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A Simple Discrete Model of Brownian Motors: Time-periodic Markov Chains

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In this paper, we consider periodically inhomogeneous Markov chains, which can be regarded as a simple version of physical model—Brownian motors. We introduce for them the concepts of periodical reversibility, detailed balance, entropy production rate and circulation distribution. We prove the equivalence of the following statements: The time-periodic Markov chain is periodically reversible; It is in detailed balance; Kolmogorov's cycle condition is satisfied; Its entropy production rate vanishes; Every circuit and its reversed circuit have the same circulation weight. Hence, in our model of Markov chains, the directed transport phenomenon of Brownian motors, i.e. the existence of net circulation, can occur only in nonequilibrium and irreversible systems. Moreover, we verify the large deviation property and the Gallavotti-Cohen fluctuation theorem of sample entropy production rates of the Markov chain.

KEY WORDS: Brownian motor, time-periodic Markov chain, periodical reversibility, detailed balance, entropy production, circulation, fluctuation theorem

1. INTRODUCTION

Noise is unavoidable for any system in thermal contact with its surroundings. In the last three decades, the creative role of noise attracts much interest of physicists and biochemists. For example, in the so-called phenomenon of Brownian motors (or say, ratchet systems),[1,2,4,6,19,22,23,30] a net current of particles can be driven by noise, providing that there is an appropriate asymmetry in the system, such as

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spatially periodic and asymmetric, so-called ratchet potential. However, in the most interesting case, such a potential is unbiased, i.e. the time-, space-, and ensemble-averaged force that it entails is required to vanish, and does not introduce a priori an obvious bias into one or the other direction of motion. Reimann[30] reviews in detail the theoretical models and experimental realizations of this phenomenon of noise-driven mass transport in spatially periodic systems out of thermal equilibrium.

Another earlier known example is the phenomenon of stochastic resonance, in which a weak periodic signal in a nonlinear system can be amplified by added noise. Stochastic resonance was introduced in refs. 3 and 24 to try to explain the Earth's ice-age cycle, but it is now recognized to be far more common, occurring for example in lasers, electronic circuits and sensory neurons. An extensive description of the phenomenon from the physical point of view can be found in ref. 11. The notion of stochastic resonance is now used in a much broader sense, and it describes a wide class of effects that the presence of noise improves some characteristics of the system.

Although several hundreds of papers on each of these two phenomena were published (see references in refs. 11 and 30), only few mathematically rigorous results are known. In many situations, the studied system is subjected to a time-periodic driving, or the temperature of the thermal noise is subjected to periodic temporal variations, which results in considering a stochastic differential equation of the following form,

$$dX_t = b(t, X_t)\,dt + \sigma(t, X_t)\,dW_t, \tag{1}$$

in which W_t is a white noise (Brownian motion), and $b(t, x)$, $\sigma(t, x)$ are periodic in the time parameter t. Its time inhomogeneity causes many difficulties in studying mathematically the property of its solution process.

In this article we consider a discrete variant of (1), a discrete-time Markov chain with time-periodic transition matrices, which will be called a periodically inhomogeneous Markov chain. We will discuss its periodical reversibility, detailed balance, entropy production rate, circulation distribution and the relationship among them. The net circulations of Markov chains and rotation numbers of diffusion processes correspond to the average particle current in Brownian motors,[17,30] which is the quantity of central interest. Imkeller and Pavlyukevich[15] introduced a model, which is a special case of ours, to study the phenomenon of stochastic resonance.

The second law of thermodynamics can be expressed as the entropy increasing principle: When a closed system evolves from one equilibrium steady state to another through an adiabatic process, the entropy of this system can not decrease; if the process is reversible, then its entropy does not change; if not, then its entropy increases.

The concept of entropy production was first put forward in nonequilibrium statistical physics to describe how far a specific state of a system is from its equilibrium state.[14,25,32] It is closely related to another concept of macroscopic irreversibility in nonequilibrium statistical physics. A macroscopic irreversible system in a steady state should have positive entropy production rate and should be in nonequilibrium.

Since 1980's, Qian, M.P., Qian, M. and Gong, G.L. [17,26–29] gave a unified measure-theoretical definition of entropy production rate of a stochastic process as the specific relative entropy of the distribution of the process with respect to that of its time reversal. Moreover, they calculated the formulae of entropy production rate and circulation distribution of homogeneous Markov chains and Q-processes, and discussed their relationship with reversibility: The chain or process is reversible if and only if its entropy production vanishes, or iff there are no net circulation.

Recently, Ruelle[31] took hyperbolic dynamical systems as the mathematical model of nonequilibrium systems, and gave the definition of entropy production rate of such a system from the perspective of statistical physics. Jiang, etc.[16] proved that the entropy production rate of Ruelle's definition can be expressed as the specific relative entropy of the system with respect to that of its time reversal, and its entropy production rate is zero iff the system is reversible.

In this article, we extend the notions and results in refs. 17 and 26–29 to the situation of a periodically inhomogeneous Markov chain, whose definition and basic properties are given in Sec. 2. Then in Sec. 3 we introduce for it the notions of periodical reversibility, detailed balance, entropy production rate and circulation distribution, calculate the expressions of its entropy production rate and circulation distribution, and discuss the relationship among the notions. To our happiness, we get the main result of this article that the following statements are equivalent, which accord excellently with the physical theory: The Markov chain is periodically reversible; It is in detailed balance; Kolmogorov's cycle condition is satisfied; Its entropy production rate vanishes; Every circuit and its reversed circuit have the same circulation weight. Hence the directed transport phenomenon of Brownian motors, i.e. the existence of net circulation in our Markov chain model, can occur only in nonequilibrium and irreversible systems.

In Sec. 4, we consider the large deviation and fluctuation theorem of sample entropy production rates of periodically inhomogeneous Markov chains. We prove that not only the sample entropy production rates converge almost surely to the average entropy production rate, but also their distributions have the large deviation property, and the large deviation rate function has a symmetry of Gallavotti-Cohen type, which is the fluctuation theorem of periodically inhomogeneous Markov chains. The fluctuation theorem was first obtained by Gallavotti and Cohen[10] for hyperbolic dynamical systems, then extended by Evans and Searles,[8,9] and extended to stochastic processes by Kurchan,[20] Lebowitz and Spohn,[21] Jiang, Qian and Zhang,[18] etc.

Section 5 contains some remarks and examples. It will be noticed that there is a close relationship between the simplified Brownian motors—periodically inhomogeneous Markov chains and Parrondo's paradoxical games.[12,13] This model involves two games, each of which played on its own results in loss for the player. But if play alternates periodically or randomly between the two games, the result is a win.

In Sec. 6, we discuss the relationship between stochastic differential equations with time-periodic coefficients (including some models of Brownian motors) and time-periodic Markov chains considered in this paper. We will see that the rocking ratchet system considered in ref. 30 can be approximated by time-periodic birth-death chains. Conversely, such a chain can be obtained by discretizing the Fokker-Planck equation of the ratchet system. Furthermore, if the time-periodic birth-death chain has periodical reversibility, then the particle current in this discrete model of Brownian motor vanishes. Therefore, for our discrete models, non-vanishing particle current exists only in systems of periodically irreversible Markov chains, which correspond to non-equilibrium steady states in statistical physics.

We believe that most results in this paper can be extended to diffusion processes, although there is still a lot to do.

2. DEFINITION AND BASIC PROPERTIES

2.1. Definition

Definition **2.1.** Suppose that $\xi = \{\xi_n : n = 0, 1, 2, \ldots\}$ is an inhomogeneous Markov chain on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ with denumerable state space S and transition probability matrix $P(m, m+1) = (p_{ij}(m, m+1))_{i,j\in S}$(we also write it as $P^m = (p^m_{ij})_{i,j\in S}$ instead for simplicity), where $p_{ij}(m, n) = P(\xi_n = j|\xi_m = i),\ \forall m \le n$. If there exists a positive integer T such that

$$p_{ij}(m, m+1) = p_{ij}(m+T, m+T+1),\ \forall i, j \in S,\ m \in \mathbb{Z}^+, \qquad (2)$$

then we call ξ a **periodically inhomogeneous Markov chain**.

Obviously, (2) implies

$$p_{ij}(m, m+n) = p_{ij}(m+T, m+T+n),\ \forall i, j \in S,\ m, n \in \mathbb{Z}^+. \qquad (3)$$

Without loss of generality, we can assume that $(\Omega, \mathcal{F}, \mathbb{P})$ is the canonical orbit space of ξ with $\Omega = \prod_{\mathbb{Z}^+} S$.

2.2. Periodically Stationary Distribution

Construct T homogeneous Markov chains as follows: $\{\eta^k_n = \xi_{nT+k} : n = 0, 1, \ldots\}$, $k = 0, 1, \ldots, T-1$. Denote their transition probability matrices by

$\tilde{P}^k = (\tilde{p}^k_{ij})_{i,j\in S}$, where

$$\begin{aligned}\tilde{p}^k_{ij} &= \mathbb{P}\big(\eta^k_{n+1} = j|\eta^k_n = i\big) = \mathbb{P}\big(\xi_{(n+1)T+k} = j|\xi_{nT+k} = i\big)\\ &= p_{ij}(nT + k, (n + 1)T + k) = p_{ij}(k, T + k).\end{aligned} \tag{4}$$

Hence,

$$\tilde{P}^k = P(k, k + 1)P(k + 1, k + 2)\cdots P(T + k - 1, T + k). \tag{5}$$

Now, we are ready to deduce several simple but useful properties of the periodically inhomogeneous Markov chain ξ.

Lemma 2.2. *If there exists an $s \in \{0, 1, 2, \ldots, T - 1\}$ such that $\{\eta^s_n\}$ is a homogenous irreducible positive recurrent Markov chain, then there exists a unique probability measure $\pi^s = (\pi^s_i)_{i\in S}$, s.t. $\pi^s\tilde{P}^s = \pi^s$.*

Definition **2.3.** Suppose that there exists a family of probability measures $\pi = \{\pi^k : k = 0, 1, 2, \ldots, T - 1\}$ on the state space S satisfying $\pi^k P(k, k + 1) = \pi^{k+1}$, $k = 0, 1, 2, \ldots, T - 2$, $\pi^{T-1}P(T - 1, T) = \pi^0$, and the periodically inhomogeneous Markov chain $\xi = \{\xi_n : n = 0, 1, 2, \ldots\}$ takes π^0 as its initial distribution, then for each $n = 0, 1, \ldots$, $k = 0, 1, \ldots, T - 1$, the distribution of ξ_{nT+k} is π^k, moreover, the distribution of $\{\xi_n : n = 0, 1, 2, \ldots\}$ is the same as its left shift $\{\xi_{lT+n} : n = 0, 1, 2, \ldots\}$ ($\forall l = 0, 1, \ldots$). In this case we call the chain ξ **periodically stationary**, and the family of probability measures $\pi = \{\pi^k : k = 0, 1, 2, \ldots, T - 1\}$ is said to be its **periodically stationary distribution** (with π^T understood to be π^0).

