil \). Then

\[ \text{Cov}[X(T)] = \text{Cov}\{X(0) + [X(\Delta t) - X(0)] + \cdots + [X(T) - X((m-1)\Delta t)]\}. \]

For two random variables \( Y, Z \), we have \(|\text{Cov}(Y, Z)| \leq \sqrt{\text{Var}[Y]\text{Var}[Z]}\).

Applying this inequality to \( \text{Cov}[X(T)] \), we have

\[ |\text{Cov}[X(T)]_{ij}| \leq D + 2m\sqrt{2DG\Delta t} + 2m^2G\Delta t \]

When \( T \) is large enough, \(|\text{Cov}[X(T)]_{ij}| \leq 3(T/\Delta t)^2G\Delta t\).

When \(|\text{Cov}[X(T)]_{ij}| \leq CT^2\), \(|\det \text{Cov}[X(T)]| \leq n!C^nT^{2n} \). Now we have

**Lemma 12.** For the diffusion process \( X(t) \) on \( \mathbb{R}^n \), assume the initial distribution \( f(x, 0) \) has finite covariance matrix. Then its entropy at time \( T \), \( h(T) \), is controlled by \( C'' \leq h(T) \leq C' \log T \) for \( T \) large enough, where \( C' \) and \( C'' \) are constants. Therefore \( \lim_{T \to \infty} h(T)/T = 0 \).

This finishes the proof of Theorem 4.

In general we do not have \( e_p(t) \to \bar{e}_p \). However, we can prove \( e_p(t) \to \bar{e}_p \) for a special case.

**Proposition 6.** For the diffusion process \( X(t) \) on \( \mathbb{R}^n \), if \( b(x) \) and \( \Gamma(x) \) are constants, initial distribution \( f(x, 0) \) has finite covariance matrix, then \( \lim_{t \to \infty} e_p(t) = \bar{e}_p \).
Proof. We need to prove \( dF^\rho(t)/dt \to 0 \). Since \( \rho(x) \) is a constant function in this case, we only need \( r(t) = dh[f(t)]/dt \to 0 \). In the following we will prove \( dr(t)/dt \leq 0 \). Then \( r(t) \) is positive and decreasing, therefore it has a limit \( c \). Thus

\[
    c = \lim_{T \to \infty} \frac{1}{T} \int_0^T r(t) dt = 0.
\]

Set \( f_0(x,t) = f(x - bt, t) \), then it is the density function of the no-drift process \( dX_0 = \Gamma dB(t) \). Entropy is invariant under translation, \( h[f(t)] = h[f_0(t)] \), therefore we can set \( b = 0 \). Since \( \Gamma \) is non-degenerate, we have singular value decomposition \( \Gamma = U \Sigma V^T \), where \( U, V \) are orthonormal, and \( \Sigma \) is diagonal and positive. Now \( dU^T X_0 = \Sigma dV^T B \). \( V^T B \) is still an \( n \)-dimensional standard Brownian motion. Since entropy is invariant under rotation, \( Y = U^T X_0 \) has the same entropy with \( X_0 \). We can set \( \Gamma \) to be diagonal and positive. Finally, set \( Z = \Sigma^{-1} X \), then \( dZ = dB \). Now the entropy of \( Z \) and \( X \) only differ by a constant \( \det(\Sigma) \), which does not affect the derivative. Therefore, we only need to prove \( d^2 h[f(t)]/dt^2 \geq 0 \) for process \( dX = dB \), where the Kolmogorov forward equation is heat equation \( f_t = \Delta f/2 \).

The following proof is from [9].

