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Fokker–Planck Equations for a Free Energy Functional or Markov Process on a Graph

Shui-Nee Chow, Wen Huang, Yao Li & Haomin Zhou

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Abstract

The classical Fokker–Planck equation is a linear parabolic equation which describes the time evolution of the probability distribution of a stochastic process defined on a Euclidean space. Corresponding to a stochastic process, there often exists a free energy functional which is defined on the space of probability distributions and is a linear combination of a potential and an entropy. In recent years, it has been shown that the Fokker–Planck equation is the gradient flow of the free energy functional defined on the Riemannian manifold of probability distributions whose inner product is generated by a 2-Wasserstein distance. In this paper, we consider analogous matters for a free energy functional or Markov process defined on a graph with a finite number of vertices and edges. If $N \geqq 2$ is the number of vertices of the graph, we show that the corresponding Fokker–Planck equation is a system of N *nonlinear* ordinary differential equations defined on a Riemannian manifold of probability distributions. However, in contrast to stochastic processes defined on Euclidean spaces, the situation is more subtle for discrete spaces. We have different choices for inner products on the space of probability distributions resulting in different Fokker–Planck equations for the same process. It is shown that there is a strong connection but there are also substantial discrepancies between the systems of ordinary differential equations and the classical Fokker–Planck equation on Euclidean spaces. Furthermore, both systems of ordinary differential equations are gradient flows for the same free energy functional defined on the Riemannian manifolds of probability distributions with different metrics. Some examples are also discussed.

1. Introduction

In this paper, we are concerned with the relationships among three concepts defined on graphs: the free energy functional, the Fokker–Planck equation and

stochastic processes. We begin by recalling some of the well-known facts about these concepts.

Consider a stochastic process defined by the following randomly perturbed differential equation,

$$\mathrm{d}x = -\nabla\Psi(x)\mathrm{d}t + \sqrt{2\beta}\mathrm{d}W_t,\ x \in \mathbb{R}^N, \tag{1}$$

where $\Psi(x)$ is a given scalar-valued potential function, β a positive constant, and $\mathrm{d}W_t$ the white noise. This stochastic differential equation (SDE) is one of the primary tools in many practical problems that involve uncertainty or incomplete information. Examples can be found in many different disciplines. Solutions of SDEs are stochastic processes. The Fokker–Planck equation is a partial differential equation describing the time evolution of the probability density function $\boldsymbol{\rho}(x,t)$ of the trajectories of the SDE (1). It has the form

$$\frac{\partial\boldsymbol{\rho}(x,t)}{\partial t} = \nabla\cdot(\nabla\Psi(x)\boldsymbol{\rho}(x,t)) + \beta\Delta\boldsymbol{\rho}(x,t), \tag{2}$$

where $\nabla\cdot(\nabla\Psi(x)\boldsymbol{\rho}(x,t))$ is called the drift term, and $\Delta\boldsymbol{\rho}(x,t)$ is the diffusion term generated by white noise. The Fokker–Planck equation plays a prominent role in many disciplines and has been studied by many authors (see, for example, [19,40,42]).

The notion of free energy is widely used in many disciplines, and it is related to the maximal amount of work that can be extracted from a system ([30,43,52] and references therein). For us, a free energy functional is a scalar-valued function defined on the space of probability distributions and is composed of a potential energy U and an entropy functional S, that is, the free energy is expressed as

$$F(\boldsymbol{\rho}) = U(\boldsymbol{\rho}) - \beta S(\boldsymbol{\rho}), \tag{3}$$

where $\beta > 0$ is a constant called temperature, and $\boldsymbol{\rho}$ is a probability density function defined on a state space X, which may be "continuous" (for example $X = \mathbb{R}^N$), or "discrete" (for example $X = \{a_1, \ldots, a_N\}$). For a system with state space $\mathbb{R}^N$, the potential functional is defined by

$$U(\boldsymbol{\rho}) := \int_{\mathbb{R}^N} \Psi(x)\boldsymbol{\rho}(x)\mathrm{d}x,$$

where $\Psi(x)$ is a given potential function. The entropy, also called Gibbs–Boltzmann entropy, is given by

$$S(\boldsymbol{\rho}) := -\int_{\mathbb{R}^N} \boldsymbol{\rho}(x)\log\boldsymbol{\rho}(x)\mathrm{d}x.$$

It is well known that the global minimizer of the free energy F is a probability distribution, called the Gibbs distribution,

$$\boldsymbol{\rho}^*(x) = \frac{1}{K}\mathrm{e}^{-\Psi(x)/\beta}, \qquad \text{where } K = \int_{\mathbb{R}^N} \mathrm{e}^{-\Psi(x)/\beta}\,\mathrm{d}x. \tag{4}$$

We note that in order for equation (4) to be well-defined, Ψ must satisfy some growth conditions to ensure that K is finite. In this paper, we consider only potentials satisfying this condition.

Although historical development of the free energy functional and that of the Fokker–Planck equation are not directly related, there are many studies that reveal some connection between them. The following two results about the relationship between them are well known [15,16,19,25,26,33,40]:

1. The free energy (3) is a Lyapunov functional for the Fokker–Planck equation (2), that is, if the probability density $\boldsymbol{\rho}(t, x)$ is a solution of (2), then $F(\boldsymbol{\rho}(t, x))$ is a decreasing function of time.
2. The Gibbs distribution (4) is the global minimizer of the free energy (3) and is the unique stationary solution of the Fokker–Planck equation (2).

In recent years, there have been many studies about the connection between the free energy, the Fokker–Planck equation, the Ricci curvature, and optimal transportation in a continuous state space. For example, Jordan et al. [26] and Otto [33] showed that the Fokker–Planck equation may be viewed as the gradient flow of the free energy functional on a Riemannian manifold of probability measures with a 2-Wasserstein metric. More precisely, let the state space X be a "suitable" complete metric space with distance d, and let $\mathscr{P}(X)$ be the space of Borel probability measures on X. For any given two elements $\mu_1, \mu_2 \in \mathscr{P}(X)$, the 2-Wasserstein distance between μ_1 and μ_2 is defined by

$$W_2(\mu_1, \mu_2)^2 = \inf_{\lambda \in \mathscr{M}(\mu_1, \mu_2)} \int_{X \times X} d(x, y)^2 d\lambda(x, y), \tag{5}$$

where $\mathscr{M}(\mu_1, \mu_2)$ is the collection of Borel probability measures on $X \times X$ with marginal measures μ_1 and μ_2 respectively. Then $(\mathscr{P}(X), W_2)$ forms a Riemannian manifold and the Fokker–Planck equation (2) can be derived by an implicit scheme which can be reinterpreted as a gradient flow of the free energy (3) on this manifold. Clearly, we have two metric spaces (X, d) and $(\mathscr{P}(X), W_2)$, and there exists an isometric embedding $X \to \mathscr{P}(X)$ given by $x \to \delta_x$. For the notion of Wasserstein distance, we refer to [13,47]. For theory and applications of the Wasserstein distance, we refer to the articles [2,7,8,10,17,18,28,34,48,49] and references therein.

We note that Otto and Westdickenberg [35] showed the relationship between 2-Wasserstein distance and minimal energy curves on $X = \mathbb{R}^N$. Moreover, the convexity of the entropy on $(\mathscr{P}(X), W_2)$ is equivalent to the non-negativity of the Ricci curvature, which induces the definition of the abstract Ricci curvature on length spaces [11,44–46,50,51]. Furthermore, it is proved in [29] that if (X, d) is a length space, then the manifold $(\mathscr{P}(X), W_2)$ is also a length space.

We summarize the relationship among the free energy, the Fokker–Planck equation and stochastic processes in the state space $\mathbb{R}^N$ in Fig. 1. From the free energy point of view, the Fokker–Planck equation is the gradient flow of the free energy on the probability space with 2-Wasserstein metric. From the viewpoint of stochastic processes, the Fokker–Planck equation describes the time evolution of the probability density function.

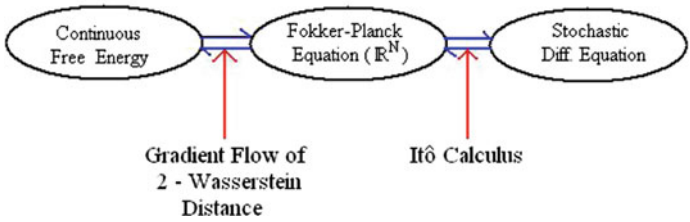

Fig. 1. Interrelations among the free energy, Fokker–Planck equation and the stochastic differential equation in $\mathbb{R}^N$

In this paper, we consider similar matters on a discrete state space which is a finite graph. For a system with a discrete state space $X = \{a_1, a_2, \ldots, a_N\}$, we let $\boldsymbol{\rho} = \{\rho_i\}_{i=1}^N$ be a probability distribution on X, that is,

$$\sum_{i=1}^N \rho_i = 1 \quad \rho_i \geqq 0,$$

where ρ_i is the probability of state a_i. Then the free energy functional has the following expression:

$$F(\boldsymbol{\rho}) = \sum_{i=1}^N \Psi_i \rho_i + \beta \sum_{i=1}^N \rho_i \log \rho_i, \tag{6}$$

where Ψ_i is the potential at the state a_i. Obviously, the potential and entropy functionals are given, respectively, by

$$U(\boldsymbol{\rho}) := \sum_{i=1}^N \Psi_i \rho_i, \quad \text{and} \quad S(\boldsymbol{\rho}) := -\sum_{i=1}^N \rho_i \log \rho_i.$$

The free energy functional has a global minimizer, the Gibbs density, given by

$$\rho_i^* = \frac{1}{K} \mathrm{e}^{-\Psi_i/\beta}, \qquad \text{where } K = \sum_{i=1}^N \mathrm{e}^{-\Psi_i/\beta}. \tag{7}$$

Despite remarkable development in the theory related to the Fokker–Planck equation in continuous state spaces, much less is known when the state space is discrete and finite. There are results in mass transport theory for discrete spaces [5,31,41]. However, to the best of our knowledge, the Fokker–Planck equation on a graph has not been established. We know that a finite metric space with more than one point is not a length space. This indicates that existing theory may not be extended directly to a finite graph. In addition, the notion of "white noise" is also not clear for a Markov process defined on a graph.

Based on recent results in continuous state spaces, it is natural to apply spatial discretization schemes, such as the central difference scheme, to the Fokker–Planck equation (2) to obtain their counterparts for discrete state spaces. The resulting

equation for a discrete state space is a system of ordinary differential equations. However, many problems arise with this approach. For instance, commonly used linear discretization schemes often lead to steady states that are different from the Gibbs density (7), which is the global minimizer of the free energy. In fact, we prove rigorously that no linear discretization scheme could achieve the Gibbs distribution at its steady state for general potentials in Theorem 1. This suggests that the equation obtained by a linear discretization scheme does not capture the real energy landscape of the free energy on a discrete space, and it is not the desired Fokker–Planck equation.

Inspired by Fig. 1, we define the Fokker–Planck equation on a graph X by two different strategies. From the free energy viewpoint, since there is no ready substitute for the Wasserstein metric on a graph, we first endow the probability space P(X) with a Riemannian metric d, which depends on the potential as well as the structure of the graph. Then, the Fokker–Planck equation can be derived as the gradient flow of the free energy F on the Riemannian manifold $(\mathscr{P}(X), d)$. From the stochastic process viewpoint, we introduce a new interpretation of white noise perturbations to a Markov process on X, and derive another Fokker–Planck equation as the time evolution equation for its probability density function. We must note that unlike the continuous state space case, we obtain two different Fokker–Planck equations on the graph following these approaches. It seems one of the reasons that we obtain different Fokker–Planck equations is that finite graphs are not length spaces, generally.

To be more precise on the approaches, we consider a graph $G = (V, E)$, where $V = \{a_1, \ldots, a_N\}$ is the set of vertices, and E the set of edges. We denote the neighborhood of a vertex $a_i \in V$ by $N(i)$:

$$N(i) = \{j \in \{1, 2, \ldots, N\} | \{a_i, a_j\} \in E\}.$$

We further assume that the graph G is a simple graph (that is, there are no self loops or multiple edges) with $|V| \geqq 2$, and G is connected. We note that results in this paper still hold after nominal modifications if the graph G is not simple.

Let $\boldsymbol{\Psi} = (\Psi_i)_{i=1}^N$ be a given potential function on V, where Ψ_i is the potential on a_i. $\beta \geqq 0$ is the strength of "white noise". Let

$$\mathscr{M} = \left\{ \boldsymbol{\rho} = (\rho_i)_{i=1}^N \in \mathbb{R}^N \,|\, \sum_{i=1}^N \rho_i = 1 \text{ and } \rho_i > 0 \text{ for } i = 1, 2, \ldots, N \right\},$$

be the space of positive probability distributions on V. Then from the free energy viewpoint, we obtain a Fokker–Planck equation on $\mathscr{M}$ (see Theorem 2):

$$\begin{aligned} \frac{\mathrm{d}\rho_i}{\mathrm{d}t} = & \sum_{j \in N(i), \Psi_j > \Psi_i} ((\Psi_j + \beta \log \rho_j) - (\Psi_i + \beta \log \rho_i))\rho_j \\ & + \sum_{j \in N(i), \Psi_j < \Psi_i} ((\Psi_j + \beta \log \rho_j) - (\Psi_i + \beta \log \rho_i))\rho_i \\ & + \sum_{j \in N(i), \Psi_j = \Psi_i} \beta(\rho_j - \rho_i) \end{aligned} \tag{8}$$

for $i = 1, 2 \ldots, N$. If we take the stochastic process viewpoint, then we obtain a different Fokker–Planck equation on $\mathscr{M}$ (see Theorem 3):

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = \sum_{j\in N(i),\bar{\Psi}_j>\bar{\Psi}_i} ((\Psi_j + \beta\log\rho_j) - (\Psi_i + \beta\log\rho_i))\rho_j + \sum_{j\in N(i),\bar{\Psi}_j<\bar{\Psi}_i} ((\Psi_j + \beta\log\rho_j) - (\Psi_i + \beta\log\rho_i))\rho_i, \tag{9}$$

where $\bar{\Psi}_i = \Psi_i + \beta\log\rho_i$ and $i = 1, 2, \ldots, N$. For convenience, we call equations (8) and (9) Fokker–Planck equation I (8) and II (9), respectively.

We will show that Fokker–Planck equation I (8) is the gradient flow of free energy (6) on a Riemannian manifold $(\mathscr{M}, d_{\boldsymbol{\Psi}})$, where $d_{\boldsymbol{\Psi}}$ is a Riemannian metric on $\mathscr{M}$ induced by Ψ, and we will give the precise definition of $(\mathscr{M}, d_{\boldsymbol{\Psi}})$ in Section 3. On the other hand, Fokker–Planck equation II (9) is derived from a Markov process on G subject to a "white noise" perturbation, for which we will give the definition in Section 5. In the continuous case, the Fokker–Planck equation obtained by these two different strategies coincides beautifully. However, in the discrete case, there are substantial differences between them, although their appearances seem to differ only a little. The connection of Fokker–Planck equation I (8) to a Markov process on the graph is still unclear. Fokker–Planck equation II (9) is not a gradient flow of the free energy on a smooth Riemannian manifold of the probability space. However, it is a "gradient flow" of the free energy on another metric space $(\mathscr{M}, d_{\bar{\boldsymbol{\Psi}}})$, which is only piecewise smooth. More precisely, we will show that $\mathscr{M}$ is divided into a finite number of segments, and $d_{\bar{\boldsymbol{\Psi}}}$ is smooth only in the interior of each segment. We also note that the manner by which we derive Fokker–Planck equation II (9) seems to be related to Onsager's flux [37–39].

Although (8) and (9) are different, they share some similar properties for $\beta > 0$:

- Free energy F decreases along solutions of both equations.
- Both equations are gradient flows of the same free energy on the same probability space $\mathscr{M}$, but with different metrics.
- The Gibbs distribution $\boldsymbol{\rho}^* = (\rho_i^*)_{i=1}^N$ is the stable stationary solution of both equations.
- Near the Gibbs distribution, the difference between the two equations is small.
- For both equations, given any initial condition $\boldsymbol{\rho}^0 \in \mathscr{M}$, there exists a unique solution $\boldsymbol{\rho}(t, \boldsymbol{\rho}^0)$ for $t \geqq 0$, and $\boldsymbol{\rho}(t, \boldsymbol{\rho}^0) \to \boldsymbol{\rho}^*$, as $t \to +\infty$.

Formally, if the graph is a lattice, both Fokker–Planck equations I (8) and II (9) can be viewed as special upwind numerical schemes of the Fokker–Planck equation on the continuous state space (2). However, they are both uncommonly used schemes. In particular, the diffusion term is discretized by two surprisingly consistent nonlinear schemes, which, to the best of our knowledge, have not been considered by other authors. It is worth mentioning that most of the commonly used consistent and stable linear schemes, such as the central difference scheme, lead to unexpected problems as demonstrated in Section 2.

