A Hamiltonian-Entropy Production Connection in the Skew-symmetric Part of a Stochastic Dynamics

Hong Qian

Department of Applied Mathematics
University of Washington, Seattle
WA 98195-2420, U.S.A.

May 1, 2014

Abstract

The infinitesimal transition probability operator for a continuous-time discrete-state Markov process, \( Q \), can be decomposed into a symmetric and a skew-symmetric parts. As recently shown for the case of diffusion processes, while the symmetric part corresponding to a gradient system stands for a reversible Markov process, the skew-symmetric part, \( \frac{d}{dt}u(t) = Au \), is mathematically equivalent to a linear Hamiltonian dynamics with Hamiltonian \( H = \frac{1}{2} u^T (A^T A) u \). It can also be transformed into a Schrödinger-like equation \( \frac{d}{dt}u = iH u \) where the “Hamiltonian” operator \( H = -iA \) is Hermitian. In fact, these two representations of a skew-symmetric dynamics emerge naturally through singular-value and eigen-value decompositions, respectively. The stationary probability of the Markov process can be expressed as \( \|u_s\|^2 \). The motion can be viewed as “harmonic” since \( \frac{d}{dt} \|u(t) - \bar{c}\|^2 = 0 \) where \( \bar{c} = (c, c, \cdots, c) \) with \( c \) being a constant. More interestingly, we discover that

\[
\text{Tr}(A^T A) = \sum_{j,\ell=1}^{n} \frac{(q_{j\ell}\pi_\ell - q_{\ell j}\pi_j)^2}{\pi_j\pi_\ell},
\]

whose right-hand-side is intimately related to the entropy production rate of the Markov process in a nonequilibrium steady state with stationary distribution \( \{\pi_j\} \). The physical implication of this intriguing connection between conservative Hamiltonian dynamics and dissipative entropy production remains to be further explored.

1 Introduction

Linear operator theory and functional analysis became the central piece of quantum mechanics in the work of Dirac and von Neumann \([1, 2, 3]\). In 1930s, Koopman, Birkhoff,
von Neumann, and others have also developed a classical dynamical systems theory, including several ergodic theorems, based on linear transformations in Hilbert space [4, 5, 6, 7]. One can find this approach to nonlinear dynamical systems in several excellent treatises [8, 9, 10, 11]. In a function space, a Koopman operator maps a function \( \phi(x) \) to \( U_t[\phi] = \phi(S_t(x)) \) where \( S_t(x) \) is the trajectory of an underlying dynamical system. Thus, it represents the dynamics in terms of a collection of arbitrary “test functions” defined on a moving coordinate system which follows a set of differential equations: “\( U_t[\phi] \) has at \( x \) the value which \( \phi \) has at the point \( S_t(x) \) into which \( x \) flows after the lapse of the time \( t \)” [4]. This is the deterministic counterpart of Kolmogorov’s backward equation; while the Perron-Frobenius operator corresponds to Kolmogorov’s forward and Liouville equations [8, 9].

Koopman [4] showed that a Hamiltonian dynamics in a certain region of \( \mathbb{R}^{2n} \) on a variety \( H(q, p) = C \) of points can be represented in terms of a unitary transformation \( U_t \) in an appropriate Hilbert space: \( (U_t[\phi], U_t[\psi]) = (\phi, \psi) \). Since \( U_t \) is a family of one-parameter group, it has an infinitesimal generator \( G \),

\[
\left[ \frac{\partial}{\partial t} U_t[\phi(x)] \right]_{t=0} = iG_\phi(x). \tag{1}
\]

\( G \) is self-adjoint, or Hermitian: \( (G_\phi, \psi) = (\phi, G_\psi) \).

This paper studies the finite-dimensional skew-symmetric linear operator derived from decomposition of continuous-time Markov processes [12]. It has been shown that for a stochastic diffusion process [12], the anti-symmetric part corresponds to a hyperbolic system whose characteristic lines follow a differential equation \( \dot{x} = j(x) \) with \( \nabla \cdot (\rho(x) j(x)) = 0 \), where \( \rho(x) \) is the stationary density of the diffusion process. Here we show that for a continuous-time, discrete-state Markov process, the skew-symmetric part in fact can be further mathematically transformed into a Hamiltonian system with a symplectic structure. This last property is the consequence of a skew-symmetric real operator \( A \) whose eigenvalues are pairs of imaginary numbers.

Based on the present result for systems with finite dimension, we suspect that an anti-symmetric operator \( A \) in an appropriate Hilbert space, derived from diffusion process decomposition, has a linear, Hamiltonian structure as well. In fact, its Hamiltonian is nothing but \( \frac{1}{2}(\phi, (A^T A)^{\frac{1}{2}} \phi) \). Note that \( (\phi, A\phi) = 0 \); and in the dynamics defined by the anti-symmetric operator \( \frac{d}{dt} \phi(t) = A\phi, ||\phi(t)||^2 = (\phi, \phi) \) is a constant of motion. In fact, any
operator $\mathcal{P}$ that commutes with $A$, $A\mathcal{P} = \mathcal{P}A$, will have

$$
\frac{d}{dt}(\phi, \mathcal{P}\phi) = (A\phi, \mathcal{P}\phi) + (\phi, \mathcal{P}A\phi) = (\phi, [-A\mathcal{P} + \mathcal{P}A]\phi) = 0.
$$

(2)

Mathematically, even for finite dimensional systems, the present analysis is far from rigorous or complete; a full treatment remains to be developed.

2 Decomposition and the skew-symmetric part

2.1 Dynamics and its different mathematical representations

When a set of variables changing with time, we say there is a “dynamics”. Classical dynamics is customly represented by the time change of the variables themselves, $x(t)$, in terms of a system of differential equations $\frac{dx}{dt} = b(x)$. In the same vein, stochastic, Markov dynamics is represented by $dx(t) = b(x)dt + \sigma dW(t)$, first appeared in the work of Langevin, now widely known as a stochastic differential equation.

The work in the 1930s by von Neumann, Koopman, and Birkhoff in USA [4, 5, 6], and Kolmogorov, Khinchin, and others in USSR [13, 7], however, represents a dynamics by a one-parameter family of linear operators in a function space. In the case of Perron-Frobenius operator [8], the corresponding Liouville equation and Kolmogorov forward equation are interpreted as the motion of a density function for a collection of particles following the classical dynamics. The interpretation of the backward equation, or Koopman operator, on the other hand, is an arbitrary “test” function in a moving coordinate system that follows the classical differential equation. These “modern” mathematical representations of dynamics ultimately became the foundation of quantum mechanics and stochastic processes. Historically, it is worth pointing out that there was a “direct personal correspondence between Schrödinger and Kolmogorov at the time” [14].

One of the insights from these earlier work is that abstract representations of dynamics, while might not have simple or intuitive interpretations, can be powerful. In fact, trajectory, forward, and backward are three different representations of a classical dynamics, deterministic or stochastic. While the relation among an ordinary differential equation, its Liouville equation and Koopman operator are unambiguously defined, the relation between a stochastic differential equation and its forward and backward equations involves Itô, Stratonovich, divergence-form, or other interpretations. This has been an important
issue in the recent work of P. Ao and his coworkers [15, 16]. It is also noted that many studies on entropy productions of diffusion processes had also employed the divergence-form elliptic operator [17, 18, 19].

2.2 Decomposition of a continuous-time Markov process

Traditionally, a continuous-time, discrete-state Markov process (CTDS-MP) is characterized by its infinitesimal transition probability rate matrix, called Q-matrix, in terms of the master equation

\[
\frac{d}{dt}p(t) = Qp(t),
\]

in which column vector \( p(t) = \{p_i(t) | i = 1, 2, \cdots, n \} \) represents the probability of a stochastic system in state \( i \) at time \( t \). If the \( p(t) \) is a matrix, Eq. 3 is also widely known as the Kolmogorov forward equation for the Markov process. It can also be understood in terms of a Markov density matrix representation. See Appendix A.

The stochastic trajectory of a CTDS-MP can be defined through a random time-changed Poisson process in terms of multi-variate independent Poisson processes with unit rate [20].

Assuming the Markov process is irreducible and recurrent, let \( \pi \) be its unique stationary distribution: \( Q\pi = 0 \). We shall denote diagonal matrix \( \Pi = \text{diag}(\pi_1, \pi_2, \cdots, \pi_n) \). Then \( Q \) can be decomposed as a forward operator: \( Q = Q_S + Q_A \) with

\[
Q_S = \frac{1}{2} \left( Q + \Pi Q^T \Pi^{-1} \right), \quad Q_A = \frac{1}{2} \left( Q - \Pi Q^T \Pi^{-1} \right).
\]

\( Q^T = Q_S^T + Q_A^T \) will be the corresponding decomposition for the backward operator. (See Appendix B for a discussion on diffusion process.)

Note a very important difference between this decomposition for CTDS-MPs and for the decomposition for diffusion processes [12]: The \( Q_A \) is no longer a proper Q-matrix; it has negative off-diagonal elements.

The dynamic equation (3) can be decomposed accordingly:

\[
\frac{d}{dt}u(t) = \left( \Pi^{-\frac{1}{2}} Q \Pi^{\frac{1}{2}} \right) \left( \Pi^{-\frac{1}{2}} p(t) \right) = (S + A) u(t)
\]

in which \( u(t) = \Pi^{-\frac{1}{2}} p(t) \). It has the dimension of the square root of probability.

The symmetric part is well understood. It corresponds to a reversible Markov process [19] with stationary solution \( u_i^s = \sqrt{\pi_i} \). Thus, \( |u_i^s|^2 = \pi_i \) is the stationary probability distribution of the Markov process. Extensive studies on the non-symmetric part in term
of a *circulation decomposition* theorem, which characterizes along the path of a process in terms of reversible and rotational motions, can be found in [19, 21, 22, 23], with applications to stationary flux analysis in physics and chemistry [24, 25, 26].