Proposition 2.4. *Under the condition of Lemma 2.2:*
(1) Let

$$\begin{aligned}&\pi^k = \pi^s P(s, s + 1)P(s + 1, s + 2)\cdots P(k - 1, k),\ k = s + 1, \ldots, T - 1;\\ &\pi^k = \pi^s P(s, s + 1)P(s + 1, s + 2)\cdots P(T + k - 1, T + k),\\ &\quad k = 0, 1, \ldots, s - 1,\end{aligned} \tag{6}$$

then for each $k \in \{0, 1, 2, \ldots, T - 1\}$, $\pi^k = (\pi^k_i)_{i\in S}$ satisfies

$$\begin{aligned}\pi^k P(k, k + 1) &= \pi^{k+1},\\ \pi^k\tilde{P}^k &= \pi^k.\end{aligned} \tag{7}$$

i.e. for each $k \in \{0, 1, 2, \ldots, T - 1\}$, π^k is the unique stationary probability measure of $\{\eta^k_n\}$; Furthermore, if there is not any column in the T matrices $P(m, m + 1)$ such that all of its elements are zero, then all the elements of π^k are positive, which implies $\{\eta^k_n\}$ is a homogenous irreducible positive recurrent Markov chain.

Meanwhile $\pi = \{\pi^k : k = 0, 1, 2, \ldots, T-1\}$ *is the unique family of periodically stationary measures of the periodically inhomogeneous Markov chain* ξ.

(2) Conversely, if for each $k \in \{0, 1, 2, \ldots, T-1\}$*, there exists a unique probability measure* π^k*, such that* $\pi^k \tilde{P}^k = \pi^k$*, then*

$$\pi^k P(k, k+1) = \pi^{k+1}, \ k = 0, 1, 2, \ldots, T-1. \tag{8}$$

Proof: (a) From Lemma 2.2 and the definition of π^k, we have (7). The uniqueness of the stationary distribution of $\{\eta_n^s\}$ guarantees the uniqueness of the stationary measures of the periodically inhomogeneous Markov chain ξ.

(b) The equality (7) implies

$$\pi^0 P(0,1) P(1,2) \cdots P(T-1, T) = \pi^0, \tag{9}$$

$$\pi^1 P(1,2) P(2,3) \cdots P(0,1) = \pi^1. \tag{10}$$

Multiply the two sides of (9) by $P(0, 1)$, then one sees that $\pi^0 P(0,1)$ is another invariant probability measure of P^1. By the uniqueness assumption $\pi^0 P(0,1) = \pi^1$. Similarly one can prove (8). □

From later on in this article, we suppose that:

(H) For each $k \in \{0, 1, \ldots, T-1\}$, $\{\eta_n^k : n = 0, 1, 2, \ldots\}$ *is a homogeneous irreducible positive recurrent Markov chain.*

2.3. Limit Theorems

From the weak limit theorem of transition matrices and the strong law of large numbers for homogeneous irreducible positive recurrent Markov chains, one can directly obtain the following results.

Proposition 2.5. *(Average Limit)*

$$(1)\ \forall k = 0, 1, 2, \ldots, T-1, \ \lim_{n\to\infty} \frac{1}{n} \sum_{l=1}^{n} p_{ij}(k, k+lT) = \pi_j^k,$$

$$(2)\ \forall k = 0, 1, 2, \ldots, T-1, \ \lim_{n\to\infty} \frac{1}{n} \sum_{l=1}^{n} p_{ij}(k, k+l) = \frac{1}{T} \sum_{s=1}^{T} \pi_j^s.$$

Obviously, the limit in (2) is independent of k.

Proposition 2.6. *If f is a bounded function on S, then with probability 1, we have*

$$\lim_{n\to\infty} \frac{1}{n} \sum_{l=0}^{n} f(\xi_l) = \frac{1}{T} \sum_{k=0}^{T-1} \sum_{i\in S} \pi_i^k f(i). \tag{11}$$

3. PERIODICAL REVERSIBILITY AND SOME EQUIVALENT CONDITIONS

3.1. Definition and Detailed Balance Condition

Definition **3.1.** If for some $k \in \{0, 1, 2, \dots, T-1\}$, the periodically inhomogeneous Markov chain ξ satisfies that $\forall n \in \mathbb{Z}^+$, $(\xi_k, \xi_{k+1}, \dots, \xi_{nT+k})$ and $(\xi_{nT+k}, \xi_{nT+k-1}, \dots, \xi_k)$ have the same distribution, then we say that the Markov chain ξ has **periodical reversibility of index k.**

If the Markov chain ξ satisfies that $\forall k = 0, 1, \dots, T-1,\ n \in \mathbb{Z}^+$, $(\xi_k, \xi_{k+1}, \dots, \xi_{nT+k})$ has the same distribution as $(\xi_{nT+k}, \xi_{nT+k-1}, \dots, \xi_k)$, then we say that ξ has **complete periodical reversibility**.

Therefore, periodically inhomogeneous Markov chain $\{\xi_n : n = 0, 1, \dots\}$ has the complete periodical reversibility if and only if $\forall k = 0, 1, \dots, T-1$, $\{\xi_n : n = 0, 1, 2, \dots\}$ has the periodical reversibility of index k.

Under the hypothesis (H), if $\xi = \{\xi_n : n = 0, 1, 2, \dots\}$ has the periodical reversibility of index k, then ξ is periodically stationary.

Proposition 3.2. *(1) Periodical reversibility of index k of the periodically stationary Markov chain ξ is equivalent to that $(\xi_k, \xi_{k+1}, \dots, \xi_{T+k})$ and $(\xi_{T+k}, \xi_{T+k-1}, \dots, \xi_k)$ have the same distribution, i.e. $\forall i_0, i_1, i_2, \dots, i_T \in S$,*

$$\pi_{i_0}^k p_{i_0 i_1}^k p_{i_1 i_2}^{k+1} \cdots p_{i_{T-1} i_T}^{k+T-1} = \pi_{i_T}^k p_{i_T i_{T-1}}^k p_{i_{T-1} i_{T-2}}^{k+1} \cdots p_{i_1 i_0}^{k+T-1}. \tag{12}$$

This is the ***detailed balance condition.***

(2) Complete periodical reversibility of the periodically stationary Markov chain ξ is equivalent to that $\forall k = 0, 1, \dots, T-1$, $(\xi_k, \xi_{k+1}, \dots, \xi_{T+k})$ and $(\xi_{T+k}, \xi_{T+k-1}, \dots, \xi_k)$ have the same distribution, i.e. $\forall k = 0, 1, \dots, T-1$, $\forall i_0, i_1, i_2, \dots, i_T \in S$,

$$\pi_{i_0}^k p_{i_0 i_1}^k p_{i_1 i_2}^{k+1} \cdots p_{i_{T-1} i_T}^{k+T-1} = \pi_{i_T}^k p_{i_T i_{T-1}}^k p_{i_{T-1} i_{T-2}}^{k+1} \cdots p_{i_1 i_0}^{k+T-1}. \tag{13}$$

Proof: We can only prove the sufficiency for the index $k = 0$, by induction for n.

(1) $n = 1$, the detailed balance condition says that $(\xi_0, \xi_1, \dots, \xi_T)$ and $(\xi_T, \xi_{T-1}, \dots, \xi_1, \xi_0)$ have the same distribution.

(2) Suppose that $(\xi_0, \xi_1, \ldots, \xi_{mT})$ has the same distribution as $(\xi_{mT}, \xi_{mT-1}, \ldots, \xi_1, \xi_0)$, then $\forall i_0, i_1, i_2, \ldots, i_{(m+1)T} \in S$,

$$\begin{aligned}
&\mathbb{P}(\xi_l = i_l, 0 \le l \le (m+1)T) \\
&\quad = \mathbb{P}(\xi_l = i_l, 0 \le l \le mT) \\
&\qquad \times \mathbb{P}(\xi_l = i_l, mT+1 \le l \le (m+1)T | \xi_{mT} = i_{mT}) \\
&\quad = \mathbb{P}(\xi_l = i_l, 0 \le l \le mT) \cdot \mathbb{P}(\xi_l = i_l, mT \le l \le (m+1)T) \\
&\qquad / \mathbb{P}(\xi_{mT} = i_{mT}) \\
&\quad = \mathbb{P}(\xi_l = i_l, 0 \le l \le mT) \cdot \mathbb{P}(\xi_{l-mT} = i_l, mT \le l \le (m+1)T) \\
&\qquad / \mathbb{P}(\xi_{mT} = i_{mT}) \\
&\quad = \mathbb{P}(\xi_l = i_{mT-l}, 0 \le l \le mT) \cdot \mathbb{P}(\xi_l = i_{l+mT}, 0 \le l \le T) / \mathbb{P}(\xi_{mT} = i_{mT}) \\
&\quad = \mathbb{P}(\xi_l = i_{(m+1)T-l}, T \le l \le (m+1)T) \cdot \mathbb{P}(\xi_l = i_{(m+1)T-l}, 0 \le l \le T) \\
&\qquad / \mathbb{P}(\xi_T = i_{mT}) \\
&\quad = \mathbb{P}(\xi_l = i_{(m+1)T-l}, T+1 \le l \le (m+1)T | \xi_T = i_{mT}) \\
&\qquad \times \mathbb{P}(\xi_l = i_{(m+1)T-l}, 0 \le l \le T) \\
&\quad = \mathbb{P}(\xi_l = i_{(m+1)T-l}, 0 \le l \le (m+1)T). \qquad \square
\end{aligned}$$

3.2. Entropy Production

Definition **3.3.** Suppose that μ and ν are two probability measures on a measurable space $(M, \mathcal{A})$. Recall that the **relative entropy** of μ with respect to ν is defined as:[33]

$$H(\mu, \nu) = \begin{cases} \int_M \log \frac{d\mu}{d\nu}(x)\mu(dx), & \text{if } \mu \ll \nu \text{ and } \log \frac{d\mu}{d\nu} \in L^1(d\mu), \\ +\infty, & \text{otherwise.} \end{cases}$$

Definition **3.4.** For each fixed $k = 0, 1, \ldots, T-1$, the **entropy production rate e_p^k of index** k of the periodically stationary Markov chain $\xi = \{\xi_n : n = 0, 1, 2, \ldots\}$ is defined as

$$e_p^k = \lim_{n\to\infty} \frac{1}{nT} H\big(\mathbb{P}_{[k,nT+k]}, \mathbb{P}^-_{[k,nT+k]}\big), \tag{14}$$

where $\mathbb{P}_{[k,nT+k]}$ is the distribution of $(\xi_k, \xi_{k+1}, \ldots, \xi_{nT+k})$, and $\mathbb{P}^-_{[k,nT+k]}$ is the distribution of $(\xi_{nT+k}, \xi_{nT+k-1}, \ldots, \xi_{k+1}, \xi_k)$. Its **complete entropy production rate** e_p is defined as $e_p = \frac{1}{T}\sum_{k=0}^{T-1} e_p^k$.

Lemma 3.5.