The results obtained in this paper are largely inspired by recent developments in the Fokker–Planck equation and the 2-Wasserstein metric, especially the theory

reported in [25,26,33]. Our results are also influenced by the upwind schemes for shock capturing in conservation laws [6,27], as well as the recent studies on Parrondo's paradox [22,23] and flashing ratchet models for molecular motors [1,14,24]. We will demonstrate a Parrondo's paradox of free energy by applying our Fokker–Planck equation (8) to a flashing ratchet model.

During the time when this paper was under review, we found that Mielke introduced a Riemannian metric independently in [32], which is similar to our Riemannian metric with a constant potential. More precisely, if we express a chemical reaction system as a graph, then Mielke's metric can be obtained by discretizing Otto's calculus in a way similar to ours. Mielke studied reaction-diffusion equations with his metric, showed that a reaction-diffusion equation with detailed balance could be written as a gradient flow of relative entropy. More recently, Hao et al. [21] gives an interesting physical explanation of the log-average term

$$\frac{\rho_i - \rho_j}{\log \rho_i - \log \rho_j},$$

which appears in both Mielke's metric and in ours. We cite from [21] that the log-average is the"conductance in the stoichiometric network theory of chemical reactions", and "the numerator is the flux and the denominator is the driving force of a transition". This new progress reveals some potential connections between our work and chemical reactions.

This paper is organized as follows: In Section 2, we discuss why we must use nonlinear Fokker–Planck equations in the discrete case. Some basic geometric properties of $\mathscr{M}$ are shown in Section 3. In Section 4, we prove that Fokker–Planck equation I (8) is the gradient flow of free energy, and show some related properties. In Section 5, we show how we interpret "white noise" in the Markov process to obtain Fokker–Planck equation II (9). In Section 6, we explain the upwind structure in Fokker–Planck equations I (8) and II (9). In the last section, we consider the flashing ratchet model as an application.

2. Why Nonlinear Fokker–Planck Equations on Graphs

Comparing the Fokker–Planck equation (2) in the continuous state space with our Fokker–Planck equations (8) and (9) on graphs, one immediately notices that our equations are nonlinear while (2) is linear. It is natural to question the nonlinearity in both equations. For example, can one just apply common discretization schemes, such as the well known central difference, to (2) and obtain linear Fokker–Planck equations in the discrete case? However, in our numerical studies, we encountered many problems. For instance, steady state solutions of linear equations derived from discretization are not the Gibbs distributions. Furthermore, the free energy does not decay along the solutions. In this section, we prove that these problems occur for all linear systems obtained from discretizing the continuous Fokker–Planck equation (2) using consistent linear schemes.

To be more precise, any given linear discretization of (2) can be written as

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = \sum_j \left(\left(\sum_k \mathrm{e}^i_{jk} \Psi_k \right) + c^i_j \right) \rho_j, \text{ for } i = 1, 2, \ldots, N, \tag{10}$$

where Ψ is the given potential and $\{\mathrm{e}^i_{jk}\}_{N\times N}$ and $\{c^i_j\}_N$ are some constants that are not all zero. Assume that the Gibbs distribution (7) is the steady state solution of (10), then we must have

$$\sum_j \left(\left(\sum_k \mathrm{e}^i_{jk} \Psi_k \right) + c^i_j \right) \mathrm{e}^{-\frac{\Psi_j}{\beta}} = 0, \text{ for } i = 1, 2, \ldots, N. \tag{11}$$

Let us denote $\mathscr{A}$ as the collection of potentials Ψ satisfying (11), that is

$$\mathscr{A} = \{(\Psi_1, \ldots, \Psi_N) \in \mathbb{R}^N : \sum_j ((\sum_k \mathrm{e}^i_{jk} \Psi_k) + c^i_j) \mathrm{e}^{-\frac{\Psi_j}{\beta}} = 0, \text{ for } 1 \leqq i \leqq N\}. \tag{12}$$

Theorem 1. *The set $\mathscr{A}$ has zero measure in $\mathbb{R}^N$, that is,*

$$\kappa(\mathscr{A}) = 0,$$

where $\kappa(\cdot)$ is the Lebesgue measure on $\mathbb{R}^N$.

To prove this theorem, we need the following lemma.

Lemma 1. *Let $g(x)$ be a function in $C^1(\mathbb{R}^N)$. Denote $\mathscr{B} = \{x \in \mathbb{R}^N : g(x) = 0\}$, and $\mathscr{B}_j = \{x \in \mathscr{B} : g_{x_j}(x) = 0\}$ for $j = 1, \ldots, N$. Then*

$$\kappa(\mathscr{B}_j) = \kappa(\mathscr{B}). \tag{13}$$

Proof. This lemma is a special case of a well known fact about functions in Sobolev spaces, see for example, Lemma 7.7 in [20].

Now, we are ready to prove Theorem 1.

Proof. For convenience of notation, let us denote $\Psi = (\Psi_1, \ldots, \Psi_N)$ and

$$f_i(\Psi) = \sum_j \left(\left(\sum_k \mathrm{e}^i_{jk} \Psi_k \right) + c^i_j \right) \mathrm{e}^{-\frac{\Psi_j}{\beta}}.$$

Clearly, we have $f_i \in C^\infty(\mathbb{R}^N)$. Then, we can consider the sets, $\mathscr{A}_\vartheta$, which collect all potentials $\Psi \in \mathscr{A}$ with vanishing ϑ-th derivatives of f_i for all $i = 1, \ldots, N$, that is,

$$\mathscr{A}_\vartheta = \{\Psi \in \mathscr{A} : D^\vartheta f_i(\Psi) = 0, \text{ for } 1 \leqq i \leqq N\},$$

where $\vartheta = (\vartheta_1, \ldots, \vartheta_N)$ is a multiple non-negative integer index, and D^ϑ is the partial derivative operator. Obviously, $\mathscr{A}$ and $\mathscr{A}_\vartheta$ are closed subsets.

Using Lemma 1 recursively, we have

$$\kappa(\mathscr{A}) = \kappa(\mathscr{A}_\vartheta), \tag{14}$$

for arbitrary multi-index ϑ. Next, we show $\kappa(\mathscr{A}) = 0$ by contradiction.

Assume that $\kappa(\mathscr{A}) > 0$, so we have $\kappa(\mathscr{A}_\vartheta) = \kappa(\mathscr{A}) > 0$ for arbitrary multi-index ϑ. This implies that there must exist a potential $\Psi^0 \in \mathscr{A}$ such that

$$f_i(\Psi^0) = 0 \quad \text{and} \quad D^\vartheta f_i(\Psi^0) = 0,$$

for arbitrary ϑ.

For any $r \in \{1, \ldots, N\}$ and $s \in \{1, \ldots, N\}$ with $r \neq s$, we have

$$\frac{\partial^3 f_i}{\partial \Psi_r^2 \partial \Psi_s}(\Psi) = \frac{\mathrm{e}^i_{rs}}{\beta^2} \mathrm{e}^{-\frac{\Psi_r}{\beta}}.$$

Therefore,

$$\frac{\partial^3 f_i}{\partial \Psi_r^2 \partial \Psi_s}(\Psi^0) = 0$$

implies $\mathrm{e}^i_{rs} = 0$ for $r \neq s$. Thus, we must have

$$f_i(\Psi) = \sum_j (\mathrm{e}^i_{jj} \Psi_j + c_j) \mathrm{e}^{-\frac{\Psi_j}{\beta}}.$$

It is easy to compute that for any $j \in \{1, \ldots, N\}$,

$$\frac{\partial^l f_i}{\partial \Psi_j^l} = \left(\frac{l \mathrm{e}^i_{jj}}{(-\beta)^{l-1}} + \frac{(\mathrm{e}^i_{jj} \Psi_j + c^i_j)}{(-\beta)^l} \right) \mathrm{e}^{-\frac{\Psi_j}{\beta}},$$

for arbitrary $l \in \mathbb{N}$. Using the fact that

$$\frac{\partial^l f_i}{\partial \Psi_j^l}(\Psi^0) = 0,$$

which is

$$-\beta l \mathrm{e}^i_{jj} + (\mathrm{e}^i_{jj} \Psi^0_j + c^i_j) = 0, \quad \text{for all } l \geqq 1.$$

This implies $\mathrm{e}^i_{jj} = 0$ and $c^i_j = 0$, and it contradicts the fact that not all of e^i_{jk} and c^i_j are zero. So we must have $\kappa(\mathscr{A}) = 0$.

Theorem 1 indicates that one cannot expect a linear system obtained by a consistent discretization of the continuous Fokker–Planck equation (2) to achieve the Gibbs distribution at its steady state for general potentials. It suggests that a Fokker–Planck equation on a graph needs to be nonlinear, in general. However, this does not imply that general linear systems cannot achieve the Gibbs distribution at their steady states. In fact, it can be verified that for any given probability vector

ρ^*, including the Gibbs distribution, there exists a "reaction matrix" A, such that the solution of the ODE system

$$\rho'(t) = \rho A$$

tends to ρ^* as time $t \to \infty$. Furthermore, the choice of A is not unique. One may choose any A with the property of $e^{At} \to P$, where $P = [\rho^*, \rho^*, \ldots, \rho^*]$ is a rank one matrix. For example, taking $A = P - I$ will work in this situation. But such a matrix A cannot be obtained by linearly discretizing the continuous Fokker–Planck equation in a consistent way, as we explained in Theorem 1.

3. Metrics on $\mathscr{M}$ and Riemannian Manifolds

Given a graph $G = (V, E)$ with $V = \{a_1, a_2, \ldots, a_N\}$, we consider all positive probability distributions on V:

$$\mathscr{M} = \left\{ \boldsymbol{\rho} = (\rho_i)_{i=1}^N \in \mathbb{R}^N \,\middle|\, \sum_{i=1}^N \rho_i = 1 \text{ and } \rho_i > 0 \text{ for } i \in \{1, 2, \ldots, N\} \right\},$$

and its closure,

$$\overline{\mathscr{M}} = \left\{ \boldsymbol{\rho} = (\rho_i)_{i=1}^N \in \mathbb{R}^N \,\middle|\, \sum_{i=1}^N \rho_i = 1 \text{ and } \rho_i \geqq 0 \text{ for } i \in \{1, 2, \ldots, N\} \right\}.$$

Let $\partial\mathscr{M}$ be the boundary of $\mathscr{M}$, that is,

$$\partial\mathscr{M} = \left\{ \boldsymbol{\rho} = \{\rho_i\}_{i=1}^N \in \mathbb{R}^N \,\middle|\, \sum_{i=1}^N \rho_i = 1,\ \rho_i \geqq 0 \text{ and } \prod_{i=1}^N \rho_i = 0 \right\}.$$

The tangent space $T_{\boldsymbol{\rho}}\mathscr{M}$ at $\boldsymbol{\rho} \in \mathscr{M}$ is defined by

$$T_{\boldsymbol{\rho}}\mathscr{M} = \left\{ \boldsymbol{\sigma} = (\sigma_i)_{i=1}^N \in \mathbb{R}^N \,\middle|\, \sum_{i=1}^N \sigma_i = 0 \right\}.$$

It is clear that the standard Euclidean metric on $\mathbb{R}^N$, d, is also a Riemannian metric on $\mathscr{M}$.

Let

$$\boldsymbol{\Phi} : (\mathscr{M}, d) \to (\mathbb{R}^N, d) \tag{15}$$

be an arbitrary smooth map given by:

$$\boldsymbol{\Phi}(\boldsymbol{\rho}) = (\Phi_i(\boldsymbol{\rho}))_{i=1}^N, \qquad \boldsymbol{\rho} \in \mathscr{M}.$$

In the following, we will endow $\mathscr{M}$ with a metric $d_{\boldsymbol{\Phi}}$, which depends on $\boldsymbol{\Phi}$ and the structure of G.

For technical reasons, we first consider the function

$$\frac{r_1 - r_2}{\log r_1 - \log r_2},$$

where $r_1 > 0, r_2 > 0$ and $r_1 \neq r_2$. We want to extend this to the closure of the first quadrant in the plane. In fact, this can be easily achieved by the following function:

$$e(r_1, r_2) = \begin{cases} \frac{r_1 - r_2}{\log r_1 - \log r_2} & \text{if } r_1 \neq r_2 \text{ and } r_1 r_2 > 0 \\ 0 & \text{if } r_1 r_2 = 0 \\ r_1 & \text{if } r_1 = r_2 \end{cases}.$$

It is easy to check that $e(r_1, r_2)$ is a continuous function on

$$\{(r_1, r_2) \in \mathbb{R}^2 : r_1 \geqq 0, r_2 \geqq 0\}$$

and satisfies

$$\min\{r_1, r_2\} \leqq e(r_1, r_2) \leqq \max\{r_1, r_2\}.$$

For simplicity, we will use its original form instead of the function $e(r_1, r_2)$ in this paper.

Next, we introduce the following equivalence relation "$\sim$" in $\mathbb{R}^N$:

$$\boldsymbol{p} \sim \boldsymbol{q} \quad \text{if and only if} \quad p_1 - q_1 = p_2 - q_2 = \cdots = p_N - q_N,$$

and let $\mathscr{W}$ be the quotient space $\mathbb{R}^N / \sim$. In other words, for $\boldsymbol{p} \in \mathbb{R}^N$ we consider its equivalent class

$$[\boldsymbol{p}] = \{(p_1 + c, p_2 + c, \ldots, p_N + c) : c \in \mathbb{R}\},$$

and all such equivalent classes form the vector space $\mathscr{W}$.

For a given $\boldsymbol{\Phi}$, and $[\boldsymbol{p}] = [(p_i)_{i=1}^N] \in \mathscr{W}$, we define an identification $\tau_{\boldsymbol{\Phi}}([\boldsymbol{p}]) = (\sigma_i)_{i=1}^N$ from $\mathscr{W}$ to $T_{\boldsymbol{\rho}}\mathscr{M}$ by,

$$\sigma_i = \sum_{j \in N(i)} \Gamma_{ij}^{\Phi}(\boldsymbol{\rho})(p_i - p_j), \tag{16}$$

where

$$\Gamma_{ij}^{\Phi}(\boldsymbol{\rho}) = \begin{cases} \rho_i & \text{if } \Phi_i > \Phi_j, j \in N(i) \\ \rho_j & \text{if } \Phi_j > \Phi_i, j \in N(i) \\ \frac{\rho_i - \rho_j}{\log \rho_i - \log \rho_j} & \text{if } \Phi_i = \Phi_j, j \in N(i) \end{cases} \tag{17}$$

for $i = 1, 2, \ldots, N$. With this identification, we can express $\boldsymbol{\sigma} \in T_{\boldsymbol{\rho}}\mathscr{M}$ by $[\boldsymbol{p}] := \tau_{\boldsymbol{\Phi}}^{-1}(\boldsymbol{\sigma}) \in \mathscr{W}$, and denote it by

$$\boldsymbol{\sigma} \simeq [(p_i)_{i=1}^N].$$

We note that this identification depends on $\boldsymbol{\Phi}$, the probability distribution $\boldsymbol{\rho}$ and the structure of the graph G. In the following lemma, we show that this identification (16) is well-defined.

Lemma 2. *If each σ_i satisfies (16), then the map $\tau_\Phi : [(p_i)_{i=1}^N] \in \mathscr{W} \mapsto \boldsymbol{\sigma} = (\sigma_i)_{i=1}^N \in T_\rho\mathscr{M}$ is a linear isomorphism.*

Proof. It is clear that

$$\tau_{\boldsymbol{\Phi}} : [(p_i)_{i=1}^N] \in \mathscr{W} \mapsto \tau_{\boldsymbol{\Phi}}([(p_i)_{i=1}^N]) = (\sigma_i)_{i=1}^N \in T_\rho\mathscr{M}$$

is a well-defined linear map. Furthermore, both $\mathscr{W}$ and $T_{\boldsymbol{\rho}}\mathscr{M}$ are $(N-1)$-dimensional real linear spaces. Thus, in order to prove that the map $\tau_{\boldsymbol{\Phi}}$ is an isomorphism, it is sufficient to show that the map $\tau_{\boldsymbol{\Phi}}$ is injective, which is equivalent to the fact that if $\boldsymbol{p} = \{p_i\}_{i=1}^N \in \mathbb{R}^N$ satisfies

$$\sigma_i = \sum_{j\in N(i)} \Gamma_{ij}^\Phi (p_i - p_j) = 0, \Longleftrightarrow p_i = \left(\sum_{j\in N(i)} \Gamma_{ij}^\Phi p_j\right) \Big/ \left(\sum_{j\in N(i)} \Gamma_{ij}^\Phi\right)$$

for $i = 1, 2, \ldots, N$, then $p_1 = p_2 = \cdots = p_N$.

Assume this is not true, and let $c = \max\{p_i : i = 1, 2, \ldots, N\}$. Then, there must exist $\{a_\ell, a_k\} \in E$ such that $p_\ell = c$ and $p_k < c$, because the graph G is connected. This gives

$$c = p_\ell = \frac{\sum_{j\in N(\ell)} \Gamma_{\ell j}^\Phi p_j}{\sum_{j\in N(\ell)} \Gamma_{\ell j}^\Phi} = c + \frac{\sum_{j\in N(\ell)} \Gamma_{\ell j}^\Phi (p_j - c)}{\sum_{j\in N(\ell)} \Gamma_{\ell j}^\Phi} \leqq c - \frac{\Gamma_{\ell k}^\Phi (c - p_k)}{\sum_{j\in N(\ell)} \Gamma_{\ell j}^\Phi} < c,$$

which is a contradiction. The proof is complete.