We shall abbreviate \( df/dx_i \) by \( f_i \) in the following to prevent double subscripts. We also assume that the initial condition is sufficiently nice to guarantee integration by parts being valid.

\[
    \frac{dh[f(t)]}{dt} = \int_{\mathbb{R}^n} \frac{\nabla f \cdot \nabla f}{2f} d\mathbf{x}.
\]

\[
    \frac{d^2 h[f(t)]}{dt^2} = \int_{\mathbb{R}^n} \left( \frac{\nabla f \cdot \nabla f_i}{f} - \frac{\nabla f \cdot \nabla f_i f_i}{2f^2} \right) d\mathbf{x}
    \]
\[
    = \int_{\mathbb{R}^n} \left( \frac{1}{2} \sum_{i,j} f_i f_{ij} - \frac{1}{4} \sum_{i,j} \frac{f_i f_i f_{jj}}{f^2} \right) d\mathbf{x}.
\]

Integrate by parts yields,

\[
    \frac{d^2 h[f(t)]}{dt^2} = \int_{\mathbb{R}^n} \left( -\frac{1}{2} \sum_{i,j} f_{ij} f_{ij} - f_{ij} f_{ij} - \frac{1}{4} \sum_{i,j} \frac{f_j f_i f_{ij} - 2f_i f_j f_i f_j}{f^4} \right) d\mathbf{x}
    \]
\[
    = -\frac{1}{2} \int_{\mathbb{R}^n} \left( f_{ij}^2 - \frac{f_i f_j f_{ij}}{f^2} + \frac{f_i f_j^2}{f^3} \right) d\mathbf{x}
    \]
\[
    = -\frac{1}{2} \int_{\mathbb{R}^n} \left( \frac{f_{ij}}{\sqrt{f}} - \frac{f_i f_j}{f \sqrt{f}} \right)^2 d\mathbf{x} \leq 0.
\]
F. Entropy production as energy dissipation

Consider the free energy with detailed balance stationary measure $\mu = \exp(-\varphi)$ (if exists)

$$F^\mu(t) = \int_{\mathbb{R}^n} f(\mathbf{x}, t) \log \frac{f(\mathbf{x}, t)}{\mu(\mathbf{x})} d\mathbf{x} = \int_{\mathbb{R}^n} f(\mathbf{x}, t) \log f(\mathbf{x}, t) d\mathbf{x} - \int_{\mathbb{R}^n} f(\mathbf{x}, t) \log \mu(\mathbf{x}) d\mathbf{x}.$$ 

Here $S(t) = -\int_{\mathbb{R}^n} f(\mathbf{x}, t) \log f(\mathbf{x}, t) d\mathbf{x}$ is the entropy, and $E(t) = \int_{\mathbb{R}^n} f(\mathbf{x}, t) \varphi(\mathbf{x}) d\mathbf{x}$ is the mean potential energy. Thus $F^\mu(t) = E(t) - S(t)$.

For $E(t)$, we have the following result:

**Proposition 7.** The time derivative of $E(t)$ converges to the negative stationary entropy production rate,

$$\frac{dE(t)}{dt} \to -\bar{e}_p.$$ 

**Proof.**

$$\frac{dE(t)}{dt} + \bar{e}_p(t) = \int_{\mathbb{R}^n} [\nabla \cdot (Df) - bf] \cdot \left(\frac{\nabla \mu}{\mu}\right) d\mathbf{x}$$

$$+ \int_{\mathbb{R}^n} [\nabla \cdot (Df) - bf] \cdot \left(\frac{\nabla \bar{f}}{\bar{f}} + D^{-1} \nabla \cdot D - D^{-1} b\right) d\mathbf{x}$$

$$= \int_{\mathbb{T}^n} [\nabla \cdot (D\bar{f}) - \bar{b}\bar{f}] \cdot \left(\frac{\nabla \bar{f}}{\bar{f}}\right) d\bar{\mathbf{x}} = -\int_{\mathbb{T}^n} \nabla \cdot [\nabla \cdot (D\bar{f}) - \bar{b}\bar{f}] \log \bar{f} d\bar{\mathbf{x}}$$

$$= -\int_{\mathbb{T}^n} \nabla \cdot [\nabla \cdot (D\bar{\rho}) - \bar{b}\bar{\rho}] \log \bar{\rho} d\bar{\mathbf{x}} = 0.$$

