Optimization of Markov process violates detailed balance condition

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(Dated: February 23, 2016)

We consider the optimization of Markovian dynamics to pursue the fastest convergence to the stationary state. The brachistochrone method is applied to the continuous-time master equation for finite-size systems. The principle of least action leads to a brachistochrone equation for the transition-rate matrix. Three-state systems are explicitly analyzed, and we find that the solution violates the detailed balance condition. The properties of the solution are studied in detail to observe the optimality of the solution. We also discuss the counterdiabatic driving for the Markovian dynamics. The transition-rate matrix is then divided into two parts, and the state is given by an eigenstate of the first part. The second part violates the detailed balance condition and plays the role of a counterdiabatic term.

PACS numbers: 02.50.-r, 05.10.Ln, 02.70.Tt, 05.70.Ln

I. INTRODUCTION

The Markov-chain Monte Carlo method is widely used in various fields of research to realize a desired distribution by simulating the stochastic dynamics. Frequently used algorithms such as Metropolis and heat-bath algorithms are under a well-known limitation called the detailed balance condition (DBC) [1, 2]. This is not a necessary condition but rather a sufficient one for convergence to the stationary distribution. Recent studies revealed that violation of the DBC can accelerate relaxation. Several algorithms were proposed in the literature to show the speed-up of convergence to the stationary state and the reduction of the correlation time of the sampling [3–6]. Ichiki and Ohzeki mathematically showed that the violation gives shorter relaxation times [7]. They provided insight into the acceleration of the relaxation to the steady state from the viewpoint of rare-event sampling [8] and developed a simple method to implement the violation in Langevin dynamics [9–11].

The preceding studies, as listed above, focused on the violation of the DBC. Although the violation actually leads to the speed-up of the convergence, we still have considerable freedom in choosing the algorithm. No general principles to determine the optimality of algorithms are known, which prevents us from developing efficient algorithms. Several studies on optimization were performed within the DBC [11–12]. In addition, the minimization of the Kullback–Leibler divergence between the original dynamics under the DBC and an alternative stochastic pathway results in a nontrivial solution without the DBC but with the common observables in the stationary state [8–13]. In the present study, we formulate a general method to generate the optimal stochastic rule by developing an optimization method in quantum mechanics.

The Markov-chain Monte Carlo method is formulated using the master equation. It is a first-order differential equation in time and is formally understood as the imaginary-time Schrödinger equation. The transition-rate matrix corresponds to the quantum Hamiltonian. We exploit this similarity to develop a formal method to optimize the stochastic dynamics. In quantum systems, the brachistochrone method has been studied to determine the optimal Hamiltonian under specified constraints [14, 15]. We may naively expect that this idea can be directly applied to the optimization of the master equation. The optimal solution yields the stochastic dynamics with the fastest convergence to the stationary state, which results in the best algorithm in the Markov-chain Monte Carlo method in terms of convergence speed.

Furthermore, the quantum brachistochrone method leads to a fascinating connection to a different type of optimization called “shortcuts to adiabaticity” [16–20]. Under some condition, the optimized quantum state obtained from the brachistochrone equation (BE) follows an adiabatic passage, which is defined by the instantaneous eigenstates of a time-dependent Hamiltonian [21]. Although we usually treat a time-independent transition-rate matrix in the master equation, studying counterdiabatic driving in the present system can provide insight to obtain the optimal algorithm.

The aim of the present work is as follows. First, we formulate a brachistochrone method to optimize the transition-rate matrix in the master equation. Second, we investigate whether the DBC is actually violated in the optimized solution. Third, we study our optimization method from the viewpoint of shortcuts to adiabaticity.

The rest of the paper is organized as follows. In Sec. II, the master equation is defined and is deformed for the convenience of our analysis. Section III is the main part of the present work, where the brachistochrone method for the master equation is formulated. The general form of the BE is derived, and we discuss its general properties. Three-state systems are studied in detail in Sec. IV. In Sec. V, we extend our method to time-dependent systems...
to observe the connection to shortcuts to adiabaticity. The summary is presented in the last section VI.

II. MASTER EQUATION

The Markov-chain Monte Carlo method is described by the master equation. The continuous-time master equation for discrete $N$ states is suitable for our purpose and is written as

$$\frac{d}{dt}p_i(t) = \sum_{j=1}^{N} q_{ij}p_j(t),$$  \hspace{1cm} (1)

where $i = 1, 2, \ldots, N$. $p(t) = (p_1(t), p_2(t), \ldots, p_N(t))$ denotes a probability distribution at time $t$ satisfying

$$\sum_{i=1}^{N} p_i(t) = 1.$$  \hspace{1cm} (2)

The coefficient $q_{ij}$ with $i \neq j$ is positive and denotes an incoming transition probability rate from the state $j$ to $i$. The diagonal element $q_{ii}$ is negative, and the magnitude represents the outgoing probability rate of state $i$. It is determined so that the following relation holds:

$$\sum_{j=1}^{N} q_{ji} = 0.$$  \hspace{1cm} (3)

By taking the sum over $i$ in Eq. (1), we see that this is a condition for the conservation of normalization.

At $t \to \infty$, we assume that the probability distribution becomes a stationary one as

$$p_i(t) \to \pi_i.$$  \hspace{1cm} (4)

Then, the balance condition requires

$$\sum_{j=1}^{N} q_{ij} \pi_j = 0.$$  \hspace{1cm} (5)

The transition-rate matrix $q$ is determined so that Eqs. (3) and (5) are satisfied. In the traditional approach, we use the DBC

$$q_{ij} \pi_j = q_{ji} \pi_i$$  \hspace{1cm} (6)

instead of the balance condition (5). This is a sufficient condition for convergence to the stationary distribution and is not necessarily satisfied. In the present study, we consider the optimization of the master equation without imposing the DBC. For convergence to the stationary distribution, we need an additional condition of irreducibility. Irreducibility can be checked by observing the obtained solution, and we do not treat the condition explicitly.