Definition 1. By the above identification (16), we define an inner product on $T_{\boldsymbol{\rho}}\mathscr{M}$ by:

$$g_{\boldsymbol{\rho}}^{\boldsymbol{\Phi}}(\boldsymbol{\sigma}^1, \boldsymbol{\sigma}^2) = \sum_{i=1}^N p_i^1 \sigma_i^2 = \sum_{i=1}^N p_i^2 \sigma_i^1.$$

It is easy to check that this definition is equivalent to

$$g_{\boldsymbol{\rho}}^{\boldsymbol{\Phi}}(\boldsymbol{\sigma}^1, \boldsymbol{\sigma}^2) = \sum_{\{a_i, a_j\}\in E} \Lambda_{ij}^\Phi (p_i^1 - p_j^1)(p_i^2 - p_j^2), \tag{18}$$

where

$$\Lambda_{ij}^\Phi(\boldsymbol{\rho}) = \begin{cases} \rho_j & \text{if } \{a_i, a_j\} \in E, \Phi_i < \Phi_j, \\ \frac{\rho_i - \rho_j}{\log \rho_i - \log \rho_j} & \text{if } \{a_i, a_j\} \in E, \Phi_i = \Phi_j, \end{cases} \tag{19}$$

for $\boldsymbol{\sigma}^1 = (\sigma_i^1)_{i=1}^N, \boldsymbol{\sigma}^2 = (\sigma_i^2)_{i=1}^N \in T_\rho\mathscr{M}$, and $[(p_i^1)_{i=1}^N], [(p_i^2)_{i=1}^N] \in \mathscr{W}$ satisfying

$$\boldsymbol{\sigma}^1 \simeq [(p_i^1)_{i=1}^N] \text{ and } \boldsymbol{\sigma}^2 \simeq [(p_i^2)_{i=1}^N].$$

In particular,

$$g_{\boldsymbol{\rho}}^{\boldsymbol{\Phi}}(\boldsymbol{\sigma}, \boldsymbol{\sigma}) = \sum_{\{a_i, a_j\}\in E} \Lambda_{ij}^\Phi(\boldsymbol{\rho})(p_i - p_j)^2 \tag{20}$$

for $\boldsymbol{\sigma} \in T_\rho\mathscr{M}$, where $\boldsymbol{\sigma} \simeq [(p_i)_{i=1}^N]$.

Since $\boldsymbol{\rho} \in \mathscr{M} \mapsto g^{\boldsymbol{\Phi}}_{\boldsymbol{\rho}}$ is measurable, using the inner product $g^{\boldsymbol{\Phi}}_{\boldsymbol{\rho}}$, we can define the distance between two points $\boldsymbol{\rho}^1$ and $\boldsymbol{\rho}^2$ in $\mathscr{M}$ by

$$d_{\boldsymbol{\Phi}}(\boldsymbol{\rho}^1, \boldsymbol{\rho}^2) = \inf_{\gamma} L(\gamma(t)) \tag{21}$$

where $\gamma : [0, 1] \to \mathscr{M}$ ranges over all continuously differentiable curves with $\gamma(0) = \boldsymbol{\rho}^1, \gamma(1) = \boldsymbol{\rho}^2$. The arc length of γ is given by

$$L(\gamma(t)) = \int_0^1 \sqrt{g^{\boldsymbol{\Phi}}_{\gamma(t)}(\dot{\gamma}(t), \dot{\gamma}(t))} \mathrm{d}t.$$

Although $g^{\boldsymbol{\Phi}}_{\boldsymbol{\rho}}$ may or may not be a smooth inner product with respect to $\boldsymbol{\rho}$, the length of any smooth curve is still well-defined because $\boldsymbol{\rho} \in \mathscr{M} \mapsto g^{\boldsymbol{\Phi}}_{\boldsymbol{\rho}}$ is measurable. It is shown by Lemma 3 that $d_{\boldsymbol{\Phi}}$ is a metric on $\mathscr{M}$. Thus we have a metric space $(\mathscr{M}, d_{\boldsymbol{\Phi}})$. In particular, if $\boldsymbol{\Phi}$ is a constant map, then the metric $d_{\boldsymbol{\Phi}}$ is a Riemannian metric on $\mathscr{M}$, since the map $\boldsymbol{\rho} \in \mathscr{M} \mapsto g^{\boldsymbol{\Phi}}_{\boldsymbol{\rho}}$ is smooth. Hence, $(\mathscr{M}, d_{\boldsymbol{\Phi}})$ is a Riemannian manifold.

Remark 1. The identification (16) is motivated by a similar identification introduced by Otto in [33] for the case of a continuous state space. We replace the differential operator in [33] by a combination of finite differences because our state space V is discrete. Since (16) adopts an upwind scheme and the structure of the Kolmogorov equation (42) in Section 5, we call the inner product $g^{\boldsymbol{\Phi}}_{\boldsymbol{\rho}}$ the upwind inner product induced by $\boldsymbol{\Phi}$.

Next, we show that the metric $d_{\boldsymbol{\Phi}}$ is bounded. Given $\boldsymbol{\rho} = (\rho_i)_{i=1}^N \in \mathscr{M}$, we define matrices

$$A = [A(i, j)]_{N\times N}, \ A_m = [A_m(i, j)]_{N\times N}, \text{ and } A_M = [A_M(i, j)]_{N\times N}$$

as follows. If $i \neq j$, we have

$$A(i, j) = \begin{cases} -\Gamma^{\Phi}_{ij}(\boldsymbol{\rho}) & \text{if } \{a_i, a_j\} \in E \\ 0 & \text{otherwise} \end{cases},$$

$$A_m(i, j) = \begin{cases} -\max\{\rho_i, \rho_j\} & \text{if } \{a_i, a_j\} \in E \\ 0 & \text{otherwise} \end{cases}$$

and

$$A_M(i, j) = \begin{cases} -\min\{\rho_i, \rho_j\} & \text{if } \{a_i, a_j\} \in E \\ 0 & \text{otherwise} \end{cases}.$$

On the diagonal, $i = j$, we define

$$\begin{cases} A(i, i) = -\sum_{k\neq i} A(i, k) \\ A_m(i, i) = -\sum_{k\neq i} A_m(i, k) \\ A_M(i, i) = -\sum_{k\neq i} A_M(i, k) \end{cases}.$$

Thus the identification (16) can be expressed by

$$\boldsymbol{\sigma}^T = A\boldsymbol{p}^T,$$

where $\boldsymbol{\sigma} = (\sigma_i)_{i=1}^N \in T_{\boldsymbol{\rho}}\mathscr{M}$ and $\boldsymbol{p} = (p_i)_{i=1}^N \in \mathbb{R}^N$.

We consider two new identifications

$$\sigma^T = A_m \boldsymbol{p}^T \tag{22}$$

and

$$\sigma^T = A_M \boldsymbol{p}^T. \tag{23}$$

Similar to the identification (16), identifications (22) and (23) are both linear isomorphisms between $T_{\boldsymbol{\rho}}\mathscr{M}$ and $\mathscr{W}$. Furthermore, they induce inner products $g_{\boldsymbol{\rho}}^m(\cdot,\cdot)$ and $g_{\boldsymbol{\rho}}^M(\cdot,\cdot)$ respectively on $T_{\boldsymbol{\rho}}\mathscr{M}$. It is not hard to see that the maps $\boldsymbol{\rho} \mapsto g_{\boldsymbol{\rho}}^m$ and $\boldsymbol{\rho} \mapsto g_{\boldsymbol{\rho}}^M$ are smooth. By using the inner products $g_{\boldsymbol{\rho}}^m$ and $g_{\boldsymbol{\rho}}^M$, we can obtain distances $d_m(\cdot,\cdot)$ and $d_M(\cdot,\cdot)$ respectively on $\mathscr{M}$. Then both $(\mathscr{M}, d_m)$ and $(\mathscr{M}, d_M)$ are smooth Riemannian manifolds.

Lemma 3. *For any smooth map* $\boldsymbol{\Phi} : (\mathscr{M}, d) \to (\mathbb{R}^N, d)$ *and* $\boldsymbol{\rho}^1, \boldsymbol{\rho}^2 \in \mathscr{M}$,

$$d_m(\boldsymbol{\rho}^1, \boldsymbol{\rho}^2) \leqq d_{\boldsymbol{\Phi}}(\boldsymbol{\rho}^1, \boldsymbol{\rho}^2) \leqq d_M(\boldsymbol{\rho}^1, \boldsymbol{\rho}^2).$$

Proof. Let $\boldsymbol{\Phi} : (\mathscr{M}, d) \to (\mathbb{R}^N, d)$ be a smooth map. Given $\boldsymbol{\rho} \in \mathscr{M}$, the identification (16) can be expressed by

$$\boldsymbol{\sigma}^T = A\boldsymbol{p}^T,$$

where $\boldsymbol{\sigma} = (\sigma_i)_{i=1}^N \in T_{\boldsymbol{\rho}}\mathscr{M}$ and $\boldsymbol{p} = (p_i)_{i=1}^N \in \mathbb{R}^N$. Since $\sum_{i=1}^N \sigma_i = 0$ for $(\sigma_i)_{i=1}^N \in T_{\boldsymbol{\rho}}\mathscr{M}$, by deleting the last row and last column of the matrix A we obtain a symmetric diagonally dominant $(N-1)\times(N-1)$-matrix B. Thus, the identification (16) becomes

$$\boldsymbol{\sigma}_*^T = B\boldsymbol{p}_*^T$$

where $\boldsymbol{\sigma}_* = (\sigma_i)_{i=1}^{N-1}$ and $\boldsymbol{p}_* = (p_i - p_N)_{i=1}^{N-1}$.

Similarly we can get symmetric diagonally dominant matrices B_m and B_M from A_m and A_M respectively. Moreover, B, B_m and B_M are all irreducible matrices since the graph G is connected. They are all nonsingular and positive definite, because they all have positive diagonal entries.

The inner products are given as

$$\begin{aligned} g_{\boldsymbol{\rho}}^{\boldsymbol{\Phi}}(\boldsymbol{\sigma},\boldsymbol{\sigma}) &= \boldsymbol{\sigma}\boldsymbol{p}^T = \boldsymbol{\sigma}_*\boldsymbol{p}_*^T = \boldsymbol{\sigma}_* B^{-1}\boldsymbol{\sigma}_*^T \\ g_{\boldsymbol{\rho}}^{m}(\boldsymbol{\sigma},\boldsymbol{\sigma}) &= \boldsymbol{\sigma}\boldsymbol{p}^T = \boldsymbol{\sigma}_*\boldsymbol{p}_*^T = \boldsymbol{\sigma}_* B_m^{-1}\boldsymbol{\sigma}_*^T \\ g_{\boldsymbol{\rho}}^{M}(\boldsymbol{\sigma},\boldsymbol{\sigma}) &= \boldsymbol{\sigma}\boldsymbol{p}^T = \boldsymbol{\sigma}_*\boldsymbol{p}_*^T = \boldsymbol{\sigma}_* B_M^{-1}\boldsymbol{\sigma}_*^T \end{aligned}$$

for $\boldsymbol{\sigma} \in T_{\boldsymbol{\rho}}\mathscr{M}$. It is well known that a symmetric diagonally dominant real matrix with nonnegative diagonal entries is positive semidefinite. Since $B_m - B$, $B - B_M$

are still symmetric diagonally dominant matrices with nonnegative diagonal entries, we have $B_m - B$ and $B - B_M$ are positive semidefinite. Now we claim that: for every $\boldsymbol{\sigma} \in T_{\boldsymbol{\rho}}\mathscr{M}$, we have

$$g_{\boldsymbol{\rho}}^{m}(\boldsymbol{\sigma}, \boldsymbol{\sigma}) \leqq g_{\boldsymbol{\rho}}^{\boldsymbol{\Phi}}(\boldsymbol{\sigma}, \boldsymbol{\sigma}) \leqq g_{\boldsymbol{\rho}}^{M}(\boldsymbol{\sigma}, \boldsymbol{\sigma}).$$

We first prove

$$g_{\boldsymbol{\rho}}^{m}(\boldsymbol{\sigma}, \boldsymbol{\sigma}) \leqq g_{\boldsymbol{\rho}}^{\boldsymbol{\Phi}}(\boldsymbol{\sigma}, \boldsymbol{\sigma}).$$

Note that

$$g_{\boldsymbol{\rho}}^{\boldsymbol{\Phi}}(\boldsymbol{\sigma}, \boldsymbol{\sigma}) - g_{\boldsymbol{\rho}}^{m}(\boldsymbol{\sigma}, \boldsymbol{\sigma}) = \boldsymbol{\sigma}_*(B^{-1} - B_m^{-1})\boldsymbol{\sigma}_*^T.$$

Therefore, to show that

$$g_{\boldsymbol{\rho}}^{m}(\boldsymbol{\sigma}, \boldsymbol{\sigma}) \leqq g_{\boldsymbol{\rho}}^{\boldsymbol{\Phi}}(\boldsymbol{\sigma}, \boldsymbol{\sigma}),$$

it is sufficient to show $(B^{-1} - B_m^{-1})$ is positive semi-definite.

Since B is a positive definite symmetric matrix, B^{-1} is also positive definite symmetric. Combining this with the fact that $(B_m - B)$ is positive semi-definite, we know that $(B^{-1} - B_m^{-1})$ is positive semi-definite from the following equality

$$B^{-1} - B_m^{-1} = B_m^{-1}\{(B_m - B)B^{-1}(B_m - B)^T + (B_m - B)\}(B_m^{-1})^T.$$

In a similar fashion, we prove $g_{\boldsymbol{\rho}}^{\boldsymbol{\Phi}}(\boldsymbol{\sigma}, \boldsymbol{\sigma}) \leqq g_{\boldsymbol{\rho}}^{M}(\boldsymbol{\sigma}, \boldsymbol{\sigma})$.

Thus we obtain

$$d_m(\boldsymbol{\rho}^1, \boldsymbol{\rho}^2) \leqq d_{\boldsymbol{\Phi}}(\boldsymbol{\rho}^1, \boldsymbol{\rho}^2) \leqq d_M(\boldsymbol{\rho}^1, \boldsymbol{\rho}^2)$$

for any $\boldsymbol{\rho}^1, \boldsymbol{\rho}^2 \in \mathscr{M}$.

Now we consider two choices of the function $\boldsymbol{\Phi}$ which are related to Fokker–Planck equations I (8) and II (9), respectively. Let the potential $\boldsymbol{\Psi} = (\Psi_i)_{i=1}^N$ on V be given and $\beta \geqq 0$, where Ψ_i is the potential on vertex a_i.

For Fokker–Planck equation I (8), we let

$$\boldsymbol{\Phi}(\boldsymbol{\rho}) \equiv \boldsymbol{\Psi},$$

where $\boldsymbol{\rho} \in \mathscr{M}$. The identification (16)

$$\boldsymbol{\sigma} \simeq [(p_i)_{i=1}^N]$$

is given by

$$\sigma_i = \sum_{j \in N(i)} (p_i - p_j)\Gamma_{ij}^{\boldsymbol{\Psi}}(\boldsymbol{\rho}) \tag{24}$$

and the corresponding norm (20) is

$$g_{\boldsymbol{\rho}}^{\boldsymbol{\Psi}}(\boldsymbol{\sigma}, \boldsymbol{\sigma}) = \sum_{\{a_i, a_j\} \in E} \Lambda_{ij}^{\boldsymbol{\Psi}}(\boldsymbol{\rho})(p_i - p_j)^2, \tag{25}$$

for $\boldsymbol{\sigma} \in T_{\boldsymbol{\rho}}\mathscr{M}$ with $\boldsymbol{\sigma} \simeq [(p_i)_{i=1}^N]$. Note that the map $\boldsymbol{\rho} \in \mathscr{M} \mapsto g_{\boldsymbol{\rho}}^{\boldsymbol{\Psi}}$ is smooth and the inner product $g^{\boldsymbol{\Psi}}$ generates a Riemannian metric space $(\mathscr{M}, d_{\boldsymbol{\Psi}})$, where $d_{\boldsymbol{\Psi}}$ comes from (21). Similar to the theory developed in [33], we will show in Section 4 that Fokker–Planck equation I (8) is the gradient flow of free energy on the Riemannian manifold $(\mathscr{M}, d_{\boldsymbol{\Psi}})$.