Suppose that $\forall i_0, i_1, \ldots, i_T \in S$, $p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+T-1}_{i_{T-1} i_T} > 0$ *if and only if* $p^k_{i_T i_{T-1}} p^{k+1}_{i_{T-1} i_{T-2}} \cdots p^{k+T-1}_{i_1 i_0} > 0$, *then* $\mathbb{P}_{[k,nT+k]}$ *and* $\mathbb{P}^-_{[k,nT+k]}$ *are absolutely continuous with respect to each other, and* $\mathbb{P}$*-almost everywhere, the Radon-Nikodym derivative is*

$$\frac{d\mathbb{P}_{[k,nT+k]}}{d\mathbb{P}^-_{[k,nT+k]}}(\omega) = \frac{\pi^k_{\xi_k(\omega)} p^k_{\xi_k(\omega)\xi_{k+1}(\omega)} \cdots p^{k-1}_{\xi_{nT+k-1}(\omega)\xi_{nT+k}(\omega)}}{\pi^k_{\xi_{nT+k}(\omega)} p^k_{\xi_{nT+k}(\omega)\xi_{nT+k-1}(\omega)} \cdots p^{k-1}_{\xi_{k+1}(\omega)\xi_k(\omega)}}. \tag{15}$$

Proposition 3.6. *The* e^k_p *in Definition 3.4 can be expressed as*

$$\frac{1}{2T} \sum_{i_0, i_1, \ldots, i_T \in S} \left\{ \begin{array}{l} \left[\pi^k_{i_0} p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+T-1}_{i_{T-1} i_T} \right. \\ \left. -\pi^k_{i_T} p^k_{i_T i_{T-1}} p^{k+1}_{i_{T-1} i_{T-2}} \cdots p^{k+T-1}_{i_1 i_0} \right] \\ \cdot \log \frac{\pi^k_{i_0} p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+T-1}_{i_{T-1} i_T}}{\pi^k_{i_T} p^k_{i_T i_{T-1}} p^{k+1}_{i_{T-1} i_{T-2}} \cdots p^{k+T-1}_{i_1 i_0}} \end{array} \right\}. \tag{16}$$

Proof: If there exist $i_0, i_1, \ldots, i_T \in S$ such that only one of $p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+T-1}_{i_{T-1} i_T}$ and $p^k_{i_T i_{T-1}} p^{k+1}_{i_{T-1} i_{T-2}} \cdots p^{k+T-1}_{i_1 i_0}$ is positive, and the other is equal to zero, then $\mathbb{P}_{[k,nT+k]}$ is not absolutely continuous with respect to $\mathbb{P}^-_{[k,nT+k]}$, hence by the definition of $H(\mathbb{P}_{[k,nT+k]}, \mathbb{P}^-_{[k,nT+k]})$, $e^k_p = +\infty$; meanwhile, in (16), at least one term is $+\infty$, and none of the others is negative, so the sum is also equal to $+\infty$.

Now we will prove the desired result under the condition that $p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k-1}_{i_{T-1} i_T}$ and $p^k_{i_T i_{T-1}} p^{k+1}_{i_{T-1} i_{T-2}} \cdots p^{k-1}_{i_1 i_0}$ are either positive or equal to 0 simultaneously. In this case, by Lemma 3.5, $\mathbb{P}_{[k,nT+k]}$ is absolutely continuous with respect to $\mathbb{P}^-_{[k,nT+k]}$, moreover,

$$\begin{aligned} e^k_p &= \lim_{n\to\infty} \frac{1}{nT} H\left(\mathbb{P}_{[k,nT+k]}, \mathbb{P}^-_{[k,nT+k]}\right) \\ &= \lim_{n\to\infty} \frac{1}{nT} \sum_{i_0, i_1, \ldots, i_{nT} \in S} \left[\begin{array}{l} \pi^k_{i_0} p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+nT-1}_{i_{nT-1} i_{nT}} \\ \cdot \log \frac{\pi^k_{i_0} p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+nT-1}_{i_{nT-1} i_{nT}}}{\pi^k_{i_{nT}} p^k_{i_{nT} i_{nT-1}} p^{k+1}_{i_{nT-1} i_{nT-2}} \cdots p^{k+nT-1}_{i_1 i_0}} \end{array} \right] \\ &= \lim_{n\to\infty} \frac{1}{nT} \cdot n \sum_{i_0, i_1, \ldots, i_T \in S} \left[\begin{array}{l} \pi^k_{i_0} p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+T-1}_{i_{T-1} i_T} \\ \cdot \log \frac{\pi^k_{i_0} p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+T-1}_{i_{T-1} i_T}}{\pi^k_{i_T} p^k_{i_T i_{T-1}} p^{k+1}_{i_{T-1} i_{T-2}} \cdots p^{k+T-1}_{i_1 i_0}} \end{array} \right] \end{aligned}$$

$$= \frac{1}{T} \sum_{i_0, i_1, \ldots, i_T \in S} \left[\begin{array}{l} \pi^k_{i_0} p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+T-1}_{i_{T-1} i_T} \\ \cdot \log \frac{\pi^k_{i_0} p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+T-1}_{i_{T-1} i_T}}{\pi^k_{i_T} p^k_{i_T i_{T-1}} p^{k+1}_{i_{T-1} i_{T-2}} \cdots p^{k+T-1}_{i_1 i_0}} \end{array} \right]$$

$$= \frac{1}{2T} \sum_{i_0, i_1, \ldots, i_T \in S} \left\{ \begin{array}{l} \left[\pi^k_{i_0} p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+T-1}_{i_{T-1} i_T} \right. \\ \left. - \pi^k_{i_T} p^k_{i_T i_{T-1}} p^{k+1}_{i_{T-1} i_{T-2}} \cdots p^{k+T-1}_{i_1 i_0} \right] \\ \cdot \log \frac{\pi^k_{i_0} p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+T-1}_{i_{T-1} i_T}}{\pi^k_{i_T} p^k_{i_T i_{T-1}} p^{k+1}_{i_{T-1} i_{T-2}} \cdots p^{k+T-1}_{i_1 i_0}} \end{array} \right\}. \qquad \square$$

Proposition 3.6 immediately implies that e^k_p is nonnegative, furthermore, $e^k_p = 0$ is equivalent to $\forall i_0, i_1, \ldots, i_T \in S$,

$$\pi^k_{i_0} p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+T-1}_{i_{T-1} i_T} = \pi^k_{i_T} p^k_{i_T i_{T-1}} p^{k+1}_{i_{T-1} i_{T-2}} \cdots p^{k+T-1}_{i_1 i_0}. \tag{17}$$

Hence, by Proposition 3.2, we get

Proposition 3.7. *(1) Periodical reversibility of index k of the periodically stationary Markov chain ξ is equivalent to $e^k_p = 0$.*

(2) Complete periodical reversibility of the periodically stationary Markov chain ξ is equivalent to $e_p = 0$, i.e. $\forall k \in \{0, 1, 2, \ldots, T-1\}$, $e^k_p = 0$.

3.3. Kolmogorov's Cycle Condition

Definition **3.8.** We can associate an integer $k = n \ mod \ T$ to a state i which appears at time n in a trajectory of the periodically inhomogeneous Markov chain ξ. It is called **the index of state i at this time**.

Remark 3.9. *(1) For simplicity, we can also use n as its index at time n. (2) If the element p^k_{ij} of the transition matrix $P(k, k+1)$ is positive, then we say that state j can be arrived from the state i by one step for index k, and we write $i \stackrel{k}{\to} j$ for simplicity.*

Definition **3.10.** A simple circuit of length nT ($\forall n \in \mathbb{N}$) in S, $i_0 \stackrel{k}{\to} i_1 \stackrel{k+1}{\to} \cdots \stackrel{k+nT-2}{\to} i_{nT-1} \stackrel{k+nT-1}{\to} i_0$ is called a **periodical circuit** of the periodically inhomogeneous Markov chain ξ. It is written as

$$C = (i_0, i_1, \ldots, i_{nT-1}; k)$$

(the index of i_0 is k). In this article, all of its cyclic permutation $(i_1, i_2, \ldots, i_{nT-1}, i_0; k+1)$, etc. are understood to be the same periodical circuit.

Definition **3.11.** The reversed circuit of a periodical circuit $C = (i_0, i_1, \ldots, i_{nT-1}; k)$ with respect to an index l ($l = 0, 1, \ldots, T-1$), which is simply called the **reversed circuit for index** l, is defined as

$$C_{l_-} = (i_0, i_{nT-1}, \ldots, i_2, i_1; 2l - k).$$

Remark 3.12. *(1) A periodical circuit has several equivalent expressions.*

(2) It is not allowed that two same states in a periodical circuit have the same index.

(3) The reversed circuits for index l defined via different expressions of C are the same, and $(C_{l_-})_{l_-} = C$. So the definition above is reasonable.

*(4) A path of length nT (no matter whether it is a circuit) $i_0 \xrightarrow{k} i_1 \xrightarrow{k+1} \cdots \xrightarrow{k-1} i_{nT}$ can be written as $[i_0, i_1, \ldots, i_{nT}; k]$, which is called **a path with index** k.*

Proposition 3.13. *The periodically stationary Markov chain ξ has periodical reversibility of index k if and only if the condition below is satisfied: for each periodical circuit $C = (i_0, i_1, \ldots, i_{nT-1}; k)$,*

$$p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+nT-1}_{i_{nT-1} i_0} = p^k_{i_0 i_{nT-1}} p^{k+1}_{i_{nT-1} i_{nT-2}} \cdots p^{k+nT-1}_{i_1 i_0}. \tag{18}$$

Now, fix an arbitrary state $i_0 \in S$. For each $i \neq i_0$, there exists a path of length nT with index k from i_0 to i, $i_0 \xrightarrow{k} i_1 \xrightarrow{k+1} \cdots \xrightarrow{k+nT-2} i_{nT-1} \xrightarrow{k+nT-1} i_{nT} = i$. Define

$$\upsilon^k_i = \prod_{m=0}^{nT-1} \frac{p^{k+m}_{i_m i_{m+1}}}{p^{k+nT-m-1}_{i_{m+1} i_m}},$$

then $0 < \upsilon^k_i < \infty$, and $\pi^k = \{\pi^k_i, i \in S\}$ in the periodically stationary measures π of ξ can be expressed as

$$\pi^k_i = \begin{cases} \alpha^{-1} \upsilon^k_i, & i \neq i_0, \\ 1/a, & i = i_0, \end{cases}$$

where $\alpha = 1 + \sum_{i \neq i_0} \upsilon^k_i$.

One can imitate the proof of Kolmogorov's cycle condition for homogeneous irreducible Markov chains[7] to show that the values of υ^k_i's are independent of the choice of the paths and that they constitute a periodically stationary measure of ξ.

Corollary 3.14. *The periodically stationary Markov chain ξ has complete periodical reversibility if and only if the condition below is satisfied:*

$\forall k = 0, 1, 2, \ldots, T-1$, *for each periodical circuit* $C = (i_0, i_1, \ldots, i_{nT-1}; k)$,

$$p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+nT-1}_{i_{nT-1} i_0} = p^k_{i_0 i_{nT-1}} p^{k+1}_{i_{nT-1} i_{nT-2}} \cdots p^{k+nT-1}_{i_1 i_0}. \tag{19}$$

Now for each $k = 0, 1, 2, \ldots, T-1$, *fix an arbitrary state* $i_0 \in S$. *For each* $i \neq i_0$, *there exists a path of length* nT *with index* k *from* i_0 *to* i, $i_0 \xrightarrow{k} i_1 \xrightarrow{k+1} \cdots \xrightarrow{k-2} i_{nT-1} \xrightarrow{k-1} i_{nT} = i$. *Define*

$$\upsilon^k_i = \prod_{m=0}^{nT-1} \frac{p^{k+m}_{i_m i_{m+1}}}{p^{k+nT-m-1}_{i_{m+1} i_m}},$$

then $0 < \upsilon^k_i < \infty$, *and* $\pi^k = (\pi^k_i)_{i \in S}$ *in the periodically stationary measures* π *of* ξ *can be expressed as*

$$\pi^k_i = \begin{cases} \alpha^{-1} \upsilon^k_i, & i \neq i_0 \\ 1/\alpha, & i = i_0 \end{cases}$$

where $\alpha = 1 + \sum_{i \neq i_0} \upsilon^k_i$.

