Diffusion equations from master equations — A discrete geometric approach —

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Abstract

In this paper, master equations with finite states employed in nonequilibrium statistical mechanics are formulated in the language of discrete geometry. In this formulation, chains in algebraic topology play roles, and master equations are described on graphs that consist of vertexes representing states and of directed edges representing transition matrices. It is then shown that master equations under the detailed balance conditions are equivalent to discrete diffusion equations, where the Laplacians are defined as self-adjoint operators with respect to introduced inner products. An isospectral property of these Laplacians is shown for non-zero eigenvalues, and its applications are given. The convergence to the equilibrium state is shown by analyzing this class of diffusion equations. In addition, a systematic way to derive closed dynamical systems for expectation values is given. For the case that the detailed balance conditions are not imposed, master equations are expressed as a form of a continuity equation.

1 Introduction

Master equations are vital in the study of nonequilibrium statistical mechanics[1, 2], since they are mathematically simple and allow to show relaxation processes towards to equilibrium states[3]. These equations describe the time evolution of the probability that discrete states are found, and they are first order differential or difference equations. In addition, these equations are used in Monte Carlo simulations[4]. Quantum mechanical case can be considered by extending classical systems[5]. Thus there have been a variety of applications in mathematical sciences, and its progress continues to attract attention in the literature[6, 7, 8].

Algebraic topology and graph theory have been applied to a variety of sciences and mathematical engineering. Several topological approaches to master equations exist in the literature[9, 10, 11]. Not only master equations, but also random walks on lattices[12], electric circuits[13, 14, 15], and so on, have been studied from the viewpoint of algebraic topology. By introducing inner products for functions on graphs, one can define adjoint operators and Laplacians as self-adjoint operators[12]. These operators are useful as proven in the literature of functional analysis[16]. An amalgamation of these mathematical disciplines may be called discrete geometry. It is then of interest to explore how above mentioned operators can be used for master equations. Also, although discrete diffusion equations are derived from master equations in some cases, the condition when such diffusion equations can be derived is not known. Since the knowledge of discrete diffusion equations has been accumulated, clarifying such a condition is expected to be fruitful for the study of master equations.

In this paper master equations are formulated in terms of functions of chains, where states and transition matrices for master equations are described by chains used in algebraic topology. In particular, probability distribution function is regarded as a function of 0-chain, and transition matrix a function of 1-chain, where a discrete state is expressed as a vertex or a 0-chain. After introducing some inner products for functions on chains and current as a function on 1-chain, it is shown that master equations are written in terms of co-derivative of the current, which is equivalent to the following.

Claim. Master equations can be written as a form of a continuity equation (See Theorem 3.1 for details).

In addition, under the assumption that the detailed balance conditions hold, an equivalence between master equations and discrete diffusion equations is shown, where the Laplacians are constructed by choosing appropriate measures for inner products:

Claim. Master equations under the detailed balance conditions are equivalent to discrete diffusion equations (See Theorem 3.2 for details).

By applying this statement, it is shown that probability distribution functions relax to the equilibrium state (See Corollary 3.1 and Proposition 3.2). By contrast, it is shown that discrete diffusion equations yield master equations (See Proposition 3.1). Also, an isospectral property for non-zero eigenvalues of these Laplacians is given (See Theorem 3.3), and this can be referred to as a supersymmetry[17]. With this supersymmetry dynamical systems for expectation variables are derived without any approximation (See Propositions 3.5 and 3.6).

These theorems, corollary, and so on should be compared with those in the existing literature. In the study of random walks on lattices, chains, functions and their Laplacians are also used[12]. In the literature the probability distribution functions are identified with functions on 1-chains, which is different to the present formalism. The differences appear since transition matrices are introduced for describing state transitions for the present study. On the other hand, similarities between the present study and existing studies appear due to the use of Laplacians. Laplacian is a self-adjoint operator with respect to an inner product, and brings several properties as well as the case of the standard Riemannian geometry.

In Section 2, some preliminaries are provided in order to keep this paper self-contained. In Section 3, master equations are formulated on graph, and the main claims of this paper and their consequences are provided.

2 Preliminaries

Let $G = (V, E)$ be a directed graph with V a vertex set and E an edge set. Throughout this paper, every graph is finite ($\#E < \infty$), connected, and allowed to have loop edges. However parallel edges that will be defined later are excluded from this contribution.

2.1 Standard operators

In this subsection, most of notions and notations follow Ref. [12]. However, some variants are also introduced.

For a given edge $e \in E$, the inverse of e, the terminus of e, and the origin of e are denoted by $\overline{e}$, $\mathrm{t}(e) \in V$, and $\mathrm{o}(e) \in V$, respectively:

$$\underset{\mathrm{o}(e)}{\bullet} \xrightarrow[e]{\qquad\qquad} \underset{\mathrm{t}(e)}{\bullet}\;, \qquad \text{and} \qquad \underset{\mathrm{t}(\overline{e})}{\bullet} \xleftarrow[\overline{e}]{\qquad\qquad} \underset{\mathrm{o}(\overline{e})}{\bullet}\;.$$

Then, it follows that

$$\mathrm{t}(\overline{e}) = \mathrm{o}(e), \qquad \text{and} \qquad \mathrm{o}(\overline{e}) = \mathrm{t}(e).$$

A *loop edge* $e \in E$ is such that $\mathrm{o}(e) = \mathrm{t}(e)$, and *parallel edges* $e_1, e_2 \in E$ are such that $e_1 \neq e_2$ with $\mathrm{o}(e_1) = \mathrm{o}(e_2)$ and $\mathrm{t}(e_1) = \mathrm{t}(e_2)$. Parallel edges are not assumed to exist in any graph in this paper.

Then one defines the groups of 0-*chains* and 1-*chains* on a graph G with coefficients $\mathbb{R}$

$$\begin{aligned} C_0(G, \mathbb{R}) &:= \left\{ \sum_{x \in V} a_x x \;\middle|\; a_x \in \mathbb{R} \right\}, \\ C_1(G, \mathbb{R}) &:= \left\{ \sum_{e \in E} a_e e \;\middle|\; a_e \in \mathbb{R} \right\}, \end{aligned}$$

respectively. The spaces of functions on $C^0(G,\mathbb{R})$ and $C^1(G,\mathbb{R})$ are denoted by

$$
\begin{aligned}
C^0(G,\mathbb{R}) &:= \{ f : V \to \mathbb{R} \}, \\
C^1(G,\mathbb{R}) &:= \{ \omega : E \to \mathbb{R} \}.
\end{aligned}
$$

Elements of the subset of $C^0(G,\mathbb{R})$ being dual to $C_0(G,\mathbb{R})$ are referred to as 0-*cochains*. Similarly, elements of the subset of $C^1(G,\mathbb{R})$ being dual to $C_1(G,\mathbb{R})$ are referred to as 1-*cochains*. The set $C^0(G,\mathbb{R})$ is also denoted by $\Lambda^0(G,\mathbb{R})$ in this paper. The subsets $\Lambda^1(G,\mathbb{R}) \subset C^1(G,\mathbb{R})$ and $S^1(G,\mathbb{R}) \subset C^1(G,\mathbb{R})$ are defined by

$$
\begin{aligned}
\Lambda^1(G,\mathbb{R}) &:= \left\{ \omega \in C^1(G,\mathbb{R}) \mid \omega(\overline{e}) = -\omega(e) \right\}, \\
S^1(G,\mathbb{R}) &:= \left\{ \mu \in C^1(G,\mathbb{R}) \mid \mu(\overline{e}) = \mu(e) \right\},
\end{aligned}
$$

where $\omega(e)$ is understood as $\omega(e) \in \mathbb{R}$. In what follows, $C_0(G,\mathbb{R})$ and $C_1(G,\mathbb{R})$ are often abbreviated as $C_0(G)$ and $C_1(G)$, respectively. Similar abbreviations will be adopted.

The *boundary operator* is defined as

$$
\partial : C_1(G) \to C_0(G), \qquad \text{so that} \qquad \partial(e) := \mathrm{t}(e) - \mathrm{o}(e),
$$

and the linearity holds:

$$
\partial(c_1 + c_2) = \partial c_1 + \partial c_2, \qquad \text{and} \qquad \partial(a\, c) = a\, \partial\, c, \qquad a \in \mathbb{R}, \quad c, c_1, c_2 \in C_1(G).
$$

The dual of the boundary operator, the *coboundary map*, is defined by

$$
\mathrm{d} : \Lambda^0(G) \to \Lambda^1(G), \qquad \text{so that} \qquad (\mathrm{d}f)(e) := f(\mathrm{t}(e)) - f(\mathrm{o}(e)),
$$

and the linearity holds:

$$
\mathrm{d}(f_1 + f_2) = \mathrm{d}f_1 + \mathrm{d}f_2, \qquad \text{and} \qquad \mathrm{d}(a\, f) = a\, \mathrm{d}f, \qquad a \in \mathbb{R}, \quad f, f_1, f_2 \in \Lambda^0(G).
$$

If f is a 0-cochain, then it follows that $(\mathrm{d}f)(e) = f(\partial e)$. For any loop edge $e \in E$, it follows from $f(\mathrm{t}(e)) = f(\mathrm{o}(e))$ that $(\mathrm{d}f)(e) = 0$. This $\mathrm{d}f$ is indeed an element belonging to $\Lambda^1(G)$, as shown below. For any $f \in \Lambda^0(G)$ and $e \in E$, one has that

$$
(\mathrm{d}f)\,(\,\overline{e}\,) = f(\,\mathrm{t}(\overline{e})\,) - f(\,\mathrm{o}(\overline{e})\,) = f(\,\mathrm{o}(e)\,) - f(\,\mathrm{t}(e)\,) = -\,(\mathrm{d}f)(\,e\,).
$$

To define inner products,

$$
\langle\ ,\ \rangle_V : \Lambda^0(G) \times \Lambda^0(G) \to \mathbb{R} \qquad \text{and} \qquad \langle\ ,\ \rangle_E : \Lambda^1(G) \times \Lambda^1(G) \to \mathbb{R},
$$

one introduces some measures. Let m_V and m_E be elements of $C^0(G)$ and $S^1(G)$, such that

$$
m_V(x) > 0, \quad \forall\, x \in V,
$$

and

$$
m_E(e) = m_E(\,\overline{e}\,) > 0, \quad \forall\, e \in E.
$$

This $m_E \in S^1(G)$ is referred to as a *reversible measure*.