For Fokker–Planck equation II (9), we let

$$\boldsymbol{\Phi}(\boldsymbol{\rho}) \equiv \bar{\boldsymbol{\Psi}}(\boldsymbol{\rho}),$$

where the new potential $\bar{\boldsymbol{\Psi}}(\boldsymbol{\rho}) = (\bar{\Psi}_i(\boldsymbol{\rho}))_{i=1}^N$ is defined by

$$\bar{\Psi}_i(\boldsymbol{\rho}) = \Psi_i + \beta \log \rho_i.$$

In this case, for a given $\boldsymbol{\rho} \in \mathscr{M}$, the identification (16) is given by

$$\sigma_i = \sum_{j \in N(i)} (p_i - p_j)\Gamma_{ij}^{\bar{\boldsymbol{\Psi}}}(\boldsymbol{\rho}), \tag{26}$$

and the inner product (18) on $T_{\boldsymbol{\rho}}\mathscr{M}$ is

$$g_{\boldsymbol{\rho}}^{\bar{\boldsymbol{\Psi}}}(\boldsymbol{\sigma}^1, \boldsymbol{\sigma}^2) = \sum_{i=1}^N p_i^1 \sigma_i^2 = \sum_{i=1}^N p_i^2 \sigma_i^1 = \sum_{\{a_i, a_j\} \in E} \Lambda_{ij}^{\bar{\boldsymbol{\Psi}}}(\boldsymbol{\rho})(p_i^1 - p_j^1)(p_i^2 - p_j^2), \tag{27}$$

for $\boldsymbol{\sigma}^1 = (\sigma_i^1)_{i=1}^N, \boldsymbol{\sigma}^2 = (\sigma_i^2)_{i=1}^N \in T_{\boldsymbol{\rho}}\mathscr{M}$, and $[(p_i^1)_{i=1}^N], [(p_i^2)_{i=1}^N] \in \mathscr{W}$ satisfying $\boldsymbol{\sigma}^1 \simeq [(p_i^1)_{i=1}^N]$ and $\boldsymbol{\sigma}^2 \simeq [(p_i^2)_{i=1}^N]$. In particular, we have

$$g_{\boldsymbol{\rho}}^{\bar{\boldsymbol{\Psi}}}(\boldsymbol{\sigma}, \boldsymbol{\sigma}) = \sum_{\{a_i, a_j\} \in E} \Lambda_{ij}^{\bar{\boldsymbol{\Psi}}}(\boldsymbol{\rho})(p_i - p_j)^2, \tag{28}$$

for $\boldsymbol{\sigma} \in T_{\boldsymbol{\rho}}\mathscr{M}$ and $\boldsymbol{\sigma} \simeq [(p_i)_{i=1}^N]$.

The inner product $g_{\boldsymbol{\rho}}^{\bar{\boldsymbol{\Psi}}}$ induces a metric space $(\mathscr{M}, d_{\bar{\boldsymbol{\Psi}}})$, where $d_{\bar{\boldsymbol{\Psi}}}$ comes from (21). However, the map $\boldsymbol{\rho} \in \mathscr{M} \mapsto g_{\boldsymbol{\rho}}^{\bar{\boldsymbol{\Psi}}}$ is not continuous due to the fact that $\bar{\boldsymbol{\Psi}}$ depends on $\boldsymbol{\rho}$. Thus, $(\mathscr{M}, d_{\bar{\boldsymbol{\Psi}}})$ is not a Riemannian manifold. On the other hand, since $g_{\boldsymbol{\rho}}^{\bar{\boldsymbol{\Psi}}}$ is a piecewise smooth function with respect to $\boldsymbol{\rho}$, the space $(\mathscr{M}, d_{\bar{\boldsymbol{\Psi}}})$ is a union of finitely many smooth Riemannian manifolds. More precisely, the space $\mathscr{M}$ is divided into components whose boundaries are given by $N(N-1)/2$ sub-manifolds

$$S_{r,t} = \{(\rho_i)_{i=1}^N \in \mathscr{M} : \Psi_r + \beta \log \rho_r = \Psi_t + \beta \log \rho_t\}, \ 1 \leqq r < t \leqq N.$$

The inner product $g_{\boldsymbol{\rho}}^{\bar{\boldsymbol{\Psi}}}$ is smooth in each component divided by $\{S_{r,t}\}_{1 \leqq r < t \leqq N}$, and gives a smooth Riemannian distance in each and every component. Moreover, all sub-manifolds $S_{r,t}$ intersect at one point which is the Gibbs distribution $\boldsymbol{\rho}^* = (\rho_i^*)_{i=1}^N$, as given in (7).

Fokker–Planck equation II (9) can also be seen as the "gradient flow" of free energy on the metric space $(\mathscr{M}, d_{\bar{\boldsymbol{\Psi}}})$, which will be shown in Section 5.

By Lemma 3, $d_{\boldsymbol{\Psi}}$ and $d_{\bar{\boldsymbol{\Psi}}}$ are bounded by d_m and d_M. The explicit expressions of these distances $d_{\boldsymbol{\Psi}}, d_{\bar{\boldsymbol{\Psi}}}, d_m$ and d_M are hard to obtain in general. In the following example, we show one explicit expression of the distance function $d_{\boldsymbol{\Psi}}$.

Example. We consider a star graph $G = (V, E)$ with

$$V = \{a_1, \ldots, a_N, a_{N+1}\},$$

and

$$E = \{\{a_i, a_{N+1}\} : i = 1, 2, \ldots, N\}.$$

Let the potential $\boldsymbol{\Psi} = (\Psi_i)_{i=1}^{N+1}$ on V satisfy:

$$\Psi_i > \Psi_{N+1}, \qquad i = 1, \ldots, N.$$

Then the identification (24) on the tangent space $T_{\boldsymbol{\rho}}\mathscr{M}$ is

$$\begin{aligned} \sigma_1 &= (p_1 - p_{N+1})\rho_1, \\ &\cdots \\ \sigma_N &= (p_N - p_{N+1})\rho_N, \\ \sigma_{N+1} &= -\sum_{i=1}^{N}(p_i - p_{N+1})\rho_i, \end{aligned}$$

where $\boldsymbol{\sigma} = (\sigma_i)_{i=1}^{N+1} \in T_{\boldsymbol{\rho}}\mathscr{M} \simeq [(p_i)_{i=1}^{N+1}] \in \mathscr{W}$.

By this identification and (25), we obtain the norm

$$g_{\boldsymbol{\rho}}^{\boldsymbol{\Psi}}(\boldsymbol{\sigma}, \boldsymbol{\sigma}) = \sum_{i=1}^{N}(p_i - p_{N+1})^2\rho_i = \sum_{i=1}^{N}\frac{\sigma_i^2}{\rho_i},$$

where $\boldsymbol{\sigma} \simeq [(p_i)_{i=1}^{N+1}]$.

Given $\boldsymbol{\rho}^1 = (\rho_1^1, \ldots, \rho_{N+1}^1)$, $\boldsymbol{\rho}^2 = (\rho_1^2, \ldots, \rho_{N+1}^2) \in \mathscr{M}$, we suppose that

$$\gamma(t) = (\rho_1(t), \ldots, \rho_N(t), \rho_{N+1}(t)) : [0, 1] \to \mathscr{M}$$

is a continuously differentiable curve from $\boldsymbol{\rho}^1$ to $\boldsymbol{\rho}^2$. Then

$$L(\gamma) = \int_0^1 \sqrt{g_{\gamma(t)}^{\boldsymbol{\Psi}}(\dot\gamma(t), \dot\gamma(t))}\mathrm{d}t = \int_0^1 \sqrt{\sum_{i=1}^{N}\frac{(\rho_i'(t))^2}{\rho_i(t)}}\mathrm{d}t = \int_0^1 \sqrt{\sum_{i=1}^{N}(x_i'(t))^2}\mathrm{d}t,$$

where we use the substitution $x_i(t) = 2\sqrt{\rho_i(t)}$ for $i = 1, \ldots, N$. Let $\alpha(t) = (x_1(t), x_2(t), \ldots, x_N(t))$ for $t \in [0, 1]$ and

$$D = \left\{(x_1, x_2, \ldots, x_N) \in \mathbb{R}^N : \sum_{i=1}^{N} x_i^2 < 4 \text{ and } x_i > 0 \text{ for } i = 1, 2, \ldots, N\right\}.$$

Then D is a convex subset of an open ball with radius 2 in $\mathbb{R}^N$, and α is a continuously differentiable curve in D from $\eta^1 = 2(\sqrt{\rho_1^1}, \ldots, \sqrt{\rho_N^1})$ to $\eta^2 = 2(\sqrt{\rho_1^2}, \ldots, \sqrt{\rho_N^2})$. Clearly, we have

$$L(\gamma) = \int_0^1 \sqrt{\sum_{i=1}^{N}(x_i'(t))^2}\mathrm{d}t \geqq \|\eta^1 - \eta^2\| = 2\sqrt{\sum_{i=1}^{N}\left(\sqrt{\rho_i^1} - \sqrt{\rho_i^2}\right)^2},$$

where $\|\cdot\|$ is the Euclidean norm.

On the other hand, we take

$$\alpha^*(t) = (x_1^*(t), \dots, x_N^*(t)) := t\eta^1 + (1-t)\eta^2$$

for $t \in [0,1]$. In fact, α^* is the straight line segment in D from η^1 to η^2. Let $\rho_i^*(t) = (x_i^*(t))^2/4$ for $i = 1, 2, \dots, N$ and $\rho_{N+1}^*(t) = 1 - (\sum_{i=1}^N \rho_i^*(t))$. Then

$$\gamma^*(t) = (\rho_i^*(t))_{i=1}^{N+1} : [0,1] \to \mathscr{M}$$

is a continuously differentiable curve from $\boldsymbol{\rho}^1$ to $\boldsymbol{\rho}^2$. This implies that

$$L(\gamma^*) = \int_0^1 \sqrt{\sum_{i=1}^N ((x_i^*(t))')^2}\mathrm{d}t = \|\eta^1 - \eta^2\| = 2\sqrt{\sum_{i=1}^N \left(\sqrt{\rho_i^1} - \sqrt{\rho_i^2}\right)^2}.$$

Thus,

$$d_{\boldsymbol{\Psi}}(\boldsymbol{\rho}^1, \boldsymbol{\rho}^2) = \inf_{\gamma} L(\gamma) = 2\sqrt{\sum_{i=1}^N \left(\sqrt{\rho_i^1} - \sqrt{\rho_i^2}\right)^2}$$

for $\boldsymbol{\rho}^1 = (\rho_1^1, \dots, \rho_{N+1}^1)$, $\boldsymbol{\rho}^2 = (\rho_1^2, \dots, \rho_{N+1}^2) \in \mathscr{M}$. Finally, we note that the metric $d_{\boldsymbol{\Psi}}$ can be extended naturally to the space $\overline{\mathscr{M}}$, that is,

$$d_{\boldsymbol{\Psi}}(\boldsymbol{\rho}^1, \boldsymbol{\rho}^2) = 2\sqrt{\sum_{i=1}^N \left(\sqrt{\rho_i^1} - \sqrt{\rho_i^2}\right)^2}$$

for $\boldsymbol{\rho}^1 = (\rho_1^1, \dots, \rho_{N+1}^1)$, $\boldsymbol{\rho}^2 = (\rho_1^2, \dots, \rho_{N+1}^2) \in \overline{\mathscr{M}}$.

4. Fokker–Planck Equation I

In this section, we show that Fokker–Planck equation I (8) defined on a graph $G = (V, E)$ with potentials $\boldsymbol{\Psi} = (\Psi_i)_{i=1}^N$ on V and $\beta \geqq 0$ is the gradient flow of the free energy F on the Riemannian manifold $(\mathscr{M}, d_{\boldsymbol{\Psi}})$ introduced in Section 3. We also show some basic properties of Fokker–Planck equation I (8).

Let $\beta \geqq 0$ be fixed and the free energy functional F be defined on the space $\overline{\mathscr{M}}$:

$$F(\boldsymbol{\rho}) = \sum_{i=1}^N \Psi_i \rho_i + \beta \sum_{i=1}^N \rho_i \log \rho_i \tag{29}$$

where $\boldsymbol{\rho} = \{\rho_i\}_{i=1}^N \in \overline{\mathscr{M}}$. Thus, we have the gradient flow of F on $(\mathscr{M}, g^{\boldsymbol{\Psi}})$ given by,

$$\frac{\mathrm{d}\boldsymbol{\rho}}{\mathrm{d}t} = -\mathrm{grad}F(\boldsymbol{\rho}), \tag{30}$$

where $\operatorname{grad} F(\boldsymbol{\rho})$ is in the tangent space $T_{\boldsymbol{\rho}}\mathscr{M}$. We show that equation (30) is the Fokker–Planck equation I (8) on $\mathscr{M}$ first.

If the differential of F, which is in the cotangent space, is denoted by $\operatorname{diff} F$, then (30) could be expressed as

$$g_{\boldsymbol{\rho}}^{\boldsymbol{\Psi}}\left(\frac{\mathrm{d}\boldsymbol{\rho}}{\mathrm{d}t}, \boldsymbol{\sigma}\right) = -\operatorname{diff} F(\boldsymbol{\rho}) \cdot \boldsymbol{\sigma} \qquad \forall \boldsymbol{\sigma} \in T_{\boldsymbol{\rho}}\mathscr{M}. \tag{31}$$

It is clear that

$$\operatorname{diff} F((\rho_i)_{i=1}^N) = (\Phi_i + \beta(1 + \log \rho_i))_{i=1}^N \tag{32}$$

for $(\rho_i)_{i=1}^N \in \mathscr{M}$. By (31) and the identification (24), we are able to obtain the explicit expression of the vector field on $\mathscr{M}$.

Now we are ready to show our first main result.

Theorem 2. *Given a graph $G = (V, E)$ with its vertex set $V = \{a_1, a_2, \ldots, a_N\}$, edge set E, a potential $\boldsymbol{\Psi} = (\Psi_i)_{i=1}^N$ on V and a constant $\beta \geqq 0$, let the neighborhood set of a vertex a_i be*

$$N(i) = \{j \in \{1, 2, \ldots, N\} | \{a_i, a_j\} \in E\},$$

then

1. *The gradient flow of free energy F,*

$$F(\boldsymbol{\rho}) = \sum_{i=1}^N \Psi_i \rho_i + \beta \sum_{i=1}^N \rho_i \log \rho_i$$

on the Riemannian manifold $(\mathscr{M}, d_{\boldsymbol{\Psi}})$ of probability densities $\boldsymbol{\rho}$ on V is

$$\begin{aligned}\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = &\sum_{j \in N(i), \Psi_j > \Psi_i} \big((\Psi_j + \beta \log \rho_j) - (\Psi_i + \beta \log \rho_i)\big)\rho_j \\ &+ \sum_{j \in N(i), \Psi_j < \Psi_i} \big((\Psi_j + \beta \log \rho_j) - (\Psi_i + \beta \log \rho_i)\big)\rho_i \\ &+ \sum_{j \in N(i), \Psi_j = \Psi_i} \beta(\rho_j - \rho_i)\end{aligned}$$

for $i = 1, 2, \ldots, N$, which is Fokker–Planck equation I (8).

2. *For all $\beta > 0$, Gibbs distribution $\boldsymbol{\rho}^* = (\rho_i^*)_{i=1}^N$ given by*

$$\rho_i^* = \frac{1}{K} \mathrm{e}^{-\Psi_i/\beta} \text{ with } K = \sum_{i=1}^N \mathrm{e}^{-\Psi_i/\beta}$$

is the unique stationary distribution of equation (8) in $\mathscr{M}$. Furthermore, the free energy F attains its global minimum at the Gibbs distribution.

3. *For all $\beta > 0$, there exists a unique solution*

$$\boldsymbol{\rho}(t) : [0, \infty) \to \mathscr{M}$$

of equation (8) with initial value $\boldsymbol{\rho}^0 \in \mathscr{M}$, and $\boldsymbol{\rho}(t)$ satisfies:
(a) *the free energy $F(\boldsymbol{\rho}(t))$ decreases as time t increases,*
(b) *$\boldsymbol{\rho}(t) \to \boldsymbol{\rho}^*$ under the Euclidean metric of $\mathbb{R}^N$ as $t \to +\infty$.*

As a direct consequence, we have the following result.

Corollary 1. *Given the graph $G = (V, E)$ with $V = \{a_1, a_2, \ldots, a_N\}$ and potential $\boldsymbol{\Psi} = (\Psi_i)_{i=1}^N$ on V, we have*

1. *If the noise level $\beta = 0$, then Fokker–Planck equation I (8) for the discrete state space is*

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = \sum_{j \in N(i), \Psi_j > \Psi_i} (\Psi_j - \Psi_i)\rho_j + \sum_{j \in N(i), \Psi_j < \Psi_i} (\Psi_j - \Psi_i)\rho_i \tag{33}$$

for $i = 1, 2, \ldots, N$.
2. *In a special case when the potential is a constant at each vertex, this equation is the master equation:*

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = \sum_{j \in N(i)} \beta(\rho_j - \rho_i) \tag{34}$$

for $i = 1, 2, \ldots, N$.

Remark 2. Given $\boldsymbol{\rho}^0 \in \overline{\mathscr{M}}$ and a continuous function

$$\boldsymbol{\rho}(t) : [0, c) \to \overline{\mathscr{M}}$$

for some $0 < c \leqq +\infty$, we call such a function a generalized solution of equation (8) with initial value $\boldsymbol{\rho}^0$, if $\boldsymbol{\rho}(0) = \boldsymbol{\rho}^0$ and $\boldsymbol{\rho}(t) \in \mathscr{M}$ satisfy equation (8) for $t \in (0, c)$. In Appendix A, we give an example of a graph G and free energy to show that a generalized solution to (8) may not exist for some $\boldsymbol{\rho}^0 \in \partial\mathscr{M} := \overline{\mathscr{M}} \setminus \mathscr{M}$. We also note that the equation (8) is not well-defined on the boundary $\partial\mathscr{M} := \overline{\mathscr{M}} \setminus \mathscr{M}$.