3.4. Circulation Distribution

From later on in this article, for simplicity, we suppose that *the state space* S *is finite* for in Sec. 6.

Construct a Markov chain $\eta = \{\eta_n : n = 0, 1, \ldots\}$, $\eta_n = (\xi_n, n \bmod T)$, with state space $\mathcal{X} = S \times \{0, 1, 2, \ldots, T-1\}$. Sort the N elements of S as $(s_1, s_2, \ldots, s_N)$, then we can sort the elements of $\mathcal{X}$ as

$$((s_1, 0), (s_2, 0), \ldots, (s_N, 0), (s_1, 1), (s_2, 1), \ldots, (s_N, 1), \ldots,$$
$$(s_1, T-1), (s_2, T-1) \cdots, (s_N, T-1)).$$

The transition probability matrix of η from step n to step $n+1$ is

$$\tilde{P}(n, n+1) = \begin{pmatrix} 0 & P(0,1) & 0 & \cdots & 0 \\ 0 & 0 & P(1,2) & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \cdots & P(T-2, T-1) \\ P(T-1, T) & 0 & \cdots & \cdots & 0 \end{pmatrix}, \tag{20}$$

which does not depend on n, so $\{\eta_n : n = 0, 1, 2, \ldots\}$ is a homogeneous Markov chain. Write $\tilde{P}(n, n+1)$ as $\tilde{P}$. Let $\tilde{\pi} = \frac{1}{T}(\pi^0, \pi^1, \ldots, \pi^{T-1}) = \frac{1}{T}(\pi_{(i,k)}, i \in S, k = 0, 1, 2, \ldots, T-1)$, then by (8), $\tilde{\pi}\tilde{P} = \tilde{\pi}$, so $\tilde{\pi}$ is the unique stationary measure of η. Therefore, η is a homogeneous irreducible positive recurrent Markov chain. Each circuit $(i_0, k) \to (i_1, k+1) \to \cdots \to (i_{nT-1}, k-1) \to (i_0, k)$ (written as $\tilde{C}$) of η in its state space $\mathcal{X} = S \times \{0, 1, 2, \ldots, T-1\}$ corresponds to the periodical circuit $C = (i_0, i_1, \dots, i_{nT-1}; k)$ of the periodically inhomogeneous Markov chain ξ. We will derive the periodical circuit distribution of the periodically inhomogeneous Markov chain ξ from the circuit distribution of the homogeneous Markov chain η. Use Theorem 1.3.3 in ref. 17, then one can directly get

Proposition 3.15. *Let $\tilde{\mathcal{C}}_n(\omega)$ be the class of all circuits occurring along the sample path $\{\eta_l(\omega) : l = 0, 1, 2, \dots\}$ until time n, and $\tilde{\lambda}_{\tilde{C},n}(\omega)$ be the number of occurrences of a circuit $\tilde{C}$ up to time n along the sample path $\{\eta_l(\omega) : l = 0, 1, 2, \dots\}$, then the sequence $(\tilde{\mathcal{C}}_n(\omega), \tilde{\lambda}_{\tilde{C},n}(\omega)/n)$ converges almost surely to a class $(\tilde{\mathcal{C}}_\infty, \tilde{\lambda}_{\tilde{C}})$. Furthermore, for any directed circuit $\tilde{C} = (i_0, k) \to (i_1, k+1) \to \cdots \to (i_{nT-1}, k-1) \to (i_0, k) \in \tilde{\mathcal{C}}_\infty$, we have*

$$\tilde{\lambda}_{\tilde{C}} = \tilde{p}_{(i_0,k)(i_1,k+1)}\tilde{p}_{(i_1,k+1)(i_2,k+2)}\cdots\tilde{p}_{(i_{nT-1},k-1)(i_0,k)} \cdot\frac{\tilde{D}(\{(i_0,k),(i_1,k+1),(i_2,k+2),\dots,(i_{nT-1},k-1)\}^c)}{\sum_{(j,l)\in\mathcal{X}}\tilde{D}(\{(j,l)\}^c)}, \qquad (21)$$

where for a subset $\tilde{S}$ of the state space $\mathcal{X}$, $\tilde{D}(\tilde{S})$ is the determinant of $\tilde{\mathbb{D}} = I - \tilde{P}$ with rows and columns indexed in the index set $\tilde{S}$. $\tilde{D}(\emptyset)$ is understood as 1.

We refer the reader to Chap. 1, Sect. 2 of ref. 17 for the rigorous definition of $\tilde{\lambda}_{\tilde{C},n}(\omega)$ using the so-called derived chain.

The following is a direct result from the elementary algebra knowledge of determinants.

Lemma 3.16. *If a matrix A can be written as the block matrix below:*

$$A = \begin{pmatrix} I & -A_0 & 0 & \cdots & \cdots & 0 \\ 0 & I & -A_1 & 0 & \cdots & 0 \\ \vdots & \ddots & \cdots & \cdots & \cdots & \vdots \\ 0 & \vdots & \vdots & \cdots & \cdots & 0 \\ 0 & \ddots & \ddots & 0 & I & -A_{m-2} \\ -A_{m-1} & 0 & \cdots & \cdots & 0 & I \end{pmatrix},$$

where I, $A_0, A_1, \dots, A_{m-1}$ are all square matrices of order M, then the determinants

$$|A| = |I - A_0 A_1 A_2 \cdots A_{m-1}|.$$

Given two subsets S_1, S_2 of S, we use $P_k^{k+1}(S_1, S_2)$ to denote the matrix which is obtained by deleting the rows with indices in S_1 and columns with indices in S_2 from P^k. Let $\mathcal{C}_n(\omega)$ be the class of all periodical circuits occurring along the sample path $\{\xi_n(\omega) : n = 0, 1, 2, \ldots\}$ until time n, and let $\lambda_{C,n}(\omega)$ be the number of occurrences of a periodical circuit C up to the time n along the sample path $\{\xi_n(\omega) : n = 0, 1, 2, \ldots\}$. Since $\tilde{\lambda}_{\tilde{C},n}(\omega) = \lambda_{C,n}(\omega)$, by Proposition 3.15 and Lemma 3.16, we can get

Corollary 3.17. *The sequence $(\mathcal{C}_n(\omega), \lambda_{C,n}(\omega)/n)$ converges almost surely to a class $(\mathcal{C}_\infty, \lambda_C)$. Furthermore, for any directed periodical circuit $C = (i_0, i_1, \ldots, i_{nT-1}; k)$, the circulation weight*

$$
\begin{aligned}
\lambda_C &= p^{k}_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+nT-1}_{i_{nT-1} i_0} \\
&\quad \times \frac{\tilde{D}(\{(i_0, k), (i_1, k+1), (i_2, k+2) \cdots, (i_{nT-1}, k-1)\}^c)}{\sum_{(j,l)\in\mathcal{X}} \tilde{D}(\{(j,l)\}^c)} \\
&= p^{k}_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k+nT-1}_{i_{nT-1} i_0} \\
&\quad \times \frac{|I - P^1_0(S_r, S_{r+1}) P^2_1(S_{r+1}, S_{r+2}) \cdots P^T_{T-1}(S_{r-1}, S_r)|}{\sum_{l=0}^{T-1} \sum_{j\in S} \tilde{D}(\{(j,l)\}^c)},
\end{aligned} \tag{22}
$$

where $r = T - k$, and $S_l = \{i_l, i_{T+l}, \ldots, i_{(n-1)T+l}\}$. The circulation weights $\{\lambda_C : C \in \mathcal{C}_\infty\}$ is called the ***circulation distribution*** *of ξ.*

Obviously, $\lambda_C = \tilde{\lambda}_{\tilde{C}}$. Apply a similar argument as the proof of Theorem 1.3.5 in ref. 17 to the homogeneous Markov chain η, then one can get

Proposition 3.18. *For the homogeneous irreducible positive recurrent Markov chain $\eta = \{\eta_l : l = 0, 1, 2, \ldots\}$, we have the following probabilistic cycle representation: $\forall i_0, i_1, \ldots, i_T \in S$, $k = 0, 1, \ldots, T-1$,*

$$
\begin{aligned}
&\frac{\pi_{(i_0,k)}}{T} \tilde{p}_{(i_0,k)(i_1,k+1)} \tilde{p}_{(i_1,k+1)(i_2,k+2)} \cdots \tilde{p}_{(i_{T-1},k-1)(i_T,k)} \\
&\quad = \sum_{\tilde{C}\in\tilde{\mathcal{C}}_\infty} \tilde{\lambda}_{\tilde{C}} J_{\tilde{C}}((i_0,k), (i_1,k+1), \ldots, (i_{T-1},k-1), (i_T,k)),
\end{aligned}
$$

where $J_{\tilde{C}}((i_0,k), (i_1,k+1), \ldots, (i_{T-1},k-1), (i_T,k))$ is defined to be 1 if $\tilde{C}$ includes the path $(i_0,k) \to (i_1,k+1) \to \cdots \to (i_T,k)$, otherwise 0.

Since $\pi_{(i,k)} = \pi^k_i$, $\tilde{\lambda}_{\tilde{C}} = \lambda_C$, by the relationship between $\tilde{P}$ and $P(0,1)$, $\cdots$, $P(T-1,T)$, we can get the corresponding *probabilistic cycle representation* of periodically inhomogeneous Markov chains:

Corollary 3.19. *For the periodically inhomogeneous Markov chain* $\xi = \{\xi_n : n = 0, 1, 2, \ldots\}$*, we have*

$$\frac{\pi^k_{i_0}}{T} p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k-1}_{i_{T-1} i_T} = \sum_{C \in \mathcal{C}_\infty} \lambda_C J_C([i_0, i_1, \ldots, i_{T-1}, i_T; k]),$$
$$\forall i_0, i_1, \ldots, i_T \in S, k = 0, 1, \ldots, T-1, \quad (23)$$

where $J_C([i_0, i_1, \ldots, i_{T-1}, i_T; k])$ *is defined to be* 1 *if* C *includes the path* $i_0 \overset{k}{\rightarrow} i_1 \overset{k+1}{\rightarrow} \cdots \overset{k+T-1}{\rightarrow} i_T$*, otherwise* 0.

Corollary 3.20. *We have the following circulation decomposition of the periodically inhomogeneous Markov chain* $\xi = \{\xi_n : n = 0, 1, 2, \ldots\}$*:*

$$\begin{aligned}
&\pi^k_{i_0} p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k-1}_{i_{T-1} i_T} - \pi^k_{i_T} p^k_{i_T i_{T-1}} \cdots p^{k-1}_{i_1 i_0} \\
&\quad = T \sum_{C \in \mathcal{C}_\infty} \lambda_C J_C([i_0, i_1, \ldots, i_{T-1}, i_T; k]) \\
&\qquad - T \sum_{C_{k_} \in \mathcal{C}_\infty} \lambda_{C_{k_}} J_{C_{k_}}([i_T, i_{T-1}, \ldots, i_1, i_0; k]) \\
&\quad = T \sum_{C \in \mathcal{C}_\infty} (\lambda_C - \lambda_{C_{k_}}) J_C([i_0, i_1, \ldots, i_{T-1}, i_T; k]).
\end{aligned} \quad (24)$$

The corollary says that any one of the T-step probability fluxes $\pi^k_{i_0} p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k-1}_{i_{T-1} i_T}$ can be decomposed into two parts: one is the part of the detailed balance

$$\min\left\{\pi^k_{i_0} p^k_{i_0 i_1} p^{k+1}_{i_1 i_2} \cdots p^{k-1}_{i_{T-1} i_T}, \pi^k_{i_T} p^k_{i_T i_{T-1}} \cdots p^{k-1}_{i_1 i_0}\right\},$$

i.e. the eliminated part of the two T-step probability fluxes; another is the part of the circulation balance, i.e. the net part of the probability flux along the path $i_0 \overset{k}{\rightarrow} i_1 \overset{k+1}{\rightarrow} \cdots \overset{k+T-1}{\rightarrow} i_T$, which is composed of a set of circulations on $\mathcal{C}_\infty$ that pass the path or its reversal.