The following are inner products

$$
\begin{aligned}
\langle\, f_1\,,\, f_2\,\rangle_V &:= \sum_{x\in V} f_1(x)\, f_2(x)\, m_V(x), \qquad \forall\, f_1, f_2\ \in \Lambda^0(G), && (1)\\
\langle\, \omega_1\,,\, \omega_2\,\rangle_E &:= \frac{1}{2}\sum_{e\in E} \omega_1(e)\, \omega_2(e)\, m_E(e), \qquad \forall\, \omega_1, \omega_2\ \in \Lambda^1(G). && (2)
\end{aligned}
$$

Associated with this set of inner products, one defines the *co-derivative* $\mathrm{d}^\dagger : \Lambda^1(G) \to \Lambda^0(G)$ such that

$$(\mathrm{d}^\dagger\omega)(x) = \frac{-1}{m_V(x)} \sum_{e\in E_x} \omega(e)\, m_E(e), \tag{3}$$

where

$$E_x := \{\, e \in E \mid \mathrm{o}(e) = x \,\}\,.$$

It follows from (3) that the linearity holds:

$$\mathrm{d}^\dagger(\omega_1 + \omega_2) = \mathrm{d}^\dagger\omega_1 + \mathrm{d}^\dagger\omega_2, \qquad \text{and} \qquad \mathrm{d}^\dagger(a\,\omega) = a\,\mathrm{d}^\dagger\omega, \qquad a \in \mathbb{R}, \quad \omega, \omega_1, \omega_2 \in \Lambda^1(G).$$

This operator $\mathrm{d}^\dagger$ is the adjoint one of d as shown below.

Lemma 2.1.

$$\langle\, \mathrm{d}f\,,\, \omega\,\rangle_E = \langle\, f\,,\, \mathrm{d}^\dagger\omega\,\rangle_V\,.$$

Proof. Straightforward calculations yield

$$\begin{aligned}
\langle\, \mathrm{d}f\,,\, \omega\,\rangle_E &= \frac{1}{2}\sum_{e\in E}(\mathrm{d}f)(e)\omega(e)\, m_E(e) = \frac{1}{2}\sum_{e\in E}[\, f(\mathrm{t}(e)) - f(\mathrm{o}(e))\,]\; \omega(e)\, m_E(e)\\
&= \frac{-1}{2}\sum_{e\in E}[\, f(\mathrm{o}(e))\,\omega(e) - f(\mathrm{t}(e))\,\omega(e)\,]\; m_E(e)\\
&= \frac{-1}{2}\sum_{e\in E}[\, f(\mathrm{o}(e))\,\omega(e)\, m_E(e) + f(\,\mathrm{o}(\overline{e})\,)\,\omega(\,\overline{e}\,)\, m_E(\,\overline{e}\,)\,]\\
&= \sum_{x\in V} f(x)\,(\,\mathrm{d}^\dagger\omega\,)(x)\, m_V(x) = \langle\, f\,,\, \mathrm{d}^\dagger\omega\,\rangle_V\,.
\end{aligned}$$

□

Remark 2.1. An operator analogous to $-\,\mathrm{d}^\dagger$ in the continuous standard Riemannian geometry is referred to as divergence. Thus, $-\,\mathrm{d}^\dagger$ can be referred to as *divergence* on graph[18]. This operator $\Lambda^1(G) \to \Lambda^0(G)$ is denoted by

$$\mathrm{div} := -\,\mathrm{d}^\dagger. \tag{4}$$

The *Laplacian acting on* $\Lambda^0(G)$, $\Delta_V : \Lambda^0(G) \to \Lambda^0(G)$, is defined as

$$\Delta_V := -\,\mathrm{d}^\dagger\mathrm{d}. \tag{5}$$

The explicit form of its action is obtained as follows. By putting $\omega = \mathrm{d}f$ for $f \in \Lambda^0(G)$, one has

$$\begin{aligned}
(\Delta_V f)(x) &= -\,(\mathrm{d}^\dagger\mathrm{d}f)(x) = -\,(\mathrm{d}^\dagger\,\omega)(x)\\
&= \frac{1}{m_V(x)}\sum_{e\in E_x}\omega(e)\, m_E(e) = \frac{1}{m_V(x)}\sum_{e\in E_x}(\,\mathrm{d}f\,)(e)\, m_E(e).
\end{aligned}$$

Since d and $\mathrm{d}^\dagger$ are linear operators, Δ_V is also a linear operator:

$$\Delta_V(f_1 + f_2) = \Delta_V f_1 + \Delta_V f_2, \qquad \text{and} \qquad \Delta_V(a\,f) = a\,\Delta_V f, \qquad a \in \mathbb{R},\; f, f_1, f_2 \in \Lambda^0(G).$$

Moreover, it follows that

$$(\Delta_V f)(x) = \frac{1}{m_V(x)}\sum_{e\in E_x}[\, f(\,\mathrm{t}(e)\,) - f(\,\mathrm{o}(e)\,)\,]\; m_E(e). \tag{6}$$

To see a link between (6) and a well-known form of discrete Laplacian, choose $m_V(x) = \delta$ and $m_E(e) = 1$ for all $x \in V$ and $e \in E$, where $\delta > 0$ is a constant. Then consider the graph

$$x' \xleftarrow{\;e'\;} x \xrightarrow{\;e''\;} x'' \,.$$

For this graph, one has that

$$(\Delta_V f)(x) = \frac{1}{\delta}\,[\, f(x') - 2f(x) + f(x'')\,]\,.$$

By taking the limit $\delta \to 0$ appropriately, one has the second derivative of f. See Ref. [20] for another link between this Laplacian Δ_V and the so-called adjacency operator.

This operator is self-adjoint as shown below.

Lemma 2.2.

$$\langle\, \Delta_V f_1\,,\, f_2\,\rangle_V = \langle\, f_1\,,\, \Delta_V f_2\,\rangle_V\,.$$

Proof. It follows that

$$\langle\, \Delta_V f_1\,,\, f_2\,\rangle_V = \left\langle -\mathrm{d}^\dagger \mathrm{d} f_1\,,\, f_2\,\right\rangle_V = \langle\, \mathrm{d} f_1\,,\, -\mathrm{d} f_2\,\rangle_E = \left\langle\, f_1\,,\, -\mathrm{d}^\dagger \mathrm{d} f_2\,\right\rangle_V = \langle\, f_1\,,\, \Delta_V f_2\,\rangle_V\,.$$

□

The *Laplacian acting on* $\Lambda^1(G)$, $\Delta_E : \Lambda^1(G) \to \Lambda^1(G)$, is defined as

$$\Delta_E := -\,\mathrm{d}\,\mathrm{d}^\dagger. \tag{7}$$

This operator is self-adjoint as shown below.

Lemma 2.3.

$$\langle\, \Delta_E\, \omega_1\,,\, \omega_2\,\rangle_E = \langle\, \omega_1\,,\, \Delta_E\, \omega_2\,\rangle_E\,.$$

Proof. It can be proven by straightforward calculations. To this end, we put $f_1 = \mathrm{d}^\dagger \omega_1 \in \Lambda^0(G)$ and then it follows that

$$\begin{aligned}
\langle\, \Delta_E\, \omega_1\,,\, \omega_2\,\rangle_E &= \left\langle -\mathrm{d}\,\mathrm{d}^\dagger\, \omega_1\,,\, \omega_2\,\right\rangle_E = \langle -\mathrm{d} f_1\,,\, \omega_2\,\rangle_E = \left\langle\, f_1\,,\, -\mathrm{d}^\dagger\, \omega_2\,\right\rangle_V \\
&= \left\langle\, \mathrm{d}^\dagger \omega_1\,,\, -\mathrm{d}^\dagger\, \omega_2\,\right\rangle_V = \left\langle\, \omega_1\,,\, -\mathrm{d}\,\mathrm{d}^\dagger\, \omega_2\,\right\rangle_E = \langle\, \omega_1\,,\, \Delta_E\, \omega_2\,\rangle_E\,.
\end{aligned}$$

□

Most of the operators and their properties discussed so far are well-known[12]. On the other hand, those discussed in the next subsection are not standard ones.

2.2 Operators for master equations

To discuss master equations, one introduces

$$\begin{aligned}
C^1_{\mathrm{A}}(G,\mathbb{R}) &:= \left\{\, \omega \in C^1(G,\mathbb{R}) \mid \omega(\overline{e}) = -(\varphi(e))^{-1}\,\omega(e), \quad \varphi \in C^1_{\mathrm{R}}(G,\mathbb{R})\,\right\}, \\
C^1_{\mathrm{R}}(G,\mathbb{R}) &:= \left\{\, \varphi \in C^1(G,\mathbb{R}) \,\middle|\, \varphi(\,\overline{e}\,) = \frac{1}{\varphi(e)} \right\}.
\end{aligned} \tag{8}$$

The operator associated with $\varphi \in C^1_{\mathrm{R}}(G)$ is defined as

$$\mathrm{d}_\varphi : C^0(G,\mathbb{R}) \to C^1_{\mathrm{A}}(G,\mathbb{R}), \qquad \text{such that} \qquad (\mathrm{d}_\varphi f)(e) := \varphi(e)\, f(\mathrm{t}(e)) - f(\mathrm{o}(e)), \tag{9}$$

and the linearity in f holds:

$$\mathrm{d}_\varphi (f_1 + f_2) = \mathrm{d}_\varphi f_1 + \mathrm{d}_\varphi f_2, \qquad \text{and} \qquad \mathrm{d}_\varphi (af) = a\,\mathrm{d}_\varphi f, \qquad a \in \mathbb{R}, \quad f, f_1, f_2 \in C^0(G).$$

Condition in (8) is to guarantee the property $\mathrm{d}_{\varphi} f \in C^{1}_{\mathrm{A}}(G)$ for $f \in C^{0}(G)$,

$$(\mathrm{d}_{\varphi} f)(\overline{e}) = \frac{-1}{\varphi(e)}(\mathrm{d}_{\varphi} f)(e).$$

The above equality is verified as

$$\begin{aligned}(\mathrm{d}_{\varphi} f)(\overline{e}) &= \varphi(\overline{e})\, f(\mathrm{t}(\overline{e})) - f(\mathrm{o}(\overline{e})) = \varphi(\overline{e})\, f(\mathrm{o}(e)) - f(\mathrm{t}(e)) = \frac{1}{\varphi(e)} f(\mathrm{o}(e)) - f(\mathrm{t}(e)) \\ &= \frac{-1}{\varphi(e)}(\mathrm{d}_{\varphi} f)(e).\end{aligned}$$

Remark 2.2. In the case that φ is such that $\varphi(e) = 1$ for any $e \in E$, one has that $\mathrm{d}_{\varphi} f = \mathrm{d}f$ for any $f \in C^{0}(G)$. The operator d_{φ} is an analogue of the one introduced in Ref. [19].