The symmetric part as an $n$-dimensional linear system

$$\frac{d}{dt} u(t) = S u = -\nabla \Phi(u),$$

has a gradient with potential $\Phi(u) = -\frac{1}{2} u^T S u$. The symmetric matrix $(-S)$ is semi-positive. More recently, the dynamics of the symmetric part has also been shown as a gradient flow in an appropriate Riemannian manifold of probability distributions under a Wasserstein metric [27, 28].

### 2.3 A linear Hamiltonian system

we now consider the skew-symmetric part as an $n$-dimensional linear system

$$\frac{d}{dt} u(t) = A u,$$

in which real matrix $A$ is skew-symmetric $A^T = -A$. Eigenvalues of $A$ are pairs of imaginary conjugate numbers or zeros, say $\pm i\lambda_1, \pm i\lambda_2, \cdots, \pm i\lambda_k, 0, \cdots, 0$. Therefore, by an orthogonal matrix $B$, $B^{-1} = B^T$, a similarity transformation relates $A$ to

$$H_1 = BAB^T = \begin{pmatrix} 0 & \lambda_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\lambda_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \lambda_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\lambda_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \lambda_k & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\lambda_k & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

(8)

(together with

$$(u_1, u_2, \cdots, u_n) B^T = (x_1, y_1, x_2, y_2, \cdots, x_k, y_k, \cdots).$$

1The orthogonal matrix $B$ is real. This will be shown in the next section. In fact, $B = V^*$ in Sec. 3.3
The matrix $H_1$ defines a linear Hamiltonian dynamical system (harmonic oscillator!)
\[
\frac{dx_j}{dt} = \frac{\partial H}{\partial y_j}, \quad \frac{dy_j}{dt} = -\frac{\partial H}{\partial x_j},
\]
with Hamiltonian
\[
H(x_1, y_2, x_2, y_2, \cdots, x_k, y_k, \cdots) = \frac{1}{2} \sum_{j=1}^{k} \lambda_j (x_j^2 + y_j^2).
\]

For the dynamics in (7), the Hamiltonian in (11) is
\[
\frac{1}{2} u^T (A^T A) \frac{1}{2} u = H(u).
\]
Furthermore, one indeed has the conservation
\[
\frac{d}{dt} u^T (A^T A) \frac{1}{2} u = H(u).
\]

2.4 A Schrödinger-like equation

Diagonalization of $H_1$ requires working with complex eigenvalues and eigenvectors. Each $2 \times 2$ block in (8) can be transformed
\[
\frac{1}{2} \begin{pmatrix} -i & -1 \\ 1 & i \end{pmatrix} \begin{pmatrix} 0 & \lambda \\ -\lambda & 0 \end{pmatrix} \begin{pmatrix} i & 1 \\ -1 & -i \end{pmatrix} = i \begin{pmatrix} \lambda & 0 \\ 0 & -\lambda \end{pmatrix}.
\]
Therefor one can denote $H_1 = iH_2$ where $H_2$ is Hermitian. Then $A$ can be written as $A = B^T H_1 B = iB^T H_2 B = iH$, where $H = B^T H_2 B$ is Hermitian since $B$ is orthogonal. The dynamics in (7) then has another, Schrödinger-like, representation
\[
\frac{d}{dt} u(t) = iHu.
\]
The Hamiltonian for (16) is $u^T (H^2)^{\frac{1}{2}} u$. Therefore, $H$ can be legitimately called a Hamiltonian operator.

From Eq. (15) it is also interesting to note that

$$H(u) = \frac{1}{2} \left( u^T (A^T A)^{\frac{1}{2}} u \right) = \text{Tr} \left[ \Sigma (B \hat{\rho} B^T) \right],$$

(17)
in which matrix $\hat{\rho} = uu^T$. This representation is analogous to that of Heisenberg’s in matrix mechanics [29].

3 Representations via decompositions of skew-symmetric matrix

We now apply two widely used matrix analysis methods, eigenvalue decomposition (EVD) and singular-value decomposition (SVD), to a skew-symmetric matrix [30]. We shall show Schrödinger-equation like and Hamiltonian dynamics naturally emerge in these two representations, respectively.

3.1 $2 \times 2$ matrix

First, let us consider skew-symmetric $2 \times 2$ matrices in the general form

$$\lambda \left( \begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} \right).$$

It has an eigenvalue decomposition (EVD) (Eq. 15):

$$\left( \begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} \right) = \frac{1}{2} \left( \begin{array}{cc} 1 & -i \\ i & -1 \end{array} \right) \left( \begin{array}{cc} i & 0 \\ 0 & -i \end{array} \right) \left( \begin{array}{cc} 1 & -i \\ -1 & i \end{array} \right) = iB \Lambda B^*,$$

(18)

and a singular-value decomposition (SVD):

$$\left( \begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} \right) = \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right) \left( \begin{array}{cc} -1 & 0 \\ 0 & 1 \end{array} \right) = U \Sigma V^T.$$  

(19)

Note that while in general $U$ and $V$ in an SVD are not unique, the $U$ and $V$ in Eq. (19) are unique.
3.2 Eigenvalue decomposition (EVD)

Let skew-symmetric, real matrix $A$ has eigenvalues and corresponding eigenvectors $A\vec{x}_\ell = i\lambda \vec{x}_\ell$, where $\lambda_\ell$ are real and $\ell = 1, 2, \cdots, n$. There is at least one $\lambda = 0$; and for even $n$, there are at least two zero eigenvalues. Furthermore, each $i\lambda$ has a conjugate $-i\lambda$. As a convention, we shall denote $\lambda_{2k} = -\lambda_{2k-1} \leq 0$. Then

$$A\vec{x}_{2k-1} = i\lambda_{2k-1}\vec{x}_{2k-1}, \quad A\vec{x}_{2k-1} = -i\lambda_{2k-1}\vec{x}_{2k-1} = i\lambda_{2k}\vec{x}_{2k-1}.$$

Therefore, $\vec{x}_{2k} = c \vec{x}_{2k-1}$ where $c$ is a complex multiplier. Note that $\vec{x}_{2k-1}$ and $\vec{x}_{2k}$ are orthonormal: $\vec{x}_{2k-1} \cdot \vec{x}_{2k} = 0$. Hence, $\vec{x}_{2k} \cdot \vec{x}_{2k} = 0$, so is $\vec{x}_{2k-1} \cdot \vec{x}_{2k-1} = 0$. For example, these are indeed the case for the column vectors of $B$ and row vectors of $B^*$ in Eq. 18.

The EVD of $A$ can then be written as

$$A = B(i\mathcal{H})B^* = \left( \begin{array}{cccc} 1 & 1 & 1 & \cdots & 1 \\ \vec{x}_1 & \vec{x}_2 & \vec{x}_3 & \cdots & \vec{x}_n \end{array} \right) \left( \begin{array}{ccc} \lambda_1 & 0 & 0 \\ 0 & -\lambda_1 & 0 \\ 0 & 0 & \lambda_3 \\ 0 & 0 & -\lambda_3 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 0 \end{array} \right) \left( \begin{array}{ccc} \vec{v}_1 & \vec{v}_2 & \vec{v}_3 \\ \vec{x}_1 & \vec{x}_2 & \vec{x}_3 \\ \vdots & \vdots & \vdots \\ \vec{x}_n \end{array} \right),$$

in which $\mathcal{H} = \left( \begin{array}{cccc} \lambda_1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -\lambda_1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & -\lambda_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 \end{array} \right)$, \hspace{1cm} (20)

and $\vec{x}_k \cdot \vec{x}_\ell = \delta_{k\ell}$.

The dynamics (7) in this representation becomes $\frac{d}{dt}\varphi(t) = i\mathcal{H}\varphi$ in which $\varphi(t) = B^*u(t)$.

3.3 Singular-value decomposition (SVD)

The SVD of $A$ gives

$$A = \left( \begin{array}{cccc} \vec{u}_1 & \vec{u}_2 & \vec{u}_3 & \cdots & \vec{u}_n \end{array} \right) \Sigma \left( \begin{array}{ccc} \vec{v}_1 & \vec{v}_2 & \vec{v}_3 \\ \vec{u}_1 & \vec{u}_2 & \vec{u}_3 \\ \vdots & \vdots & \vdots \\ \vec{u}_n \end{array} \right),$$

in which

$$\Sigma = \left( \begin{array}{cccc} \lambda_1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -\lambda_1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & -\lambda_3 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & -\lambda_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 \end{array} \right).$$
in which the square diagonal

\[
\Sigma = \begin{pmatrix}
|\lambda_1| & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & |\lambda_2| & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & |\lambda_3| & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & |\lambda_4| & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0
\end{pmatrix},
\]

(21)

and \( A^T A \vec{u}_\ell = |\lambda_\ell|^2 \vec{u}_\ell \) with \(|\lambda_{2k-1}| = |\lambda_{2k}| \). Similarly, \( A^T A \vec{v}_\ell = |\lambda_\ell|^2 \vec{v}_\ell \). Both \( U \) and \( V \) are themselves orthogonal matrices. Furthermore, \( \vec{v}_{2k-1} = \vec{u}_{2k} \) and \( \vec{v}_{2k} = -\vec{u}_{2k-1} \). Therefore, we have

\[
\begin{pmatrix}
-\vec{v}_1 \\
-\vec{v}_2 \\
\vdots \\
-\vec{v}_n
\end{pmatrix}
\begin{pmatrix}
\vec{u}_1 \\
\vec{u}_2 \\
\vec{u}_3 \\
\vdots \\
\vec{u}_n
\end{pmatrix}
\begin{pmatrix}
|\lambda_1| & |\lambda_2| & \cdots & |\lambda_n|
\end{pmatrix}
\begin{pmatrix}
0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & \cdots & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & \cdots & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\triangleq \tilde{\mathcal{H}}_1.
\]

(22)

The dynamics (7) in this representation then becomes

\[
\frac{d}{dt} \xi(t) = V^* U \Sigma \xi = \tilde{\mathcal{H}}_1 \Sigma \xi,
\]

(23)

in which \( \xi(t) = V^* u(t) \). \( \tilde{\mathcal{H}}_1 \) reveals a symplectic structure of the dynamics. \( \tilde{\mathcal{H}}_1 \Sigma = \mathcal{H}_1 \) in Eq. 8.