Remark 3. Equation (33) describes the time evolution of the probability distribution due to the potential energy and is also the probability distribution of a time homogeneous Markov process on the graph G. The master equation is a first order differential equation that describes the time evolution of the probability distribution at every vertex in the discrete state space. Its entropy increases along with the master equation. In this sense, Fokker–Planck equation I (8) is a generalization of the master equation. We refer to [12] for more details on the master equation.

Proof of Theorem 2. (1). We know that the gradient flow of free energy F on $(\mathscr{M}, d_{\boldsymbol{\Psi}})$ is given by equation (31),

$$g_{\boldsymbol{\rho}}^{\boldsymbol{\Psi}}\left(\frac{\mathrm{d}\boldsymbol{\rho}}{\mathrm{d}t}, \boldsymbol{\sigma}\right) = -\mathrm{diff}\, F(\boldsymbol{\rho}) \cdot \boldsymbol{\sigma} \quad \forall \boldsymbol{\sigma} \in T_{\boldsymbol{\rho}}\mathscr{M}.$$

The left-hand side of equation (31) is

$$g_{\boldsymbol{\rho}}^{\boldsymbol{\Psi}}\left(\frac{\mathrm{d}\boldsymbol{\rho}}{\mathrm{d}t},\boldsymbol{\sigma}\right)=\sum_{i=1}^{N}\frac{\mathrm{d}\rho_i}{\mathrm{d}t}p_i \tag{35}$$

where $\boldsymbol{\sigma}=(\sigma_i)_{i=1}^N\simeq[(p_i)_{i=1}^N]$. By (32), the right-hand side of equation (31) is

$$-\operatorname{diff}F(\rho)\cdot\boldsymbol{\sigma}=-\sum_{i=1}^{N}(\Psi_i+\beta(1+\log\rho_i))\sigma_i. \tag{36}$$

Using the identification (24), we have

$$\begin{aligned}
&\sum_{i=1}^{N}(\Psi_i+\beta(1+\log\rho_i))\sigma_i=\sum_{i=1}^{N}(\Psi_i+\beta\log\rho_i)\sigma_i\\
&\quad=\sum_{i=1}^{N}(\Psi_i+\beta\log\rho_i)\left(\sum_{j\in N(i)}\Gamma_{ij}^{\boldsymbol{\Psi}}(\boldsymbol{\rho})(p_i-p_j)\right)\\
&\quad=\sum_{\{a_i,a_j\}\in E,\,\Psi_i<\Psi_j}\{(\Psi_i-\Psi_j)+\beta(\log\rho_i-\log\rho_j)\}\rho_j(p_i-p_j)\\
&\qquad+\beta\sum_{\{a_i,a_j\}\in E,\,\Psi_i=\Psi_j}(\rho_i-\rho_j)(p_i-p_j)\\
&\quad=\sum_{i=1}^{N}\Bigg\{\sum_{j\in N(i),\,\Psi_j>\Psi_i}\big((\Psi_i-\Psi_j)\rho_j+\beta(\log\rho_i-\log\rho_j)\rho_j\big)\\
&\qquad+\sum_{j\in N(i),\,\Psi_j<\Psi_i}\big((\Psi_i-\Psi_j)\rho_i+\beta(\log\rho_i-\log\rho_j)\rho_i\big)\\
&\qquad+\beta\sum_{j\in N(i),\,\Psi_j=\Psi_i}(\rho_i-\rho_j)\Bigg\}p_i.
\end{aligned}$$

Combining this equation with equations (31), (35) and (36), we have

$$\begin{aligned}
\sum_{i=1}^{N}\frac{\mathrm{d}\rho_i}{\mathrm{d}t}p_i=\sum_{i=1}^{N}\Bigg\{&\sum_{j\in N(i),\,\Psi_j>\Psi_i}\big((\Psi_j-\Psi_i)\rho_j+\beta(\log\rho_j-\log\rho_i)\rho_j\big)\\
&+\sum_{j\in N(i),\,\Psi_j<\Psi_i}\big((\Psi_j-\Psi_i)\rho_i+\beta(\log\rho_j-\log\rho_i)\rho_i\big)\\
&+\beta\sum_{j\in N(i),\,\Psi_j=\Psi_i}(\rho_j-\rho_i)\Bigg\}p_i.
\end{aligned}$$

Since the above equality stands for any $(p_i)_{i=1}^N\in\mathbb{R}^N$, we obtain Fokker–Planck equation I (8). This completes the proof of (1).

(2). It is well known that F attains its minimum at Gibbs density. By a direct computation, we have that the Gibbs distribution is a stationary solution. Let $\boldsymbol{\rho} = (\rho_i)_{i=1}^N$ be a stationary solution of equation (8) in $\mathscr{M}$. For $\boldsymbol{\sigma} = (\sigma_i)_{i=1}^N \in T_\rho \mathscr{M}$, we let $\boldsymbol{\sigma} \simeq [(p_i)_{i=1}^N]$ for some $(p_i)_{i=1}^N \in \mathbb{R}^N$. Since $\boldsymbol{\rho}$ is the stationary solution, it implies that

$$\begin{aligned}
&\sum_{i=1}^N (\Psi_i + \beta(1+\log\rho_i))\sigma_i \\
&= \sum_{i=1}^N \Bigg\{ \sum_{j\in N(i), \Psi_j > \Psi_i} \big((\Psi_i - \Psi_j)\rho_j + \beta(\log\rho_i - \log\rho_j)\rho_j\big) \\
&\quad + \sum_{j\in N(i), \Psi_j < \Psi_i} \big((\Psi_i - \Psi_j)\rho_i + \beta(\log\rho_i - \log\rho_j)\rho_i\big) \\
&\quad + \sum_{j\in N(i), \Psi_j = \Psi_i} \beta(\rho_i - \rho_j) \Bigg\} p_i \\
&= 0.
\end{aligned}$$

We note that for any $(\sigma_i)_{i=1}^{N-1} \in \mathbb{R}^{N-1}$, if we take

$$\sigma_N = -\sum_{i=1}^{N-1} \sigma_i$$

then $(\sigma_i)_{i=1}^N \in T_{\boldsymbol{\rho}} \mathscr{M}$. Thus one has

$$\sum_{i=1}^{N-1} \{(\Psi_i + \beta(1+\log\rho_i)) - (\Psi_N + \beta(1+\log\rho_N))\}\sigma_i = 0$$

for any $(\sigma_i)_{i=1}^{N-1} \in \mathbb{R}^{N-1}$. This implies

$$(\Psi_i + \beta\log\rho_i) - (\Psi_N + \beta\log\rho_N) = 0,$$

which is

$$\rho_i = \mathrm{e}^{\frac{\Psi_N - \Psi_i}{\beta}} \rho_N$$

for $i = 1, 2, \ldots, N-1$.

Combining this fact with $\sum_{i=1}^N \rho_i = 1$, we have $\rho_i = \frac{1}{K}\mathrm{e}^{-\Psi_i/\beta} = \rho_i^*$ for $i = 1, 2, \ldots, N$, where $K = \sum_{i=1}^N \mathrm{e}^{-\frac{\Psi_i}{\beta}}$. This completes the proof of (2).

(3). Let a continuous function

$$\boldsymbol{\rho}(t) : [0, c) \to \mathscr{M}$$

for some $0 < c \leqq +\infty$ be a solution of equation (8) with initial value $\boldsymbol{\rho}^0 \in \mathscr{M}$. For any $\boldsymbol{\rho}^0 \in \mathscr{M}$, there exists a maximal interval of existence $[0, c(\boldsymbol{\rho}^0))$ and $0 < c(\boldsymbol{\rho}^0)) \leqq +\infty$. We will show that for any $\boldsymbol{\rho}^0$, $c(\boldsymbol{\rho}^0) = +\infty$. In fact, this follows from the following claim.

Claim. Given $\boldsymbol{\rho}^0 \in \mathscr{M}$, there exists a compact subset B of $\mathscr{M}$ with respect to the Euclidean metric such that $\boldsymbol{\rho}^0 \in \mathrm{int}(B)$, where $\mathrm{int}(B)$ is the interior of B in $\mathscr{M}$. If

$$\boldsymbol{\rho}(t) : [0, c(\boldsymbol{\rho}^0)) \to \mathscr{M}$$

is the solution of equation (8) with initial value $\boldsymbol{\rho}^0$ on its maximal interval of existence, then $c(\boldsymbol{\rho}^0) = +\infty$ and $\boldsymbol{\rho}(t) \in \mathrm{int}(B)$ for $t > 0$.

Proof of Claim. Let $\boldsymbol{\rho}^0 = (\rho_i^0)_{i=1}^N \in \mathscr{M}$ be fixed and $\boldsymbol{\rho}(t) : [0, c(\boldsymbol{\rho})) \to \mathscr{M}$ be the solution to equation (8) with initial value $\boldsymbol{\rho}^0$ on its maximal interval of existence. First, we construct a compact subset B of $\mathscr{M}$ with respect to the Euclidean metric such that $\boldsymbol{\rho}^0 \in \mathrm{int}(B)$. Then we show that $c(\boldsymbol{\rho}^0) = +\infty$ and $\boldsymbol{\rho}(t) \in \mathrm{int}(B)$ for all $t > 0$.

Let us denote

$$\begin{aligned} M &= \max\{\mathrm{e}^{2|\Psi_i|} : i = 1, 2, \ldots, N\}, \\ \varepsilon_0 &= 1, \end{aligned}$$

and

$$\varepsilon_1 = \frac{1}{2} \min \left\{ \frac{\varepsilon_0}{(1 + (2M)^{\frac{1}{\beta}})}, \min\{\rho_i^0 : i = 1, \ldots, N\} \right\}.$$

For $\ell = 2, 3, \ldots, N-1$, we let

$$\varepsilon_\ell = \frac{\varepsilon_{\ell-1}}{1 + (2M)^{\frac{1}{\beta}}}.$$

We define

$$B = \left\{ \boldsymbol{\rho} = (\rho_i)_{i=1}^N \in \mathscr{M} : \sum_{r=1}^{\ell} \rho_{i_r} \leqq 1 - \varepsilon_\ell \text{ where } \ell \in \{1, \ldots, N-1\}, \right. \\ \left. 1 \leqq i_1 < \cdots < i_\ell \leqq N \right\}.$$

Then B is a compact subset of $\mathscr{M}$ with respect to the Euclidean metric,

$$\mathrm{int}(B) = \left\{ \boldsymbol{\rho} = (\rho_i)_{i=1}^N \in \mathscr{M} : \sum_{r=1}^{\ell} \rho_{i_r} < 1 - \varepsilon_\ell, \text{ where } \ell \in \{1, \ldots, N-1\}, \right. \\ \left. 1 \leqq i_1 < \cdots < i_\ell \leqq N \right\},$$

and $\boldsymbol{\rho}^0 \in \mathrm{int}(B)$.

Let $t_0 \in [0, c(\boldsymbol{\rho}^0))$ with $\boldsymbol{\rho}(t_0) \in \mathrm{int}(B)$. Then for any $\ell \in \{1, 2, \ldots, N-1\}$ and $1 \leqq i_1 < i_2 < \cdots i_\ell \leqq N$, one has

$$\sum_{r=1}^{\ell} \rho_{i_r}(t_0) < 1 - \varepsilon_\ell.$$

Moreover,

$$\sum_{r=1}^{\ell} \rho_{i_r}(t) < 1 - \varepsilon_\ell$$

for small enough $t > t_0$ by continuity. Thus $\boldsymbol{\rho}(t) \in \mathrm{int}(B)$ for small enough $t > t_0$.

With the above discussion and the compactness of B, we are ready to prove that $c(\boldsymbol{\rho}^0) = +\infty$. To show this, it is sufficient to prove that $\boldsymbol{\rho}(t) \in \mathrm{int}(B)$ for all $t > 0$. Let us assume this is not true, which means the solution $\boldsymbol{\rho}(t)$ hits the boundary. In this case, there exists $t_1 > 0$ such that $\boldsymbol{\rho}(t_1) \in \partial B$ and $\boldsymbol{\rho}(t) \in \mathrm{int}(B)$ for all $t \in [0, t_1)$. Since $\boldsymbol{\rho}(t_1) \in \partial B$, we can find $1 \leqq i_1 < \cdots < i_l \leqq N$ such that $1 \leqq l \leqq N - 1$ and

$$\sum_{r=1}^{l} \rho_{i_r}(t_1) = 1 - \varepsilon_l. \tag{37}$$

Let $A = \{i_1, i_2, \ldots, i_\ell\}$ and $A^c = \{1, 2, \ldots, N\} \setminus A$. Then for any $j \in A^c$,

$$\rho_j(t_1) \leqq 1 - \left(\sum_{r=1}^{\ell} \rho_{i_r}(t_1) \right) = \varepsilon_\ell. \tag{38}$$

Since $\boldsymbol{\rho}(t_1) \in B$, we have

$$\sum_{j=1}^{\ell-1} \rho_{s_j}(t_1) \leqq 1 - \varepsilon_{\ell-1},$$

for any $1 \leqq s_1 < s_2 < \cdots < s_{\ell-1} \leqq N$. Hence for each $i \in A$,

$$\rho_i(t_1) \geqq 1 - \varepsilon_\ell - (1 - \varepsilon_{\ell-1}) = \varepsilon_{\ell-1} - \varepsilon_\ell. \tag{39}$$

Combining equations (38), (39) and the fact

$$\varepsilon_\ell \leqq \frac{\varepsilon_{\ell-1}}{1 + (2M)^{\frac{1}{\beta}}},$$

one has, for any $i \in A$, $j \in A^c$,

$$\begin{aligned} &\Psi_j - \Psi_i + \beta(\log \rho_j - \log \rho_i) \leqq \Psi_j - \Psi_i + \beta(\log \varepsilon_\ell - \log(\varepsilon_{\ell-1} - \varepsilon_\ell)) \\ &\leqq -\log 2. \end{aligned} \tag{40}$$

Since the graph G is connected, there exists $i_* \in A$, $j_* \in A^c$ such that $\{a_{i_*}, a_{j_*}\} \in E$. Thus

$$\sum_{i \in A, j \in A^c, \{a_i, a_j\} \in E} \Gamma_{ij}^{\boldsymbol{\Psi}}(\boldsymbol{\rho}(t_1)) \geqq \Gamma_{i_* j_*}^{\boldsymbol{\Psi}}(\boldsymbol{\rho}(t_1)) > 0. \tag{41}$$

Now, by (40) and (41), one has

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\sum_{r=1}^{\ell}\rho_{i_r}(t)\mid_{t=t_1} &= \sum_{i\in A}\sum_{j\in N(i)}\Gamma_{ij}^{\Psi}(\boldsymbol{\rho}(t_1))\left(\Psi_j-\Psi_i+\beta(\log\rho_j(t_1)-\log\rho_i(t_1))\right)\\
&= \sum_{i\in A}\left\{\sum_{j\in A\cap N(i)}\Gamma_{ij}^{\Psi}(\boldsymbol{\rho}(t_1))\left(\Psi_j-\Psi_i+\beta(\log\rho_j(t_1)-\log\rho_i(t_1))\right)\right.\\
&\quad \left.+\sum_{j\in A^c\cap N(i)}\Gamma_{ij}^{\Psi}(\boldsymbol{\rho}(t_1))\left(\Psi_j-\Psi_i+\beta(\log\rho_j(t_1)-\log\rho_i(t_1))\right)\right\}\\
&= \sum_{i\in A}\sum_{j\in A^c\cap N(i)}\Gamma_{ij}^{\Psi}(\boldsymbol{\rho}(t_1))\left(\Psi_j-\Psi_i+\beta(\log\rho_j(t_1)-\log\rho_i(t_1))\right)\\
&\leqq -\log 2\sum_{i\in A}\sum_{j\in A^c\cap N(i)}\Gamma_{ij}^{\Psi}(\boldsymbol{\rho}(t_1))\\
&= -\log 2\sum_{i\in A,\, j\in A^c,\{a_i,a_j\}\in E}\Gamma_{ij}^{\Psi}(\boldsymbol{\rho}(t_1))\\
&\leqq -\log 2\,\Gamma_{i_*j_*}^{\Psi}(\boldsymbol{\rho}(t_1))<0.
\end{aligned}$$

Combining this with (37), it is clear that

$$\sum_{i=1}^{l}\rho_{i_r}(t_1-\delta)>1-\varepsilon_l$$

for sufficiently small $\delta>0$. This implies $\boldsymbol{\rho}(t_1-\delta)\notin B$, and it contradicts the fact that $\boldsymbol{\rho}(t)\in\mathrm{int}(B)$ for $t\in[0,t_1)$. This completes the proof of the Claim.