As well as the case for $\langle\ ,\ \rangle_{E}$, one introduces an *inner product on* $C^{1}_{\mathrm{A}}(G)$

$$\langle\ ,\ \rangle^{\varphi}_{E} : C^{1}_{\mathrm{A}}(G) \times C^{1}_{\mathrm{A}}(G) \to \mathbb{R},$$

associated with a reversible measure $m_{E} \in S^{1}(G)$. The value of the inner product is the same as (2):

$$\langle \omega_{1}, \omega_{2} \rangle^{\varphi}_{E} := \frac{1}{2}\sum_{e\in E} \omega_{1}(e)\, \omega_{2}(e)\, m_{E}(e) = \langle \omega_{1}, \omega_{2} \rangle_{E}.$$

With this inner product, one introduces the *co-derivative on* $C^{1}_{\mathrm{R}}(G)$, $\mathrm{d}^{\dagger}_{\varphi} : C^{1}_{\mathrm{A}}(G) \to C^{0}(G)$ with $\varphi \in C^{1}_{\mathrm{R}}(G)$ such that

$$(\mathrm{d}^{\dagger}_{\varphi}\omega)(x) := \frac{-1}{m_{V}(x)} \sum_{e\in E_{x}} \omega(e)\, m_{E}(e).$$

Lemma 2.4. *For* $\varphi \in C^{1}_{\mathrm{R}}(G)$, $\omega \in C^{1}_{\mathrm{A}}(G)$, *and* $f \in C^{0}(G)$, *one has*

$$\langle \mathrm{d}_{\varphi} f, \omega \rangle^{\varphi}_{E} = \left\langle f, \mathrm{d}^{\dagger}_{\varphi}\omega \right\rangle_{V},$$

Proof. Substituting

$$\varphi(e) = \frac{1}{\varphi(\overline{e})}, \qquad \omega(e) = -\varphi(\overline{e})\, \omega(\overline{e}), \qquad \text{and} \qquad m_{E}(e) = m_{E}(\overline{e}),$$

into

$$\begin{aligned}\langle \mathrm{d}_{\varphi} f, \omega \rangle^{\varphi}_{E} &= \frac{1}{2}\sum_{e\in E} [\, \varphi(e) f(\mathrm{t}(e)) - f(\mathrm{o}(e))\,]\, \omega(e)\, m_{E}(e) \\ &= \frac{-1}{2}\sum_{e\in E} [\, f(\mathrm{o}(e))\, \omega(e) - \varphi(e) f(\mathrm{t}(e))\, \omega(e)\,]\, m_{E}(e),\end{aligned}$$

one has

$$\begin{aligned}\langle \mathrm{d}_{\varphi} f, \omega \rangle^{\varphi}_{E} &= \frac{-1}{2}\sum_{e\in E} \left[f(\mathrm{o}(e))\, \omega(e) - \frac{1}{\varphi(\overline{e})} f(\mathrm{o}(\overline{e}))\, (-\varphi(\overline{e})\, \omega(\overline{e}))\right] m_{E}(e) \\ &= \frac{-1}{2}\sum_{e\in E} [\, f(\mathrm{o}(e))\, \omega(e)\, m_{E}(e) + f(\mathrm{o}(\overline{e}))\, \omega(\overline{e})\, m_{E}(e)\,] = \left\langle f, \mathrm{d}^{\dagger}_{\varphi}\, \omega \right\rangle_{V}.\end{aligned}$$

□

Although the following operators will not be used in Section 3, the Laplacian is discussed for the sake of completeness. The Laplacian $\Delta_V^{\varphi} : C^0(G) \to C^0(G)$ is defined as

$$\Delta_V^{\varphi} := -\,\mathrm{d}_{\varphi}^{\dagger}\,\mathrm{d}_{\varphi}.$$

The explicit form of its action is obtained as follows. By putting $\omega = \mathrm{d}_{\varphi} f$ for $f \in C^0(G)$, one has

$$\begin{aligned}
(\Delta_V^{\varphi} f)(x) &= -\,(\mathrm{d}_{\varphi}^{\dagger}\,\mathrm{d}_{\varphi} f)(x) = -\,(\mathrm{d}_{\varphi}^{\dagger}\,\omega)(x) \\
&= \frac{1}{m_V(x)} \sum_{e \in E_x} \omega(e)\, m_E(e) = \frac{1}{m_V(x)} \sum_{e \in E_x} (\,\mathrm{d}_{\varphi} f\,)(e)\, m_E(e) \\
&= \frac{1}{m_V(x)} \sum_{e \in E_x} [\,\varphi(e)\, f(\,\mathrm{t}(e)\,) - f(\,\mathrm{o}(e)\,)\,]\; m_E(e).
\end{aligned}$$

This operator is self-adjoint:

$$\langle\, \Delta_V^{\varphi} f_1\,,\, f_2\,\rangle_V = \langle\, f_1\,,\, \Delta_V^{\varphi} f_2\,\rangle_V\,,$$

since

$$\langle\, \Delta_V^{\varphi} f_1\,,\, f_2\,\rangle_V = \left\langle -\,\mathrm{d}_{\varphi}^{\dagger}\,\mathrm{d}_{\varphi} f_1\,,\, f_2\,\right\rangle_V = \langle\, \mathrm{d}_{\varphi} f_1\,,\, -\,\mathrm{d}_{\varphi}\, f_2\,\rangle_E = \left\langle\, f_1\,,\, -\,\mathrm{d}_{\varphi}^{\dagger}\,\mathrm{d}_{\varphi}\, f_2\,\right\rangle_V = \langle\, f_1\,,\, \Delta_V^{\varphi} f_2\,\rangle_V\,.$$

3 Master equations

Master equations are written as

$$\frac{\mathrm{d}}{\mathrm{d}t} p_t(x) = -\lambda(x) p_t(x) + \sum_{x'} w_{x' \to x}\, p_t(x'), \qquad \text{with} \quad \lambda(x) = \sum_{x'} w_{x \to x'}, \tag{10}$$

where $\{x\}$ are discrete states, $\{w_{x\to y}\}$ a transition matrix that describes the transition rate from a state x to another y. The equilibrium state at x is denoted by $p^{\mathrm{eq}}(x)$. In what follows, these objects, $\{x\}$, $\{w_{x\to y}\}$, and $\{p^{\mathrm{eq}}(x)\}$, are treated as given data.

In this section, a graph formulation of master equations is shown in terms of objects developed in Section 2. Main claims of this paper and their consequences are then provided.

3.1 Graph formulation

Introduce a graph $G = (V, E)$ associated with the given data $\{x\}$ and $\{w_{x\to y}\}$ so that

- $x \in V$
- $w(e) = w_{x\to y}$ for $e \in E$ such that $\mathrm{t}(e) = y$ and $\mathrm{o}(e) = x$
- $\overline{e} \in E$ for any $e \in E$. Also, if $w(\overline{e}) = w_{y\to x}$ does not exist, then let w be such that $w(\overline{e}) = 0$.

Then, regard p_t and w as follows.

- $p_t \in \Lambda^0(G)$ so that $p_t(x) \in \mathbb{R}$ for any $x \in V$.
- $w \in C^1(G)$ so that $w(e) \in \mathbb{R}$ for any $e \in E$.

The master equations (10) can be written in terms of these graph terminologies as

$$\frac{\mathrm{d}}{\mathrm{d}t} p_t(x) = \sum_{e \in E_x} [\,-\,p_t(\mathrm{o}(e))\, w(e) + p_t(\mathrm{t}(e))\, w(\,\overline{e}\,)\,]\,. \tag{11}$$

An example of this set of the procedures is given below.

Example 3.1. Consider the set of master equations whose total number of states is 2,

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t(x_1) = -w_{1\to 2}\,p_t(x_1), \qquad \frac{\mathrm{d}}{\mathrm{d}t}p_t(x_2) = w_{1\to 2}\,p_t(x_1),$$

where $w_{1\to 2}$ is a positive constant. This set of equations can be written in terms of the graph

$$\begin{tikzcd} \underset{x_1}{\bullet} \arrow[r, bend left, "e'"] & \underset{x_2}{\bullet} \arrow[l, bend left, "e''"] \end{tikzcd}, \qquad \text{where} \quad w(e') = w_{1\to 2}, \quad \text{and} \quad w(e'') = 0.$$

A consistency between this graph expression and the given set of master equations is verified as follows. Since $\{e'\} = E_1$,$\{e''\} = E_2$, $x_1 = \mathrm{o}(e') = \mathrm{t}(e'')$, $x_2 = \mathrm{t}(e') = \mathrm{o}(e'')$, and $\overline{e''} = e'$, (11) yields

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t(x_1) = \big[-p_t(\mathrm{o}(e'))\,w(e') + p_t(\mathrm{t}(e'))\,w(\,\overline{e'}\,)\big] = -p_t(x_1)w_{1\to 2},$$

and

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t(x_2) = \big[-p_t(\mathrm{o}(e''))\,w(e'') + p_t(\mathrm{t}(e''))\,w(\,\overline{e''}\,)\big] = p_t(x_1)w_{1\to 2}.$$

In what follows, master equations are rewritten. To this end, one defines $J_t \in C^1(G)$ and $I_t \in \Lambda^1(G)$ so that

$$\begin{aligned} J_t(e) &:= -p_t(\,\mathrm{o}(e)\,)\,w(e), \\ I_t(e) &:= J_t(e) - J_t(\,\overline{e}\,). \end{aligned}$$

One verifies that $J_t(\overline{e}) = -J_t(e)$, and that $I(e)$ is the summand in the right hand side of (11),

$$I_t(e) = J_t(e) - J_t(\,\overline{e}\,) = -p_t(\,\mathrm{o}(e)\,)\,w(e) + p_t(\,\mathrm{o}(\overline{e})\,)\,w(\,\overline{e}\,) = -p_t(\,\mathrm{o}(e)\,)\,w(e) + p_t(\,\mathrm{t}(e)\,)\,w(\,\overline{e}\,),$$

and then,

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t(x) = \sum_{e\in E_x} I_t(e).$$

The physical meaning of the case of $I_t(e) = 0$ for a given $e \in E$ is that the probability flow or current is locally balanced. If the condition $w(\overline{e}) = w(e)$ is satisfied for all $e \in E$, then one has

$$I_t(e) = w(e)\,(\mathrm{d}p_t)(e).$$

To describe some measures, introduce

$$1_V \in \Lambda^0(G), \quad \text{and} \quad 1_E \in S^1(G) \qquad \text{such that} \qquad 1_V(x) = 1 \ \text{ and } 1_E(e) = 1, \quad \forall x \in V,\ \forall e \in E.$$

In terms of these objects, one has the following.