For the convenience of notation, we change the variables as

$$P_i(t) = \frac{1}{\sqrt{\pi_i}}p_i(t),$$  \hspace{1cm} (7)

$$W_{ij} = \frac{1}{\sqrt{\pi_i}}q_{ij}\sqrt{\pi_j}.$$  \hspace{1cm} (8)

Then, the form of the master equation is unchanged:

$$\frac{d}{dt}P_i(t) = \sum_{j=1}^{N} W_{ij}P_j(t).$$  \hspace{1cm} (9)

The normalization condition for $P_i(t)$ is given by

$$\sum_{i=1}^{N} \sqrt{\pi_i}P_i(t) = 1.$$  \hspace{1cm} (10)

By definition, the transition rate $W_{ij}$ satisfies

$$\sum_{i=1}^{N} \sqrt{\pi_i}W_{ij} = 0.$$  \hspace{1cm} (11)

This condition is equivalent to Eq. (3). We note that the diagonal elements of $W$ are negative and the off-diagonal elements are positive.

The stationary distribution is given by

$$P_i(t) \to \sqrt{\pi_i}.$$  \hspace{1cm} (12)

The balance condition (5) and DBC (6) are rewritten, as

$$\sum_{j=1}^{N} W_{ij}\sqrt{\pi_j} = 0,$$  \hspace{1cm} (13)

$$W_{ij} = W_{ji}.$$  \hspace{1cm} (14)

The advantage of representation (9) is that the DBC is represented simply by the symmetry of the matrix $W$.

Since the transition-rate matrix $W$ is asymmetric in general, the eigenvalue equations are written by using the right and left eigenstates.

$$W|R_i\rangle = \Lambda_i |R_i\rangle,$$  \hspace{1cm} (15)

$$\langle L_i|W = \langle L_i|\Lambda_i.$$  \hspace{1cm} (16)

These vectors are orthonormalized with each other:

$$\langle L_i|R_j\rangle = \delta_{ij}.$$  \hspace{1cm} (17)

We also know that $|\pi\rangle = (\sqrt{\pi_1}, \sqrt{\pi_2}, \ldots, \sqrt{\pi_N})^T$ and $\langle \pi| = (\sqrt{\pi_1}, \sqrt{\pi_2}, \ldots, \sqrt{\pi_N})$ are the right and left eigenstates with zero eigenvalue, respectively. They satisfy the normalization $\langle \pi|\pi\rangle = 1$ and are orthogonal to the other eigenstates. The spectral decomposition of $W$ is written as

$$W = \sum_{i=1}^{N-1} \Lambda_i |R_i\rangle\langle L_i| + 0 \cdot |\pi\rangle\langle \pi|.$$  \hspace{1cm} (18)

The formal solution of the probability distribution $|P(t)\rangle = (P_1(t), \ldots, P_N(t))^T$ is given by

$$|P(t)\rangle = e^{Wt} |P(0)\rangle$$  \hspace{1cm} (19)

$$= \sum_{i=1}^{N-1} e^{\Lambda_i t} |R_i\rangle \langle L_i|P(0)\rangle + |\pi\rangle,$$
where we use the property $\langle \pi | P(t) \rangle = 1$. In order for the system to approach the stationary distribution $\pi$, we require the condition $\Re \Lambda_i < 0$. This property is mathematically described by the Perron–Frobenius theorem.

Representation \cite{12} shows that the relaxation time is given by $\text{Max}(-1/\Re \Lambda_i)$. Smaller values of the relaxation time accelerate the relaxation to the stationary distribution.

III. BRACHISTOCHROME EQUATION

A. Kullback–Leibler divergence

The main idea of the present work is to use the similarity between the master equation and the Schrödinger equation. We naively expect that the formulation used in quantum mechanics can be directly applied to the Markovian dynamics. The brachistochrone method requires a quantity to be optimized using the variational principle. Here, we optimize the duration between the initial and final states. This means that our aim is to derive the optimal solution with the fastest convergence between the initial and final states. This means that our aim is to define the velocity, we obtain the duration in an integral form as

$$T = \int \frac{ds}{v} = \int dt \sqrt{\sum_{i=1}^{N} \frac{\sqrt{P_i \pi_i}}{\sum_{j=1}^{N} W_{ij} P_j}}. \quad (27)$$

We note that the master equation is not imposed in this expression. When we impose the master equation, the integrand tends to unity, and we obtain a trivial integral. To determine the optimal solution, we perform the variational method in a larger space. The master equation is imposed as a constraint.

In the context of the quantum brachistochrone method, the form of the BE is shown to be insensitive to the measure \cite{13}. It is not obvious whether the same property holds in the present formulation. Therefore, we adopt the above measure for optimization.

B. Brachistochrone equation

In the brachistochrone method, the Euler–Lagrange equation of motion is derived by considering the variation with respect to dynamical variables. In the present case, we consider the variations with respect to the probability distribution $P(t)$ and the transition-rate matrix $W$ under some constraints. The constraints to be imposed are as follows: (i) master equation \cite{9}; (ii) normalization \cite{10}; (iii) conservation of normalization \cite{11}; (iv) balance condition \cite{13}; and (v) other constraints for $W$ represented as

$$f_a(W) = 0 \quad (a = 1, 2, \ldots). \quad (28)$$

By introducing multipliers, we define the action to be minimized as $S = T + S_c$, where

$$S_c = \int dt \sum_{i=1}^{N} \lambda_i^{(i)}(t) \left( \frac{d}{dt} P_i(t) - \sum_{j=1}^{N} W_{ij} P_j(t) \right) + \int dt \lambda^{(i)}(t) \left( 1 - \sum_{i=1}^{N} \sqrt{\pi_i P_i(t)} \right)$$

$$= \int dt \sum_{i=1}^{N} \lambda_i^{(i)}(t) \left( \frac{d}{dt} P_i(t) - \sum_{j=1}^{N} W_{ij} P_j(t) \right) + \int dt \lambda^{(i)}(t) \left( 1 - \sum_{i=1}^{N} \sqrt{\pi_i P_i(t)} \right) \quad (29)$$

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We note that the multipliers $\lambda^{(i)}(t)$ and $\lambda^{(ii)}(t)$ are real functions of $t$ and the other multipliers, $\lambda^{(iii)}_j$, $\lambda^{(iv)}$, and $\lambda^{(v)}_a$, are time-independent real constants.