Lemma 3.21. *If* A *and* B *are both square matrices of order* M*, then* $|I - AB| = |I - BA|$.

Theorem 3.22. *The periodically stationary Markov chain* ξ *has the periodical reversibility of index* k *if and only if for each periodical circuit* $C = (i_0, i_1, \ldots, i_{nT-1}; k) \in \mathcal{C}_\infty$*, the circulation weights* λ_C *of* C *and* $\lambda_{C_{k\_}}$ *of its reversed circuit* $C_{k\_} = (i_0, i_{nT-1}, \ldots, i_1; k)$ *are equal to each other.*

Proof: Necessity: At first, we prove the necessity for $k = 0$. By Proposition 3.13 and Corollary 3.17, we only need to prove

$$
\begin{aligned}
&\left|I - P_0^1(S_0, S_1)P_1^2(S_1, S_2)\cdots P_{T-1}^T(S_{T-1}, S_0)\right| \\
&\quad = \left|I - P_0^1(S_0, S_{T-1})P_1^2(S_{T-1}, S_{T-2})\cdots P_{T-1}^T(S_1, S_0)\right|.
\end{aligned}
$$

Write $\Lambda = \operatorname{diag}(\pi_i^0)_{i\notin S_0}$, then $\Lambda^{-1} = \operatorname{diag}(\frac{1}{\pi_j^0})_{j\notin S_0}$. From

$$
\begin{aligned}
&\pi_i^0 \cdot \left[P_0^1(S_0, S_1)P_1^2(S_1, S_2)\cdots P_{T-1}^T(S_{T-1}, S_0)\right]_{ij} \cdot \frac{1}{\pi_j^0} \\
&= \sum_{\substack{k_l\notin S_l, l=1,2\cdots,T-1 \\ i,j\notin S_0}} \pi_i^0 \cdot p_{ik_1}^0 p_{k_1k_2}^1 \cdots p_{k_{T-1}j}^{T-1} \cdot \frac{1}{\pi_j^0} \\
&= \sum_{\substack{k_l\notin S_l, l=1,2\cdots,T-1 \\ i,j\notin S_0}} p_{jk_{T-1}}^0 p_{k_{T-1}k_{T-2}}^1 \cdots p_{k_1 i}^{T-1} \\
&= \left[P_0^1(S_0, S_{T-1})P_1^2(S_{T-1}, S_{T-2})\cdots P_{T-1}^T(S_1, S_0)\right]_{ji}
\end{aligned}
$$

follows that

$$
\begin{aligned}
&\Lambda P_0^1(S_0, S_1)P_1^2(S_1, S_2)\cdots P_{T-1}^T(S_{T-1}, S_0)\Lambda^{-1} \\
&\quad = \left[P_0^1(S_0, S_{T-1})P_1^2(S_{T-1}, S_{T-2})\cdots P_{T-1}^T(S_1, S_0)\right]'.
\end{aligned}
$$

So, we immediately get

$$
\begin{aligned}
&\left|I - P_0^1(S_0, S_1)P_1^2(S_1, S_2)\cdots P_{T-1}^T(S_{T-1}, S_0)\right| \\
&\quad = \left|\Lambda(I - P_0^1(S_0, S_1)P_1^2(S_1, S_2)\cdots P_{T-1}^T(S_{T-1}, S_0))\Lambda^{-1}\right| \\
&\quad = \left|I - \Lambda P_0^1(S_0, S_1)P_1^2(S_1, S_2)\cdots P_{T-1}^T(S_{T-1}, S_0)\Lambda^{-1}\right| \\
&\quad = \left|I - P_0^1(S_0, S_{T-1})P_1^2(S_{T-1}, S_{T-2})\cdots P_{T-1}^T(S_1, S_0)\right|.
\end{aligned}
$$

For the case $k > 0$, use Lemma 3.21, and imitate the proof for the case $k = 0$. The sufficiency follows obviously from Proposition 3.2 and Corollary 3.20. □

Corollary 3.23. *The periodically stationary Markov chain $\{\xi_n : n \geq 0\}$ has the complete periodical reversibility if and only if $\forall k = 0, 1, \ldots, T-1$ and for each periodical circuit $C = (i_0, i_1, \ldots, i_{nT-1}; k) \in \mathcal{C}_\infty$, the circulation weight λ_C of C and the circulation weight $\lambda_{C_{k-}}$ of its reversed circuit with index k, $C_{k-} = (i_0, i_{nT-1}, \ldots, i_1; k)$ satisfy the equation $\lambda_C = \lambda_{C_{k-}}$.*

4. LARGE DEVIATION OF SAMPLE ENTROPY PRODUCTION AND FLUCTUATION THEOREM

In this section, fix an arbitrary $k \in \{0, 1, \ldots, T-1\}$.

4.1. Large Deviation

Define a new Markov chain $\{\psi_n^k = (\xi_{nT+k}, \xi_{nT+k+1}, \ldots, \xi_{(n+1)T+k}) : n = 0, 1, 2, \ldots\}$ from the periodically stationary Markov chain $\xi = \{\xi_n : n = 0, 1, 2, \ldots\}$. The state space of $\{\psi_n^k\}$ can be taken as $\Gamma = \{(i_0, i_1, \ldots, i_T) \in S^{T+1} : p_{i_0i_1}^k p_{i_1i_2}^{k+1} \cdots p_{i_{T-1}i_T}^{k-1} > 0\}$.

Proposition 4.1. *$\{\psi_n^k : n = 0, 1, 2, \ldots\}$ is a homogeneous irreducible Markov chain with stationary distribution*

$$\mu(i_0, i_1, \ldots, i_T) = \pi_{i_0}^k p_{i_0i_1}^k p_{i_1i_2}^{k+1} \cdots p_{i_{T-1}i_T}^{k-1} > 0.$$

Obviously, $\{\psi_n^k : n = 0, 1, 2, \ldots\}$ is also positive recurrent.

Proof: By the time periodicity of the transition matrix of ξ and our basic hypothesis (H), we get that $\{\psi_n^k : n = 0, 1, 2, \ldots\}$ is a homogeneous irreducible Markov chain with transition probability $P_{(i_0,i_1,\ldots,i_T)(j_0,j_1,\ldots,j_T)} = \delta_{i_Tj_0} p_{j_0j_1}^k p_{j_1j_2}^{k+1} \cdots p_{j_{T-1}j_T}^{k-1}$.

Since π is the periodically stationary distribution of $\{\xi_n : n = 0, 1, 2 \ldots\}$,

$$\begin{aligned}
&\sum_{(j_0,j_1,\ldots,j_T)\in\Gamma} \mu(j_0, j_1, \ldots, j_T) P_{(j_0,j_1,\ldots,j_T)(i_0,i_1,\ldots,i_T)} \\
&= \sum_{(j_0,j_1,\ldots,j_T)\in\Gamma} \pi_{j_0}^k p_{j_0j_1}^k p_{j_1j_2}^{k+1} \cdots p_{j_{T-1}j_T}^{k-1} \cdot \delta_{j_Ti_0} p_{i_0i_1}^k p_{i_1i_2}^{k+1} \cdots p_{i_{T-1}i_T}^{k-1} \\
&= \sum_{(j_0,j_1,\ldots,j_{T-1})} \pi_{j_0}^k p_{j_0j_1}^k p_{j_1j_2}^{k+1} \cdots p_{j_{T-1}i_0}^{k-1} \cdot p_{i_0i_1}^k p_{i_1i_2}^{k+1} \cdots p_{i_{T-1}i_T}^{k-1} \\
&= \sum_{(j_1,\ldots,j_{T-1})} \pi_{j_1}^{k+1} p_{j_1j_2}^{k+1} \cdots p_{j_{T-1}i_0}^{k-1} \cdot p_{i_0i_1}^k p_{i_1i_2}^{k+1} \cdots p_{i_{T-1}i_T}^{k-1} \\
&= \sum_{(j_2,\ldots,j_{T-1})} \pi_{j_2}^{k+2} p_{j_2j_3}^{k+2} \cdots p_{j_{T-1}i_0}^{k-1} p_{i_0i_1}^k p_{i_1i_2}^{k+1} \cdots p_{i_{T-1}i_T}^{k-1} \\
&= \sum_{j_{T-1}} \pi_{j_{T-1}}^{k-1} p_{j_{T-1}i_0}^{k-1} p_{i_0i_1}^k p_{i_1i_2}^{k+1} \cdots p_{i_{T-1}i_T}^{k-1} \\
&= \pi_{i_0}^k p_{i_0i_1}^k p_{i_1i_2}^{k+1} \cdots p_{i_{T-1}i_T}^{k-1} \\
&= \mu(i_0, i_1, \ldots, i_T).
\end{aligned}$$

So, $\mu(i_0, i_1, \ldots, i_T) = \pi_{i_0}^k p_{i_0i_1}^k p_{i_1i_2}^{k+1} \cdots p_{i_{T-1}i_T}^{k-1} > 0$ is the unique stationary distribution of $\{\psi_n^k\}$. □

In the discussion below we will assume that the state space S is finite and the following condition is satisfied: $p_{i_0i_1}^k \cdots p_{i_{T-1}i_T}^{k-1}$ and $p_{i_Ti_{T-1}}^k \cdots p_{i_1i_0}^{k-1}$ are either positive or equal to zero at the same time. Then, by Lemma 3.5,

$$\frac{d\mathbb{P}_{[k,nT+k]}}{d\mathbb{P}^{-}_{[k,nT+k]}}(\omega) = \frac{\pi^k_{\xi_k(\omega)} p^k_{\xi_k(\omega)\xi_{k+1}(\omega)} \cdots p^{k-1}_{\xi_{nT+k-1}(\omega)\xi_{nT+k}(\omega)}}{\pi^k_{\xi_{nT+k}(\omega)} p^k_{\xi_{nT+k}(\omega)\xi_{nT+k-1}(\omega)} \cdots p^{k-1}_{\xi_{k+1}(\omega)\xi_k(\omega)}}.$$

Let $W^k_n(\omega) = \log \frac{d\mathbb{P}_{[k,nT+k]}}{d\mathbb{P}^{-}_{[k,nT+k]}}(\omega)$.