### 3.4 Relationships between \( \vec{x} \) and \( \vec{u} \)

While vector \( \vec{x}_\ell \) are complex, vector \( \vec{u}_\ell \) are real. We have \( A \vec{x}_\ell = i\lambda_\ell \vec{x}_\ell \), \( A^T A \vec{x}_\ell = \lambda_\ell^2 \vec{x}_\ell \)

Noting \( \lambda_{2k-1}^2 = \lambda_{2k}^2 \), we therefore have,

\[
\vec{u}_{2k-1} = \alpha_{11} \vec{x}_{2k-1} + \alpha_{12} \vec{x}_{2k},
\]

(24a)
\[
\vec{u}_{2k} = \alpha_{21} \vec{x}_{2k-1} + \alpha_{22} \vec{x}_{2k}.
\] 

(24b)

According to the example in (18) and (19),

\[
\begin{pmatrix}
\alpha_{11} & \alpha_{12} \\
\alpha_{21} & \alpha_{22}
\end{pmatrix} = \begin{pmatrix}
-i/2 & -i/2 \\
1/2 & i/2
\end{pmatrix}.
\]

4 Trace, Hamiltonian, and entropy production

In terms of the original Markov process with infinitesimal transition rate matrix \( Q \), the elements of matrix \( A = \Pi^{-1} Q \Pi - \Pi^T Q^T \Pi^{-1} \) is:

\[
a_{ij} = \frac{q_{ij} \pi_j - q_{ji} \pi_i}{\sqrt{\pi_i \pi_j}}.
\]

(25)

It turns out that the trace of \( A^T A \) is:

\[
\text{Tr}(A^T A) = \sum_{i,j=1}^{n} a_{ij}^2 = \sum_{i,j=1}^{n} \frac{(q_{ij} \pi_j - q_{ji} \pi_i)^2}{\pi_i \pi_j}.
\]

(26)

Therefore, we have

\[
\text{Tr}(A^T A) = \sum_{\ell=1}^{n} ||\lambda_{\ell}||^2 = \sum_{i,j=1}^{n} a_{ij}^2.
\]

(27)

The implication of the mathematical equation in (26) is very intriguing since according to the nonequilibrium steady state (NESS) theory of a Markov process, its entropy production \([19, 31, 32]\) is

\[
e_p = \sum_{i>j} (q_{ij} \pi_j - q_{ji} \pi_i) \ln \left( \frac{q_{ij} \pi_j}{q_{ji} \pi_i} \right).
\]

(28)

In particular, when a system is near an equilibrium, \( q_{ij} \pi_j \simeq q_{ji} \pi_i \), then

\[
e_p \simeq \frac{1}{2} \sum_{i,j=1}^{n} \frac{(q_{ij} \pi_j - q_{ji} \pi_i)^2}{q_{ji} \pi_i}.
\]

(29)

5 Discussion

Since 1930s, it has been known that three different types of dynamics, classical deterministic, quantum, and stochastic dynamics, can all be represented in terms of linear operators in function space. While Schrödinger, Dirac, von Neumann’s quantum mechanics, and
Kolmogorov’s forward and backward equations for stochastic processes are widely known, Koopman’s powerful approach to classical dynamics has been mainly limited in mathematical literature. While Newton and Hamiltonian’s classical dynamics are conservative for mechanical energy, Fourier’s analytical theory of heat, together with the heat equation which turns out to the Kolmogorov equation for pure Brownian motion, has been a canonical example of dissipative systems.

There is a growing interest in treating stochastic dynamics and statistical thermodynamics in a unified framework [33, 34, 10, 35, 36, 37, 38, 39, 40]. Recently, a decomposition of general stochastic diffusion dynamics in function space into symmetric and anti-symmetric parts has shown that the former generalizes precisely Fourier’s heat equation, while the latter generalizes Newtonian conservative dynamics [12]. Furthermore, the dynamics decomposition fits perfectly with a recently discovered free energy balance equation: The symmetric part has “free energy decreasing = entropy production”, as was known to Helmholtz and Gibbs, and the anti-symmetric dynamics has free energy conservation.

A mathematical investigation of anti-symmetric dynamics in a Hilbert space will be desirable. In the present work, we seek insights on the anti-symmetric, or skew-symmetric dynamics from finite dimensional systems. It is shown that both Hamiltonian representation and Schrödinger-like representation naturally emerge in the singular-value decomposition and eigen-value decomposition of an skew-symmetric matrix. Finally, we discover an intriguing connection between the Hamiltonian for the skew-symmetric dynamics and the entropy production rate of the original irreversible Markov process. This observation calls for re-thinking of the nature of dissipation and time reversibility [12].

ACKNOWLEDGEMENTS. I thank Ping Ao, Rafael De La Madrid, Hao Ge, Eli Shlizerman, Jin Wang, and Wen-An Yong for helpful discussions.

References

[1] Dirac, P.A.M. (1930) *The Principles of Quantum Mechanics*. Cambridge Univ. Press, U.K.

[2] von Neumann, J. (1932) *Mathematical Foundations of Quantum Mechanics*, Beyer, R.T. transla., Princeton Univ. Press, NJ.
[3] Jordan, T.F. (2006) *Linear Operators for Quantum Mechanics*, Dover, New York.

[4] Koopman, B.O. (1931) Hamiltonian systems and transformation in Hilbert space. *Proc. Natl. Acad. Sci. USA* **17**, 315–318.

[5] Koopman, B.O. and von Neumann, J. (1932) Dynamical systems of continuous spectra. *Proc. Natl. Acad. Sci. USA* **18**, 255–263.

[6] Birkhoff, G.D. and Koopman, B.O. (1932) Recent contributions to the ergodic theory. *Proc. Natl. Acad. Sci. USA* **18**, 279–282.

[7] Khintchine, A. (1933) The method of spectral reduction in classical dynamics. *Proc. Natl. Acad. Sci. USA* **19**, 567–573.

[8] Lasota, A. and Mackey, M.C. (1993) *Chaos, Fractals, and Noise: Stochastic Aspects of Dynamics*, 2nd ed., Appl. Math. Sci. vol. 97, Springer, New York.

[9] Gaspard, P. (1998) *Chaos, Scattering and Statistical Mechanics*, Cambridge Univ. Press, U.K.

[10] Mackey, M.C. (1989) The dynamic origin of increasing entropy. *Rev. Mod. Phys.* **61**, 981–1016.

[11] Mezić, I. and Banaszuk, A. (2004) Comparison of systems with complex behavior. *Physica D*, **197**, 101–133.

[12] Qian, H. (2012) A decomposition of irreversible diffusion processes without detailed balance. *arxiv.org/abs/1204.6496*.

[13] Kolmogorov, A. (1931) Über die analytischen Methoden in der Wahrscheinlichkeitrechnung (On analytical methods in the theory of probability). *Mathematische Annalen*, **104**, 415–458.

[14] Nagasawa, M. (2000) *Stochastic Processes in Quantum Physics*, Birkhäuser, Boston.

[15] Shi, J., Chen, T., Yuan, R., Yuan, B. and Ao, P. (2011) Relation of biologically motivated new interpretation of stochastic differential equations to Itô process. *arxiv.org/abs/1111.2987*.  

12
[16] Yuan, R. and Ao, P. (2012) Beyond Itô vs. Stratonovich. arxiv.org/abs/1203.6600.

[17] van den Broeck, C. and Esposito, M. (2010) Three faces of the second law. II. Fokker-Planck formulation. Phys. Rev. E 82, 011144.

[18] Maes, C., Netočný, K. and Wynants, B. (2008) Steady state statistics of driven diffusions. Physica A 387, 2675–2689.

[19] Jiang, D.-Q., Qian, M. and Qian, M.-P. (2004) Mathematical Theory of Nonequilibrium Steady States, LNM 1833, Springer, New York.

[20] Kurtz, T.G. (1980) Representations of Markov processes as multiparameter time changes. Ann. Prob. 8, 682–715.

[21] Qian, M.-P. and Qian, M. (1982) Circulation for recurrent Markov chains. Z. Wahrsch. Verw. Gebiete., 59, 203–210.

[22] Qian, M.-P., Qian M. and Gong, G.-L. (1991) The reversibility and the entropy production of Markov processes. Contemp. Math. 118, 255–261.

[23] Kalpazidou, S.L. (2006) Cycle Representations of Markov Processes, 2nd ed., Springer, New York.

[24] Hill, T.L. (2004) Free Energy Transduction and Biochemical Cycle Kinetics, Dover, New York.

[25] Wang, J., Xu, L. and Wang, E. (2008) Potential landscape and flux framework of nonequilibrium networks: Robustness, dissipation, and coherence of biochemical oscillations. Proc. Natl. Acad. Sci. U.S.A. 105, 12271–12276.

[26] Li, C., Wang, E. and Wang, J. (2011) Landscape and flux decomposition for exploring global natures of non-equilibrium dynamical systems under intrinsic statistical fluctuations. Chem. Phys. Lett. 505, 75–80.