Theorem 3.1. *(Continuity equation for master equations). Choose $m_V \in \Lambda^0(G)$ and $m_E \in S^1(G)$ to be*

$$m_V = 1_V, \qquad \textit{and} \qquad m_E = 1_E. \tag{12}$$

Then (11) is identical to

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t = -\,\mathrm{d}^\dagger I_t. \tag{13}$$

Proof. With the choices m_V and m_E, the co-derivative $\mathrm{d}^\dagger$ defined in (3) reduces to the one such that

$$(\,\mathrm{d}^\dagger\omega\,)(x) = -\sum_{e\in E_x}\omega(e), \qquad \omega \in \Lambda^1(G).$$

From this and (11), one has

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t(x) = \sum_{e\in E_x} I_t(e) = -\,(\mathrm{d}^\dagger I_t)(x),$$

for any $x \in V$. Thus, the desired expression is obtained. $\square$

It is worth mentioning that (13) is written as a form of a continuity equation in continuum mechanics

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t + \mathrm{div}(-I_t) = 0,$$

where $\mathrm{div} : \Lambda^1(G) \to \Lambda^0(G)$ has been defined in (4).

Theorem 3.1 deals with $p_t \in \Lambda^0(G)$. On the other hand, an equality on $\Lambda^1(G)$ associated with the master equations is obtained from (13) as

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d}p_t = -\,\mathrm{d}\mathrm{d}^\dagger I_t = \Delta_E I_t, \tag{14}$$

where Δ_E has been defined in (7).

3.1.1 Expectation values

Much attention is devoted to expectation values with respect to p_t in applications of master equations. To discuss such expectation values, one introduces $\mathcal{O}^0 \in \Lambda^0(G)$ that is to be summed over vertexes at fixed time. In this subsection, $m_V \in \Lambda^0(G)$ and $m_E \in S^1(G)$ are chosen as (12).

The expectation value of $\mathcal{O}^0$ with respect to p_t is denoted by

$$\mathbb{E}_p[\,\mathcal{O}^0\,] := \sum_{x\in V} p_t(x)\,\mathcal{O}^0(x), \tag{15}$$

which is written in terms of the inner product with (12) as

$$\mathbb{E}_p[\,\mathcal{O}^0\,] = \left\langle\, p_t\,,\,\mathcal{O}^0\,\right\rangle_V.$$

From the master equations (13) and Lemma 2.1, the time-development of $\left\langle\,\mathcal{O}^0\,\right\rangle_V := \mathbb{E}_p[\,\mathcal{O}^0\,]$ is described by

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\,\mathcal{O}^0\,\right\rangle_V = -\left\langle\,\mathrm{d}^\dagger I_t\,,\,\mathcal{O}^0\,\right\rangle_V = -\left\langle\, I_t\,,\,\mathrm{d}\mathcal{O}^0\,\right\rangle_E. \tag{16}$$

Remark 3.1. Combining the sum over vertexes at fixed time t,

$$\mathbb{E}_p\,[\,1_V\,] = \langle\, p_t\,,\,1_V\,\rangle_V = \sum_{x\in V} p_t(x),$$

the identity

$$(\mathrm{d}1_V)(e) = 1_V(\mathrm{t}(e)) - 1_V(\mathrm{o}(e)) = 1-1 = 0,$$

and (16), one verifies that the derivative of $\langle\,1_V\,\rangle_V = \mathbb{E}_p\,[\,1_V\,]$ with respect to time vanishes:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}_p\,[\,1_V\,] = \frac{\mathrm{d}}{\mathrm{d}t}\langle\,1_V\,\rangle_V = \langle\,\dot{p}_t\,,\,1_V\,\rangle_V = -\,\langle\, I_t\,,\,\mathrm{d}1_V\,\rangle_V = 0,$$

where $\dot{p}_t$ denotes derivative of p_t with respect to time t, $\dot{p}_t = \mathrm{d}p_t/\mathrm{d}t$.

Remark 3.2. For $\mathcal{O}' = \mathcal{O} + c\,1_V \in \Lambda^0(G)$ with $c \in \mathbb{R}$ being constant, one has

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\,\mathcal{O}'\,\rangle_V = -\,\langle\, I_t\,,\,\mathrm{d}\mathcal{O}'\,\rangle_E = \frac{\mathrm{d}}{\mathrm{d}t}\langle\,\mathcal{O}\,\rangle_V.$$

The inner product for $\mathcal{O}^1_A \in \Lambda^1(G)$ and $\mathcal{O}^1_B \in \Lambda^1(G)$ is $\left\langle\,\mathcal{O}^1_A\,,\,\mathcal{O}^1_B\,\right\rangle_E$. In the case where $\mathcal{O}^1_B = \mathrm{d}\dot{p}_t$ and $\mathcal{O}^1_A$ that does not depend on time t, one uses (14) to obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\,\mathcal{O}^1_A\,,\,\mathrm{d}p_t\,\right\rangle_E = \left\langle\,\mathcal{O}^1_A\,,\,\mathrm{d}\dot{p}_t\,\right\rangle_E = \left\langle\,\mathcal{O}^1_A\,,\,\Delta_E I_t\,\right\rangle_E.$$

3.2 Detailed balance conditions

Let $p^{\,\mathrm{eq}}$ be a probability distribution function so that

$$\sum_x p^{\,\mathrm{eq}}(x) = 1.$$

Impose for any connected states x and y

$$p^{\,\mathrm{eq}}(x)\, w_{\,x\to y} = p^{\,\mathrm{eq}}(y)\, w_{\,y\to x}, \tag{17}$$

which are known as the *detailed balance conditions*. For the stationary solution $p^{\,\mathrm{eq}}(x)$ of the master equations, $\mathrm{d}p^{\,\mathrm{eq}}(x)/\mathrm{d}t = 0$, one has from (10) that

$$\sum_{x'} [\, w_{\,x\to x'} p^{\,\mathrm{eq}}(x) - w_{\,x'\to x}\, p^{\,\mathrm{eq}}(x'\,)\,] = 0. \tag{18}$$

If (17) holds, then (18) is satisfied.

These conditions are written in the graph theoretic language as

$$\sum_{x\in V} p^{\,\mathrm{eq}}(x) = 1,$$

and

$$p^{\,\mathrm{eq}}(\mathrm{o}(e))\, w(e) = p^{\,\mathrm{eq}}(\mathrm{t}(e))\, w(\,\overline{e}\,). \tag{19}$$

The later leads to

$$w(\,\overline{e}\,) = \pi(e)\, w(e), \qquad \text{where} \qquad \pi(e) := \frac{p^{\,\mathrm{eq}}(\mathrm{o}(e))}{p^{\,\mathrm{eq}}(\mathrm{t}(e))} = \frac{1}{\pi(\,\overline{e}\,)}.$$

Thus, $\pi(e) = 1$ for any loop edge $e\in E$, and

$$\pi \in C^{\,1}_{\,\mathrm{R}}(G).$$

Also, the $m_{\,E}\in S^{\,1}(G)$ specified such that

$$m_{\,E}(e) = p^{\,\mathrm{eq}}(\mathrm{o}(e))\, w(e),$$

has the property that $m_{\,E}(e) = m_{\,E}(\,\overline{e}\,) > 0$ due to (19). Thus, this $m_{\,E}\in S^{\,1}(G)$ can be used for a reversible measure defining (2).

The master equations (11) under the detailed balance conditions are written as

$$\frac{\mathrm{d}}{\mathrm{d}t}p(x) = \sum_{e\in E_{\,x}} w(e)\, [\, \pi(e)\, p(\mathrm{t}(e)) - p(\mathrm{o}(e))\,]\,. \tag{20}$$

This can be written in terms of d_π, that is (9) with $\varphi = \pi$, as

$$\frac{\mathrm{d}}{\mathrm{d}t}p(x) = \sum_{e\in E_{\,x}} w(e)\, [\, (\mathrm{d}_\pi\, p)\,(e)\,] = -\sum_{e\in E_{\,x}} w(\,\overline{e}\,)\, [\, (\mathrm{d}_\pi p)(\overline{e})\,]\,. \tag{21}$$

The above equations involve d_π. In (21), there is no loop edge contribution since $\pi(e) = 1$ and $(\mathrm{d}_\pi\, p)(e) = 0$ for any loop edge $e\in E$, (See Remark 2.2). Although there is no self-adjoint operator in (21), there exists a way to express master equations in terms of a Laplacian, which is accomplished by a change of variables.

The following is the main theorem in this paper.

Theorem 3.2. *(Diffusion equations from master equations). Choose the measures $m_V \in \Lambda^0(G)$ and $m_E \in S^1(E)$ to be*

$$m_V(x) = p^{\rm eq}(x), \qquad \text{and} \qquad m_E(e) = w(e)\, p^{\rm eq}(\mathrm{o}(e)), \tag{22}$$

respectively, where $w(e)$ satisfies (19). Then introduce $\psi_t \in \Lambda^0(G)$ such that

$$p_t(x) = p^{\rm eq}(x)\, \psi_t(x), \qquad \forall\, x \in V. \tag{23}$$

This function ψ_t satisfies the diffusion equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\psi_t = \Delta_V\, \psi_t, \tag{24}$$

where Δ_V has been defined in (5).

Proof. Substituting (23) into (20), and using the definition of the Laplacian (5), one can complete the proof. The details are as follows.