Proposition 4.2. *Almost surely, one has*

$$\lim_{n\to\infty} \frac{W^k_n(\omega)}{nT} = e^k_p. \tag{25}$$

Proof: Define a real function on the state space Γ,

$$f(i_0, i_1, \ldots, i_T) = \frac{1}{T} \log \frac{\pi^k_{i_0} p^k_{i_0 i_1} \cdots p^{k-1}_{i_{T-1} i_T}}{\pi^k_{i_T} p^k_{i_T i_{T-1}} \cdots p^{k-1}_{i_1 i_0}}.$$

Apply the strong law of large numbers for homogeneous irreducible Markov chains to $\{\psi^k_n : n = 0, 1, 2, \ldots\}$, then we can get that almost surely

$$\begin{aligned}
&\lim_{n\to\infty} \frac{W^k_n}{nT} \\
&= \lim_{n\to\infty} \frac{1}{nT} \log \frac{\pi^k_{\xi_k} p^k_{\xi_k \xi_{k+1}} \cdots p^{k-1}_{\xi_{nT+k-1}\xi_{nT+k}}}{\pi^k_{\xi_{nT+k}} p^k_{\xi_{nT+k}\xi_{nT+k-1}} \cdots p^{k-1}_{\xi_{k+1}\xi_k}} \\
&= \lim_{n\to\infty} \frac{1}{n} \sum_{l=0}^{n-1} \frac{1}{T} \log \frac{\pi^k_{\xi_{lT+k}} p^k_{\xi_{lT+k}\xi_{lT+k+1}} \cdots p^{k-1}_{\xi_{(l+1)T+k-1}\xi_{(l+1)T+k}}}{\pi^k_{\xi_{(l+1)T+k}} p^k_{\xi_{(l+1)T+k}\xi_{(l+1)T+k-1}} \cdots p^{k-1}_{\xi_{lT+k+1}\xi_{lT+k}}} \\
&= \lim_{n\to\infty} \frac{1}{n} \sum_{l=0}^{n-1} f\left(\psi^k_l\right) \\
&= \sum_{(i_0, i_1, \ldots, i_T)\in\Gamma} \mu(i_0, i_1, \ldots, i_T) f(i_0, i_1, \ldots, i_T) \\
&= \frac{1}{T} \sum_{i_0, i_1, \ldots, i_T \in S} \pi^k_{i_0} p^k_{i_0 i_1} \cdots p^{k-1}_{i_{T-1} i_T} \log \frac{\pi^k_{i_0} p^k_{i_0 i_1} \cdots p^{k-1}_{i_{T-1} i_T}}{\pi^k_{i_T} p^k_{i_T i_{T-1}} \cdots p^{k-1}_{i_1 i_0}} = e^k_p. \qquad \square
\end{aligned}$$

Let $c^k_n(\lambda) = \frac{1}{n} \log E e^{\lambda W^k_n}$.

Proposition 4.3. *There exists a real differentiable function $c^k(\lambda)$ such that $\lim_{n\to\infty} c_n^k(\lambda) = c^k(\lambda)$. So the family of the distributions of $\{\frac{W_n^k(\omega)}{n} : n \in \mathbb{N}\}$ has a large deviation property with rate function $I^k(z) = \sup_{\lambda\in R}\{\lambda z - c^k(\lambda)\}$.*

Proof:

$$
\begin{aligned}
&Ee^{\lambda W_n^k}\\
&= E\left(\frac{d\mathbb{P}_{[k,nT+k]}}{d\mathbb{P}^-_{[k,nT+k]}}(\omega)\right)^\lambda\\
&= E\left(\frac{\pi^k_{\xi_k(\omega)}p^k_{\xi_k(\omega)\xi_{k+1}(\omega)}\cdots p^{k-1}_{\xi_{nT-1+k}(\omega)\xi_{nT+k}(\omega)}}{\pi^k_{\xi_{nT+k}(\omega)}p^k_{\xi_{nT+k}(\omega)\xi_{nT+k-1}(\omega)}\cdots p^{k-1}_{\xi_{k+1}(\omega)\xi_k(\omega)}}\right)^\lambda\\
&= \sum_{\substack{i_0,i_1,\ldots,i_{nT}\in S:\\ p^k_{i_0i_1}\cdots p^{k-1}_{i_{nT-1}i_{nT}}>0}}\left[\pi^k_{i_0}p^k_{i_0i_1}\cdots p^{k-1}_{i_{nT-1}i_{nT}}\left(\frac{\pi^k_{i_0}p^k_{i_0i_1}\cdots p^{k-1}_{i_{nT-1}i_{nT}}}{\pi^k_{i_{nT}}p^k_{i_{nT}i_{nT-1}}\cdots p^{k-1}_{i_1i_0}}\right)^\lambda\right]\\
&= \sum_{\substack{i_0,i_1,\ldots,i_{nT}\in S:\\ p^k_{i_0i_1}\cdots p^{k-1}_{i_{nT-1}i_{nT}}>0}}\left[\begin{array}{l}\pi^k_{i_0}p^k_{i_0i_1}\cdots p^{k-1}_{i_{T-1}i_T}\left(\frac{\pi^k_{i_0}p^k_{i_0i_1}\cdots p^{k-1}_{i_{T-1}i_T}}{\pi^k_{i_T}p^k_{i_Ti_{T-1}}\cdots p^{k-1}_{i_1i_0}}\right)^\lambda\\ \cdots p^k_{i_{(n-1)T}i_{(n-1)T+1}}\cdots p^{k-1}_{i_{nT-1}i_{nT}}\\ \left(\frac{\pi^k_{i_{(n-1)T}}p^k_{i_{(n-1)T}i_{(n-1)T+1}}\cdots p^{k-1}_{i_{nT-1}i_{nT}}}{\pi^k_{i_{nT}}p^k_{i_{nT}i_{nT-1}}\cdots p^{k-1}_{i_{(n-1)T+1}i_{(n-1)T}}}\right)^\lambda\end{array}\right].
\end{aligned}
\tag{26}
$$

Let

$$
a_{ij}(\lambda) = \sum_{\substack{i_1,i_2,\ldots,i_{T-1}\in S:\\ p^k_{ii_1}\cdots p^{k-1}_{i_{T-1}j}>0}}\left[p^k_{ii_1}p^{k+1}_{i_1i_2}\cdots p^{k-1}_{i_{T-1}j}\left(\frac{\pi^k_i p^k_{ii_1}\cdots p^{k-1}_{i_{T-1}j}}{\pi^k_j p^k_{ji_{T-1}}\cdots p^{k-1}_{i_1i}}\right)^\lambda\right],
$$

Obviously,

$$
\begin{aligned}
a_{ij}(\lambda) > 0 &\Leftrightarrow \exists i_1, i_2, \ldots, i_{T-1} \in S,\ s.t.\ p^k_{ii_1}\cdots p^{k-1}_{i_{T-1}j} > 0\\
&\Leftrightarrow \tilde{p}^k_{ij} > 0.
\end{aligned}
$$

So $A(\lambda) = (a_{ij}(\lambda))_{i,j\in S}$ is an irreducible nonnegative matrix. By the Perron-Frobenius theorem, its spectral radius $e(\lambda)$ is a positive eigenvalue of $A(\lambda)$ with one-dimensional eigenspace, whose correspondent eigenvector is supposed to be $\alpha = (\alpha_1, \ldots, \alpha_N)^T$, $\alpha_i > 0, \forall i \in S$. Write $M = \max_i(\alpha_i)$, $m = \min_i(\alpha_i)$, then, by (26), for any fixed λ, we have

$$
M^{-1}\pi^k A(\lambda)^n\alpha \le Ee^{\lambda W_n^k} = \pi^k A(\lambda)^n\mathbf{1} \le m^{-1}\pi^k A(\lambda)^n\alpha,
$$

in which $\mathbf{1} = (1, \ldots, 1)^T$. Hence,

$$\lim_{n\to\infty} c_n^k(\lambda) = \lim_{n\to\infty} \frac{1}{n} \log Ee^{\lambda W_n^k} = \lim_{n\to\infty} \frac{1}{n} \log \pi^k A(\lambda)^n \alpha = e(\lambda) \triangleq c^k(\lambda).$$

Then, by Remark 1.5.6 in ref. 17, we come to the conclusion that $e(\lambda)$ is differentiable, and the large deviation property follows from the Gärtner-Ellis Theorem (see Theorem 1.5.2 in ref. 17). □

4.2. Fluctuation Theorem

Theorem 4.4. *(Fluctuation Theorem) The free energy function $c^k(\lambda)$ and the large deviation rate function $I^k(z)$ have the following properties:*

$$c^k(\lambda) = c^k(-(1+\lambda)), \quad I^k(z) = I^k(-z) - z. \tag{27}$$

Proof: One only needs to prove that $c_n^k(\lambda) = c_n^k(-(1+\lambda))$.

$$\begin{aligned}
&Ee^{\lambda W_n^k} \\
&= \sum_{\substack{i_0, i_1, \cdots, i_{nT} \in S: \\ p^k_{i_0 i_1} \cdots p^{k-1}_{i_{nT-1} i_{nT}} > 0}} \left[\pi^k_{i_0} p^k_{i_0 i_1} \cdots p^{k-1}_{i_{nT-1} i_{nT}} \left(\frac{\pi^k_{i_0} p^k_{i_0 i_1} \cdots p^{k-1}_{i_{nT-1} i_{nT}}}{\pi^k_{i_{nT}} p^k_{i_{nT} i_{nT-1}} \cdots p^{k-1}_{i_1 i_0}} \right)^{\lambda} \right] \\
&= \sum_{\substack{i_0, i_1, \cdots, i_{nT} \in S: \\ p^k_{i_0 i_1} \cdots p^{k-1}_{i_{nT-1} i_{nT}} > 0}} \left[\begin{array}{l} \pi^k_{i_{nT}} p^k_{i_{nT} i_{nT-1}} \cdots p^{k-1}_{i_1 i_0} \\ \left(\dfrac{\pi^k_{i_{nT}} p^k_{i_{nT} i_{nT-1}} \cdots p^{k-1}_{i_1 i_0}}{\pi^k_{i_0} p^k_{i_0 i_1} \cdots p^{k-1}_{i_{nT-1} i_{nT}}} \right)^{\lambda} \end{array} \right] \\
&= \sum_{\substack{i_0, i_1, \cdots, i_{nT} \in S: \\ p^k_{i_0 i_1} \cdots p^{k-1}_{i_{nT-1} i_{nT}} > 0}} \left[\begin{array}{l} \pi^k_{i_0} p^k_{i_0 i_1} \cdots p^{k-1}_{i_{nT-1} i_{nT}} \\ \left(\dfrac{\pi^k_{i_0} p^k_{i_0 i_1} \cdots p^{k-1}_{i_{nT-1} i_{nT}}}{\pi^k_{i_{nT}} p^k_{i_{nT} i_{nT-1}} \cdots p^{k-1}_{i_1 i_0}} \right)^{-1-\lambda} \end{array} \right] \\
&= Ee^{(-1-\lambda) W_n^k}.
\end{aligned}$$

Hence

$$\begin{aligned}
I^k(z) &= \sup_{\lambda\in R} \{\lambda z - c^k(\lambda)\} = \sup_{\lambda \in R} \{(-1-\lambda) z - c^k(-1-\lambda)\} \\
&= \sup_{\lambda \in R} \{\lambda(-z) - c^k(\lambda)\} - z = I^k(-z) - z.
\end{aligned}$$

□

Corollary 4.5. *It holds that*

$$\mathbb{P}\left(\frac{W_n^k}{n}=z\right)=e^{nz}\mathbb{P}\left(\frac{W_n^k}{n}=-z\right). \tag{28}$$