[27] Chow, S.-N., Huang, W., Li, Y. and Zhou, H. (2012) Fokker-Planck equations for a free energy functional or Markov process on a graph. Arch. Ratl. Mech. Anal. 203, 969–1008.
[28] Jordan, R., Kinderlehrer, D. and Otto, F. (1998) The variational formulation of the Fokker-Planck equation. *SIAM J. Math. Anal.* **29**, 1–17.

[29] Louisell, W.H. (1973) *Quantum Statistical Properties of Radiation*, John Wiley & Sons, New York.

[30] Xu, H. (2003) An SVD-like matrix decomposition and its applications. *Linear Algebra Appl.* **368**, 1-24.

[31] Zhang, X.-J., Qian, H. and Qian, M. (2012) Stochastic theory of nonequilibrium steady states and its applications (Part I). *Phys. Rep.* **510**, 1–86.

[32] Ge, H., Qian, M. and Qian, H. (2012) Stochastic theory of nonequilibrium steady states (Part II): Applications in chemical biophysics. *Phys. Rep.* **510**, 87–118.

[33] Spohn, H. (1978) Entropy production for quantum dynamical semigroups. *J. Math. Phys.* **19**, 1227–1230.

[34] Misra, B., Prigogine, I. and Courbage, M (1979) From deterministic dynamics to probabilistic descriptions. *Proc. Natl. Acad. Sci. USA* **76**, 3607–3611.

[35] Bedeaux, D. and Mazur, P. (2001) Mesoscopic non-equilibrium thermodynamics for quantum systems. *Physica A* **298**, 81–100.

[36] Reguera, D., Rubí, J.M. and Vilar, J.M.G. (2005) The mesoscopic dynamics of thermodynamic systems. *J. Chem. Phys. B* **109**, 21502–21515.

[37] Ao, P. (2005) Laws of Darwinian evolutionary theory. *Phys. Life Rev.* **2**, 117–156.

[38] Qian, H. (2006) Open-system nonequilibrium steady state: Statistical thermodynamics, fluctuations, and chemical oscillations. *J. Chem. Phys. B* **110**, 15063–15074.

[39] Ao, P. (2008) Emerging of stochastic dynamical equalities and steady state thermodynamics from Darwinian dynamics. *Commun. Theor. Phys.* **49**, 1073–1090.

[40] Qian, H. (2010) Cellular biology in terms of stochastic nonlinear biochemical dynamics: Emergent properties, isogenetic variations and chemical system inheritability. *J. Stat. Phys.* **141**, 990–1013.
6 Appendices

6.1 Appendix A: Density matrix for a Markov process

The solution to Eq. 3 can be formally written as

\[ p(t) = e^{Qt}p(0). \]  (30)

One can introduce a Markov density matrix:

\[ \rho_M(t) = e^{Qt}|p(0)\rangle\langle 1| \]  (31)

in which \( |p(0)\rangle \) is an \( n \times 1 \) matrix, i.e., a column vector, and \( \langle 1| \) is a row vector consisting of 1s. Therefore, \( \rho_M(t) \) is a matrix with \( \text{Tr}(\rho_M) = \langle 1|p(t)\rangle = 1 \). Furthermore,

\[ \rho_M^2 = e^{Qt}|p(0)\rangle\langle 1| = \rho_M. \]  (32)

Then we have \( \rho_M(t) \) satisfying the same dynamic equation as the Kolmogorov forward equation

\[ \frac{d}{dt}\rho(t) = Q\rho, \]  (33)

with a difference in the initial data \( \rho(0) \): It gives a transition probability matrix if \( \rho(0) = I \); and it gives a density matrix if \( \rho_M(0) = |p(0)\rangle\langle 1| \).

Similarly, a density matrix approach can be formulated for Eq. 16. It yields

\[ \frac{d}{dt}\rho(t) = i[\mathcal{H}\rho - \rho\mathcal{H}]. \]  (34)

6.2 Appendix B

The recently introduced “canonical conservative dynamics” [12] had been discussed in [4], in which the inner product in a Hilbert space is defined with \( \rho(x) \) as a weight [19]: \( \rho(x) \) being a positive, single-valued, analytic function on \( \mathbb{R}^n \). In the contrary, the weight used in [12] is \( \rho^{-1}(x) \). This difference can be seen in the matrix theory: Both \( \Pi Q \) and \( Q\Pi^{-1} \) are symmetric for reversible Markov process with generator \( Q \), but only \( \Pi^{-\frac{1}{2}} Q\Pi^{\frac{1}{2}} \) transforms the master equation into a gradient system. In fact, Koopman operator and Perron-Frobenius operator belong to two different Hilbert spaces with inner products

\[ (\phi, \psi)_K = \int_{\mathbb{R}^n} \rho(x)\phi(x)\psi(x)dx, \]  (35)
and
\[
(\phi, \psi)_{PF} = \int_{\mathbb{R}^n} \rho^{-1}(x)\phi(x)\psi(x)dx,
\]
respectively. Therefore, the symmetric operator in the Koopman (backward) space is
\[
\mathcal{L}_S^*[u] = \frac{1}{2} \left( \mathcal{L}^*[u] + \rho^{-1} \mathcal{L}[\rho u] \right) = \nabla \cdot \left( A(x) \nabla u \right) + \left( \nabla \ln \rho \right) A(x) \left( \nabla u \right),
\]
while in the Perron-Frobenius (forward) space is \[12\]
\[
\mathcal{L}_S[u] = \frac{1}{2} \left( \mathcal{L}[u] + \rho \mathcal{L}^* [\rho^{-1} u] \right) = \nabla \cdot A(x) \left( \nabla u - \left( \nabla \ln \rho \right) u \right).
\]
Indeed, \( \mathcal{L}_S \) and \( \mathcal{L}_S^* \) correspond to the Kolmogorov forward and backward equations of a reversible diffusion.
A Hamiltonian-Entropy Production Connection in the Skew-symmetric Part of a Stochastic Dynamics

Hong Qian

Department of Applied Mathematics
University of Washington, Seattle
WA 98195-2420, U.S.A.

May 1, 2014

Abstract

The infinitesimal transition probability operator for a continuous-time discrete-state Markov process, \( Q \), can be decomposed into a symmetric and a skew-symmetric parts. As recently shown for the case of diffusion processes, while the symmetric part corresponding to a gradient system stands for a reversible Markov process, the skew-symmetric part, \( \frac{d}{dt} u(t) = Au \), is mathematically equivalent to a linear Hamiltonian dynamics with Hamiltonian \( H = \frac{1}{2} u^T (A^T A) u \). It can also be transformed into a Schrödinger-like equation \( \frac{d}{dt} u = i\mathcal{H} u \) where the “Hamiltonian” operator \( \mathcal{H} = -iA \) is Hermitian. In fact, these two representations of a skew-symmetric dynamics emerge naturally through singular-value and eigen-value decompositions, respectively. The stationary probability of the Markov process can be expressed as \( \|u_s\|^2 \). The motion can be viewed as “harmonic” since \( \frac{d}{dt} \|u(t) - \vec{c}\|^2 = 0 \) where \( \vec{c} = (c, c, \cdots, c) \) with \( c \) being a constant. More interestingly, we discover that

\[
\text{Tr}(A^T A) = \sum_{j,\ell=1}^n \left( \frac{q_{j\ell} \pi_{j\ell} - q_{\ell j} \pi_{\ell j}}{\pi_j \pi_\ell} \right)^2,
\]

whose right-hand-side is intimately related to the entropy production rate of the Markov process in a nonequilibrium steady state with stationary distribution \( \{\pi_j\} \). The physical implication of this intriguing connection between conservative Hamiltonian dynamics and dissipative entropy production remains to be further explored.

1 Introduction

Linear operator theory and functional analysis became the centerpiece of quantum mechanics in the work of Dirac and von Neumann [1,2,3]. In 1930s, Koopman, Birkhoff, von
Neumann, and others have also developed a classical dynamical systems theory, including several ergodic theorems, based on linear transformations in Hilbert space \([4, 5, 6, 7]\). One can find this approach to nonlinear dynamical systems in several excellent treatises \([8, 9, 10, 11]\). In a function space, a Koopman operator maps a function \(\phi(x)\) to
\[
U_t[\phi] = \phi(S_t(x))
\]
where \(S_t(x)\) is the trajectory of an underlying dynamical system. Thus, it represents the dynamics in terms of a collection of arbitrary “test functions” defined on a moving coordinate system which follows a set of differential equations: “\(U_t[\phi]\) has at \(x\) the value which \(\phi\) has at the point \(S_t(x)\) into which \(x\) flows after the lapse of the time \(t\)” \([4]\). This is the deterministic counterpart of Kolmogorov’s backward equation; while the Perron-Frobenius operator corresponds to Kolmogorov’s forward and Liouville equations \([8, 9]\).

Koopman \([4]\) showed that a Hamiltonian dynamics in a certain region of \(\mathbb{R}^{2n}\) on a variety \(H(q, p) = C\) of points can be represented in terms of a unitary transformation \(U_t\) in an appropriate Hilbert space: \((U_t[\phi], U_t[\psi]) = (\phi, \psi)\). Since \(U_t\) is a family of one-parameter group, it has an infinitesimal generator \(G\),
\[
\left[ \frac{\partial}{\partial t} U_t[\phi(x)] \right]_{t=0} = iG\phi(x).
\]
\(G\) is self-adjoint, or Hermitian: \((G\phi, \psi) = (\phi, G\psi)\).