We first consider the variation $P_i \to P_i + \delta P_i$. The condition $\left. \frac{\delta S}{\delta P_i(t)} \right|_{t} = 0$ yields

$$\frac{d}{dt} \left( \frac{\pi_i^0}{\sqrt{\frac{\pi_i^0}{\sum_{j=1}^{N} \pi_j^0 P_j^2}}} - \sum_{k=1}^{N} \frac{\sqrt{\pi_k^0 P_k^2}}{\sqrt{\frac{\pi_k^0}{\sum_{j=1}^{N} \pi_j^0 P_j^2}}}, \right) - \sum_{j=1}^{N} \lambda_j^{(i)} W_{ji} - \lambda^{(ii)} \sqrt{\pi_i} = 0. \quad (30)$$

To eliminate the multiplier constant $\lambda^{(ii)}$, we multiply $\sqrt{\pi_i}$ and take the sum over $i$. Thus, we obtain

$$\lambda^{(ii)} = - \frac{d}{dt} \left( \frac{\sum_{i=1}^{N} \pi_i^0 P_i^2}{\sum_{j=1}^{N} \pi_j^0 P_j^2} \right) - \sum_{i=1}^{N} \delta W_{ji} \lambda^{(i)}_i \sqrt{\pi_i}. \quad (31)$$

Equation (31) is written in vector form as

$$(1 - Q)|\lambda^{(i)}(t)| + W^T |\lambda^{(i)}(t)| = -(1 - Q)|\delta(t) - W^T |\delta(t)|, \quad (32)$$

where $|\lambda^{(i)}(t)|$ is the $N$-component vector, the elements of which are given by $\lambda^{(i)}_1, \lambda^{(i)}_2, \ldots, \lambda^{(i)}_N$, respectively. Here, $|\delta\rangle$ is defined in the same manner, and the ith element is given by

$$\delta_i = \frac{\pi_i^0 P_i^2}{\sum_{j=1}^{N} \pi_j^0 P_j^2}. \quad (33)$$

We also define the projection matrix

$$Q = |\pi\rangle \langle \pi|. \quad (34)$$

Then, Eq. (32) is formally solved as

$$|\lambda^{(i)}(t)| + |\delta(t)| = e^{-W^T t} \left( |\lambda^{(i)}(0)| + |\delta(0)| \right). \quad (35)$$

We note that $(1 - Q)W^T = W^T$. By the multiplication of $W^T$, a state is projected onto the space excluding $|\pi\rangle$.

Next, we consider the variation $W_{ij} \to W_{ij} + \delta W_{ij}$ and impose the condition $\partial S/\partial W_{ij} = 0$. We obtain

$$+ \sum_{i,j=1}^{N} \left( \sqrt{\pi_i} W_{ij} \lambda^{(iii)}_j + \lambda^{(iv)}_i W_{ij} \sqrt{\pi_j} \right)$$

$$+ \sum_{a} \lambda^{(v)}_a f_a(W). \quad (29)$$

$\lambda^{(iii)}_j$ and $\lambda^{(iv)}_j$ can be eliminated using the corresponding constraints, as was the case for $\lambda^{(i)}$. Then, we have

$$\int dt \left[ \lambda^{(i)}_i + \delta_i - \sqrt{\pi_i} \sum_{k=1}^{N} \sqrt{\pi_k} (\lambda^{(i)}_k + \delta_k) \right] (P_j - \sqrt{\pi_j})$$

$$= \sum_{a} \lambda^{(v)}_a \left( \frac{\partial f_a}{\partial W_{ij}} - \sum_{k=1}^{N} \frac{\partial f_a}{\partial W_{jk}} \sqrt{\pi_k} \sqrt{\pi_j} \right) \sqrt{\pi_i} \sum_{k=1}^{N} \frac{\partial f_a}{\partial W_{kj}} \sqrt{\pi_k} \sqrt{\pi_j}. \quad (37)$$

By inserting the solution of $\lambda^{(i)}_i$ into Eq. (35) to this equation, we obtain the result in matrix form,

$$(1 - Q)F(1 - Q) = \int dt |\pi(t) - |\pi\rangle\rangle \left( |\lambda^{(i)}(0)| + |\delta(0)| \right) e^{-W^T t} (1 - Q), \quad (38)$$

where $F$ is the $N \times N$ matrix, the elements of which are given by

$$F_{ij} = \sum_{a} \lambda^{(v)}_a \frac{\partial f_a}{\partial W_{ji}}. \quad (39)$$

Using the formal representation of the master equation (11), we obtain the BE

$$F_\perp = \int_0^T dt e^{W^T t} G_\perp e^{-W^T t}, \quad (40)$$

where

$$F_\perp = (1 - Q)F(1 - Q), \quad (41)$$

$$G_\perp = (|P(0) - |\pi\rangle\rangle |\lambda_\perp\rangle, \quad (42)$$

and $|\lambda_\perp\rangle$ is an arbitrary and constant vector satisfying

$$Q|\lambda_\perp\rangle = 0. \quad (43)$$

We also have

$$QF_\perp = F_\perp Q = 0, \quad (44)$$

$$QG_\perp = G_\perp Q = 0. \quad (45)$$

The BE (40) is the main result of the present work.

C. General properties of the brachistochrone equation

The constraints (28) determine the form of the matrix $F$, and the BE (40) is solved under given initial and final states with constraints (i)–(v), in principle. It should be noted that the result strongly depends on the constraints. This property is reasonable because we will have an infinitely small duration if we do not impose any constraints. Conversely, the result seems to be insensitive to
the measure in Eq. (27). It is reflected in the definition of \( \delta_i \) in Eq. (33), but the explicit form is not important for the final BE (40). These properties are the same as in the case of the quantum BE.

Generally, it is a difficult task to parametrize the final state. Here, we proceed as follows. We set the parameters in \( G \) to find an appropriate final state \( p(T) \). The transition-rate matrix \( W \) is parametrized under the constraints (i)-(v), and the unknown parameters are obtained by solving the BE. This procedure corresponds to specifying the initial position and velocity, instead of fixing the initial and final positions in the variational method, as is the case for classical mechanics.