Given $\boldsymbol{\rho}^0\in\mathscr{M}$, by the above Claim, there exists a unique solution

$$\boldsymbol{\rho}(t):[0,\infty)\to\mathscr{M}$$

to equation (8) with initial value $\boldsymbol{\rho}^0$, and we can find a compact subset B of $\mathscr{M}$ with respect to the Euclidean metric such that $\{\boldsymbol{\rho}(t):t\in[0,+\infty)\}\subset B$. For $t\in(0,+\infty)$,

$$\frac{\mathrm{d}F(\boldsymbol{\rho}(t))}{\mathrm{d}t}=\mathrm{diff}\,F(\boldsymbol{\rho}(t))\cdot\frac{\mathrm{d}\boldsymbol{\rho}}{\mathrm{d}t}(t)=-g^{\Psi}_{\rho(t)}\left(\frac{\mathrm{d}\boldsymbol{\rho}}{\mathrm{d}t}(t),\frac{\mathrm{d}\boldsymbol{\rho}}{\mathrm{d}t}(t)\right)\leqq 0$$

and thus

$$\frac{\mathrm{d}F(\boldsymbol{\rho}(t))}{\mathrm{d}t}=0\quad\text{if and only if}\quad\frac{\mathrm{d}\boldsymbol{\rho}(t)}{\mathrm{d}t}=0.$$

This is equivalent to $\boldsymbol{\rho}(t)=(\rho_i^*)_{i=1}^N$ by (2). This implies that the free energy $F(\boldsymbol{\rho}(t))$ decreases as time t increases.

Finally, we show that $\boldsymbol{\rho}(t)\to\boldsymbol{\rho}^*$ under the Euclidean metric of $\mathbb{R}^N$ as $t\to+\infty$. We let

$$\omega(\boldsymbol{\rho}^0)=\left\{\boldsymbol{\rho}\in\mathbb{R}^N:\exists\, t_i\to+\infty\text{ such that }\lim_{i\to+\infty}\boldsymbol{\rho}(t_i)=\boldsymbol{\rho}\ \text{ in Euclidean metric}\right\}$$

be the ω-limit set of $\boldsymbol{\rho}^0$. Clearly, $\omega(\boldsymbol{\rho}^0) \subset B$ is a compact set of $\mathbb{R}^N$ with respect to the Euclidean metric.

To show $\boldsymbol{\rho}(t) \to \boldsymbol{\rho}^*$ under the Euclidean metric of $\mathbb{R}^N$ when $t \to +\infty$, it is sufficient to show that $\omega(\boldsymbol{\rho}^0) = \{\boldsymbol{\rho}^*\}$. Since $\omega(\boldsymbol{\rho}^0)$ is a compact set and the free energy F is continuous on $\overline{\mathscr{M}}$, we can find $\boldsymbol{\rho}^1 \in \omega(\boldsymbol{\rho}^0)$ such that $F(\boldsymbol{\rho}^1) = \max\{F(\boldsymbol{\rho}) : \boldsymbol{\rho} \in \omega(\boldsymbol{\rho}^0)\}$. Then there exists $t_i \to +\infty$ such that $\lim_{i\to+\infty} \boldsymbol{\rho}(t_i) = \boldsymbol{\rho}^1$ and $\lim_{i\to+\infty} \boldsymbol{\rho}(t_i - 1) = \boldsymbol{\rho}^2$ for some $\boldsymbol{\rho}^2 \in \mathscr{M}$. If we let $\boldsymbol{\rho}^2(t)$ be the solution to equation (8) with initial value $\boldsymbol{\rho}^2$, then $\boldsymbol{\rho}^2(0) = \boldsymbol{\rho}^2$ and $\boldsymbol{\rho}^2(1) = \boldsymbol{\rho}^1$. Note that

$$\frac{\mathrm{d}F(\boldsymbol{\rho}^2(t))}{\mathrm{d}t} = \operatorname{diff} F(\boldsymbol{\rho}^2(t)) \cdot \frac{\mathrm{d}\boldsymbol{\rho}^2}{\mathrm{d}t}(t) = -g^{\Psi}_{\boldsymbol{\rho}^2(t)}\left(\frac{\mathrm{d}\boldsymbol{\rho}^2}{\mathrm{d}t}(t), \frac{\mathrm{d}\boldsymbol{\rho}^2}{\mathrm{d}t}(t)\right) \leqq 0$$

and thus

$$\frac{\mathrm{d}F(\boldsymbol{\rho}^2(t))}{\mathrm{d}t} = 0 \quad \text{if and only if} \quad \frac{\mathrm{d}\boldsymbol{\rho}^2(t)}{\mathrm{d}t} = 0,$$

which is equivalent to $\boldsymbol{\rho}^2(t) = \boldsymbol{\rho}^*$ by (2). Hence if $\boldsymbol{\rho}^1 \neq \boldsymbol{\rho}^*$, then $F(\boldsymbol{\rho}^2) > F(\boldsymbol{\rho}^1)$, which is a contradiction with $F(\boldsymbol{\rho}^1) = \max\{F(\boldsymbol{\rho}) : \boldsymbol{\rho} \in \omega(\boldsymbol{\rho}^0)\}$. So we must have $\boldsymbol{\rho}^1 = \boldsymbol{\rho}^*$. Thus,

$$\max\{F(\boldsymbol{\rho}) : \boldsymbol{\rho} \in \omega(\boldsymbol{\rho}^0)\} = F(\boldsymbol{\rho}^*).$$

It is well known that $\boldsymbol{\rho}^*$ is the unique minimal value point of F. This implies $\omega(\boldsymbol{\rho}^0) = \{\boldsymbol{\rho}^*\}$. This completes the proof of (3).

There are many reasons why we consider Fokker–Planck equation I (8) on the manifold $\mathscr{M}$ instead of its closure. One of the main reasons is that $\overline{\mathscr{M}}$ is a manifold with boundary and its tangent space is only well-defined in its interior. Another reason is that the free energy is not differentiable when $\rho_i = 0$ for some i, and it is also not clear how the Riemannian metric d_{Ψ} on $\mathscr{M}$ can be extended to $\overline{\mathscr{M}}$. Moreover, even if the distance is well-defined on $\overline{\mathscr{M}}$, there may not be a solution to the equation (8) with initial value on the boundary ∂M (see the example in Appendix A).

Theorem 2 (3) guarantees that the solution of (8) can never attain the boundary $\partial\mathscr{M}$ if the initial value is in $\mathscr{M}$. In practice, we still need an equation to describe the transient process if the initial value is on the boundary. However, we think that the study of this important aspect is beyond the scope of this paper. The discussion on it will be given in a sequel paper.

5. Fokker–Planck Equation II

Given a graph $G = (V, E)$, we consider a time homogeneous Markov process $X(t)$ on the set V. We assume that $X(t)$ is generated by a potential function

$\boldsymbol{\Psi} = (\Psi_i)_{i=1}^N$ on V as a "gradient flow". If the process starts at a vertex a_i at time t, then the transition probability to the vertex a_j at time $t+h$ is given by

$$Pr(X(t+h) = a_j | X(t) = a_i)$$
$$= \begin{cases} (\Psi_i - \Psi_j)h + o(h) & \text{if} \quad j \in N(i), \Psi_j < \Psi_i, \\ 1 - \sum\limits_{k \in N(i), \Psi_k < \Psi_i} (\Psi_i - \Psi_k)h + o(h) & \text{if} \quad j = i, \\ 0 & \text{otherwise,} \end{cases}$$

where $o(h)/|h| \to 0$ as $h \to 0$.

The generating matrix $Q = [Q_{ij}]_{N \times N}$ for the Markov process can be defined by

$$Q_{ij} = \begin{cases} \Psi_i - \Psi_j & \text{if } \{a_i, a_j\} \in E, \Psi_j < \Psi_i, \\ 0 & \text{otherwise,} \end{cases}$$

which is the transition rate from i to j, and $Q_{ii} = -\sum_{j \neq i} Q_{ij}$.

Let $\boldsymbol{\rho}(t) = (\rho_i(t))_{i=1}^N$, where $\rho_i(t) = Pr(X(t) = a_i)$ for $i = 1, 2, \ldots, N$. The time evolution of probability distribution $\boldsymbol{\rho}(t)$ is given by a forward Kolmogorov equation:

$$\begin{cases} \frac{\partial \boldsymbol{\rho}}{\partial t}(t) = \boldsymbol{\rho}(t) Q \\ \boldsymbol{\rho}(0) = \{\rho_i^0\}_{i=1}^N, \end{cases}$$

or in an explicit form,

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = \sum_{j \in N(i), \Psi_j > \Psi_i} (\Psi_j - \Psi_i)\rho_j + \sum_{j \in N(i), \Psi_j < \Psi_i} (\Psi_j - \Psi_i)\rho_i \tag{42}$$

for $i = 1, 2, \ldots, N$.

We can consider $X(t)$ as an analog of the following gradient flow in Euclidean space:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\nabla \Psi(x), \quad x \in \mathbb{R}^N \tag{43}$$

and the forward Kolmogorov equation (42) is an analog of the corresponding degenerate Fokker–Planck equation without noise,

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (\nabla \Psi \rho). \tag{44}$$

For this reason, we call the Markov process $X(t)$ the gradient Markov process generated by discrete potential function $\boldsymbol{\Psi}$ on the graph G. Equation (42) can also be considered as a discretization of equation (44) with an upwind scheme [27].

An important observation is that in the continuous state space $\mathbb{R}^N$, Fokker–Planck equation (2) can be obtained by adding "white noise" to the degenerate Fokker–Planck equation (44). As an analog, we will obtain the Fokker–Planck

equation on a discrete space by adding "white noise" with strength $\sqrt{2\beta}$ to equation (42).

Suppose we rewrite Fokker–Planck equation (2) in the following degenerate fashion:

$$\rho_t = \nabla \cdot (\nabla \Psi \rho) + \beta \Delta \rho = \nabla \cdot [\nabla(\Psi + \beta \log \rho)\rho],$$

and its corresponding free energy in the following:

$$F = \int_{\mathbb{R}^N} (\Psi + \beta \log \rho)\rho \mathrm{d}x.$$

This indicates that if white noise $\sqrt{2\beta}\mathrm{d}W_t$ is added to system (43) on $\mathbb{R}^N$, it is equivalent to considering a new potential

$$\bar{\Psi}(x, t) = \Psi(x) + \beta \log \rho(x, t)$$

in the gradient flow (44).

Remark 4. This new potential function $\Psi + \beta \log \rho(x, t)$ is called Onsager's potential, and its derivative is called the Onsager thermodynamic flux [4,37].

As an analog, adding "white noise" to a time homogeneous Markov process $X(t)$ on a graph is equivalent to "changing the potential" to a new potential defined by:

$$\bar{\Psi}_i(t) = \Psi_i + \beta \log \rho_i(t)$$

for $i = 1, 2, \ldots, N$. For this modified potential $\bar{\Psi}$ we have a new Markov process $X_\beta(t)$, which is time inhomogeneous and may be considered as a "white noise" perturbation from the original homogeneous Markov process $X(t)$. More precisely, the conditional distribution of a_j at time $t + h$ given a_i at time t is given by

$$Pr(X_\beta(t + h) = a_j | X_\beta(t) = a_i) = \begin{cases} (\bar{\Psi}_i(t) - \bar{\Psi}_j(t))h + o(h), & \text{if } j \in N(i), \bar{\Psi}_j(t) < \bar{\Psi}_i(t), \\ 1 - \sum\limits_{k \in N(i), \bar{\Psi}_k(t) < \bar{\Psi}_i(t)} (\bar{\Psi}_i(t) - \bar{\Psi}_k(t))h + o(h) & \text{if } j = i, \\ 0, & \text{otherwise.} \end{cases}$$

The time evolution of probability distribution $(\rho_i(t))_{i=1}^N$ of $X_\beta(t)$ satisfies the following forward Kolmogorov equation:

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = \sum_{j \in N(i), \bar{\Psi}_j > \bar{\Psi}_i} ((\Psi_j + \beta \log \rho_j) - (\Psi_i + \beta \log \rho_i))\rho_j + \sum_{j \in N(i), \bar{\Psi}_j < \bar{\Psi}_i} ((\Psi_j + \beta \log \rho_j) - (\Psi_i + \beta \log \rho_i))\rho_i,$$

which is exactly Fokker–Planck equation II (9). On the other hand, we can also consider Fokker–Planck equation II (9) as a gradient flow of the free energy on the

space $\mathscr{M}$ with an appropriate inner product. Let us define the inner product $g^{\bar{\Psi}}_{\boldsymbol{\rho}}$ based on the new potential $\bar{\Psi}_i(t)$, and use it to induce a distance $d_{\bar{\Psi}}$ as shown in Section 3. The free energy F on the space $\mathscr{M}$ is given by:

$$F(\boldsymbol{\rho}) = \sum_{i=1}^{N} \Psi_i \rho_i + \beta \sum_{i=1}^{N} \rho_i \log \rho_i$$

where $\boldsymbol{\rho} = (\rho_i)_{i=1}^N \in \mathscr{M}$.

Since $\boldsymbol{\rho} \in \mathscr{M} \mapsto g^{\bar{\Psi}}_{\boldsymbol{\rho}}$ may not be continuous, there may not exist a gradient flow of F on $(\mathscr{M}, d_{\bar{\Psi}})$. However, we can consider a *generalized gradient flow* of F on $(\mathscr{M}, d_{\bar{\Psi}})$ because of the special relationship between $\mathscr{M}$ and its tangent spaces. More precisely, the derivative $\frac{\mathrm{d}\boldsymbol{\rho}(t)}{\mathrm{d}t} \in T_{\boldsymbol{\rho}(t)}\mathscr{M}$ is the same as the one computed using Euclidean metric. Thus, we can consider the following equation as our generalized gradient flow:

$$g^{\bar{\Psi}}_{\boldsymbol{\rho}}\left(\frac{\mathrm{d}\boldsymbol{\rho}}{\mathrm{d}t}(t), \boldsymbol{\sigma}\right) = -\mathrm{diff}\, F(\boldsymbol{\rho}(t)) \cdot \boldsymbol{\sigma} \qquad \forall \boldsymbol{\sigma} \in T_{\boldsymbol{\rho}}\mathscr{M}, \tag{45}$$

where $\mathrm{diff}\, F$ is the differential of F (see (32)). This also implies:

$$\frac{\mathrm{d}F(\boldsymbol{\rho}(t))}{\mathrm{d}t} = \mathrm{diff}\, F(\boldsymbol{\rho}(t)) \cdot \frac{\mathrm{d}\boldsymbol{\rho}(t)}{\mathrm{d}t} = -g^{\bar{\Psi}}_{\boldsymbol{\rho}(t)}\left(\frac{\mathrm{d}\boldsymbol{\rho}(t)}{\mathrm{d}t}, \frac{\mathrm{d}\boldsymbol{\rho}(t)}{\mathrm{d}t}\right). \tag{46}$$

We have the following theorem:

Theorem 3. *Given the graph $G = (V, E)$ with $V = \{a_1, a_2, \ldots, a_N\}$, potential $\boldsymbol{\Psi} = (\Psi_i)_{i=1}^N$ on V and $\beta \geqq 0$, we consider the gradient Markov process $X(t)$ generated by the potential $\boldsymbol{\Psi}$. Then we have*

1. *Fokker–Planck equation II (9)*

$$\begin{aligned}\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = &\sum_{j \in N(i), \bar{\Psi}_j > \bar{\Psi}_i} ((\Psi_j + \beta \log \rho_j) - (\Psi_i + \beta \log \rho_i))\rho_j \\ &+ \sum_{j \in N(i), \bar{\Psi}_j < \bar{\Psi}_i} ((\Psi_j + \beta \log \rho_j) - (\Psi_i + \beta \log \rho_i))\rho_i\end{aligned}$$

   describes the time evolution of probability distribution of $X_\beta(t)$, where $X_\beta(t)$ is the time inhomogeneous Markov process perturbed by "white noise" from the original Markov process $X(t)$.
2. *Fokker–Planck equation II (9) is the generalized gradient flow (45) of the free energy F on the metric space $(\mathscr{M}, d_{\bar{\Psi}})$ of probability densities $\boldsymbol{\rho}$ on V.*
3. *For all $\beta > 0$, Gibbs distribution $\boldsymbol{\rho}^* = (\rho_i^*)_{i=1}^N$*

$$\rho_i^* = \frac{1}{K}\mathrm{e}^{-\Psi_i/\beta} \text{ with } K = \sum_{i=1}^{N} \mathrm{e}^{-\Psi_i/\beta}$$

   is the unique stationary distribution of equation (9) in $\mathscr{M}$, and the free energy F attains a minimum at the Gibbs distribution.

4. *For all $\beta > 0$, there exists a unique solution $\boldsymbol{\rho}(t) : [0, \infty) \to \mathscr{M}$ to equation (9) with initial value $\boldsymbol{\rho}^0 \in \mathscr{M}$, and $\boldsymbol{\rho}(t)$ satisfies*
   (a) *The free energy $F(\boldsymbol{\rho}(t))$ decreases when time t increases.*
   (b) *$\boldsymbol{\rho}(t) \to \boldsymbol{\rho}^*$ under the Euclid metric of $\mathbb{R}^N$ when $t \to +\infty$.*

Proof. (1) The result in (1) comes from the discussion in the beginning of this section.