From (23) and (20), and $\mathrm{d}p^{\rm eq}(x)/\mathrm{d}t = 0$, one has

$$\begin{aligned} p^{\rm eq}(x)\frac{\mathrm{d}}{\mathrm{d}t}\psi_t(x) &= \sum_{e\in E_x} w(e)\left[\frac{p^{\rm eq}(\mathrm{o}(e))}{p^{\rm eq}(\mathrm{t}(e))}\, p^{\rm eq}(\mathrm{t}(e))\,\psi_t(\mathrm{t}(e)) - p^{\rm eq}(\mathrm{o}(e))\,\psi_t(\mathrm{o}(e))\right] \\ &= \sum_{e\in E_x} w(e)\left[p^{\rm eq}(\mathrm{o}(e))\,\psi_t(\mathrm{t}(e)) - p^{\rm eq}(\mathrm{o}(e))\,\psi_t(\mathrm{o}(e))\right], \end{aligned}$$

from which

$$\frac{\mathrm{d}}{\mathrm{d}t}\psi_t(x) = \frac{1}{p^{\rm eq}(x)}\sum_{e\in E_x} w(e)\, p^{\rm eq}(\mathrm{o}(e))\,\left[\psi_t(\mathrm{t}(e)) - \psi_t(\mathrm{o}(e))\right].$$

Since the action of the Laplacian (6) with (22) on ψ_t is

$$(\Delta_V\, \psi_t)(x) = \frac{1}{p^{\rm eq}(x)}\sum_{e\in E_x} p^{\rm eq}(\mathrm{o}(e))\, w(e)\left[\psi_t(\mathrm{t}(e)) - \psi_t(\mathrm{o}(e))\right], \tag{25}$$

one obtains (24). □

Remark 3.3. The explicit expression (25) reduces further. It follows from $\mathrm{o}(e) = x$ for $e \in E_x$ that

$$(\Delta_V\, \psi_t)(x) = \sum_{e\in E_x} w(e)\left[\psi_t(\mathrm{t}(e)) - \psi_t(\mathrm{o}(e))\right] = \sum_{e\in E_x} w(e)\,(\mathrm{d}\psi_t)(e). \tag{26}$$

Remark 3.4. The conservation law of the sum

$$\sum_{x\in V} p_t(x) = 1, \qquad \forall t \in \mathbb{R}$$

can be shown below. With (24), one can show

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\sum_{x\in V} p_t(x) &= \sum_{x\in V} p^{\rm eq}(x)\left(\frac{\mathrm{d}}{\mathrm{d}t}\psi_t\right)(x) = \sum_{x\in V} p^{\rm eq}(x)\,(\Delta_V\psi_t)\,(x) \\ &= \langle\, \Delta_V\psi_t\,,\, 1_V\,\rangle_V = \langle\, \psi_t\,,\, \Delta_V 1_V\,\rangle_V = 0. \end{aligned} \tag{27}$$

Remark 3.5. Theorem 3.2 and (6) indicate that (24) does not involve any loop edge. This property also holds for the equations written in terms of $p_t(x)$, (20).

The following is an example of how this formulation can be applied to a model studied in nonequilibrium statistical mechanics.

Example 3.2. (Kinetic Ising model without spin-coupling, [21]). Let $\sigma = \pm 1$ be a spin variable, and $p_{\text{Ising}}^{\text{eq}}(\sigma)$ an equilibrium distribution of σ. Consider the master equations

$$\frac{\mathrm{d}}{\mathrm{d}t} p_{t,\text{Ising}}(\sigma) = -w_{\sigma\to-\sigma}\, p_{t,\text{Ising}}(\sigma) + w_{-\sigma\to\sigma}\, p_{t,\text{Ising}}(-\sigma), \qquad \sigma = \pm 1,$$

where the detailed balance condition is satisfied:

$$w_{\sigma\to-\sigma}\, p_{\text{Ising}}^{\text{eq}}(\sigma) = w_{-\sigma\to\sigma}\, p_{\text{Ising}}^{\text{eq}}(-\sigma).$$

This set of master equations can be written in terms of the graph

$$\begin{tikzcd} \underset{\sigma}{\bullet} \arrow[r, bend left, "e'"] & \underset{-\sigma}{\bullet} \arrow[l, bend left, "e''"] \end{tikzcd}, \quad w(e') = w_{\sigma\to-\sigma}, \quad w(e'') = w_{-\sigma\to\sigma}, \quad \{e'\} = E_{\sigma}, \quad \{e''\} = E_{-\sigma}.$$

Introduce $\psi_{t,\text{Ising}}$ such that

$$p_{t,\text{Ising}}(\sigma) = p_{\text{Ising}}^{\text{eq}}(\sigma)\psi_{t,\text{Ising}}(\sigma), \qquad \sigma = \pm 1.$$

With these variables and the detailed balance condition

$$w_{-\sigma\to\sigma} = w_{\sigma\to-\sigma}\frac{p_{\text{Ising}}^{\text{eq}}(\sigma)}{p_{\text{Ising}}^{\text{eq}}(-\sigma)},$$

one has that

$$p_{\text{Ising}}^{\text{eq}}(\sigma)\frac{\mathrm{d}}{\mathrm{d}t}\psi_{t,\text{Ising}}(\sigma) = w_{\sigma\to-\sigma}\left[-p_{\text{Ising}}^{\text{eq}}(\sigma)\psi_{t,\text{Ising}}(\sigma) + \frac{p_{\text{Ising}}^{\text{eq}}(\sigma)}{p_{\text{Ising}}^{\text{eq}}(-\sigma)}p_{\text{Ising}}^{\text{eq}}(-\sigma)\psi_{t,\text{Ising}}(-\sigma)\right],$$

from which

$$\frac{\mathrm{d}}{\mathrm{d}t}\psi_{t,\text{Ising}}(\sigma) = w_{\sigma\to-\sigma}\left[\psi_{t,\text{Ising}}(-\sigma) - \psi_{t,\text{Ising}}(\sigma)\right], \qquad \sigma = \pm 1. \tag{28}$$

This derived set of equations is consistent with (26).

To investigate the long-time behavior of the system

$$\frac{\mathrm{d}}{\mathrm{d}t}\psi_t = \mathcal{F}(\psi_t), \qquad \text{where} \qquad \mathcal{F}(\psi) := \Delta_V\psi, \in \Lambda^0(G) \tag{29}$$

that is (24), the following Lemmas will be used.

Lemma 3.1. *The non-trivial solutions, $\psi^{(0)}(x) \neq 0$, to the equations $(\Delta_V\psi^{(0)})(x) = 0$ for any $x \in V$ are $\psi^{(0)}(x) = \psi_0^{(0)}$, where $\psi_0^{(0)}$ is constant.*

Proof. For general ψ, it follows that

$$\langle \Delta_V\psi, \psi\rangle_V = -\langle \mathrm{d}\psi, \mathrm{d}\psi\rangle_E \le 0.$$

The equality holds only when $\mathrm{d}\psi = 0$. It implies that

$$\Delta_V\psi^{(0)} = 0 \qquad \Longleftrightarrow \qquad \mathrm{d}\psi^{(0)} = 0.$$

Since

$$(\mathrm{d}\psi^{(0)})(e) = \psi^{(0)}(\mathrm{t}(e)) - \psi^{(0)}(\mathrm{o}(e)) = 0, \qquad \forall e \in E,$$

and the assumption that the graph is connected, the solution is $\psi^{(0)}(x) = \psi_0^{(0)}$ with $\psi_0^{(0)}$ being constant. $\square$

Lemma 3.1 states that the steady state $\psi^{(0)}$ for (24), $\mathrm{d}\psi^{(0)}/\mathrm{d}t = 0$, is $\psi^{(0)} = \psi_0^{(0)} 1_V$. In other words, this $\psi_0^{(0)} 1_V$ forms a fixed point set for this system. The following describes the stability for $\psi = \psi_0^{(0)} 1_V$.

Lemma 3.2. *The state $\psi = \psi_0^{(0)} 1_V$ is asymptotically stable for (29).*

Proof. Introduce the dynamical system for $\widetilde{\psi} \in \Lambda^0(G)$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\psi}_t = \widetilde{\mathcal{F}}\left(\widetilde{\psi}_t\right), \qquad \widetilde{\mathcal{F}}\left(\widetilde{\psi}\right) := \Delta_V\left(\widetilde{\psi} + \psi_0^{(0)} 1_V\right) \ \in\ \Lambda^0(G) \tag{30}$$

where $\widetilde{\psi} = \psi_0^{(0)} 1_V$ forms a fixed point set for (29). It follows from Lemma 3.1 that this $\widetilde{\mathcal{F}}(\widetilde{\psi})$ has the properties that

$$\widetilde{\mathcal{F}}\left(\widetilde{\psi}\right) = \mathcal{F}\left(\widetilde{\psi} + \psi_0^{(0)} 1_V\right), \qquad \text{and} \qquad \widetilde{\mathcal{F}}(0) = \mathcal{F}(\phi_0^{(0)} 1_V) = \Delta_V(\psi_0^{(0)} 1_V) = 0_V,$$

where 0_V is the element of $\Lambda^0(G)$ such that $0_V(x) = 0$ for any $x \in V$. The later states that the fixed point set for (30) is expressed by $\widetilde{\psi} = 0_V$.

Then define $\mathcal{L}$ acting on $\Lambda^0(G)$ such that

$$\mathcal{L}\left(\widetilde{\psi}_t\right) = \frac{1}{2}\left\langle \widetilde{\psi}_t, \widetilde{\psi}_t \right\rangle_V.$$

It immediately follows that $\mathcal{L}(\widetilde{\psi}_t) \geq 0$ for any $t \in \mathbb{R}$. In addition, one has that $\mathrm{d}\mathcal{L}(\widetilde{\psi}_t)/\mathrm{d}t \leq 0$ for any $t \in \mathbb{R}$, since

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{L}\left(\widetilde{\psi}_t\right) = \left\langle \dot{\widetilde{\psi}}_t, \widetilde{\psi}_t \right\rangle_V = \left\langle \Delta_V\left(\widetilde{\psi}_t + \psi_0^{(0)} 1_V\right), \widetilde{\psi}_t \right\rangle_V = -\left\langle \mathrm{d}^\dagger \mathrm{d}\,\widetilde{\psi}_t, \widetilde{\psi}_t \right\rangle_V = -\left\langle \mathrm{d}\widetilde{\psi}_t, \mathrm{d}\widetilde{\psi}_t \right\rangle_E \leq 0.$$

From these properties, $\mathcal{L}(\widetilde{\psi}_t)$ is a Lyapunov function. Applying these statements to the Lyapunov stability theorem, one has that $\widetilde{\psi}_t = 0_V$ in the dynamical system (30) is asymptotically stable. This yields that $\psi_0^{(0)} 1_V$ is asymptotically stable for (29). □

Then one has the following.