We also mention here the difference between the present BE and the quantum BE. In the quantum case, we usually consider a time-dependent Hamiltonian, and the BE represents an equation of motion satisfied at all values of \( t \). Consequently, the optimized solution is characterized by a dynamical invariant \( 21, 22 \). This is not the case in the present system, and the corresponding invariant does not exist. To clarify the meaning of the quantity \( F \), we study the BE in Sec. IV by allowing time-dependent fluctuations of the transition matrix \( W \).

Below, we show how to solve the BE (40). By using the eigenstates introduced in Sec. II, we write

\[
|P(0)\rangle - |\pi\rangle = \sum_{i=1}^{N-1} p_i |R_i\rangle,
\]

\[
\langle \lambda_\perp \rangle = \sum_{i=1}^{N-1} \lambda_i \langle L_i \rangle.
\]

The coefficients \( p_i \) and \( \lambda_i \) are determined from the initial condition.

Possible general forms of the operator \( F \) are considered as follows. As a constraint, we assume the form

\[
f_a = \text{Tr} W X_a,
\]

where \( X_a \) represents a matrix. For example, when we specify the \( ji \) component of \( W \), we use \( \langle X \rangle_{\mu \nu} = \delta_{\mu j} \delta_{\nu i} \). Then \( F \) is written as

\[
F = \sum_a \lambda_a^{(v)} X_a.
\]

By using the spectral decomposition, we write the BE as

\[
\sum_a \lambda_a^{(v)} \langle L_i | X_a | R_j \rangle = e^{(L_i - L_j)T} - 1 \frac{1}{L_i - L_j} \nu_j \nu_i.
\]

\( W \) and \( \lambda_a^{(v)} \) are determined for given \( p = (p_1, \ldots, p_{N-1}) \), \( \lambda = (\lambda_1, \ldots, \lambda_{N-1}) \), and \( T \). In \( N \)-dimensional space, \( W \) has \((N - 1)^2\) degrees of freedom if we consider constraints (iii) and (iv). Constraint (v) does not change the number of undetermined parameters, because a multiplier constant is introduced for each constraint.

Some of their parameters are determined by considering the trace of the equation. We have

\[
\sum_a \lambda_a^{(v)} \text{Tr} X_a - \langle \pi | X_a | \pi \rangle = T \sum_{i=1}^{N-1} p_i \lambda_i,
\]

\[
\sum_a \lambda_a^{(v)} \text{Tr} W^k X_a = T \sum_{i=1}^{N-1} \Lambda^k \nu_i \lambda_i,
\]

where \( k \) is an integer. These relations determine \( N - 1 \) parameters. For the remaining parameters, we cannot derive any general formula without explicitly calculating the eigenstates of \( W \). In the following, we study a simple system with \( N = 3 \) to observe how the parameters are determined from the BE.

## IV. THREE-STATE SYSTEM

### A. Parametrization

In the case of \( N = 3 \), \( W \) is parametrized as

\[
W = \begin{pmatrix}
-\frac{\pi_2 a + \pi_3 b}{\pi_2 \pi_1 a + \pi_3 \delta} & \sqrt{\pi_1} \pi_2 a - \sqrt{\pi_3} \delta & \sqrt{\pi_1} \pi_3 b + \sqrt{\pi_3} \delta \\
\sqrt{\pi_2 \pi_1 a + \sqrt{\pi_3} \delta} & \pi_3 c + \pi_1 a & \pi_2 \pi_3 c - \sqrt{\pi_1} \delta \\
\pi_3 \pi_1 b - \sqrt{\pi_2} \delta & \sqrt{\pi_3 \pi_2 c + \pi_1 \delta} & \pi_1 b + \pi_2 c
\end{pmatrix},
\]

which ensures non-negative values of the off-diagonal elements.

The initial distribution is parametrized as

\[
|P(0)\rangle = \begin{pmatrix}
p_1 / \sqrt{\pi_1} \\
p_2 / \sqrt{\pi_2} \\
p_3 / \sqrt{\pi_3}
\end{pmatrix},
\]

where \( p_{1,2,3} \) are non-negative numbers satisfying \( p_1 + p_2 + p_3 = 1 \). In what follows, we consider the uniform distribution \( p_1 = p_2 = p_3 = 1/3 \). It is difficult to parametrize
the BE explicitly by using parameters in \( |P(T)\rangle \), as mentioned in the previous section. Therefore, we use a different parameter to characterize the BE. It is naturally defined in the course of the following calculations.

The transition-rate matrix \( W \) can be diagonalized as
\[
W = \Lambda_+ |R_+\rangle \langle L_+| + \Lambda_- |R_-\rangle \langle L_-|,
\]
where \( |R_\pm\rangle \) and \( \langle L_\pm| \) are the right and left eigenstates, respectively. Their negative eigenvalues are given by
\[
\Lambda_\pm = -\frac{A}{2} \pm \frac{\Delta}{2}.
\]
We define
\[
\Delta = \sqrt{A^2 - 4B},
\]
\[
A = (1 - \pi_3)a + (1 - \pi_2)b + (1 - \pi_1)c,
\]
\[
B = \pi_1 ab + \pi_3 bc + \pi_2 ca + \delta^2,
\]
where \( \Delta \) represents the gap between two states \( \pm \). In the general formulation, \( \Delta \) is not necessarily real, but the following analysis shows that it is real in the present three-state case. We also note that \( A \geq 0 \) and \( B \geq 0 \). By using the eigenstates of \( W \), we parametrize \( |P(0)\rangle \) and \( |\lambda_\perp\rangle \) as
\[
|P(0)\rangle - |\pi\rangle = |R_+\rangle p_+ + |R_-\rangle p_-,
\]
\[
|\lambda_\perp\rangle = \lambda_+ |L_+\rangle + \lambda_- |L_-\rangle.
\]