Proof:

$$\begin{aligned}
&\mathbb{P}\left(\frac{W_n^k}{n}=z\right)\\
&=\mathbb{P}_{[k,nT+k]}\left(\frac{d\mathbb{P}_{[k,nT+k]}}{d\mathbb{P}^-_{[k,nT+k]}}(\omega)=e^{nz}\right)\\
&=\sum_{\substack{i_m\in S,\ m=0,1,2,\ldots,nT:\\ \frac{\pi^k_{i_0}p^k_{i_0i_1}\cdots p^{k-1}_{i_{nT-1}i_{nT}}}{\pi^k_{i_{nT}}p^k_{i_{nT}i_{nT-1}}\cdots p^{k-1}_{i_1i_0}}=e^{nz}}}\pi^k_{i_0}p^k_{i_0i_1}\cdots p^{k-1}_{i_{nT-1}i_{nT}}\\
&=\sum_{\substack{i_m\in S,\ m=0,1,2,\ldots,nT:\\ \frac{\pi^k_{i_0}p^k_{i_0i_1}\cdots p^{k-1}_{i_{nT-1}i_{nT}}}{\pi^k_{i_{nT}}p^k_{i_{nT}i_{nT-1}}\cdots p^{k-1}_{i_1i_0}}=e^{nz}}}e^{nz}\pi^k_{i_{nT}}p^k_{i_{nT}i_{nT-1}}\cdots p^{k-1}_{i_1i_0}\\
&=\sum_{\substack{i_m\in S,\ m=0,1,2,\ldots,nT:\\ \frac{\pi^k_{i_{nT}}p^k_{i_{nT}i_{nT-1}}\cdots p^{k-1}_{i_1i_0}}{\pi^k_{i_0}p^k_{i_0i_1}\cdots p^{k-1}_{i_{nT-1}i_{nT}}}=e^{nz}}}e^{nz}\pi^k_{i_0}p^k_{i_0i_1}\cdots p^{k-1}_{i_{nT-1}i_{nT}}\\
&=e^{nz}\mathbb{P}_{[k,nT+k]}\left(\frac{d\mathbb{P}^-_{[k,nT+k]}}{d\mathbb{P}_{[k,nT+k]}}(\omega)=e^{nz}\right)\\
&=e^{nz}\mathbb{P}\left(\frac{W_n^k}{n}=-z\right).
\end{aligned}$$

□

Remark 4.6. *Roughly speaking, the fluctuation theorem gives a formula for the probability ratio that the sample entropy production rate* $\frac{W_n^k}{n}$ *takes a value* z *to that of* $-z$*, and the ratio is roughly* e^{nz}*. Under the condition of periodical irreversibility for index* k*, for* $z>0$ *in a certain range, the sample entropy production rate* $\frac{W_n^k}{n}$ *has a positive probability to take the value* z *as well as the value* $-z$*, but the fluctuation theorem tells that the former probability is greater, which accords with the second law of thermodynamics.*

5. SEVERAL REMARKS OF PERIODICAL REVERSIBILITY

5.1. Remark 1

Even if $\forall k \in \{0, 1, 2, \ldots, T-1\}$, $\{\eta_n^k : n = 0, 1, 2, \ldots\}$ is a reversible Markov chain, and all the $P(m, m+1)$ have reversible distributions when regarded as the transition probability matrix of a homogeneous Markov chain, $\{\xi_n : n = 0, 1, 2, \ldots\}$ may still be periodically irreversible. This fact of periodically inhomogeneous Markov chain is similar to Parrondo's paradoxical games.[12,13] We expect that the results obtained in this article can be applied to provide a new rigorous mathematical analysis of the paradox.

For fixed m, $P(m, m+1)$ having a reversible distribution corresponds to that in (1), for fixed t, $(\sigma(t,x)\sigma^T(t,x))^{-1}b(t,x)$ has a potential.[17]

Example 5.1 Let $T = 3$,

$$P(0,1) = P(1,2) = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}, \quad P(2,3) = \begin{pmatrix} 0 & \frac{5}{12} & \frac{7}{12} \\ \frac{1}{3} & \frac{1}{12} & \frac{7}{12} \\ \frac{1}{3} & \frac{5}{12} & \frac{1}{4} \end{pmatrix}.$$

$$\tilde{P}^0 = P(0,1)P(1,2)P(2,3) = \begin{pmatrix} \frac{1}{6} & \frac{1}{3} & \frac{1}{2} \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{2} \\ \frac{1}{4} & \frac{1}{3} & \frac{5}{12} \end{pmatrix}$$

has a reversible distribution $(\frac{3}{13}, \frac{4}{13}, \frac{6}{13})$,

$$\tilde{P}^1 = P(1,2)P(2,3)P(0,1) = \begin{pmatrix} \frac{1}{3} & \frac{3}{8} & \frac{7}{24} \\ \frac{5}{12} & \frac{7}{24} & \frac{7}{24} \\ \frac{5}{12} & \frac{3}{8} & \frac{5}{24} \end{pmatrix}$$

has a reversible distribution $(\frac{5}{13}, \frac{9}{26}, \frac{7}{26})$, and

$$\tilde{P}^2 = P(2,3)P(0,1)P(1,2) = \begin{pmatrix} \frac{1}{4} & \frac{17}{48} & \frac{19}{48} \\ \frac{1}{3} & \frac{13}{48} & \frac{19}{48} \\ \frac{1}{3} & \frac{17}{48} & \frac{5}{16} \end{pmatrix}$$

has a reversible distribution $(\frac{4}{13}, \frac{17}{52}, \frac{19}{52})$. But the periodically stationary Markov chain determined by $P(0,1)$, $P(1,2)$, $P(2,3)$ is not periodically reversible. For instance, consider the path $1 \to 2 \to 3 \to 2$:
index 0: $\frac{3}{13} \times \frac{1}{2} \times \frac{1}{2} \times \frac{5}{12} \neq \frac{4}{13} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{3}$,
index 1: $\frac{5}{13} \times \frac{1}{2} \times \frac{7}{12} \times \frac{1}{2} \neq \frac{9}{26} \times \frac{1}{2} \times \frac{5}{12} \times \frac{1}{2}$,

index 2: $\frac{4}{13} \times \frac{5}{12} \times \frac{1}{2} \times \frac{1}{2} \neq \frac{17}{52} \times \frac{7}{12} \times \frac{1}{2} \times \frac{1}{2}$.

5.2. Remark 2

There exists completely periodically reversible Markov chains.

Example 5.2 Let $T = 2$,

$$P(0,1) = \begin{pmatrix} 0 & \frac{1}{3} & \frac{2}{3} \\ \frac{1}{3} & 0 & \frac{2}{3} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}, \quad P(1,2) = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}.$$

They determine a completely periodically reversible inhomogeneous Markov chain.

5.3. Remark 3

Periodical reversibility for different indices are not equivalent.

Example 5.3 Let $T = 3$,

$$P(0,1) = P(1,2) = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}, \quad P(2,3) = \begin{pmatrix} \frac{1}{3} & \frac{2}{3} \\ \frac{1}{3} & \frac{2}{3} \end{pmatrix}.$$

When the initial distribution is $\pi = (\frac{1}{2}, \frac{1}{2})$, the Markov chain is periodically reversible for index 0, but periodically irreversible for index 1. Consider the path for index 1: $1 \xrightarrow{1} 1 \xrightarrow{2} 2 \xrightarrow{0} 1$ and its reversal $1 \xrightarrow{1} 2 \xrightarrow{2} 1 \xrightarrow{0} 1$,

$$\frac{1}{2} \times \frac{1}{2} \times \frac{2}{3} \times \frac{1}{2} \neq \frac{1}{2} \times \frac{1}{2} \times \frac{1}{3} \times \frac{1}{2}.$$

6. RELATIONSHIP BETWEEN BROWNIAN MOTORS AND TIME-PERIODIC MARKOV CHAINS

6.1. Discrete Model of Rocking Ratchet

In Chapter 5 of ref. 30, Reimann proposed the rocking ratchet model of Brownian motor with periodic driving, i.e. the one-dimensional overdamped stochastic system

$$\eta \dot{x}(t) = -V'(x(t)) + y(t) + \xi(t),$$

where $\xi(t)$ is the white noise, η is the viscous friction coefficient, $V'(x) = \frac{\partial V(x)}{\partial x}$, and $y(t)$ is assumed to be a periodic function of time t with some period J, i.e.

$y(t+J) = y(t),\ \forall t$. Moreover, the potential V is always assumed to be spatially periodic with certain period L, i.e. $V(x+L) = V(x)$ for all x.

To make our discussion more general, we study the master equation of Brownian motors in (1):

$$dX_t = b(t, X_t)\,dt + \sigma(t, X_t)\,dW_t,$$

in which W_t is a Brownian motion, and $b(t,x)$, $\sigma(t,x)$ are periodic in both the time parameter t and the spatial parameter x.

For (1), we have the Kolmogorov's forward equation, also called the Fokker-Planck equation for the probability density $\rho(t,y)$ of X_t:

$$\begin{cases} \frac{\partial \rho(t,y)}{\partial t} = \frac{1}{2}\frac{\partial^2}{\partial y^2}(\sigma(t,y)^2\rho(t,y)) - \frac{\partial}{\partial y}(b(t,y)\rho(t,y)) \\ \rho(0,y) = \delta_{xy} \end{cases} \tag{29}$$

for some initial fixed point x.

Let $\frac{\partial}{\partial y}$ and $\frac{\partial^2}{\partial y^2}$ be replaced respectively by the finite difference operator δ and δ^2 on $S = \{0, \pm\Delta, \pm 2\Delta, \ldots\}$ with space step $\Delta > 0$, and let $\frac{\partial}{\partial t}$ be replaced by the finite difference operator τ on $\Theta = \{0, \epsilon, 2\epsilon, \ldots\}$ with time step $\epsilon = \frac{\Delta^2}{c} > 0$, where c is specified in Remark 6.3 below:

$$\begin{aligned} \delta f(i\Delta) &= \frac{f((i+1)\Delta) - f((i-1)\Delta)}{2\Delta}, \\ \delta^2 f(i\Delta) &= \frac{f((i+1)\Delta) + f((i-1)\Delta) - 2f(i\Delta)}{\Delta^2}, \\ \tau f(n\epsilon) &= \frac{f((n+1)\epsilon) - f(n\epsilon)}{\epsilon}. \end{aligned}$$

Then we can get the difference equation, which is just the discretized version of the Fokker-Planck equation from the point view of numerical analysis:

$$\tau\rho^{(\Delta)}(n\epsilon, i\Delta) = -\delta\big[b(n\epsilon, i\Delta)\rho^{(\Delta)}(n\epsilon, i\Delta)\big] + \frac{1}{2}\delta^2\big[\sigma^2(n\epsilon, i\Delta)\rho^{(\Delta)}(n\epsilon, i\Delta)\big], \tag{30}$$

i.e.

$$\begin{aligned} &\frac{\rho^{(\Delta)}((n+1)\epsilon, i\Delta) - \rho^{(\Delta)}(n\epsilon, i\Delta)}{\epsilon} \\ &= \frac{b(n\epsilon, (i-1)\Delta)\rho^{(\Delta)}(n\epsilon, (i-1)\Delta) - b(n\epsilon, (i+1)\Delta)\rho^{(\Delta)}(n\epsilon, (i+1)\Delta)}{2\Delta} \\ &\quad + \frac{1}{2\Delta^2}\big[\sigma^2(n\epsilon, (i+1)\Delta)\rho^{(\Delta)}(n\epsilon, (i+1)\Delta) - 2\sigma^2(n\epsilon, i\Delta)\rho^{(\Delta)}(n\epsilon, i\Delta) \\ &\quad + \sigma^2(n\epsilon, (i-1)\Delta)\rho^{(\Delta)}(n\epsilon, (i-1)\Delta)\big]. \end{aligned} \tag{31}$$

Following the next two theorems, one can see that (31) is also the master equation of a time-periodic Markov chain $\{Y_n^{(\Delta)} : n = 0, 1, 2, \ldots\}$, which converges in distribution to the inhomogeneous diffusion $\{X_t : t \geq 0\}$ in (1) as $\Delta \downarrow 0$.