This paper studies the skew-symmetric linear operator derived from decomposition of continuous-time Markov processes \([12]\). It has been shown that for a stochastic diffusion process \([12]\), the anti-symmetric part corresponds to a hyperbolic system whose characteristic lines follow a differential equation \(\dot{x} = j(x)\) with \(\nabla \cdot (\rho(x) j(x)) = 0\), where \(\rho(x)\) is the stationary density of the diffusion process. Here we show that, as a finite-dimensional analogue of the \(G\), the skew-symmetric part of a continuous-time, discrete-state Markov process in fact can be further mathematically transformed into a Hamiltonian system with a symplectic structure. This is the consequence of a skew-symmetric real operator \(A\) whose eigenvalues are pairs of imaginary numbers.

Based on the present result for systems with finite dimension, we suspect that an anti-symmetric operator \(A\) in an appropriate Hilbert space, derived from diffusion process decomposition, has a linear, Hamiltonian structure as well, with its Hamiltonian being \(\frac{1}{2}(\phi, (A^T A)^{\frac{1}{2}} \phi)\). Note that \((\phi, A\phi) = 0\); and in the dynamics defined by the anti-symmetric operator \(\frac{d}{dt}\phi(t) = A\phi\), \(\|\phi(t)\|^2 = (\phi, \phi)\) is a constant of motion. In fact, any
operator $\mathcal{P}$ that commutes with $\mathcal{A}$, $\mathcal{A}\mathcal{P} = \mathcal{P}\mathcal{A}$, will have

$$
\frac{d}{dt}(\phi, \mathcal{P}\phi) = (\mathcal{A}\phi, \mathcal{P}\phi) + (\phi, \mathcal{P}\mathcal{A}\phi) = (\phi, [\mathcal{A}\mathcal{P}, \mathcal{P}\mathcal{A}]\phi) = 0.
$$

(2)

Mathematically, even for finite dimensional systems, the present analysis is far from rigorous or complete; a full treatment remains to be developed.

2 Decomposition and the skew-symmetric part

2.1 Dynamics and its different mathematical representations

When a set of variables changing with time, we say there is a “dynamics”. Classical dynamics is customly represented by the time change of the variables themselves, $x(t)$, in terms of a system of differential equations $\frac{dx}{dt} = b(x)$. In the same vein, stochastic, Markov dynamics is represented by $dx(t) = b(x)dt + \sigma dW(t)$, first appeared in the work of Langevin, now widely known as a stochastic differential equation.

The work in the 1930s by von Neumann, Koopman, and Birkhoff in USA [4, 5, 6], and Kolmogorov, Khinchin, and others in USSR [13, 7], however, represents a dynamics by a one-parameter family of linear operators in a function space. In the case of Perron-Frobenius operator [8], the corresponding Liouville equation and Kolmogorov forward equation are interpreted as the motion of a density function for a collection of particles following the classical dynamics. The interpretation of the backward equation, or Koopman operator, on the other hand, is an artitary “test” function in a moving coordinate system that follows the classical differential equation. These “modern” mathematical representations of dynamics ultimately became the foundation of quantum mechanics and stochastic processes. Historically, it is worth pointing out that there was a “direct personal correspondence between Schrödinger and Kolmogorov at the time” [14].

One of the insights from these earlier work is that abstract representations of dynamics, while might not have simple or intuitive interpretations, can be powerful. In fact, trajectory, forward, and backward are three different representations of a classical dynamics, deterministic or stochastic. While the relation among an ordinary differential equation, its Liouville equation and Koopman operator are unambiguously defined, the relation between a stochastic differential equation and its forward and backward equations involves Itô, Stratonovich, divergence-form, or other interpretations. This has been an important
issue in the recent work of P. Ao and his coworkers [15, 16]. It is also noted that many studies on entropy productions of diffusion processes had also employed the divergence-form elliptic operator [17, 18, 19].

2.2 Decomposition of a continuous-time Markov process

Traditionally, a continuous-time, discrete-state Markov process (CTDS-MP) is characterized by its infinitesimal transition probability rate matrix, called Q-matrix, in terms of the master equation

$$\frac{d}{dt}p(t) = Qp(t),$$

(3)

in which column vector \( p(t) = \{p_i(t)\} \) represents the probability of a stochastic system in state \( i \) at time \( t \). If the \( p(t) \) is a matrix, Eq. 3 is also widely known as the Kolmogorov forward equation for the Markov process. It can also be understood in terms of a Markov density matrix representation. See Appendix A.

The stochastic trajectory of a CTDS-MP can be defined through a random time-changed Poisson process in terms of multi-variate independent Poisson processes with unit rate [20]. Assuming the Markov process is irreducible and recurrent, let \( \pi \) be its unique stationary distribution: \( Q\pi = 0 \). We shall denote diagonal matrix \( \Pi = \text{diag}(\pi_1, \pi_2, \cdots, \pi_n) \). Then \( Q \) can be decomposed as a forward operator: \( Q = QS + QA \) with

$$Q_S = \frac{1}{2} \left( Q + \Pi Q^T \Pi^{-1} \right), \quad Q_A = \frac{1}{2} \left( Q - \Pi Q^T \Pi^{-1} \right).$$

(4)

\( Q_T = Q_S^T + Q_A^T \) will be the corresponding decomposition for the backward operator. (See Appendix B for a discussion on the diffusion process.)

Note a very important difference between this decomposition for CTDS-MPs and for the decomposition for diffusion processes [12]: The \( Q_A \) is no longer a proper Q-matrix; it has negative off-diagonal elements.

The dynamic equation (3) can be decomposed accordingly:

$$\frac{d}{dt} u(t) = \left( \Pi^{-\frac{1}{2}} Q \Pi^{\frac{1}{2}} \right) \left( \Pi^{-\frac{1}{2}} p(t) \right) = (S + A) u(t)$$

(5)

in which \( u(t) = \Pi^{-\frac{1}{2}} p(t) \). It has the dimension of the square root of probability.

The symmetric part is well understood. It corresponds to a reversible Markov process [19] with stationary solution \( u_i^s = \sqrt{\pi_i} \). Thus, \( |u_i^s|^2 = \pi_i \) is the stationary probability distribution of the Markov process. Extensive studies on the non-symmetric part in term
of a *circulation decomposition* theorem, which characterizes along the path of a process in terms of reversible and rotational motions, can be found in [19, 21, 22, 23], with applications to stationary flux analysis in physics and chemistry [24, 25, 26].

The symmetric part as an $n$-dimensional linear system

$$\frac{d}{dt}u(t) = Su = -\nabla \Phi(u), \quad (6)$$

has a gradient with potential $\Phi(u) = -\frac{1}{2}u^T Su$. The symmetric matrix $(-S)$ is semi-positive. More recently, the dynamics of the symmetric part has also been shown as a gradient flow in an appropriate Riemannian manifold of probability distributions under a Wasserstein metric [27, 28].

### 2.3 A linear Hamiltonian system

we now consider the skew-symmetric part as an $n$-dimensional linear system

$$\frac{d}{dt}u(t) = Au, \quad (7)$$

in which real matrix $A$ is skew-symmetric $A^T = -A$. Eigenvalues of $A$ are pairs of imaginary conjugate numbers or zeros, say $\pm i \lambda_1, \pm i \lambda_2, \cdots, \pm i \lambda_k, 0, \cdots, 0$. Therefore, by an orthogonal matrix $B$, $B^{-1} = B^T$, a similarity transformation relates $A$ to

\[
\mathcal{H}_1 = BAB^T = \begin{pmatrix}
0 & \lambda_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-\lambda_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \lambda_2 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -\lambda_2 & 0 & 0 & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & 0 & 0 & 0 & \lambda_k & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -\lambda_k & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{pmatrix}, \quad (8)
\]

\[
(u_1, u_2, \cdots, u_n)B^T = (x_1, y_1, x_2, y_2, \cdots, x_k, y_k, \cdots). \quad (9)
\]

\[\text{1 The orthogonal matrix } B \text{ is real. This will be shown in the next section. In fact, } B = V^* \text{ in Sec. 3.3}\]
Note that the matrix transformation reveals canonical pairs of variables \((x_i, y_i)\) which are hidden under the original representation with \(u\)'s. The matrix \(H_1\) defines a linear Hamiltonian dynamical system (harmonic oscillator!)

\[
\frac{dx_j}{dt} = \frac{\partial H}{\partial y_j}, \quad \frac{dy_j}{dt} = -\frac{\partial H}{\partial x_j}, \tag{10}
\]

with Hamiltonian

\[
H(x_1, y_2, x_2, y_2, \cdots, x_k, y_k, \cdots) = \frac{1}{2} \sum_{j=1}^{k} \lambda_j (x_j^2 + y_j^2). \tag{11}
\]

For the dynamics in \((7)\), the Hamiltonian in \((11)\) is \(\frac{1}{2} u^T (A^T A)^{\frac{1}{2}} u\), where we introduce the notion,

\[
(A^T A)^{\frac{1}{2}} = B^{-1}(BA^T B^{-1}BAB^{-1})^{\frac{1}{2}} B = B^{-1}(H_1^T H_1)^{\frac{1}{2}} B. \tag{12}
\]

In Eq. \((12)\) \((H_1^T H_1)^{\frac{1}{2}} = \Sigma = \text{diag}(\lambda_1, \lambda_1, \lambda_2, \lambda_2, \cdots, \lambda_k, \lambda_k, 0, \cdots, 0)\) is the singular value matrix of \(A\) (see Sec. 3.3). Then following Eq. \((9)\) we have,

\[
\frac{1}{2} u^T (A^T A)^{\frac{1}{2}} u = H(u). \tag{13}
\]