The right-hand side of the BE is calculated as
\[
\int_0^T dt e^{Wt} G \circ e^{-Wt} = T \left( \begin{array}{cc} p_+ \lambda_+ & p_+ \lambda_- (e^-) \\ p_- \lambda_+ (e^-) & p_- \lambda_- \end{array} \right),
\]
where
\[
\langle e^- \rangle = \frac{1}{T} \int_0^T dt e^{-\Delta t} = \frac{1 - e^{-\Delta T}}{\Delta T},
\]
\[
\langle e \rangle = \frac{1}{T} \int_0^T dt e^{\Delta t} = \frac{e^{\Delta T} - 1}{\Delta T}.
\]

In the following analysis, we set \( a = 1 \) as a constraint. Then, the matrix \( F \) is written as
\[
F = \lambda^{(v)} X = \lambda^{(v)} \left( \begin{array}{ccc} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{array} \right).
\]
The BE reads
\[
\lambda^{(v)} \left( \begin{array}{c} \langle L_+ |X|R_+\rangle \\ \langle L_- |X|R_-\rangle \end{array} \right) = T \left( \begin{array}{cc} p_+ \lambda_+ & p_+ \lambda_- (e^-) \\ p_- \lambda_+ (e^-) & p_- \lambda_- \end{array} \right).
\]

### B. Analysis of the brachistochrone equation

To find the explicit form of Eq. (57), we first use Eq. (61). By taking the trace of Eq. (67), we obtain
\[
\frac{\lambda^{(v)}}{T} = -\frac{p_+ \lambda_+ + p_- \lambda_-}{2\sqrt{\pi_1 \pi_2}}.
\]
This relation determines the multiplier \( \lambda^{(v)} \). Next, we consider Eq. (62) with \( k = 1 \), which gives
\[
A = 2a + \frac{1 - z}{1 + z},
\]
where
\[
z = \frac{p_- \lambda_+}{p_+ \lambda_-}.
\]
Equations (58) and (59) are obtained from the diagonal elements of the BE.

One of the remaining two equations is obtained by taking the trace of the square of Eq. (67). After some calculations, we arrive at the expression
\[
\left( \frac{\sinh \frac{\Delta T}{2}}{\frac{\Delta T}{2}} \right)^2 = 1 + \frac{\pi_3}{\pi_1 \pi_2} \frac{(1 + z)^2}{4z}.
\]
The derived equation is parameterized by \( z \), which is defined in Eq. (70). We take this variable as a natural parameter characterizing the distribution at \( t = 0 \).

To determine the last equation, we need to know the explicit form of the eigenfunctions \( \langle L_\pm | \) and \( |R_\pm\rangle \). We consider the ratio of the off-diagonal parts of the BE, which is written as
\[
\frac{\langle L_+ |X|R_-\rangle}{\langle L_- |X|R_+\rangle} = \frac{p_+ \lambda_- e^{\Delta T}}{p_- \lambda_+}.
\]
The explicit form of this equation is discussed in what follows.

For given parameters \( a \), \( p_{1,2,3} \), \( \pi_{1,2,3} \), and \( z \), other parameters \( b \), \( c \), and \( T \) are obtained from Eqs. (60), (71), and (72). It is impossible to determine four parameters from three equations. This uncertainty is resolved by demanding the minimum possible value of \( T \).

The quantity \( \Delta T \) is determined using Eq. (71). As shown in Fig. 1, we can determine a real solution for an arbitrary value of \( z \) with \( z \geq 0 \). To observe other possibilities, we consider the definition of \( \Delta \) in Eq. (55). We find that \( \Delta \) can be purely imaginary when \( A^2 < 4B \). By inserting the expression \( \Delta = i\Delta \) into Eq. (71), we see that the equation can be solved by using a negative \( z \). However, Eq. (59) shows that \( (1 - z)/(1 + z) \) must be purely imaginary because \( A \) is always real. We put
\[
\frac{1 - z}{1 + z} = -i\alpha,
\]
where $\alpha$ is real. Equation (74) is written as

$$
\left( \sin \frac{\Delta T}{2} \right)^2 = 1 + \frac{\pi_3}{\pi_1 \pi_2} \frac{1}{1 + \alpha^2}.
$$

(74)

This has no solution, and we conclude that the BE does not give complex eigenvalues in the present case. This result is reasonable because the imaginary part of the eigenvalues of the transition-rate matrix does not accelerate relaxation.

The variable $A$ is written as Eq. (69) and $B = \frac{1}{4} (A^2 - \Delta^2)$. As these quantities must be non-negative, we have

$$
\Delta \leq \frac{1 + z}{z} a.
$$

(75)

We seek the smallest $T$, which means that $\Delta$ takes the largest possible value. When the equality holds in Eq. (73), $B = 0$, and we obtain a trivial solution $b = c = \delta = 0$. Therefore, to find the nontrivial result, we take a $\Delta$ smaller than the maximum possible value. It is parametrized as

$$
\Delta = \frac{1 + z}{z} a g.
$$

(76)

where $0 \leq g \leq 1$. Then

$$
A = a \left( 2 + \frac{1 - z}{z} g \right).
$$

(77)

We also introduce $\tau$ with the condition $0 \leq \tau \leq 1$ to write

$$
b = \frac{A - (1 - \pi_3) a}{1 - \pi_2} \tau,
$$

(78)

$$
c = \frac{A - (1 - \pi_3) a}{1 - \pi_1} (1 - \tau).
$$

(79)

Using these parametrizations, we can rewrite Eq. (72) in the form

$$
\delta = f(g, \tau, \delta^2, z),
$$

(80)

where $f$ is a function of the specified variables. The detailed calculation and the explicit form of $f$ are presented in the Appendix. Here, we simply mention that the parameters $p_{\pm}$ and $\lambda_{\pm}$ appear only through $z$.

For given $a$, $p_{1,2,3}$, and $\pi_{1,2,3}$, the solution is obtained as follows.