Just as the well-known Donsker's invariance principle (the symmetric simple random walk approximates the Brownian motion under proper scaling of states and time), the homogeneous diffusions can be derived as the limit of discrete-parameter birth-death chains with decreasing step size and increasing frequencies. Here we only state Theorem 4.1 in Chapter V of ref. 5 without proof, where $[r]$ is the integer part of r.

Theorem 6.1. *Given two real-valued bounded functions $b(x)$, $\sigma(x)$ on $\mathbb{R}$, assume $b(x)$ continuously differentiable with bounded derivatives, and σ'' exists and is continuous, also $\sigma^2(x) > 0$ for all x. Let $\{Y_n^{(\Delta)} : n = 0, 1, 2, \ldots\}$ be a discrete-parameter birth-death chain on $S = \{0, \pm\Delta, \pm 2\Delta, \ldots\}$ with one-step transition probabilities p_{ij} from $i\Delta$ to $j\Delta$ given by*

$$p_{i,i-1} = \delta_i^{(\Delta)} = \frac{\sigma^2(i\Delta)\epsilon}{2\Delta^2} - \frac{b(i\Delta)\epsilon}{2\Delta},$$

$$p_{i,i+1} = \beta_i^{(\Delta)} = \frac{\sigma^2(i\Delta)\epsilon}{2\Delta^2} + \frac{b(i\Delta)\epsilon}{2\Delta},$$

$$p_{ii} = 1 - \delta_i^{(\Delta)} - \beta_i^{(\Delta)} = 1 - \frac{\sigma^2(i\Delta)\epsilon}{\Delta^2}.$$

where $\epsilon = \frac{\Delta^2}{\sigma_0^2}$ with $\sigma_0^2 = \sup_x \sigma^2(x)$. Let $Y_0^{(\Delta)} = [x_0/\Delta]\Delta$ where x_0 is an initial fixed point. Define

$$X_t^{(\Delta)} = Y_{[t/\epsilon]}^{(\Delta)}, \quad \forall t \geq 0.$$

(Remember $[t/\epsilon]$ is the integer part of t/ϵ.) Then, as $\Delta \downarrow 0$, the process $\{X_t^{(\Delta)}\}$ converges in distribution to the diffusion process $\{X_t\}$ with drift $b(x)$ and diffusion coefficient $\sigma^2(x)$, starting at x_0.

Following the same step as in ref. 5, one can also get the corresponding theorem for inhomogeneous diffusions, including the time-periodic case.

Theorem 6.2. *Given two real-valued bounded functions $b(t, x)$, $\sigma(t, x)$ on $\mathbb{R}^+ \times \mathbb{R}$, assume $b(t, x)$ continuously differentiable with bounded derivatives, and σ_x'' exists and is continuous, also $\sigma^2(t, x) > 0$ for all t and x. Let $\{Y_n^{(\Delta)} : n = 0, 1, 2, \ldots\}$ be a discrete-parameter birth-death chain on $S = \{0, \pm\Delta, \pm 2\Delta, \ldots\}$ with transition probabilities*

$$p_{ij}(n) = P\left(Y_{n+1}^{(\Delta)} = j\Delta | Y_n^{(\Delta)} = i\Delta\right)$$

given by

$$p_{i,i-1}(n) = \delta_i^{(\Delta)}(n) = \frac{\sigma^2(n\epsilon, i\Delta)\epsilon}{2\Delta^2} - \frac{b(n\epsilon, i\Delta)\epsilon}{2\Delta},$$

$$p_{i,i+1}(n) = \beta_i^{(\Delta)}(n) = \frac{\sigma^2(n\epsilon, i\Delta)\epsilon}{2\Delta^2} + \frac{b(n\epsilon, i\Delta)\epsilon}{2\Delta},$$

$$p_{ii}(n) = 1 - \delta_i^{(\Delta)}(n) - \beta_i^{(\Delta)}(n) = 1 - \frac{\sigma^2(n\epsilon, i\Delta)\epsilon}{\Delta^2}. \tag{32}$$

where $\epsilon = \frac{\Delta^2}{\sigma_0^2}$ *with* $\sigma_0^2 = \sup_{t,x} \sigma^2(t, x)$. *Let* $Y_0^{(\Delta)} = [x_0/\Delta]\Delta$ *where* x_0 *is an initial fixed point. Define*

$$X_t^{(\Delta)} = Y_{[t/\epsilon]}^{(\Delta)}, \ \forall t \geq 0.$$

Then, as $\Delta \downarrow 0$*, the process* $\{X_t^{(\Delta)}\}$ *converges in distribution to the diffusion process* $\{X_t\}$ *with drift* $b(t, x)$ *and diffusion coefficient* $\sigma^2(t, x)$*, starting at* x_0.

Remark 6.3. The condition $\epsilon = \frac{\Delta^2}{\sigma_0^2}$ in the above two theorems can be replaced by the condition that $\epsilon = \frac{\Delta^2}{c}$, for some constant $c \geq \sigma_0^2$.

In the time-periodic case, consider a subsequence $\{\Delta_k : k = 1, 2, \ldots\}$ of $\Delta \downarrow 0$, where $\Delta_k = \sqrt{cJ/k}$. Then for each k, the birth-death chain $\{Y_n^{(\Delta_k)} : n = 0, 1, 2, \ldots\}$ is a time-periodic Markov chain with temporal period k. We have known that $\{X_t^{(\Delta_k)}\}$ converges in distribution to the diffusion $\{X_t\}$. That is to say, we can approximate the diffusion process in (1) by time-periodic Markov chains, which are much more easy to study.

As $\Delta_k \downarrow 0$ the state space $S = \{0, \pm\Delta_k, \pm 2\Delta_k, \ldots\}$ approximates $\mathbb{R}$, provided that one takes it for granted that the state $j\Delta_k$ represents an interval of width Δ_k around $j\Delta_k$. Accordingly, one can spread the probability $\rho_i^{(n)} = P(Y_n^{(\Delta_k)} = i\Delta_k)$ over this interval. Thus, one can introduce the approximate density $\rho^{(\Delta_k)}(t, y)$ at time $t = n\epsilon$ for states $y = i\Delta_k$ by

$$\rho^{(\Delta_k)}(n\epsilon, i\Delta_k) = \frac{\rho_i^{(n)}}{\Delta_k}. \tag{33}$$

For each k, we have the master equation of the time-periodic Markov chain $\{Y_n^{(\Delta_k)}\}$:

$$\rho^{(n+1)} = \rho^{(n)} P(n), \tag{34}$$

i.e.

$$\rho_i^{(n+1)} = \rho_i^{(n)} p_{ii}(n) + \rho_{i+1}^{(n)} p_{i+1,i}(n) + \rho_{i-1}^{(n)} p_{i-1,i}(n), \ \ \forall i \in \mathbb{Z}. \tag{35}$$

where the row vector $\rho^{(n)} = \{\rho_i^n\}$ denotes the distribution of $Y_n^{(\Delta_k)}$, and $P(n) = \{p_{ij}(n)\}$ denotes the transition probability matrix.

Rearrange (35) with (32) and (33), then one can also arrive at the difference equation (31).

Now we come to the conclusion that for each $k \in \mathbb{N}$, the time-periodic Markov chain $\{Y_n^{(\Delta_k)} : n = 0, 1, 2, \ldots\}$ is really a simple discrete model of rocking ratchet.

6.2. Particle Current and Circulation Weights

The quantity of most interest in the context of Brownian motor is the particle current $\langle \dot{x} \rangle = \langle \dot{x}(t) \rangle = \lim_{t\to\infty} \frac{x(t)}{t}$. By Theorem 6.2, the particle current $\langle \dot{x} \rangle$ can be regarded as a limit of the particle current of $\{Y_n^{(\Delta_k)}\}$, i.e. $\lim_{n\to\infty} \frac{Y_n^{(\Delta_k)}}{n\epsilon}$, when k tends to infinity.

Remark 6.4. By the ergodic theory, one can prove that both $\frac{x(t)}{t}$ and $\frac{Y_n^{(\Delta_k)}}{n\epsilon}$ converge to a constant with probability 1.

Note that $\{Y_n^{(\Delta_k)}\}$ is a time-periodic Markov chain with period k, and the spatial periodicity of $b(t, x)$ and $\sigma(t, x)$, then we can define another time-periodic Markov chain $\{Z_n^k : Z_n^k = Y_n^{(\Delta_k)} \bmod L\}$ with finite state space $\tilde{S} = \{0, \Delta_k, 2\Delta_k, \ldots, (N - 1)\Delta_k\}$, where $N = \frac{L}{\Delta_k}$. Technically, one can replace σ_0^2 in Theorem 6.2 by another constant $c > 0$ which is larger than σ_0^2, so that $N = \frac{L}{\Delta_k}$ is an integer with $\Delta_k = \sqrt{cJ/k}$.

As in Sec. 3, we can define periodical circuits of $\{Z_n^k\}$. We also denote the reversed circuit of a periodical circuit C for index l by $C_{l\_}$ and the circulation weights of them by λ_C and $\lambda_{C_{l\_}}$.

Since $\{Y_n^{(\Delta_k)}\}$ and $\{Z_n^k\}$ are birth-death chains, every periodical circuit C completed by $\{Z_n^k\}$ corresponds to that $\{Y_n^{(\Delta_k)}\}$ walks forward or backward with a certain length, denoted as $\kappa_C \geq 0$. For instance, let $C = (0, \Delta_k, 2\Delta_k, \ldots, (N - 1)\Delta_k; m)$, whose reversed circuit for index l is $C_{l\_} = (0, (N-1)\Delta_k, (N - 2)\Delta_k, \ldots, \Delta_k; 2l - m)$, then $\kappa_C = \kappa_{C_{l\_}} = N\Delta_k$, for any $m = 0, 1, 2, \ldots, k - 1$. Notice that each trajectory of $\{Z_n^k\}$ can be decomposed into a set of periodical circuits, then it is easy to conclude that

$$\lim_{n\to\infty} \frac{Y_n^{(\Delta_k)}}{n\epsilon} = \frac{1}{\epsilon} \sum_{C\in C_\infty^+} \kappa_C(\lambda_C - \lambda_{C_{l\_}}) \tag{36}$$

for any fixed $l = 0, 1, 2, \ldots, k - 1$, where C_∞^+ denotes the set of periodical circuits of $\{Z_n^k\}$ that corresponds to $\{Y_n^{(\Delta_k)}\}$ walking forward rather than backward. So, when k is large enough,

$$\langle \dot{x} \rangle \approx \frac{1}{\epsilon} \sum_{C \in C_\infty^+} \kappa_C (\lambda_C - \lambda_{C_{l-}}).$$

Finally, Theorem 3.22 implies the very interesting result that if the periodic Markov chain $\{Z_n^k\}$ has periodical reversibility for certain index $l = 0, 1, 2, \ldots, k-1$ (i.e. $\lambda_C = \lambda_{C_{l-}}, \forall C \in C_\infty$), then vanishes the particle current in the discrete model $\{Y_n^{(\Delta_k)}\}$ of Brownian motors. So, if one hope that a non-vanishing particle current exists, he must consider periodically irreversible Markov chains, which correspond to non-equilibrium steady states in statistical physics.

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