Corollary 3.1. (Convergence of master equations).

$$\psi_0^{(0)} = 1, \qquad \text{and} \qquad \lim_{t\to\infty} p_t(x) = p^{\mathrm{eq}}(x), \qquad \forall x \in V.$$

Proof. It follows from Lemmas 3.1 and 3.2 that

$$\lim_{t\to\infty} p_t(x) = p^{\mathrm{eq}}(x) \lim_{t\to\infty} \psi_t(x) = p^{\mathrm{eq}}(x)\, \psi_0^{(0)}.$$

This and the normalization condition $\sum_{x\in V} p^{\mathrm{eq}}(x) = 1$ lead to

$$\sum_{x\in V} \lim_{t\to\infty} p_t(x) = \psi_0^{(0)} \sum_{x\in V} p^{\mathrm{eq}}(x) = \psi_0^{(0)}.$$

On the other hand, the conservation law (27) holds. Thus, the left hand side of the equation above is unity:

$$\psi_0^{(0)} = 1.$$

Therefore,

$$\lim_{t\to\infty} p_t(x) = p^{\mathrm{eq}}(x).$$

□

It has been shown that discrete diffusion equations are derived from master equations under the conditions that the detailed balance conditions are satisfied. Its converse statement under these conditions also holds.

Proposition 3.1. *(From diffusion equations to master equations). Let $w \in C^1(G)$ be a transition matrix, and $p^{\rm eq} \in \Lambda^0(G)$ an equilibrium distribution function. Assume that the detailed balance conditions (19) hold. Choose $m_V \in \Lambda^0(G)$ and $m_E \in S^1(G)$ so that $m_V(x) = p^{\rm eq}(x)$ and $m_E(e) = w(e)p^{\rm eq}({\rm o}(e))$ as in (22). Then, the diffusion equations (24) yield the master equations.*

Proof. Introduce the inner products (1) and (2). Also, introduce $p_t \in \Lambda^0(G)$ that depends on $t \in \mathbb{R}$ such that $p_t(x) = p^{\rm eq}(x)\psi_t(x)$. Then multiplying both sides of the diffusion equations by $p^{\rm eq}(x)$, one has

$$p^{\rm eq}(x)\frac{\rm d}{{\rm d}t}\psi_t(x) = \sum_{e\in E_x} p^{\rm eq}(\,{\rm o}(e)\,)w(e)\,\left[\,\psi_t(\,{\rm t}(e)\,) - \psi_t(\,{\rm o}(e)\,)\,\right], \qquad \forall\, x \in V.$$

With (19), the equations above can be written as

$$p^{\rm eq}(x)\frac{\rm d}{{\rm d}t}\psi_t(x) = \sum_{e\in E_x} \left[\,p^{\rm eq}(\,{\rm t}(e)\,)w(\overline{e})\psi_t(\,{\rm t}(e)\,) - p^{\rm eq}(\,{\rm o}(e)\,)w(e)\psi_t(\,{\rm o}(e)\,)\,\right].$$

This can also be written in terms of $p_t(x) = p^{\rm eq}(x)\psi_t(x)$ as

$$\frac{\rm d}{{\rm d}t}p_t(x) = \sum_{e\in E_x} \left[\,-p_t(\,{\rm o}(e)\,)w(e) + p_t(\,{\rm t}(e)\,)w(\overline{e})\,\right].$$

□

So far, basic statements of the system have been given. These include asymptotic behaviour of the diffusion equations, Lemma 3.2. Furthermore, if the eigenvalues and eigenfunctions of the Laplacian Δ_V are known, then an explicit solution for the initial value problem of the diffusion equations (24) can be obtained. Since the diffusion equations are linear, it is enough to consider the case where the solution space is a linear space of $\Lambda^0(G)$. Also, from Theorem 3.2, one has the equation on $\Lambda^1(G)$ as

$$\frac{\rm d}{{\rm d}t}{\rm d}\psi_t = \Delta_E\,{\rm d}\psi_t. \tag{31}$$

Since (31) is linear, eigenvalues and eigenfunctions of Δ_E play roles. Thus in what follows $\Lambda^0(G)$ and $\Lambda^1(G)$ denote linear spaces. Then how to construct an explicit solution to the diffusion equations is argued below.

Let A be a linear operator acting on a finite-dimensional vector space $\mathcal{U}$, and λ_A a non-zero number satisfying

$$A\,\phi = \lambda_A\phi,$$

where $\phi \in \mathcal{U}$ is not 0. Then λ_A and ϕ are referred to as an *non-zero eigenvalue* and its associated or corresponding *eigenfunction*, respectively. For a self-adjoint operator A, it is known that all the eigenvalues are real, $\lambda_A \in \mathbb{R}$. In addition, if all the non-zero eigenvalues are positive, then A is referred to as a *positive operator*. If $A\,\phi = 0$ with non-zero ϕ, then ϕ is referred to as the *eigenfunction* associated with the *zero-eigenvalue*.

Since the Laplacian Δ_V is a linear operator acting on $\Lambda^0(G)$ and is self-adjoint as shown in Lemma 2.2, one can discuss if $-\Delta_V$ is a positive operator or not. Then one has the following.

Lemma 3.3. *The negative of the Laplacian acting on $\Lambda^0(G)$, $-\Delta_V$, is a positive operator.*

Proof. Let $\widetilde{\lambda}_V^{(s)}$ be a non-zero eigenvalue labeled by s, and $\widetilde{\phi}_V^{(s)}$ an associated eigenfunction of $-\Delta_V$ so that $-\Delta_V\widetilde{\phi}_V^{(s)} = \widetilde{\lambda}_V^{(s)}\widetilde{\phi}_V^{(s)}$. Then it follows that

$$\widetilde{\lambda}_V^{(s)}\left\langle\,\widetilde{\phi}_V^{(s)}\,,\,\widetilde{\phi}_V^{(s)}\,\right\rangle_V = \left\langle\,\widetilde{\lambda}_V^{(s)}\widetilde{\phi}_V^{(s)}\,,\,\widetilde{\phi}_V^{(s)}\,\right\rangle_V = \left\langle\,-\Delta_V\widetilde{\phi}_V^{(s)}\,,\,\widetilde{\phi}_V^{(s)}\,\right\rangle_V = \left\langle\,{\rm d}\widetilde{\phi}_V^{(s)}\,,\,{\rm d}\widetilde{\phi}_V^{(s)}\,\right\rangle_E > 0,$$

for all $\widetilde{\phi}_V^{(s)} \neq 0_V$. Applying $\left\langle\,\widetilde{\phi}_V^{(s)}\,,\,\widetilde{\phi}_V^{(s)}\,\right\rangle_V > 0$ to the obtained inequality $\widetilde{\lambda}_V^{(s)}\left\langle\,\widetilde{\phi}_V^{(s)}\,,\,\widetilde{\phi}_V^{(s)}\,\right\rangle_V > 0$, one concludes that $\widetilde{\lambda}_V^{(s)} > 0$. □

Remark 3.6. Repeating similar arguments in the proof of Lemma 3.3, one has that all the eigenvalues of Δ_V are negative or zero,

$$\Delta_V \phi_V^{(s)} = \lambda_V^{(s)} \phi_V^{(s)}, \qquad \lambda_V^{(s)} \leq 0,$$

where $\phi_V^{(s)} \in \Lambda^0(G)$ is the eigenfunction associated with $\lambda_V^{(s)}$. In particular, $\phi_V^{(0)}$ denotes the eigenfunction associated with the zero-eigenvalue $\lambda_V^{(0)} = 0$.

Moreover, given a self-adjoint operator A acting on a linear space $\mathcal{U}$, it is known that an element of $\mathcal{U}$ has an orthonormal decomposition. By applying this, one has the decomposition

$$\psi_t = \sum_s a^{(s)}(t)\phi_V^{(s)} = \sum_{s\in\mathcal{N}_V} a^{(s)}(t)\phi_V^{(s)} + a^{(0)}(t)\phi_V^{(0)}, \qquad \text{with} \qquad \left\langle \phi_V^{(s)}, \phi_V^{(s')} \right\rangle_V = \delta^{ss'}, \tag{32}$$

where s denotes a label for eigenfunction, $\mathcal{N}_V$ the totality of labels for non-zero eigenfunctions, $a^{(s)}$ the real-valued function labeled by s of t, and $\delta^{ss'}$ the Kronecker delta, giving unity if $s = s'$ and zero otherwise.

The normalized eigenfunction associated with the zero-eigenvalue $\phi_V^{(0)}$ is obtained as follows.

Lemma 3.4. *The normalized zero-eigenfunction is* $\phi_V^{(0)} = 1_V$*:*

$$\Delta_V \phi_V^{(0)} = 0, \qquad \textit{and} \qquad \left\langle \phi_V^{(0)}, \phi_V^{(0)} \right\rangle_V = 1.$$

Proof. It follows that $\Delta_V 1_V = -\mathrm{d}^\dagger \mathrm{d} 1_V = 0$. Then, the normalization condition is verified as

$$\left\langle \phi_V^{(0)}, \phi_V^{(0)} \right\rangle_V = \langle 1_V, 1_V \rangle_V = \sum_{x\in V} p^{\mathrm{eq}}(x) = 1.$$

□

With this Lemma, the solution for ψ_t is obtained as follows.

Proposition 3.2. *(Spectrum decomposition). Let* $\{\lambda_V^{(s)}\}$ *be the totality of non-zero eigenvalues of* Δ_V*, and* $\{\phi_V^{(s)}\}$ *that of the corresponding eigenfunctions. Then*

$$\psi_t = \sum_{s\in\mathcal{N}_V} a^{(s)}(0)\, \mathrm{e}^{-|\lambda_V^{(s)}|t} \phi_V^{(s)} + 1_V, \tag{33}$$

is a solution to the diffusion equations (24) derived from the master equations.