(2) A continuously differentiable function $\boldsymbol{\rho}(t) : [0, c) \to \mathscr{M}$ for some $c > 0$ or $c = +\infty$ is called a solution of equation (9) with initial value $\boldsymbol{\rho} \in \mathscr{M}$, if $\boldsymbol{\rho}(0) = \boldsymbol{\rho}$ and $\boldsymbol{\rho}(t)$ satisfies equation (9) for $t \in [0, c)$. Since the Fokker–Planck equation II (9) is Lipschitz continuous, by the existence and uniqueness theorem of ordinary differential equations, it is clear that for any $\boldsymbol{\rho} \in \mathscr{M}$, there exists a maximal interval $[0, c(\boldsymbol{\rho}))$ in which the solution to equation (9) with initial value ρ is uniquely defined with $c(\boldsymbol{\rho}) > 0$ or $c(\boldsymbol{\rho}) = +\infty$.

Let $\boldsymbol{\rho}(t) : [0, c) \to \mathscr{M}$ be a solution of (9). For $\boldsymbol{\sigma} = (\sigma_i)_{i=1}^N \in T_{\boldsymbol{\rho}(t)}\mathscr{M}$, we take $(p_i)_{i=1}^N \in \mathbb{R}^N$ such that $\boldsymbol{\sigma} \simeq [(p_i)_{i=1}^N]$. Then by (32), we have

$$\begin{aligned}
&\sum_{i=1}^N (\Psi_i + \beta(1 + \log \rho_i))\sigma_i = \sum_{i=1}^N (\Psi_i + \beta \log \rho_i)\sigma_i \\
&= \sum_{i=1}^N (\Psi_i + \beta \log \rho_i) \left(\sum_{j \in N(i)} \Gamma_{ij}^{\boldsymbol{\Psi}}(\boldsymbol{\rho}) \right) (p_i - p_j) \\
&= \sum_{\{a_i, a_j\} \in E, \bar{\Psi}_i < \bar{\Psi}_j} \{(\Psi_i - \Psi_j) + \beta(\log \rho_i - \log \rho_j)\}\rho_j (p_i - p_j) \\
&\quad + \beta \sum_{\{a_i, a_j\} \in E, \bar{\Psi}_i = \bar{\Psi}_j} (\bar{\Psi}_i - \bar{\Psi}_j)(p_i - p_j) \\
&= \sum_i \Bigg\{ \sum_{j \in N(i), \bar{\Psi}_j > \bar{\Psi}_i} \big((\Psi_i - \Psi_j)\rho_j + \beta(\log \rho_i - \log \rho_j)\rho_j\big) \\
&\quad + \sum_{j \in N(i), \bar{\Psi}_j < \bar{\Psi}_i} \big((\Psi_i - \Psi_j)\rho_i + \beta(\log \rho_i - \log \rho_j)\rho_i\big) \Bigg\} p_i. \qquad (47)
\end{aligned}$$

Combining this equation with Fokker–Planck equation II (9), and by identifications (26) and (28), we have

$$\begin{aligned}
\operatorname{diff} F(\boldsymbol{\rho}(t)) \cdot \boldsymbol{\sigma} &= \sum_{i=1}^N (\Psi_i + \beta(1 + \log \rho_i))\sigma_i \\
&= \sum_{i=1}^N \Bigg\{ \sum_{j \in N(i), \bar{\Psi}_j > \bar{\Psi}_i} \big((\Psi_i - \Psi_j)\rho_j + \beta(\log \rho_i - \log \rho_j)\rho_j\big)
\end{aligned}$$

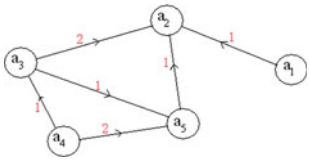

Fig. 2. "Gradient-like" transition graph

$$+\sum_{j\in N(i),\bar{\Psi}_j<\bar{\Psi}_i}\left((\Psi_i-\Psi_j)\rho_i+\beta(\log\rho_i-\log\rho_j)\rho_i\right)\Bigg\}p_i$$
$$=-\sum_{i=1}^{N}\frac{\mathrm{d}\rho_i}{\mathrm{d}t}p_i=-g^{\bar{\Psi}}_{\boldsymbol{\rho}(t)}\left(\frac{\mathrm{d}\boldsymbol{\rho}(t)}{\mathrm{d}t},\boldsymbol{\sigma}\right).$$

Hence (45) is true, and this finishes the proof of (2).

(3) Using (47) and replacing identification (24) by identification (26), the proof of (3) is completely similar to the proof of (2) in Theorem 2.

(4) Using (46) and replacing $\Gamma^{\Psi}_{ij}(\boldsymbol{\rho})$ by $\Gamma^{\bar{\Psi}}_{ij}(\boldsymbol{\rho})$ in the proof of (3) in Theorem 2, we get the proof of (4) in a similar way.

Remark 5. We note that Fokker–Planck equation I and Fokker–Planck equation II are very different even though they differ only by one term. In fact, Fokker–Planck equation II is not a gradient flow of the free energy on a smooth Riemannian manifold of the probability space, but it is a gradient flow if we allow the Riemannian manifold of probability space to be piecewise smooth. More importantly, Fokker–Planck equation II is based on two important concepts, white noise and the "nonlinear" Laplace operator for Markov processes on graphs.

Remark 6. In the above discussion, a time-homogeneous Markov process is given as the gradient Markov process generated by a potential $\boldsymbol{\Psi}$ on a graph $G = (V, E)$. On the other hand, if the potential is not given but a time-homogeneous Markov process is given, then we may reconstruct its potential function under some conditions. Let G be a weighted directed simple graph without self-loop or multi-edge. Suppose we have a time-homogeneous Markov process on G; the Markov process is called *gradient-like* if every directed loop from a_i to itself has zero total weight. In this case, a potential energy function can be defined on this graph, and it is unique up to a constant. To better illustrate this, we use the following example.

Example. We consider a graph $G = (V, E)$ with a time-homogeneous Markov process as shown in Fig. 2, which is directed and weighted. In this graph, $V = \{a_1, a_2, a_3, a_4, a_5\}$ and the number on each directed edge is the transition rate. Since the underlying weighted directed graph is gradient-like, we may associate the potential energy on each vertex as in Fig. 3. With this potential function, we can find its free energy and the Fokker–Planck equation.

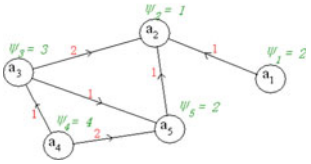

Fig. 3. Associated potential function

The transition probability rate matrix Q of this Markov process induced by Fig. 2 is:

$$\mathbf{Q} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 2 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

6. Connections to Upwind Schemes

From discussions in previous sections, it is clear that Fokker–Planck equations I (8) and II (9) on a graph are not typical discretizations of the Fokker–Planck equation in continuous state space. Moreover, one cannot obtain a Fokker–Planck equation in discrete state space with the desired properties by simply discretizing the Fokker–Planck equation in continuous state space with commonly used finite difference schemes. However, it is worth mentioning that Fokker–Planck equations (8) and (9) are motivated by the well-known strategies in finite difference methods, namely the upwind schemes for hyperbolic equations. In this section, we explain these connections in detail, and show that our discrete Fokker–Planck equations are actually consistent with the Fokker–Planck equation in continuous state space, provided that the discrete spaces are discretizations of the continuous state space.

For simplicity, let us demonstrate the connections on a 1-D lattice $G = (V, E)$ with vertex set $V = \{a_1, \ldots, a_N\}$ ($N \geqq 3$) and $E = \{\{a_i, a_{i+1}\} : i = 1, 2, \ldots, N-1\}$. We view the lattice as equal partition points of the interval $[0, 1]$ with mesh size h. We also assume that the potential function on V does not have equal values on adjacent points. Then our discrete Fokker–Planck equation I at vertex a_i, $i \in \{2, 3, \ldots, N-1\}$, is given by,

$$\begin{aligned} \frac{\mathrm{d}\rho_i}{\mathrm{d}t} &= ((\Psi_{i+1} - \Psi_i)\rho_{i+1} - (\Psi_i - \Psi_{i-1})\rho_i) \\ &\quad + \beta((\log \rho_{i+1} - \log \rho_i)\rho_{i+1} - (\log \rho_i - \log \rho_{i-1})\rho_i) \\ &\quad \text{if} \quad \Psi_{i+1} > \Psi_i > \Psi_{i-1}, \\ \frac{\mathrm{d}\rho_i}{\mathrm{d}t} &= ((\Psi_{i+1} - \Psi_i)\rho_i - (\Psi_i - \Psi_{i-1})\rho_{i-1}) \\ &\quad + \beta((\log \rho_{i+1} - \log \rho_i)\rho_i - (\log \rho_i - \log \rho_{i-1})\rho_{i-1}) \\ &\quad \text{if} \quad \Psi_{i+1} < \Psi_i < \Psi_{i-1}, \end{aligned}$$

$$\begin{aligned}\frac{\mathrm{d}\rho_i}{\mathrm{d}t} &= ((\Psi_{i+1}-\Psi_i)\rho_{i+1}-(\Psi_i-\Psi_{i-1})\rho_{i-1})\\ &\quad +\beta((\log\rho_{i+1}-\log\rho_i)\rho_{i+1}-(\log\rho_i-\log\rho_{i-1})\rho_{i-1})\\ &\quad \text{if}\quad \Psi_{i+1}>\Psi_i,\Psi_{i-1}>\Psi_i,\\ \frac{\mathrm{d}\rho_i}{\mathrm{d}t} &= ((\Psi_{i+1}-\Psi_i)\rho_i-(\Psi_i-\Psi_{i-1})\rho_i)\\ &\quad +\beta((\log\rho_{i+1}-\log\rho_i)\rho_i-(\log\rho_i-\log\rho_{i-1})\rho_i)\\ &\quad \text{if}\quad \Psi_{i+1}<\Psi_i,\Psi_{i-1}<\Psi_i.\end{aligned}$$

First, we consider the drift terms, that is, those involving the potentials, on the right-hand sides of the equations. It is obvious that when the potential is increasing at vertex a_i, which corresponds to the first scenario as $\Psi_{i+1}>\Psi_i>\Psi_{i-1}$, the term $(\Psi_{i+1}-\Psi_i)\rho_{i+1}-(\Psi_i-\Psi_{i-1})\rho_i$ involves density values ρ_{i+1} and ρ_i, which are from the right-hand side of position i. If one views the differences in potentials $(\Psi_i-\Psi_{i-1})$ and $(\Psi_{i+1}-\Psi_i)$, which are all positive, as the convection coefficient, then it indicates that the characteristic line goes from right to the left. In other words, in this situation the information propagates to the left, which is like "wind blowing" toward the left. Thus the right-hand side of the equation involves information only from the upwind (higher potential in this case) direction. Similarly, the upwind direction for the decreasing potential case with $\Psi_{i+1}<\Psi_i<\Psi_{i-1}$ is from the left to the right. And the Fokker–Planck equation relies only on the values ρ_i and ρ_{i-1}, which are from its upwind direction. In the other two cases, there are no clear upwind directions and therefore central differences are used. Moreover, one can see that the evolution of ρ_i depends only on its neighboring values with higher potentials, and this is also true for general graphs.

The appearance of upwind directions in Fokker–Planck equations I and II becomes natural if we take a closer look at the working mechanism of the drift terms. If we ignore the diffusion terms by taking $\beta=0$, then the probability density ρ_i evolves according to the gradient descent direction. The consequence is that the probability is clustered on local minima of the potentials, and, therefore, their corresponding density functions are combinations of Dirac Delta functions sitting on the minima. This is very similar to the shock (discontinuities in solutions) formation in nonlinear hyperbolic conservation laws, in which the upwind idea is considered as a fundamental strategy in designing shock capturing schemes. On the other hand, if one uses central differences in shock formation, numerical oscillations, which are called Gibbs' phenomena, are inevitable. For more discussions on numerical schemes for nonlinear conservation laws, readers are referred to books such as [6,27].

7. Parrondo's Paradox

It is known in game theory that it is possible to construct a winning strategy by playing two losing strategies alternately. This is often referred as Parrondo's paradox [1,22–24,36,38,39]. In this section, we explain, by using a discrete Fokker–Planck equation, the paradox of free energy for the flashing ratchet model [1,3,24,38,39] on a simple graph.

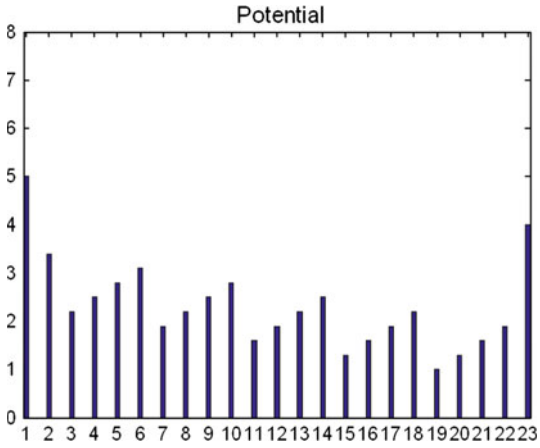

Fig. 4. Potential function Ψ^A

Table 1. Potential function Ψ^A

a_i	1	2	3	4	5	6	7	8	9	10	11	12
Ψ_i^A	5	3.4	2.2	2.5	2.8	3.1	1.9	2.2	2.5	2.8	1.6	1.9
a_i	13	14	15	16	17	18	19	20	21	22	23	
Ψ_i^A	2.2	2.5	1.3	1.6	1.9	2.2	1	1.3	1.6	1.9	4	

We consider a graph $G = (V, E)$ having 23 vertices:

$$V = \{a_1, a_2, \ldots, a_{23}\} \text{ and } E = \{\{a_i, a_{i+1}\} : i = 1, \ldots, 22\},$$

with two different potential functions Ψ^A and Ψ^B given on the graph. Ψ^A is defined as shown in Fig. 4 and $\Psi_i^B = 0$ for $i = 1, 2, \ldots, 23$. The values of Ψ^A are listed in Table 1.

Here we fix the temperature $\beta = 0.05$. For any probability density $\boldsymbol{\rho} = (\rho_i)_{i=1}^{23}$ on V, we consider two free energy functionals:

$$F_A(\boldsymbol{\rho}) = \sum_{i=1}^{23} \Psi_i^A \rho_i + 0.05 \sum_{i=1}^{23} \rho_i \log \rho_i$$

$$F_B(\boldsymbol{\rho}) = \sum_{i=1}^{23} \Psi_i^B \rho_i + 0.05 \sum_{i=1}^{23} \rho_i \log \rho_i = 0.05 \sum_{i=1}^{23} \rho_i \log \rho_i.$$

Free energy $F_A(\boldsymbol{\rho})$ induces a Markov process called Process A. Using Theorem 2 (1) with Ψ^A, we obtain a discrete Fokker–Planck equation, denoted as Equation A for Process A. (Here we omit the detailed expression of Equation A for simplicity.) Similarly, free energy $F_B(\boldsymbol{\rho})$ induces another Markov process called Process B, and its Fokker–Planck equation is given by

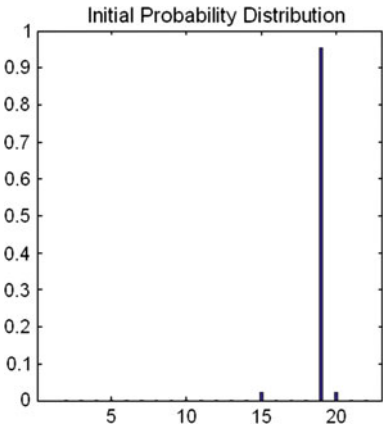

Fig. 5. Initial distribution

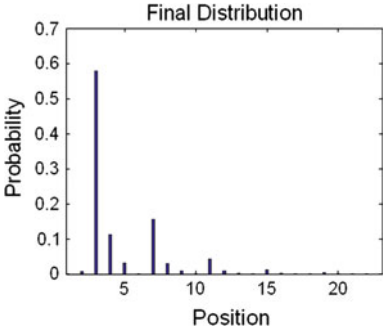

Fig. 6. Final distribution

$$\begin{cases} \dfrac{\mathrm{d}\rho_1}{\mathrm{d}t} = 0.05(\rho_2 - \rho_1) \\ \dfrac{\mathrm{d}\rho_i}{\mathrm{d}t} = 0.05(\rho_{i+1} + \rho_{i-1} - 2\rho_i), \quad 1 < i < 23. \\ \dfrac{\mathrm{d}\rho_{23}}{\mathrm{d}t} = 0.05(\rho_{22} - \rho_{23}) \end{cases}$$

We call this Equation B.

By Theorem 2 (3), free energy functionals F_A and F_B decrease monotonically along the solutions of Equations A and B, respectively, as time increases. Both processes are energy dissipative. However, if we apply processes A and B alternatingly, which is the classical flashing ratchet model, then we will observe an energy gaining process. In another word, in this viewpoint, the flashing ratchet is also a Parrondo's paradox of free energy.