Furthermore, one indeed has the conservation

\[
\frac{d}{dt} u^T (A^T A)^{\frac{1}{2}} u = u^T \left( A^T (A^T A)^{\frac{1}{2}} + (A^T A)^{\frac{1}{2}} A \right) u = (Bu)^T \left( H_1^T (H_1^T H_1)^{\frac{1}{2}} + (H_1^T H_1)^{\frac{1}{2}} H_1 \right) (Bu) = (Bu)^T \left( (H_1^T H_1)^{\frac{1}{2}} (H_1^T + H_1) \right) (Bu) = 0. \tag{14}
\]

### 2.4 A Schrödinger-like equation

Diagonalization of \(H_1\) requires working with complex eigenvalues and eigenvectors. Each 2 \(\times\) 2 block in \((8)\) can be transformed

\[
\frac{1}{2} \begin{pmatrix} -i & -1 \\ 1 & i \end{pmatrix} \begin{pmatrix} 0 & \lambda \\ -\lambda & 0 \end{pmatrix} \begin{pmatrix} i & 1 \\ -1 & -i \end{pmatrix} = i \begin{pmatrix} \lambda & 0 \\ 0 & -\lambda \end{pmatrix}. \tag{15}
\]

Therefor one can denote \(H_1 = iH_2\) where \(H_2\) is Hermitian. Then \(A\) can be written as \(A = B^T H_1 B = iB^T H_2 B = iH\), where \(H = B^T H_2 B\) is Hermitian since \(B\) is orthogonal. The dynamics in \((7)\) then has another, Schrödinger-like, representation

\[
\frac{d}{dt} u(t) = iHu. \tag{16}
\]
The Hamiltonian for (40) is $\frac{1}{2} u^T (H^2)^{\frac{1}{2}} u$. Therefore, $H$ can be legitimately called a Hamiltonian operator.

From Eq. [18] it is also interesting to note that

$$H(u) = \frac{1}{2} \left( u^T (A^T A)^{\frac{1}{2}} u \right) = \text{Tr} \left[ \Sigma (B \hat{\rho} B^T) \right], \quad (17)$$

in which matrix $\hat{\rho} = uu^T$. This representation is analogous to that of Heisenberg’s in matrix mechanics [29].

3 Representations via decompositions of skew-symmetric matrix

We now apply two widely used matrix analysis methods, eigenvalue decomposition (EVD) and singular-value decomposition (SVD), to a skew-symmetric matrix [30]. We shall show Schrödinger-equation like and Hamiltonian dynamics naturally emerge in these two representations, respectively.

3.1 $2 \times 2$ matrix

First, let us consider skew-symmetric $2 \times 2$ matrices in the general form

$$\lambda \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$  

It has an eigenvalue decomposition (EVD) (Eq. [15]):

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix} \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \begin{pmatrix} 1 & -i \\ i & -1 \end{pmatrix} = iB \Lambda B^*, \quad (18)$$

and a singular-value decomposition (SVD):

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} = U \Sigma V^T. \quad (19)$$

Note that $U$ and $V$ in an SVD are not unique in general. However, for the $2 \times 2$ problem, the general forms for orthogonal $U$ and $V$ are

$$U = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix}, \quad V^T = \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix} \quad (20)$$

with $\theta + \phi = \frac{\pi}{2}$. Hence, $UV^T$ always gives the left-hand-side of Eq. [19]. Furthermore, $V^TU = UV^T$ and $VU^T = U^TV = -UV^T$.  

7
3.2 Eigenvalue decomposition (EVD)

Let skew-symmetric, real matrix $A$ has eigenvalues and corresponding eigenvectors $A \vec{x}_\ell = i\lambda \vec{x}_\ell$, where $\lambda_\ell$ are real and $\ell = 1, 2, \cdots, n$. There is at least one $\lambda = 0$; and for even $n$, there are at least two zero eigenvalues. Furthermore, each $i\lambda$ has a conjugate $-i\lambda$. As a convention, we shall denote $\lambda_{2k} = -\lambda_{2k-1} \leq 0$. Then

$$A \vec{x}_{2k-1} = i\lambda_{2k-1} \vec{x}_{2k-1}, \quad A \overline{\vec{x}_{2k-1}} = -i\lambda_{2k-1} \overline{\vec{x}_{2k-1}} = i\lambda_{2k} \overline{\vec{x}_{2k-1}}.$$  

Therefore, $\vec{x}_{2k} = c \overline{\vec{x}_{2k-1}}$ where $c$ is a complex multiplier. Note that $\vec{x}_{2k-1}$ and $\vec{x}_{2k}$ are orthonormal: $\vec{x}_{2k-1} \cdot \vec{x}_{2k} = 0$. Hence, $\vec{x}_{2k} \cdot \vec{x}_{2k} = 0$, so is $\overline{\vec{x}_{2k-1}} \cdot \overline{\vec{x}_{2k-1}} = 0$. For example, these are indeed the case for the column vectors of $B$ and row vectors of $B^*$ in Eq. 18.

The EVD of $A$ can then be written as

$$A = B (i\mathcal{H}) B^* = \begin{pmatrix} \lambda_1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -\lambda_1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \lambda_3 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & -\lambda_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix} \begin{pmatrix} \vec{x}_1 \\ \vec{x}_2 \\ \vec{x}_3 \\ \vdots \\ \vec{x}_n \end{pmatrix} (i\mathcal{H}) \begin{pmatrix} \vec{v}_1 \\ \vec{v}_2 \\ \vec{v}_3 \\ \vdots \\ \vec{v}_n \end{pmatrix},$$

in which

$$\mathcal{H} = \begin{pmatrix} \lambda_1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -\lambda_1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \lambda_3 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & -\lambda_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}, \quad (21)$$

and $\vec{x}_k \cdot \vec{x}_\ell = \delta_{k\ell}$.

The dynamics (7) in this representation becomes $\frac{d}{dt} \varphi(t) = i\mathcal{H} \varphi$ in which $\varphi(t) = B^* u(t)$.

3.3 Singular-value decomposition (SVD)

The SVD of $A$ gives

$$A = \begin{pmatrix} \vec{u}_1 & \vec{u}_2 & \vec{u}_3 & \cdots & \vec{u}_n \end{pmatrix} \Sigma \begin{pmatrix} \vec{v}_1 & \vec{v}_2 & \vec{v}_3 & \cdots & \vec{v}_n \end{pmatrix},$$
in which the square diagonal

\[
\Sigma = \begin{pmatrix}
|\lambda_1| & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & |\lambda_2| & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & |\lambda_3| & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & |\lambda_4| & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0
\end{pmatrix}, \tag{22}
\]

and \(A^T A \vec{u}_\ell = |\lambda_\ell|^2 \vec{u}_\ell\) with \(|\lambda_{2k-1}| = |\lambda_{2k}|\). Similarly, \(A^T A \vec{v}_\ell = |\lambda_\ell|^2 \vec{v}_\ell\). Both \(U\) and \(V\) are themselves orthogonal matrices. Furthermore, \(\vec{v}_{2k-1} = \vec{u}_{2k}\) and \(\vec{v}_{2k} = -\vec{u}_{2k-1}\). Therefore, we have

\[
\begin{pmatrix}
\vec{v}_1 \\
\vec{v}_2 \\
\vdots \\
\vec{v}_n
\end{pmatrix}
= \begin{pmatrix}
0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & \cdots & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & \cdots & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\triangleq \tilde{H}_1. \tag{23}
\]

The dynamics (7) in this representation then becomes

\[
\frac{d}{dt} \xi(t) = V^* U \Sigma \xi = \tilde{H}_1 \Sigma \xi, \tag{24}
\]

in which \(\xi(t) = V^* u(t)\). \(\tilde{H}_1\) reveals a symplectic structure of the dynamics. \(\tilde{H}_1 \Sigma = \mathcal{H}_1\) in Eq. 8.

### 3.4 Relationships between \(\vec{x}\) and \(\vec{u}\)

While vector \(\vec{x}_\ell\) are complex, vector \(\vec{u}_\ell\) are real. We have \(A \vec{x}_\ell = i \lambda_\ell \vec{x}_\ell\), \(A^T A \vec{x}_\ell = \lambda_\ell^2 \vec{x}_\ell\)

Noting \(\lambda_{2k-1}^2 = \lambda_{2k}^2\), we therefore have,

\[
\vec{u}_{2k-1} = \alpha_{11} \vec{x}_{2k-1} + \alpha_{12} \vec{x}_{2k}, \tag{25a}
\]
\[ \vec{u}_{2k} = \alpha_{21} \vec{x}_{2k-1} + \alpha_{22} \vec{x}_{2k}. \]  

(25b)

According to the example in (18) and (19),

\[
\begin{pmatrix}
\alpha_{11} & \alpha_{12} \\
\alpha_{21} & \alpha_{22}
\end{pmatrix} = \begin{pmatrix}
-i & -1 \\
1 & i
\end{pmatrix}.
\]

4 Trace, Hamiltonian, and entropy production

In terms of the original Markov process with infinitesimal transition rate matrix \( Q \), the elements of matrix \( A = \Pi^{-\frac{1}{2}} Q \Pi^{\frac{1}{2}} - \Pi^{\frac{1}{2}} Q T \Pi^{-\frac{1}{2}} \) is:

\[ a_{ij} = \frac{q_{ij} \pi_j - q_{ji} \pi_i}{\sqrt{\pi_i \pi_j}}. \]  

(26)

It turns out that the trace of \( A^T A \) is:

\[ \text{Tr}(A^T A) = \sum_{i,j=1}^{n} a_{ij}^2. \]

(27)

Therefore, we have

\[ \text{Tr}(A^T A) = \sum_{\ell=1}^{n} \|\lambda_{\ell}\|^2 = \sum_{i,j=1}^{n} a_{ij}^2. \]  

(28)

The implication of the mathematical equation in (27) is very intriguing since according to the nonequilibrium steady state (NESS) theory of a Markov process, its entropy production \[19, 31, 32] is

\[ e_p = \sum_{i>j} (q_{ij} \pi_j - q_{ji} \pi_i) \ln \left( \frac{q_{ij} \pi_j}{q_{ji} \pi_i} \right). \]  

(29)

In particular, when a system is near an equilibrium, \( q_{ij} \pi_j \simeq q_{ji} \pi_i \), then

\[ e_p \simeq \frac{1}{2} \sum_{i,j=1}^{n} \frac{(q_{ij} \pi_j - q_{ji} \pi_i)^2}{q_{ji} \pi_i}. \]  

(30)

5 Discussion

Since 1930s, it has been known that three different types of dynamics, classical deterministic, quantum, and stochastic dynamics, can all be represented in terms of linear operators in function space. While Schrödinger, Dirac, von Neumann’s quantum mechanics, and
Kolmogorov’s forward and backward equations for stochastic processes are widely known, Koopman’s powerful approach to classical dynamics has been mainly limited in mathematical literature. While Newton and Hamiltonian’s classical dynamics are conservative for mechanical energy, Fourier’s analytical theory of heat, together with the heat equation which turns out to the Kolmogorov equation for pure Brownian motion, has been a canonical example of dissipative systems.