1. Fix the parameter $z$ with $z > 0$.
2. Calculate $\Delta T$ from Eq. (71).
3. Take $\tau$ between 0 and 1.
4. Take $g$ between 0 and 1.
5. Calculate $A$, $\Delta$, $B$, $b$, $c$, and $\delta^2$ using Eqs. (58), (60), (77), (78), and (79).
6. Check the positivity of the off-diagonal elements of $W$. If not, go back to step 4 and repeat the calculation with a different $g$.
7. Calculate $\delta$ from Eq. (80). Determine $g$ so that $\delta^2$ coincides with that calculated in Eq. (60). Thus, $g$ is determined for a fixed $z$ and $\tau$.
8. Change $\tau$ and repeat the calculation. Choose the solution with the largest $g$ ($\Delta$). The parameters $g$ and $\tau$ are determined for a fixed $z$.
9. Obtain $T$ from $T = (\Delta T) / \Delta$.
10. Change $z$ and repeat the calculation.

We numerically solve the BE according to this algorithm. In what follows, we set parameters $a = 1$ and $(\pi_1, \pi_2, \pi_3) = (0.5, 0.3, 0.2)$.

To find the solution of Eq. (80), we plot $|\delta - f(g, \tau, \delta^2, z)|$ as a function of $g$ and $\tau$ for a fixed $z$ in Fig. 2. The result is plotted only when the $\delta^2$ obtained from Eq. (60) is positive. We also need to impose the condition of non-negativity of the off-diagonal elements of $q$ in Eq. (54). Equation (80) has many solutions, and we select, in principle, the one with the largest value of $g$. We see from Fig. 2 that the solutions are classified into left and right branches. The solutions in the left branch are aligned along a single curve, and those in the right branch appear to be more complicated. We consider the left branch in the following calculations, and the meaning of the branches is discussed afterwards.

By taking the optimum $g$ and $\tau$, we can obtain $\delta$ and calculate other parameters. In Fig. 3 we plot the result of $b$, $c$, and $\delta$ for a given $z$. Nonzero values of $\delta$ show violation of the DBC. We expect from the previous analysis that a larger $\delta$ accelerates relaxation [7]. However, each matrix element of $q$ must be non-negative. As we see in Fig. 4, where all matrix elements are plotted, one of the
FIG. 2. |δ − f(g, τ, δ^2, z)| (Eq. (80)) as a function of g and τ. Top: The result with z = 0.2. Bottom: The result with z = 7.0. Points satisfying condition (54) are specified by the region surrounded by the dashed curves. For z = 0.2, the optimal solution is denoted by the circle. For z = 7.0, the solution is denoted by point (B). Point (A) is used as a suboptimal solution in the following analysis.

FIG. 3. Parameters b, c, and δ in the transition-rate matrix W. We take the solution with b < c.

FIG. 4. Off-diagonal elements of q representing transition rates.

FIG. 5. Eigenvalues of matrix W.

elements q_{13} is almost equal to zero. This means that |δ| takes the maximum possible value, and the violation of DBC is maximal.

We also show the nonzero eigenvalues of W in Fig. 5 and the duration T and probability distribution at t = T in Fig. 6. If the value of z is not so small, the probability distribution p(T) is very close to the stationary distribution π at t → ∞. This is a practically useful property because we usually do not set the distribution at a finite duration.

As mentioned above, the solutions of the BE are classified into two parts. To determine the meaning of the solutions, we take the solutions in both parts for z = 7.0, which are shown in Fig. 7. Solutions (A) and (B) represent the points in Fig. 2, respectively. We see that solution (A) in the left branch gives a flow 3 → 2 → 1, and the direct transition between 1 and 3 is suppressed. This is a reasonable result because the stationary distribution in the present calculation satisfies π_3 > π_2 > π_1. On the other hand, the right branch satisfies b > c, and the transition between 2 and 3 is suppressed. In other words, the flow is not in a single direction and becomes complicated. This is considered to be the reason why the solutions of the right branch in Fig. 2 are more complicated than those of the left branch.
FIG. 6. Duration $T$ (rightmost grid line) and probability distribution function $p = (p_1, p_2, p_3)$ at $t = T$ (leftward grid lines).

FIG. 7. Flow diagrams for $z = 7.0$. Top: Solution (A) in Fig. 2. Bottom: Solution (B) in Fig. 2. The width of the arrow from state $j$ to $i$ indicates the transition rate $q_{ij}$, which is also specified by the corresponding number.

C. Optimality of the solution

To see the optimality of the solution, we calculate the Kullback–Leibler divergence $D(p(T)|\pi)$ between state $p(T)$ and $\pi$. This value is compared with the same quantity with $\delta = 0$ and the other parameters unchanged. The result is plotted in Fig. 8 and shows that $D(p(T;\delta)|\pi) < D(p(T;0)|\pi)$. The inclusion of the violation parameter indeed accelerates relaxation, as discussed in Ref. 7.

In principle, our optimization is performed to minimize the duration between $p(0)$ and $p(T)$. Although $p(T)$ is very close to the stationary distribution $\pi$, as we show in Fig. 8, the optimality of the approach to $\pi$ is not guaranteed. Therefore, the use of $D(p(T)|\pi)$ is not justified to prove the optimality of the solution.

We consider the distance between the final distribution $p_{\text{opt}} = p(T)$ and the distribution $p(t, \delta)$ as a function of $t$ and $\delta$. The other parameters $a, b,$ and $c$ are the same as those in $p_{\text{opt}}$. We change $\delta$ within the region where $\Delta$ becomes real. That is, we have

$$\delta^2 \leq \frac{1}{4}(A^2 - 4B_0),$$

(81)

$$B_0 = \pi_1ab + \pi_2ca + \pi_3bc.$$  

(82)

We also require that $W_{ij} \geq 0 \ (i \neq j)$. The result is plotted in Fig. 9. The color map represents $-\ln D(p(t,\delta)|p_{\text{opt}})$ as a function of $t$ and $\delta$. We see that the solution of the BE takes the minimum value of $D(p(t,\delta)|p_{\text{opt}})$, which indeed represents the optimality of the solution.

Further confirmation of the optimization is obtained by solving the BE within the DBC. In this case, we set $\delta = 0$, and $g$ and $\tau$ are related to each other by Eq. (60), which is a quadratic equation that is easily solved to obtain $g = g(\tau)$. In Fig. 10, we plot the function $f(g(\tau), \tau, \delta, z)$ on the right-hand side of Eq. (80). The solution is given by the value of $\tau$ satisfying $f = 0$. We see that it is independent of $z$. By using the relation between $g$ and $\tau$, we obtain $g = 0$. This solution represents the boundary point between the left and right branches in Fig. 2. We have that $\Delta = 0$ and $T$ tends to $\infty$. Thus, the BE with the DBC does not give any solution. This means that we cannot reach the final state determined by $z$ with a finite duration in the algorithm with DBC.