Proof. From (32), it follows that

$$\left\langle \frac{\mathrm{d}}{\mathrm{d}t}\psi_t, \phi_V^{(s)} \right\rangle_V = \frac{\mathrm{d}a^{(s)}}{\mathrm{d}t}, \quad \text{and} \quad \left\langle \Delta_V \psi_t, \phi_V^{(s)} \right\rangle_V = \lambda_V^{(s)} a^{(s)}.$$

With these equations and (24), one has

$$\left\langle \frac{\mathrm{d}}{\mathrm{d}t}\psi_t - \Delta_V \psi_t, \phi_V^{(s)} \right\rangle_V = \frac{\mathrm{d}a^{(s)}}{\mathrm{d}t} - \lambda_V^{(s)} a^{(s)} = 0,$$

from which $a^{(s)}(t) = a^{(s)}(0)\exp(\lambda_V^{(s)} t)$. Taking into account Remark 3.6, one can write $\lambda_V^{(s)} = -|\lambda_V^{(s)}| \leq 0$. Combining these arguments, one has

$$\psi_t = \sum_{s\in\mathcal{N}_V} a^{(s)}(0)\, \mathrm{e}^{-|\lambda_V^{(s)}|t} \phi_V^{(s)} + a^{(0)}(0) 1_V.$$

Finally it follows from Corollary 3.1 that $a^{(0)}(0)$ above is unity. This completes the proof. □

Notice that

$$\frac{\mathrm{d}a^{(s)}}{\mathrm{d}t} = \lambda_V^{(s)} a^{(s)}, \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}t}\psi_t = \sum_s \frac{\mathrm{d}a^{(s)}(t)}{\mathrm{d}t}\phi_V^{(s)} = \sum_s \lambda_V^{(s)} a^{(s)}(t)\phi_V^{(s)} = \sum_{s\in\mathcal{N}_V} \lambda_V^{(s)} a^{(s)}(t)\phi_V^{(s)}. \tag{34}$$

An example of the spectrum decomposition of ψ_t is given below.

Example 3.3. (Eigen system for kinetic Ising model without spin-coupling). Consider Example 3.2. The matrix form of (28) is immediately obtained as

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} \psi_{t,\mathrm{Ising}}(-1) \\ \psi_{t,\mathrm{Ising}}(+1) \end{pmatrix} = M_{\mathrm{Ising}} \begin{pmatrix} \psi_{t,\mathrm{Ising}}(-1) \\ \psi_{t,\mathrm{Ising}}(+1) \end{pmatrix}, \qquad \text{where} \qquad M_{\mathrm{Ising}} := \begin{pmatrix} -w_{-1\to+1} & w_{-1\to+1} \\ w_{+1\to-1} & -w_{+1\to-1} \end{pmatrix}.$$

Two eigenvalues of M_{Ising} are obtained as

$$\lambda_{\mathrm{Ising}}^{(0)} = 0, \qquad \text{and} \qquad \lambda_{\mathrm{Ising}}^{(1)} = -\left(w_{+1\to-1} + w_{-1\to+1} \right).$$

Their eigenfunctions are

$$\phi_{\mathrm{Ising}}^{(0)} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad \text{and} \qquad \phi_{\mathrm{Ising}}^{(1)} = c_{\mathrm{Ising}}^{(1)} \begin{pmatrix} w_{-1\to+1} \\ -w_{+1\to-1} \end{pmatrix},$$

where

$$c_{\mathrm{Ising}}^{(1)} := \left[(w_{-1\to+1})^2 p_{\mathrm{Ising}}^{\mathrm{eq}}(-1) + (w_{+1\to-1})^2 p_{\mathrm{Ising}}^{\mathrm{eq}}(1) \right]^{-1/2}.$$

The orthonormality is verified as

$$\begin{aligned}
\left\langle \phi_{\mathrm{Ising}}^{(0)}, \phi_{\mathrm{Ising}}^{(0)} \right\rangle_V &= \sum_{\sigma=\pm1} p_{\mathrm{Ising}}^{\mathrm{eq}}(\sigma) = 1, \\
\left\langle \phi_{\mathrm{Ising}}^{(0)}, \phi_{\mathrm{Ising}}^{(1)} \right\rangle_V &= \sum_{\sigma=\pm1} \phi_{\mathrm{Ising}}^{(0)}(\sigma)\,\phi_{\mathrm{Ising}}^{(1)}(\sigma)\,p_{\mathrm{Ising}}^{\mathrm{eq}}(\sigma) \\
&= c_{\mathrm{Ising}}^{(1)} \left[w_{-1\to+1}\, p_{\mathrm{Ising}}^{\mathrm{eq}}(-1) - w_{+1\to-1}\, p_{\mathrm{Ising}}^{\mathrm{eq}}(1) \right] = 0, \\
\left\langle \phi_{\mathrm{Ising}}^{(1)}, \phi_{\mathrm{Ising}}^{(1)} \right\rangle_V &= \sum_{\sigma=\pm1} \phi_{\mathrm{Ising}}^{(1)}(\sigma)\,\phi_{\mathrm{Ising}}^{(1)}(\sigma)\,p_{\mathrm{Ising}}^{\mathrm{eq}}(\sigma) \\
&= c_{\mathrm{Ising}}^{(1)\,2} \left[(w_{-1\to+1})^2 p_{\mathrm{Ising}}^{\mathrm{eq}}(-1) + (w_{+1\to-1})^2 p_{\mathrm{Ising}}^{\mathrm{eq}}(1) \right] = 1,
\end{aligned}$$

where the normalization of $p_{\mathrm{Ising}}^{\mathrm{eq}}$ and the detailed balance condition have been used. In Ref. [21], the equilibrium distribution $p_{\mathrm{Ising}}^{\mathrm{eq}}$ and $w_{\sigma\to-\sigma}$ were chosen so that they depend on parameters $\theta \in \mathbb{R}$ and $\gamma \in \mathbb{R}_+$ as

$$p_{\mathrm{Ising}}^{\mathrm{eq}}(\sigma;\theta) = \frac{\exp(\theta\sigma)}{2\cosh\theta}, \qquad \text{and} \qquad w_{\sigma\to-\sigma}(\theta,\gamma) = \frac{\gamma}{2}\left(1 - \sigma\tanh\theta\right).$$

The physical meaning of θ is a quantity that is proportional to the inverse temperature, and that of γ is a characteristic relaxation time. The non-zero eigenvalue and its corresponding eigenfunction for this case are

$$\lambda_{\mathrm{Ising}}^{(1)} = -\gamma, \qquad \text{and} \qquad \phi_{\mathrm{Ising}}^{(1)} = c_{\mathrm{Ising}}^{(1)}(\theta,\gamma)\,\frac{\gamma}{2}\begin{pmatrix} 1+\tanh\theta \\ -1+\tanh\theta \end{pmatrix}.$$

So far eigenvalues and eigenfunctions of Δ_V have been investigated. There exists a link between eigenvalues of Δ_V and those of Δ_E. To state this, notations are introduced as follows. Let $\mathcal{N}_E$ be the totality of labels for non-zero eigenfunctions of Δ_E, $\mathrm{Spec}'\Delta_V$ and $\mathrm{Spec}'\Delta_E$ the totalities of eigenvalues in $\mathcal{N}_V$ and $\mathcal{N}_E$, respectively. Also, let

$$\ker\Delta_V := \{\, \phi_V \in \Lambda^0(G) \,|\, \Delta_V\,\phi_V = 0 \,\}, \qquad \ker\Delta_E := \{\, \phi_E \in \Lambda^1(G) \,|\, \Delta_E\,\phi_E = 0 \,\},$$

$$\ker\mathrm{d} := \{\, \phi_V \in \Lambda^0(G) \,|\, \mathrm{d}\phi_V = 0 \,\}, \qquad \text{and} \qquad \ker\mathrm{d}^\dagger := \{\, \phi_E \in \Lambda^1(G) \,|\, \mathrm{d}^\dagger\phi_E = 0 \,\}.$$

First, one has the following.

Lemma 3.5.

$$\ker \mathrm{d} = \ker \Delta_V .$$

Proof. This proof can be split into two steps. First, $\ker \mathrm{d} \subseteq \ker \Delta_V$ is shown. Then, $\ker \Delta_V \subseteq \ker \mathrm{d}$ is shown. From these, one completes the proof.

(Proof of $\ker \mathrm{d} \subseteq \ker \Delta_V$): Take $\phi_V^{(0)} \in \ker \mathrm{d}$, i.e., $\mathrm{d}\phi_V^{(0)} = 0$. Then it follows that

$$\Delta_V \phi_V^{(0)} = -\mathrm{d}^\dagger \mathrm{d}\phi_V^{(0)} = 0,$$

from which $\ker \mathrm{d} \subseteq \ker \Delta_V$.

(Proof of $\ker \Delta_V \subseteq \ker \mathrm{d}$): Take $\phi_V^{(0)} \in \ker \Delta_V$, i.e., $\Delta_V \phi_V^{(0)} = 0$. Then it follows from

$$0 = \left\langle \Delta_V \phi_V^{(0)}, \phi_V^{(0)} \right\rangle_V = -\left\langle \mathrm{d}^\dagger \mathrm{d}\, \phi_V^{(0)}, \phi_V^{(0)} \right\rangle_V = -\left\langle \mathrm{d}\, \phi_V^{(0)}, \mathrm{d}\phi_V^{(0)} \right\rangle_E \le 0$$

that $\mathrm{d}\phi_V^{(0)} = 0$. Thus, $\ker \Delta_V \subseteq \ker \mathrm{d}$.

These two steps yield $\ker \mathrm{d} = \ker \Delta_V$. □

Similar to Lemma 3.5, one has the following.

Lemma 3.6.

$$\ker \mathrm{d}^\dagger = \ker \Delta_E .$$

Proof. A way to prove this is analogous to that of Lemma 3.5. □

Then one has the following property, referred to as *supersymmetry* [17].

Theorem 3.3. *(Supersymmetry of Laplacians).*

$$\mathrm{Spec}'\Delta_V = \mathrm{Spec}'\Delta_E .$$

Proof. This proof can be split into two steps. First, $\mathrm{Spec}'\Delta_V \subseteq \mathrm{Spec}'\Delta_E$ is shown. Then, $\mathrm{Spec}'\Delta_E \subseteq \mathrm{Spec}'\Delta_V$ is shown. From these, one completes the proof.

(Proof of $\mathrm{Spec}'\Delta_V \subseteq \mathrm{Spec}'\Delta_E$): Assume that $\Delta_V \phi_V^{(s)} = \lambda_V^{(s)} \phi_V^{(s)}$, $(s \in \mathcal{N}_V)$. Then, $\{\lambda_V^{(s)}\} = \mathrm{Spec}'\Delta_V$. From this assumption and Lemma 3.5, it follows that $\mathrm{d}\,\phi_V^{(s)} \neq 0$. Since

$$\Delta_E (\mathrm{d}\,\phi_V^{(s)}) = \mathrm{d}\,\Delta_V \phi_V^{(s)} = \lambda_V^{(s)} (\mathrm{d}\,\phi_V^{(s)}), \qquad \text{with} \quad \mathrm{d}\,\phi_V^{(s)} \neq 0,$$

one has that $\lambda_V^{(s)} \in \mathrm{Spec}'\Delta_E$ for each $s \in \mathcal{N}_V$. This yields that $\mathrm{Spec}'\Delta_V \subseteq \mathrm{Spec}'\Delta_E$.