There is a growing interest in treating stochastic dynamics and statistical thermodynamics in a unified framework [33] [34] [10] [35] [36] [37] [38] [39] [40]. Recently, a decomposition of general stochastic diffusion dynamics in function space into symmetric and anti-symmetric parts has shown that the former generalizes precisely Fourier’s heat equation, while the latter generalizes Newtonian conservative dynamics [12]. Furthermore, the dynamics decomposition fits perfectly with a recently discovered free energy balance equation: The symmetric part has “free energy decreasing = entropy production”, as was known to Helmholtz and Gibbs, and the anti-symmetric dynamics has free energy conservation.

A mathematical investigation of anti-symmetric dynamics in a Hilbert space will be desirable. In the present work, we seek insights on the anti-symmetric, or skew-symmetric dynamics from finite dimensional systems. It is shown that both Hamiltonian representation and Schrödinger-like representation naturally emerge in the singular-value decomposition and eigen-value decomposition of an skew-symmetric matrix. Finally, we discover an intriguing connection between the Hamiltonian for the skew-symmetric dynamics and the entropy production rate of the original irreversible Markov process. This observation calls for re-thinking of the nature of dissipation and time reversibility [12].

ACKNOWLEDGEMENTS. I thank Ping Ao, Zhen-qing Chen, Rafael De La Madrid, Hao Ge, Eli Shlizerman, Jin Wang, and Wen-An Yong for helpful discussions.

References

[1] Dirac, P.A.M. (1930) *The Principles of Quantum Mechanics*. Cambridge Univ. Press, U.K.

[2] von Neumann, J. (1932) *Mathematical Foundations of Quantum Mechanics*, Beyer, R.T. transla., Princeton Univ. Press, NJ.
[3] Jordan, T.F. (2006) *Linear Operators for Quantum Mechanics*, Dover, New York.

[4] Koopman, B.O. (1931) Hamiltonian systems and transformation in Hilbert space. *Proc. Natl. Acad. Sci. USA* **17**, 315–318.

[5] Koopman, B.O. and von Neumann, J. (1932) Dynamical systems of continuous spectra. *Proc. Natl. Acad. Sci. USA* **18**, 255–263.

[6] Birkhoff, G.D. and Koopman, B.O. (1932) Recent contributions to the ergodic theory. *Proc. Natl. Acad. Sci. USA* **18**, 279–282.

[7] Khintchine, A. (1933) The method of spectral reduction in classical dynamics. *Proc. Natl. Acad. Sci. USA* **19**, 567–573.

[8] Lasota, A. and Mackey, M.C. (1993) *Chaos, Fractals, and Noise: Stochastic Aspects of Dynamics*, 2nd ed., Appl. Math. Sci. vol. 97, Springer, New York.

[9] Gaspard, P. (1998) *Chaos, Scattering and Statistical Mechanics*, Cambridge Univ. Press, U.K.

[10] Mackey, M.C. (1989) The dynamic origin of increasing entropy. *Rev. Mod. Phys.* **61**, 981–1016.

[11] Mezić, I. and Banaszuk, A. (2004) Comparison of systems with complex behavior. *Physica D*, **197**, 101–133.

[12] Qian, H. (2012) A decomposition of irreversible diffusion processes without detailed balance. *arXiv.org/abs/1204.6496*.

[13] Kolmogorov, A. (1931) Über die analytischen Methoden in der Wahrscheinlichkeitsrechnung (On analytical methods in the theory of probability). *Mathematische Annalen*, **104**, 415–458.

[14] Nagasawa, M. (2000) *Stochastic Processes in Quantum Physics*, Birkhäuser, Boston.

[15] Shi, J., Chen, T., Yuan, R., Yuan, B. and Ao, P. (2012) Relation of biologically motivated new interpretation of stochastic differential equations to Itô process. *J. Stat. Phys.* **148**, 579–590.
[16] Yuan, R. and Ao, P. (2012) Beyond Itô vs. Stratonovich. *J. Stat. Mech. Th. Exp.* **2012**, P07010.

[17] van den Broeck, C. and Esposito, M. (2010) Three faces of the second law. II. Fokker-Planck formulation. *Phys. Rev. E* **82**, 011144.

[18] Maes, C., Netočný, K. and Wynants, B. (2008) Steady state statistics of driven diffusions. *Physica A* **387**, 2675–2689.

[19] Jiang, D.-Q., Qian, M. and Qian, M.-P. (2004) *Mathematical Theory of Nonequilibrium Steady States*, LNM 1833, Springer, New York.

[20] Kurtz, T.G. (1980) Representations of Markov processes as multiparameter time changes. *Ann. Prob.* **8**, 682–715.

[21] Qian, M.-P. and Qian, M. (1982) Circulation for recurrent Markov chains. *Z. Wahrsch. Verw. Gebiete.*, **59**, 203–210.

[22] Qian, M.-P., Qian M. and Gong, G.-L. (1991) The reversibility and the entropy production of Markov processes. *Contemp. Math.* **118**, 255–261.

[23] Kalpazidou, S.L. (2006) *Cycle Representations of Markov Processes*, 2nd ed., Springer, New York.

[24] Hill, T.L. (2004) *Free Energy Transduction and Biochemical Cycle Kinetics*, Dover, New York.

[25] Wang, J., Xu, L. and Wang, E. (2008) Potential landscape and flux framework of nonequilibrium networks: Robustness, dissipation, and coherence of biochemical oscillations. *Proc. Natl. Acad. Sci. U.S.A.* **105**, 12271–12276.

[26] Li, C., Wang, E. and Wang, J. (2011) Landscape and flux decomposition for exploring global natures of non-equilibrium dynamical systems under intrinsic statistical fluctuations. *Chem. Phys. Lett.* **505**, 75–80.

[27] Chow, S.-N., Huang, W., Li, Y. and Zhou, H. (2012) Fokker-Planck equations for a free energy functional or Markov process on a graph. *Arch. Ratl. Mech. Anal.* **203**, 969–1008.
[28] Jordan, R., Kinderlehrer, D. and Otto, F. (1998) The variational formulation of the Fokker-Planck equation. SIAM J. Math. Anal. 29, 1–17.

[29] Louisell, W.H. (1973) Quantum Statistical Properties of Radiation, John Wiley & Sons, New York.

[30] Xu, H. (2003) An SVD-like matrix decomposition and its applications. Linear Algebra Appl. 368, 1-24.

[31] Zhang, X.-J., Qian, H. and Qian, M. (2012) Stochastic theory of nonequilibrium steady states and its applications (Part I). Phys. Rep. 510, 1–86.

[32] Ge, H., Qian, M. and Qian, H. (2012) Stochastic theory of nonequilibrium steady states (Part II): Applications in chemical biophysics. Phys. Rep. 510, 87–118.

[33] Spohn, H. (1978) Entropy production for quantum dynamical semigroups. J. Math. Phys. 19, 1227–1230.

[34] Misra, B., Prigogine, I. and Courbage, M (1979) From deterministic dynamics to probabilistic descriptions. Proc. Natl. Acad. Sci. USA 76, 3607–3611.

[35] Bedeaux, D. and Mazur, P. (2001) Mesoscopic non-equilibrium thermodynamics for quantum systems. Physica A 298, 81–100.

[36] Reguera, D., Rubí, J.M. and Vilar, J.M.G. (2005) The mesoscopic dynamics of thermodynamic systems. J. Chem. Phys. B 109, 21502–21515.

[37] Ao, P. (2005) Laws of Darwinian evolutionary theory. Phys. Life Rev. 2, 117–156.

[38] Qian, H. (2006) Open-system nonequilibrium steady state: Statistical thermodynamics, fluctuations, and chemical oscillations. J. Chem. Phys. B 110, 15063–15074.

[39] Ao, P. (2008) Emerging of stochastic dynamical equalities and steady state thermodynamics from Darwinian dynamics. Commun. Theor. Phys. 49, 1073–1090.