D. Optimization and detailed balance condition

In the above example, we have studied the case $a = 1$. We find that one of the elements of the transition-rate matrix tends to 0, which means that the violation of the
DBC is maximal. We further investigate whether it is a general property of the solution. To answer this question, we take the simple case \( a = b = c \). Then, the constraint matrix is given by

\[
F = \sum_{a=1}^{3} \lambda_a^{(v)} X_a,
\]

where \( \sum_{a=1}^{3} \lambda_a^{(v)} = 0 \), \((X_1)_{ij} = \delta_{i1} \delta_{j2} + \delta_{i2} \delta_{j3}, (X_2)_{ij} = \delta_{i1} \delta_{j3} + \delta_{i3} \delta_{j1}, \) and \((X_3)_{ij} = \delta_{i2} \delta_{j3} + \delta_{i3} \delta_{j2} \). The eigenvalues of \( W \) are given by

\[
\Lambda_{\pm} = -a \pm \sqrt{-\delta^2}.
\]

Then, Eq. (83) is replaced by

\[
-2 \left( \sqrt{\pi_1 \pi_2} \lambda_1^{(v)} + \sqrt{\pi_1 \pi_3} \lambda_2^{(v)} + \sqrt{\pi_2 \pi_3} \lambda_3^{(v)} \right)
= T(p_+ \lambda_+ + p_- \lambda_-),
\]

and Eq. (69) by

\[
\frac{1 - z}{1 + z} = \frac{1 - z}{1 + z} \sqrt{-4\delta^2} = 0.
\]

The latter equation implies \( \delta = 0 \). This means that the optimized solution in the case with the constraint \( a = b = c \) does not violate the DBC.

This example may be too simple, but it is instructive to find a solution respecting the DBC. For example, if we specify \( a, b, \) and \( c \) with \( a = b > c \), the result becomes different and we can have nonzero \( \delta \). Thus, the result is highly sensitive to the constraints, as mentioned above, and the optimized solution does not necessarily violate the DBC. This is not a surprising result, because the previous study of the optimization to reduce the rejection rate in the Markov-chain Monte Carlo method yielded a trivial solution satisfying the DBC in a simple case [3].

**V. SHORTCUTS TO ADIABATICITY**

In our BE, the matrix \( F \) constructed from constraint functions as Eq. (69) plays an important role to describe the optimized solution. However, the physical meaning of \( F \) was unclear in the above analysis. This is considered to be due to the strong restriction of the transition-rate matrix \( W \). If we allow time-dependent fluctuations of \( W \), we expect from the analysis of the quantum BE that \( F \) represents the dynamical invariant [21]. We can, in principle, formulate the BE for nonstatic systems. By examining the problem from a more general perspective, we can learn the general properties of the solution. We can also expect that the present analysis is applied to simulated annealing [23].

When \( W \) has time dependence, all the constraints are locally imposed in time. We modify the action in a local form by using the Lagrangian \( L \) as \( S = \int dt \ L \). The constraint part of the Lagrangian is given by

\[
L_c = \sum_{i=1}^{N} \lambda_i^{(i)}(t) \left( \frac{d}{dt} P_i(t) - \sum_{j=1}^{N} W_{ij}(t) P_j(t) \right) + \lambda^{(ii)}(t) \left( 1 - \sum_{i=1}^{N} \sqrt{\pi_i} P_i(t) \right)
+ \sum_{i,j=1}^{N} \left( \sqrt{\pi_i} W_{ij}(t) \lambda_{ij}^{(iii)}(t) + \lambda_{ij}^{(iv)}(t) W_{ij}(t) \sqrt{\pi_j} \right)
+ \sum_{a} \lambda_a^{(v)}(t) f_a(W(t)).
\]

Each constraint is the same as in the time-independent...
case. We note that constraint (iv) is represented as
\[ \sum_{j=1}^{N} W_{ij}(t) \sqrt{\pi_j} = 0. \tag{88} \]

In principle, the balance condition is expressed as \[ \sum_{j} W_{ij}(\infty) \sqrt{\pi_j} = 0, \] and it is not necessary to impose the balance condition at each \( t \). However, we find that it is difficult to construct a general solution if we do not impose condition \[ \text{[22]} \]. In what follows, we consider this special case with Eq. \[ \text{[85]} \].

The variational procedure is the same as in the time-independent case. We finally obtain the form
\[ F_{\perp}(t) = U(t) G_{\perp} U^{-1}(t), \tag{89} \]
where \( U(t) \) is the time-evolution operator:
\[ U(t) = T \exp \left( \int_{0}^{t} dt' W(t') \right). \tag{90} \]
The symbol \( T \) denotes the time-ordered product. The definitions of \( G_{\perp} \) and \( F_{\perp} \) are the same as before. We see that this result \[ \text{[89]} \] is a natural extension of Eq. \[ \text{[10]} \].