In the integral $\int_{\mathbb{T}^n} \cdots d\mathbf{x}$, $\bar{f}(\mathbf{x})$ is the 1-periodic extension of $\bar{f}(\bar{\mathbf{x}})$. We also apply the facts that $\nabla \cdot [\nabla \cdot (D\bar{\rho}) - \bar{b}\bar{\rho}] = 0$ and $\frac{\nabla \mu}{\mu} + D^{-1} \nabla \cdot D - D^{-1} b = 0$. 

$$\Box$$

In the decomposition of free energy $F^\mu(t) = E(t) - S(t)$, the first term is asymptotically linear with $t$, and the second term is sub-linear with $t$ (controlled by $C \log t$).

The entropy production of the diffusion process on $\mathbb{T}^n$, which cannot be described by system status quantities directly, is reflected by the free energy/potential energy dissipation of the lifted diffusion process on $\mathbb{R}^n$. 

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V. DISCUSSION AND SUMMARY OF CONCLUSIONS

A. Gibbs potential and Kirkwood’s potential of mean force

Relative entropy w.r.t. the Lebesgue measure, e.g., Gibbs-Shannon’s entropy, is not the most appropriate information characteristics for system with a nontrivial invariant measure. This insight has already in the work of classical thermodynamics, where entropy as the “thermodynamic potential” of an isolated system with a priori equal probability is replaced by the free energy as the proper thermodynamic potential for an isothermal system. In Gibbs’ theory of chemical thermodynamics, chemical potential of a chemical special $i$ has actually three parts:

$$\mu_i = \mu_i^0 + k_B T \log x_i = h^0 - T s^0 + k_B T \log x_i.$$ 

B. The nature of nonequilibrium dissipation

The nature of “thermodynamic dissipation” has long been debated. A notion that is generally agreed upon was put forward by Onsager [22], who clearly identified a dissipation with a transport process, with both nonzero thermodynamic force and thermodynamic flux. In fact, they are necessarily vanishing simultaneously in a thermodynamic equilibrium with detailed balance. This gives rise to the reciprocal relation in the linear regime near equilibrium. Macroscopic transport processes, however, can be classified into two gross types: Those induced by a nonequilibrium initial condition and those driven by an active forcing. This distinction, we believe, is precisely behind Clausius’ and Kelvin’s statements of the Second Law of thermodynamics, as well as behind the irreversibility formulated by Boltzmann and I. Prigogine, respectively. Still, in the latter case, the precise physical step(s) at which dissipation occurs has generated a wide range of arguments: It is attributed to the external driving force, to the transport processes themselves inside a system, and to the “boundary” where a system in contact with its nonequilibrium environment [2]. Our mathematical theory clearly indicates that all these perspectives are not incorrect, but a more precise, complete notion really is to identify nonequilibrium cycles which have been independently discovered by T. L. Hill [15] and by Laudauer and Bennett [4], in biochemistry and computation respectively.

A cyclic macroscopic transport process driven by a sustained nonequilibrium environment is of course an idealization of the reality: A battery has to be re-charged, the chemical solution that sustains a chemostat has to be replenished. In fact, almost all engineering systems do not use a
continuously charged energy source, but rather rely on the principle of quasi-stationarity \([11]\): A narrow range of decreasing external driving force is acceptable. Therefore, by clearly recognizing the source of a driving force, the cycles inside a finite driven system can and should be identified with a spontaneous “downhill” of an external process, as clearly shown in the present paper. In fact, a perfect stationary driving force, which is represented by the house-keeping heat in the present work, corresponds to an unbounded potential energy function on a non-compact space.

Mathematically, this lifting of a driven system with discrete state space or continuous \(n\)-torus state spaces has been rigorously established in the present work. Generalization of this result to \(\mathbb{R}^n\) without local potential is technically challenging, but that should not prevent our understanding of the nature of the physics of nonequilibrium dissipation. In fact, we propose a modernized, combined Clausius-Kelvin statement:

“A mesoscopic engine that works in completing irreversible internal cycles statistically has necessarily an external effect that passes heat from a warmer to a colder body.”

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