(Proof of $\mathrm{Spec}'\Delta_E \subseteq \mathrm{Spec}'\Delta_V$): Assume that $\Delta_E \phi_E^{(s)} = \lambda_E^{(s)} \phi_E^{(s)}$, $(s \in \mathcal{N}_E)$. Then, $\{\lambda_E^{(s)}\} = \mathrm{Spec}'\Delta_E$. From this assumption and Lemma 3.6, it follows that $\mathrm{d}^\dagger \phi_E^{(s)} \neq 0$. Since

$$\Delta_V (\mathrm{d}^\dagger \phi_E^{(s)}) = \mathrm{d}^\dagger \Delta_E \phi_E^{(s)} = \lambda_E^{(s)} (\mathrm{d}^\dagger \phi_E^{(s)}), \qquad \text{with} \quad \mathrm{d}^\dagger \phi_E^{(s)} \neq 0,$$

one has that $\lambda_E^{(s)} \in \mathrm{Spec}'\Delta_V$ for each $s \in \mathcal{N}_E$. This yields that $\mathrm{Spec}'\Delta_E \subseteq \mathrm{Spec}'\Delta_V$.

These two steps yield the desired equality. □

Due to Theorem 3.3, non-zero eigenvalues $\lambda_V^{(s)}, (s \in \mathcal{N}_V)$ and $\lambda_E^{(s)}, (s \in \mathcal{N}_E)$ are not distinguished. In what follows they are denoted $\lambda^{(s)}$.

3.2.1 Expectation values

For the case where the detailed balance conditions are not imposed, how expectation values are described has been argued in Section 3.1.1. It is also of interest to formulate how expectation values are described for the case that the detailed balance conditions are satisfied. To establish such a formulation, a relation between an expectation value and the inner product on $\Lambda^0(G)$ is shown first. Second, inequalities for sums involving ψ_t over vertexes are shown. Finally some identities for such sums are shown.

The expectation value of $\mathcal{O}^0 \in \Lambda^0(G)$ is denoted by $\mathbb{E}_p[\,\mathcal{O}^0\,]$ as in (15). This expectation value is written in terms of the inner product with (22) as

$$\mathbb{E}_p[\,\mathcal{O}^0\,] = \sum_{x\in V} \mathcal{O}^0(x)\,p_t(x) = \langle\,\mathcal{O}^0\,,\,\psi_t\,\rangle_V\,,$$

where $p_t(x) = p^{\mathrm{eq}}(x)\psi_t(x)$ in (23) has been used. The time-development of $\left\langle\,\mathcal{O}^0\,\right\rangle_V := \mathbb{E}_p[\,\mathcal{O}^0\,]$ for $\mathcal{O}^0 \in \Lambda^0(G)$ is then described by

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\,\mathcal{O}^0\,\right\rangle_V = \left\langle\,\mathcal{O}^0\,,\,\dot{\psi}_t\,\right\rangle_V = \left\langle\,\mathcal{O}^0\,,\,\Delta_V\psi_t\,\right\rangle_V = \left\langle\,\Delta_V\,\mathcal{O}^0\,,\,\psi_t\,\right\rangle_V.$$

Entropy defined by

$$H[p_t] := \mathbb{E}_p[\,-\ln\,p_t\,] = \langle\,-\ln p_t\,,\,\psi_t\,\rangle_V\,,$$

plays a central role in information theory. It is well-known that

$$\frac{\mathrm{d}}{\mathrm{d}t}H[p_t] > 0.$$

It is then of interest to explore similar inequalities for sums involving ψ_t over vertexes. Define $S_t \in \Lambda^0(G)$ to be

$$S_t := -\ln\psi_t.$$

Then one has the following.

Proposition 3.3. *(Inequality for S_t).*

$$\langle\,S_t\,,\,1_V\,\rangle_V \geq 0, \qquad \forall t\in\mathbb{R}.$$

Proof. By applying the inequality

$$\exp(-\,c) \geq 1 - c, \qquad c\in\mathbb{R},$$

to the equality

$$1 = \sum_{x\in V} p_t(x) = \sum_{x\in V} p^{\mathrm{eq}}(x)\exp(-S_t(x)) = \langle\,\exp(-S_t)\,,\,1_V\,\rangle_V\,,$$

one has

$$\langle\,S_t\,,\,1_V\,\rangle_V \geq 0.$$

□

Also one defines

$$H[\psi_t] := \mathbb{E}_p[\,S_t\,] = \mathbb{E}_p[\,-\ln\,\psi_t\,] = \langle\,S_t\,,\,\psi_t\,\rangle_V\,. \tag{35}$$

Then one has the following.

Proposition 3.4. *(Inequality for time-derivative of $H[\psi_t]$).*

$$\frac{\mathrm{d}}{\mathrm{d}t}H[\psi_t] \geq \sum_s |\,\lambda^{(s)}\,|\,(\,a^{(s)}(t)\,)^2 > 0.$$

Proof. Substituting the inequality

$$1+\ln\psi_t(x)\leq\psi_t(x),\qquad\forall x\in V$$

and (24) into (35), one has

$$\begin{aligned}-\frac{\mathrm{d}}{\mathrm{d}t}H[\psi_t] &= \sum_{x\in V}p^{\mathrm{eq}}(x)\,(1+\ln\psi_t(x))\,\dot{\psi}_t(x)\\ &\leq \sum_{x\in V}p^{\mathrm{eq}}(x)\,\psi_t(x)\,\dot{\psi}_t(x)=\langle\,\psi_t\,,\,\Delta_V\psi_t\,\rangle_V\,.\end{aligned}$$

With this and (32), one has

$$-\frac{\mathrm{d}}{\mathrm{d}t}H[\psi_t]\leq\sum_s\sum_{s'}\lambda^{(s')}\,a^{(s)}(t)a^{(s')}(t)\,\left\langle\,\phi_V^{(s)}\,,\,\phi_V^{(s')}\,\right\rangle_V=\sum_s\lambda^{(s)}\,(\,a^{(s)}(t)\,)^2,$$

from which

$$\frac{\mathrm{d}}{\mathrm{d}t}H[\psi_t]\geq-\sum_s\lambda^{(s)}\,(\,a^{(s)}(t)\,)^2=-\sum_{s\in\mathcal{N}_V}\lambda^{(s)}\,(\,a^{(s)}(t)\,)^2.$$

Since $\lambda^{(s)}=-|\lambda^{(s)}|<0$ for $s\in\mathcal{N}_V$ (See Remark 3.6), one has that

$$\frac{\mathrm{d}}{\mathrm{d}t}H[\psi_t]\geq\sum_{s\in\mathcal{N}_V}|\,\lambda^{(s)}\,|\,(\,a^{(s)}(t)\,)^2>0.$$

□

There exist closed dynamical systems for expectation variables $\mathbb{E}_p[\,\mathcal{O}^0\,]$ with some appropriately chosen $\mathcal{O}^0$. Such systems are given as follows.

Proposition 3.5. *(Dynamical systems for expectation variables 1). Consider the case where*

$$\mathcal{O}^0=\phi_V^{(s)},\qquad s\in\mathcal{N}_V.$$

Then,

$$\left\langle\,\phi_V^{(s)}\,\right\rangle_V(t):=\mathbb{E}_p[\,\phi_V^{(s)}\,],$$

follows the dynamical system

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\,\phi_V^{(s)}\,\right\rangle_V=\lambda^{(s)}\left\langle\,\phi_V^{(s)}\,\right\rangle_V.\tag{36}$$

Proof. It follows from (34) and (32) that

$$\left\langle\,\phi_V^{(s)}\,\right\rangle_V=\left\langle\,\phi_V^{(s)}\,,\,\psi_t\,\right\rangle_V=a^{(s)}(t).$$

From this and (34), one has the closed form

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\,\phi_V^{(s)}\,\right\rangle_V=\dot{a}^{(s)}(t)=\lambda^{(s)}\left\langle\,\phi_V^{(s)}\,\right\rangle_V.$$

□

In the context of dynamical systems theory in information geometry, the dynamical system

$$\frac{\mathrm{d}}{\mathrm{d}t}\eta_j=-\{\,\eta_j-\eta_j'\,\},\tag{37}$$

has been studied in [22, 23, 24, 25]. The variables $\{\eta_j\}$ in (37) denote the expectation values for an exponential family. Notice that the system (37) with $\{\eta'_j\}=0$ is obtained by replacing $\lambda^{(s)}$ with -1 in (36).

Similar to this proposition, one can have closed equations on $\Lambda^1(G)$ as follows. Define for $\mathcal{O}^1\in\Lambda^1(G)$,

$$\langle\,\mathcal{O}^1\,\rangle_E := \langle\,\mathcal{O}^1\,,\,\mathrm{d}\psi_t\,\rangle_E\,.$$

Differentiating this equation with respect to t and using (31), one has

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\,\mathcal{O}^1\,\rangle_E = \langle\,\mathcal{O}^1\,,\,\Delta_E\,\mathrm{d}\psi_t\,\rangle_E = \langle\,\Delta_E\,\mathcal{O}^1\,,\,\mathrm{d}\psi_t\,\rangle_E\,.$$

Then one has the following.

Proposition 3.6. *(Dynamical systems for expectation variables 2). Consider the case where*

$$\mathcal{O}^1 = \mathrm{d}\phi_V^{(s)},\qquad s\in\mathcal{N}_E$$

Then, one has the closed dynamical system

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\,\mathrm{d}\phi_V^{(s)}\,\right\rangle_E = \lambda^{(s)}\left\langle\,\mathrm{d}\phi_V^{(s)}\,\right\rangle_E\,.$$

Proof. It follows from that

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\,\mathrm{d}\phi_V^{(s)}\,\right\rangle_E = \left\langle\,\Delta_E\,\mathrm{d}\phi_V^{(s)}\,,\,\mathrm{d}\psi_t\,\right\rangle_E = \left\langle\,\lambda^{(s)}\mathrm{d}\phi_V^{(s)}\,,\,\mathrm{d}\psi_t\,\right\rangle_E = \lambda^{(s)}\left\langle\,\mathrm{d}\phi_V^{(s)}\,\right\rangle_E\,.$$

□

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