[40] Qian, H. (2010) Cellular biology in terms of stochastic nonlinear biochemical dynamics: Emergent properties, isogenetic variations and chemical system inheritability. J. Stat. Phys. 141, 990–1013.
6 Appendices

6.1 Appendix A: Density matrix for a Markov process

The solution to Eq. 3 can be formally written as

$$p(t) = e^{Qt}p(0).$$  \hspace{1cm} (31)

One can introduce a Markov density matrix:

$$\rho_M(t) = e^{Qt}|p(0)\rangle\langle 1|$$ \hspace{1cm} (32)

in which $|p(0)\rangle$ is an $n \times 1$ matrix, i.e., a column vector, and $\langle 1|$ is a row vector consisting of 1s. Therefore, $\rho_M(t)$ is a matrix with $\text{Tr}(\rho_M) = \langle 1|p(t)\rangle = 1$. Furthermore,

$$\rho_M^2 = e^{Qt}|p(0)\rangle\langle 1| = \rho_M.$$ \hspace{1cm} (33)

Then we have $\rho_M(t)$ satisfying the same dynamic equation as the Kolmogorov forward equation

$$\frac{d}{dt}\rho(t) = Q\rho,$$ \hspace{1cm} (34)

with a difference in the initial data $\rho(0)$: It gives a transition probability matrix if $\rho(0) = I$; and it gives a density matrix if $\rho_M(0) = |p(0)\rangle\langle 1|$. Similarly, a density matrix approach can be formulated for Eq. 40. It yields

$$\frac{d}{dt}\rho(t) = i[\mathcal{H}\rho - \rho\mathcal{H}].$$ \hspace{1cm} (35)

6.2 Appendix B

The recently introduced “canonical conservative dynamics” [12] had been discussed in [4], in which the inner product in a Hilbert space is defined with $\rho(x)$ as a weight [19]; $\rho(x)$ being a positive, single-valued, analytic function on $\mathbb{R}^n$. In the contrary, the weight used in [12] is $\rho^{-1}(x)$. This difference can be seen in the matrix theory: Both $\Pi Q$ and $Q \Pi^{-1}$ are symmetric for reversible Markov process with generator $Q$, but only $\Pi^{-\frac{1}{2}} Q \Pi^{\frac{1}{2}}$ transforms the master equation into a gradient system. In fact, Koopman operator and Perron-Frobenius operator belong to two different Hilbert spaces with inner products

$$(\phi, \psi)_K = \int_{\mathbb{R}^n} \rho(x)\phi(x)\psi(x)dx,$$ \hspace{1cm} (36)
and
\[
(\phi, \psi)_{PF} = \int_{\mathbb{R}^n} \rho^{-1}(x)\phi(x)\psi(x)dx,
\]
respectively. Therefore, the symmetric operator in the Koopman (backward) space is
\[
\mathcal{L}_S^*[u] = \frac{1}{2} (\mathcal{L}^*[u] + \rho^{-1}\mathcal{L}[\rho u]) = \nabla \cdot (A(x)\nabla u) + (\nabla \ln \rho) A(x)(\nabla u),
\]
while in the Perron-Frobenius (forward) space is
\[
\mathcal{L}_S[u] = \frac{1}{2} (\mathcal{L}[u] + \rho\mathcal{L}^* [\rho^{-1}u]) = \nabla \cdot A(x)(\nabla u - (\nabla \ln \rho) u).
\]
Indeed, \(\mathcal{L}_S\) and \(\mathcal{L}_S^*\) correspond to the Kolmogorov forward and backward equations of a reversible diffusion.

### 6.3 Appendix C: Examples of skew-symmetric dynamics

**Simple continuous skew-symmetric operator: Schrödinger equation.** Let us consider the Schrödinger equation in free space without potential:
\[
\frac{\partial \psi(x, t)}{\partial t} = \frac{i}{2} \left( \frac{\hbar}{2m} \right) \frac{\partial^2}{\partial x^2} \psi(x, t),
\]
with initial value
\[
\psi(x, 0) = \frac{1}{(2\pi\sigma_0^2)^{1/4}} e^{-x^2/(4\sigma_0^2)}.
\]
The solution is
\[
\psi(x, t) = (8\pi\sigma_0^2)^{1/4} \sqrt{\frac{1}{4\sigma_0^2 + i2\pi\hbar t/m}} \exp \left[ -\frac{x^2}{4\sigma_0^2 + i2\pi\hbar t/m} \right].
\]
Then,
\[
\|\psi(x, t)\|^2 = \sqrt{\frac{8\sigma_0^2/\pi}{(4\sigma_0^2)^2 + (2\hbar t/m)^2}} \exp \left[ -\left( \frac{8\sigma_0^2 x^2}{(4\sigma_0^2)^2 + (2\hbar t/m)^2} \right) \right].
\]
This is a normalized Gaussian distribution with variance
\[
\sigma^2(t) = \sigma_0^2 + \left( \frac{\hbar t}{2m\sigma_0} \right)^2.
\]
The variance is not growing with \(t\), but \(t^2\): This is not diffusion. The “apparent velocity” is \(\pm \hbar/(2m\sigma_0)\). The factor \(\sigma_0\) means Heisenberg’s uncertainty principle: If the initial data has an “accuracy” of \(\sigma_0\), then the uncertainty in the velocity is \(\hbar/\sigma_0\).
The solution to Eqn. (40) has a Fourier representation in time:

\[
\psi(x, t) = \int_0^\infty \left\{ \left( \alpha_1 e^{\sqrt{2m\omega/\hbar}x} + \beta_1 e^{-\sqrt{2m\omega/\hbar}x} \right) e^{i\omega t} + \left( \alpha_2 \cos \sqrt{2m\omega/\hbar}x + \beta_2 \sin \sqrt{2m\omega/\hbar}x \right) e^{-i\omega t} \right\} d\omega
\]

\[
= \int_0^\infty \left\{ \left[ \alpha_1 e^{\sqrt{2m\omega/\hbar}x} + \beta_1 e^{-\sqrt{2m\omega/\hbar}x} + \alpha_2 \cos \sqrt{2m\omega/\hbar}x + \beta_2 \sin \sqrt{2m\omega/\hbar}x \right] \cos \omega t
\]

\[
+ \left[ \alpha_1 e^{\sqrt{2m\omega/\hbar}x} + \beta_1 e^{-\sqrt{2m\omega/\hbar}x} - \alpha_2 \cos \sqrt{2m\omega/\hbar}x - \beta_2 \sin \sqrt{2m\omega/\hbar}x \right] \sin \omega t \right\} d\omega
\]

(45)

Therefore, if \(\psi(x, 0)\) is an even, real-valued function of \(x\), we keep only the \(\alpha_2(\omega)\) term:

\[
\psi(x, t) = \left( 8\pi\sigma_0^2 \right)^{1/4} \int_0^\infty e^{-\sigma_0^2\omega^2} \cos \sqrt{2m\omega/\hbar}x \left( \cos \omega t - i \sin \omega t \right) d\omega. \quad (46)
\]

Then

\[
\|\psi(x, t)\|^2 = \left( 8\pi\sigma_0^2 \right)^{1/2} \int_0^\infty \int_0^\infty e^{-\sigma_0^2(\omega^2 + \omega'^2)} \cos \sqrt{2m\omega/\hbar}x \cos \sqrt{2m\omega'/\hbar}x
\]

\[
\left\{ \cos \omega t \cos \omega' t + \sin \omega t \sin \omega' t \right\} d\omega d\omega'. \quad (47)
\]

**A discrete skew-symmetric dynamics.** Consider anti-symmetric dynamics

\[
\frac{dx}{dt} = Ax \quad \text{(48)}
\]

with

\[
A = \begin{pmatrix}
0 & -\lambda_1 & 0 & 0 \\
\lambda_1 & 0 & 0 & 0 \\
0 & 0 & 0 & -\lambda_2 \\
0 & 0 & \lambda_2 & 0
\end{pmatrix}. \quad (49)
\]

Then the solution to equation is

\[
x(t) = e^{At} x(0) \quad \text{in which} \quad e^{At} = \begin{pmatrix}
\cos \lambda_1 t & -\sin \lambda_1 t & 0 & 0 \\
\sin \lambda_1 t & \cos \lambda_1 t & 0 & 0 \\
0 & 0 & \cos \lambda_2 t & -\sin \lambda_2 t \\
0 & 0 & \sin \lambda_2 t & \cos \lambda_2 t
\end{pmatrix}. \quad (50)
\]

\[\text{More precisely, we only know the } \|\psi(x, 0)\|^2, \text{ but this does not uniquely specify the } \psi(x, 0). \text{ Therefore, there is a uncertainty in the initial value for } \psi(x, t). \text{ Different choices here lead to different behaviour in the following dynamics for } t > 0.\]
Therefore, if \( x(0) = \left( \frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}, 0 \right)^T \), then
\[
\begin{pmatrix}
\|x_1(t)\|^2 \\
\|x_2(t)\|^2 \\
\|x_3(t)\|^2 \\
\|x_4(t)\|^2
\end{pmatrix}
= \frac{1}{2}
\begin{pmatrix}
\cos^2 \lambda_1 t \\
\sin^2 \lambda_1 t \\
\cos^2 \lambda_2 t \\
\sin^2 \lambda_2 t
\end{pmatrix}.
\]
(51)

However, if \( x(0) = \left( \frac{1}{2}, \frac{1}{2}, \frac{1}{\sqrt{2}}, 0 \right)^T \), then
\[
\begin{pmatrix}
\|x_1(t)\|^2 \\
\|x_2(t)\|^2 \\
\|x_3(t)\|^2 \\
\|x_4(t)\|^2
\end{pmatrix}
= \begin{pmatrix}
\frac{1-\sin 2\lambda_1 t}{4} \\
\frac{1+\sin 2\lambda_1 t}{4} \\
\frac{\cos^2 \lambda_2 t}{2} \\
\frac{\sin^2 \lambda_2 t}{2}
\end{pmatrix}.
\]
(52)

If \( \lambda_1 \) and \( \lambda_2 \) are non-commensurate, then the \( x(t) \) is not periodic. If dimension of \( A \) is odd, then it has a zero eigenvalue.

The finite dimensional Eqn. (52) should be compared with the infinite dimensional Eqn. (47). Heisenberg’s uncertainty in the continuous dynamics is a consequence of infinite number of non-commensurate frequencies.