More precisely, we choose an initial distribution $\boldsymbol{\rho}^0$ as shown in Fig. 5. The peak of $\boldsymbol{\rho}^0$ is on the right. We choose time interval length $T = 0.3$, and we use Equation A when $0 \leqq t < T$, and Equation B when $T \leqq t < 2T$. Then we repeat the processes. After taking $ABABAB\ldots$ for 400-times, the peak of probability distribution moves to the left-hand side (Fig. 6). This indicates a directed motion

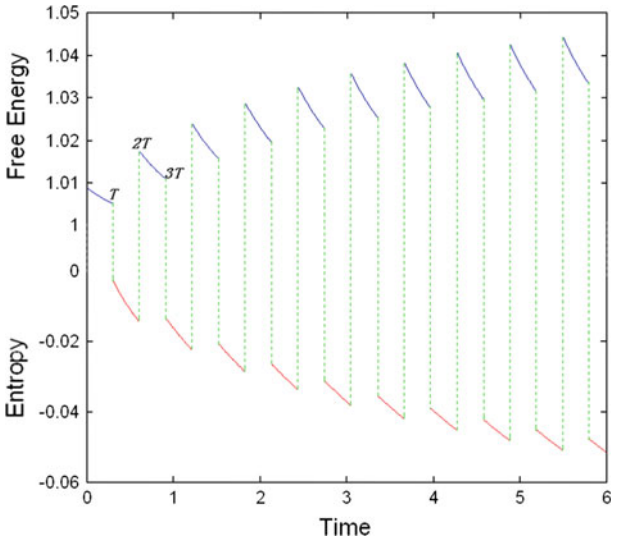

Fig. 7. First 10 process

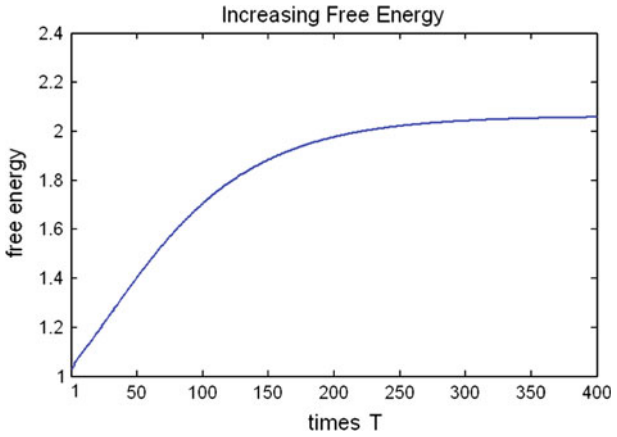

Fig. 8. The free energy at the end of Process A for the first 400 iterations

from the lower potential places to higher potential regions. This can be used to explain the directed motions by molecular motors.

To better illustrate this process, we show the free energy changes in Figs. 7 and 8. Figure 7 shows the free energy in the first 10 iterations. Process A ends at time T, and Process B begins. At time $2T$, Process B ends, and another Process A starts. These steps are repeated. Although the free energy functionals decrease on each process A and B, the free energy function $F_A(\boldsymbol{\rho})$ at time $3T$ is still higher than that at time T. So applying the two processes A and B alternatingly, we observe an energy gaining process at the end of process A, that is, at times $T, 3T, 5T, \ldots$. We show this energy gaining phenomenon in Fig. 8. For a similar example in a continuous state space, see [9].

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Appendix A. A Counterexample

Applying Theorem 2 (1) to a graph G with $\boldsymbol{\Psi}$ and $\beta > 0$, we obtain Fokker–Planck equation (8) on $\mathscr{M}$. For $\boldsymbol{\rho}^0 \in \overline{\mathscr{M}}$, a continuous function $\boldsymbol{\rho}(t) : [0, c) \to \overline{\mathscr{M}}$ for some $c > 0$ or $c = +\infty$ is defined to be a solution of equation (8) with initial value $\boldsymbol{\rho}^0$ if $\boldsymbol{\rho}(0) = \boldsymbol{\rho}^0$ and $\boldsymbol{\rho}(t) \in \mathscr{M}$ satisfies equation (8) for $t \in (0, c)$. In the following, we present an example, for which there does not exist a solution, of equation (8) for an initial value $\boldsymbol{\rho}^0 \in \partial\mathscr{M} := \overline{\mathscr{M}} \setminus \mathscr{M}$.

Example. We consider a graph with 3 vertices:

$$V = \{a_1, a_2, a_3\} \text{ and } E = \{\{a_1, a_3\}, \{a_2, a_3\}\}.$$

In this case, we have

$$\mathscr{M} = \{\boldsymbol{\rho} = (\rho_i)_{i=1}^3 \in \mathbb{R}^3 : \rho_1 + \rho_2 + \rho_3 = 1 \text{ and } \rho_i > 0 \text{ for } i = 1, 2, 3\}$$

and

$$\overline{\mathscr{M}} = \{\boldsymbol{\rho} = (\rho_i)_{i=1}^3 \in \mathbb{R}^3 : \rho_1 + \rho_2 + \rho_3 = 1 \text{ and } \rho_i \geqq 0 \text{ for } i = 1, 2, 3\}.$$

We assign potential $\boldsymbol{\Psi} = (\Psi_i)_{i=1}^3$ on V with $\Psi_1 > \Psi_3$ and $\Psi_2 > \Psi_3$, and fix $\beta > 0$. Applying Theorem 2 (1) for G, Ψ_i and β, we obtain Fokker–Planck equation I (8) on $\mathscr{M}$ as follow:

$$\begin{cases} \dfrac{\mathrm{d}\rho_1}{\mathrm{d}t} = (\Psi_3 - \Psi_1 + \beta(\log\rho_3 - \log\rho_1))\,\rho_1 \\ \dfrac{\mathrm{d}\rho_2}{\mathrm{d}t} = (\Psi_3 - \Psi_2 + \beta(\log\rho_3 - \log\rho_2))\,\rho_2 \\ \dfrac{\mathrm{d}\rho_3}{\mathrm{d}t} = \sum_{i=1}^2 (\Psi_i - \Psi_3 + \beta(\log\rho_i - \log\rho_3))\,\rho_i \end{cases} \tag{A.48}$$

Now let $\boldsymbol{\rho}^0 = (0, 1, 0) \in \partial\mathscr{M}$. Then we claim that there is no solution to equation (A.48) with initial value $\boldsymbol{\rho}^0$.

In fact, if the claim is not true, then there exists a continuous function

$$\boldsymbol{\rho}(t) = (\rho_1(t), \rho_2(t), \rho_3(t)) : [0, c) \to \overline{\mathscr{M}}$$

for some $c > 0$ or $c = +\infty$ such that $\boldsymbol{\rho}(0) = \boldsymbol{\rho}^0$ and $\boldsymbol{\rho}(t) \in \mathscr{M}$ satisfying equation (A.48) for $t \in (0, c)$. By (A.48), one has

$$\frac{\mathrm{d}\log\rho_1(t)}{\mathrm{d}t} = (\Psi_3 - \Psi_1) + \beta(\log\rho_3(t) - \log\rho_1(t))$$
$$\frac{\mathrm{d}\log\rho_2(t)}{\mathrm{d}t} = (\Psi_3 - \Psi_2) + \beta(\log\rho_3(t) - \log\rho_2(t))$$

for $t \in (0, c)$. Let $x(t) = \log\rho_1(t) - \log\rho_2(t)$ for $t \in (0, c)$, then one gets

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = \Psi_2 - \Psi_1 - \beta x(t)$$

for $t \in (0, c)$. Fix $T \in (0, c)$. It is clear that for any $0 < s < T$,

$$\mathrm{e}^{\beta T}x(T) = \mathrm{e}^{\beta s}x(s) + \int_s^T \mathrm{e}^{(\Psi_2-\Psi_1)t}\mathrm{d}t. \tag{A.49}$$

Since $\lim_{s\searrow 0}\mathrm{e}^{\beta s}x(s) = -\infty$ and $\lim_{s\searrow 0}\int_s^T \mathrm{e}^{(\Psi_2-\Psi_1)t}\mathrm{d}t = \int_0^T \mathrm{e}^{(\Psi_2-\Psi_1)t}\mathrm{d}t$, if one lets $s \searrow 0$ in (A.49), then one has $\mathrm{e}^{\beta T}x(T) = -\infty$, that is, $\rho_1(T) = -\infty$. This is a contradiction to $(\rho_1(T), \rho_2(T), \rho_3(T)) \in \mathscr{M}$.

References

1. AIT-HADDOU, R., HERZOG, W.: Brownian ratchet models of molecular motors. *Cell Bioch. Biophys.* **38**(2), 191–213 (2003)
2. AMBROSIO, L., GIGLI, N., SAVARÉ, G.: *Gradient Flows: in Metric Spaces and in the Space of Probability Measures*. Birkhäuser, 2008
3. ASTUMIAN, R.D.: Thermodynamics and kinetics of a Brownian motor. *Science* **276**(5314), 917 (1997)
4. BERGMANN, P.G., LEBOWITZ, J.L.: New approach to nonequilibrium processes. *Phys. Rev.* **99**(2), 578 (1955)
5. BONCIOCAT, A.I., STURM, K.T.: Mass transportation and rough curvature bounds for discrete spaces. *J. Funct. Anal.* **256**(9), 2944–2966 (2009)
6. BUET, C., CORDIER, S.: Numerical analysis of conservative and entropy schemes for the Fokker-Planck-Landau equation. *SIAM J. Numerical Anal.* **36**, 953–973 (1999)
7. CARLEN, E.A., GANGBO, W.: Constrained steepest descent in the 2-Wasserstein metric. *Ann. Math.* **157**, 807–846 (2003)
8. CARLEN, E.A., GANGBO, W.: Solution of a model boltzmann equation via steepest descent in the 2-Wasserstein metric. *Arch. Rational Mech. Anal.* **172**(1), 21–64 (2004)
9. CHOW, S.N., HUANG, W., LI, Y., ZHOU, H.: A free energy based mathematical study for molecular motors. *Regular Chaotic Dyn.* **16**(1), 117–127 (2011)
10. CORDERO-ERAUSQUIN, D., GANGBO, W., HOUDRÉ, C.: Inequalities for generalized entropy and optimal transportation. *Recent Advances in the Theory and Applications of Mass Transport: Summer School on Mass Transportation Methods in Kinetic Theory and Hydrodynamics*, September 4–9, 2000, Ponta Delgada, Azores, Portugal **353**, 73 (2004)
11. CORDERO-ERAUSQUIN, D., MCCANN, R.J., SCHMUCKENSCHLÄGER, M.: A Riemannian interpolation inequality à la Borell, Brascamp and Lieb. *Invent. Math.* **146**(2), 219–257 (2001)
12. VAN DEN BROECK, C.: The master equation and some applications in physics. *Stoch. Process. Appl. Phys.* 1–28 (1985)

13. Dobrushin, R.L.: Prescribing a system of random variables by conditional distributions. *Theory Probab. Appl.* **15**, 458 (1970)
14. Dolbeault, J., Kinderlehrer, D., Kowalczyk, M.: Remarks about the flashing rachet. *Partial Differential Equations and Inverse Problems*, 167–175. Contemp. Math., vol. 362
15. Ellis, R.S.: *Entropy, Large Deviations, and Statistical Mechanics*, vol. 271. Springer, 1985
16. Evans, L.C.: *Entropy and Partial Differential Equations*. Lecture Notes at UC Berkeley
17. Evans, L.C.: Partial differential equations and Monge-Kantorovich mass transfer. *Current Developments in Mathematics*, 65–126 (1997)
18. Evans, L.C., Gangbo, W.: *Differential Equations Methods for the Monge-Kantorovich Mass Transfer-Problem*, vol. 137. American Mathematical Society, 1999
19. Gardiner, C.W.: *Handbook of Stochastic Methods for Physics, Chemistry and Natural Sciences*, 4th printing of the 2nd edn, 1997
20. Gilbarg, D., Trudinger, N.S.: *Elliptic Partial Differential Equations of Second Order*, 2001
21. Hao, G., Kim, W.H., Qian, H.: *Thermodynamics and Geometry of Reversible and Irreversible Markov Processes*. Preprint
22. Harmer, G.P., Abbott, D.: Game theory: losing strategies can win by Parrondo's paradox. *Nature* **402**(6764), 864–864 (1999)
23. Harmer, G.P., Abbott, D.: A review of Parrondos paradox. *Fluct. Noise Lett.* **2**(2), R71–R107 (2002)
24. Heath, D., Kinderlehrer, D., Kowalczyk, M.: Discrete and continuous ratchets: from coin toss to molecular motor. *Discrete Contin. Dyn. Syst. B* **2**(2), 153–168 (2002)
25. Jordan, R., Kinderlehrer, D., Otto, F.: Free energy and the Fokker-Planck equation. *Physica D: Nonlinear Phenom.* **107**(2–4), 265–271 (1997)
26. Jordan, R., Kinderlehrer, D., Otto, F.: The variational formulation of the Fokker-Planck equation. *SIAM J. Math. Anal.* **29**(1), 1–17 (1998)
27. LeVeque, R.J.: *Numerical Methods for Conservation Laws*. Birkhäuser, 1992
28. Lott, J.: Some geometric calculations on Wasserstein space. *Commun. Math. Phys.* **277**(2), 423–437 (2008)
29. Lott, J., Villani, C.: Ricci curvature for metric-measure spaces via optimal transport. *Ann. Math.* **169**, 903–991 (2009)
30. Mathews, D.H., Turner, D.H.: Prediction of rna secondary structure by free energy minimization. *Curr. Opin. Struct. Biol.* **16**(3), 270–278 (2006)
31. McCann, R.J.: Exact solutions to the transportation problem on the line. *Proc. R. Soc. Lond. A: Math. Phys. Eng. Sci.* **455**(1984), 1341 (1999)
32. Mielke, A.: A gradient structure for reaction–diffusion systems and for energy-drift-diffusion systems. *Nonlinearity* **24**, 1329 (2011)
33. Otto, F.: The geometry of dissipative evolution equations: the porous medium equation. *Commun. Partial Differ. Equ.* **26**(1–2), 101–174 (2001)
34. Otto, F., Villani, C.: Generalization of an inequality by Talagrand and links with the logarithmic Sobolev inequality. *J. Funct. Anal.* **173**(2), 361–400 (2000)
35. Otto, F., Westdickenberg, M.: Eulerian calculus for the contraction in the Wasserstein distance. *SIAM J. Math. Anal.* **37**(4), 1227–1255 (2005)
36. Percus, O.E., Percus, J.K.: Can two wrongs make a right? Coin-tossing games and Parrondos paradox. *Math. Intell.* **24**(3), 68–72 (2002)
37. Qian, H.: Motor protein with nonequilibrium potential: its thermodynamics and efficiency. *Phys. Rev. E* **69**(1), 012901 (2004)
38. Qian, H.: Cycle kinetics, steady state thermodynamics and motors—a paradigm for living matter physics. *J. Phys. Condens. Matter* **17**, S3783 (2005)
39. Qian, M., Zhang, X., Wilson, R.J., Feng, J.: Efficiency of Brownian motors in terms of entropy production rate. *Europhys. Lett.* **84**, 10014 (2008)
40. Risken, H.: *The Fokker-Planck Equation: Methods of Solution and Applications*, vol. 18. Springer, 1996

41. SAMMER, M., TETALI, P.: Concentration on the discrete torus using transportation. *Combin. Probab. Comput.* **18**(5), 835–860 (2009)
42. SCHUSS, Z.: Singular perturbation methods in stochastic differential equations of mathematical physics. *SIAM Rev.* **22**, 119–155 (1980)
43. SMOLKA, B., WOJCIECHOWSKI, K.: Contrast enhancement of badly illuminated images based on Gibbs distribution and random walk model. *CAIP'1997*, 271–278, 1997
44. STURM, K.T.: Generalized Ricci bounds and convergence of metric measure spaces. *Comptes Rendus Math.* **340**(3), 235–238 (2005)
45. STURM, K.T.: On the geometry of metric measure spaces. *Acta Math.* **196**(1), 65–131 (2006)
46. STURM, K.T.: On the geometry of metric measure spaces, II. *Acta Math.* **196**(1), 133–177 (2006)
47. VASERSTEIN, L.N.: Markov processes over denumerable products of spaces, describing large systems of automata. *Problemy Peredachi Informatsii* **5**(3), 64–72 (1969)
48. VILLANI, C.: *Topics in Optimal Transportation*, vol. 58. American Mathematical Society, 2003
49. VILLANI, C.: *Optimal Transport: Old and New*, vol. 338. Springer, 2009
50. VON RENESSE, M.K., STURM, K.T.: Transport inequalities, gradient estimates, entropy and Ricci curvature. *Commun. Pure Appl. Math.* **58**(7), 923–940 (2005)
51. VON RENESSE, M.K., STURM, K.T.: Entropic measure and Wasserstein diffusion. *Ann. Probab.* **37**(3), 1114–1191 (2009)
52. WU, Y., HUA, G., YU, T.: Tracking articulated body by dynamic Markov network. *Proceedings of Ninth IEEE International Conference on Computer Vision, 2003*. IEEE, 1094–1101, 2003

School of Mathematics,
Georgia Institute of Technology,
Atlanta, GA 30332, USA.
e-mail: chow@math.gatech.edu
e-mail: yli@math.gatech.edu
e-mail: hmzhou@math.gatech.edu

and

Department of Mathematics,
University of Science and Technology of China,
Hefei 230026, Anhui, People's Republic of China.
e-mail: wenh@mail.ustc.edu.cn

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