The difference from the previous case is that the constraint matrix \( F \) is time-dependent and we can consider the time derivative of \( F \), which satisfies the equation of motion
\[ \frac{dF_{\perp}(t)}{dt} = [W(t), F_{\perp}(t)]. \tag{91} \]
In this case, \( F \) has a clear meaning: it is a dynamical invariant \[ \text{[22]} \]. We consider the symmetric case \( F = F^T \). This means that the constraints are imposed only on the part with DBC. In this case, the matrix is diagonalized as
\[ F_{\perp}(t) = \sum_{n} f_n |n(t)\rangle \langle n(t)|. \tag{92} \]
We can easily show from Eq. \[ \text{[91]} \] that the eigenvalues \( f_n \) are time independent. By using the eigenstates, we can also show that
\[ \langle m(t)|W(t)|n(t)\rangle = \langle m(t)|\dot{n}(t)\rangle, \tag{93} \]
where \( m \neq n \). This relation means that \( W \) is written as
\[ W(t) = \sum_{n} w_n(t) |n(t)\rangle \langle n(t)| \\
+ \sum_{m \neq n} |m(t)\rangle \langle m(t)|\dot{n}(t)\rangle \langle n(t)| \\
= \sum_{n} (w_n(t) - \langle n(t)\rangle \langle n(t)|\dot{n}(t)\rangle) |n(t)\rangle \langle n(t)| \\
+ \sum_{n} |\dot{n}(t)\rangle \langle n(t)|, \tag{94} \]
where \( w_n(t) \) is a function of \( t \) and cannot be determined from Eq. \[ \text{[11]} \]. We note that the second term in Eq. \[ \text{[94]} \] is asymmetric:
\[ \left( \sum_{n} |\dot{n}(t)\rangle \langle n(t)| \right)^T = - \sum_{n} |\dot{n}(t)\rangle \langle n(t)|. \tag{95} \]
This property shows that the optimal transition-rate matrix violates the DBC.

The present result is interpreted as the counterdiabatic driving. The probability distribution is given by
\[ |P(t)| = \sum_{n} |n(t)\rangle \exp \left( \int_{0}^{t} dt' w_n(t') \right) + |\pi\rangle. \tag{96} \]
This means that the probability distribution is given by the instantaneous eigenstate of the first term in Eq. \[ \text{[94]} \]. The second term represents the counterdiabatic term and prevents nonadiabatic transitions to different states. The counterdiabatic term explicitly violates the DBC. This is the main result of the present section. In quantum systems, the counterdiabatic term usually takes an operator that is absent in the original Hamiltonian. The same is true for the Markovian dynamics. We need to break the DBC to prevent non-adiabatic transitions.

VI. DISCUSSION AND CONCLUSIONS

We performed optimization for Markovian dynamics through the brachistochrone method. The master equation, which represents the classical stochastic dynamics, has a formal similarity to the Schrödinger equation in quantum systems. Therefore, we applied the formalism of the quantum brachistochrone method to our case by replacing the measure with a proper one. We derived the BE and showed that the optimized solution can violate the DBC. We took a simple case with three states to demonstrate our method and various properties of the optimal solution in detail. We also found that the optimized solution was interpreted as the counterdiabatic driving by considering the time-dependent transition-rate matrix. In this case, the solution is characterized by the dynamical invariant. The probability distribution follows an adiabatic passage, and the counterdiabatic term in the transition-rate matrix violates the DBC.

Our result shows that the optimized solution significantly depends on the constraints to be used. A part of the optimized solution satisfies the DBC, but in general, the optimized solution violates the DBC. This means that the violation of the DBC does not necessarily optimize the time evolution. The same property was obtained by Suwa and Todo in Ref. \[ \text{[3]} \], where they optimized the stochastic dynamics with respect to the rejection rate and found that the DBC is not violated in some simple cases. On the other hand, if we allow time dependence in the transition-rate matrix, the general solution violates the DBC. The violation originates from the counterdiabatic term to keep the system in the instantaneous stationary state. In other words, violation of the DBC immediately relaxes the system to the instantaneous stationary state in the time-dependent case.

The starting point of our analysis is to use the Kullback–Leibler divergence as the measure of optimization, and we pursue the “fastest” solution. However, by using the defined action, we found that the general form...
of the BE is not sensitive to the form of the measure, as in the case of quantum systems. This property is very convenient to us because we can avoid the uncertainty caused by the fact that the meaning of “fastest” depends on the choice of measure. There exists a geometrical interpretation in the quantum brachistochrone method [24]. We expect that a similar interpretation holds in the present case of classical stochastic dynamics.

Originally, we aimed at the optimal solution leading to the fastest convergence to the stationary distribution. Although the stationary state can be achieved after infinite-time relaxation, in our formulation, the optimization is performed between states at a finite duration. In this sense, we do not directly attain the optimal pathway between the initial and stationary states. This is due to the limitation of the original quantum brachistochrone method. Thus, we focused not on the relaxation time but on the finite duration. Nevertheless, in this formulation, we found that the optimal solution violates the DBC to reach the specified final distribution. Furthermore, in three-state systems, the distribution $p(T)$ at the final time is very close to the stationary distribution $\pi$, which means that our optimization practically makes sense in finding the optimal solution to the stationary state. We hope that future studies fulfill the gap in the formulation.

Considering the above properties of our analysis, we offer possible applications of our method. Certainly, it will be difficult to optimize the dynamics fully in large systems. However, it is possible to optimize a portion of the elements in the transition-rate matrix by imposing several constraints. In principle, we can implement any constraint in our method. This flexibility is one of the advantages of our approach and will be useful for practical applications.

Before closing the last section, we list below possible directions for future research in the subject of the present study. The adiabatic passage is translated into a quasi-static process to maintain system equilibrium in the context of the classical counterpart. The time-dependent driving appears in the cases of simulated annealing to find an optimal solution in the rugged landscape of the energy [25] and in the case of machine learning to estimate optimal parameters characterizing the stationary distribution by driving the stochastic dynamics many times [25, 27]. We can develop a more efficient algorithm for these applications by utilizing the brachistochrone method for the classical stochastic dynamics, as in our study. Actually, the dynamics modified by violating the DBC leads to an efficient algorithm in learning [27].

As shown in our study, use of the BE can be a useful method to design the transition-rate matrix. It is straightforward to generalize our scheme to the case of the Fokker–Planck equation, which is also interpreted as the imaginary-time Schrödinger equation. We naturally expect that the BE leads to the special force to accelerate convergence to the stationary state, as proposed in Refs. 9, 10, and beyond. Finally, future studies may expand the present analysis to the case of discrete-time evolution by changing the implementation of the quantum brachistochrone because the implementation in numerical computations can be realized in discrete time. In this sense, the present study is merely a starting point to construct the best algorithm simulating the optimal stochastic dynamics. After various studies on the subject of the present study, we hope that a type of constructive concept to generate an algorithm more efficient than DBC emerges in the future.

ACKNOWLEDGMENTS

The authors are grateful to A. Ichiki for useful comments. KT was supported by JSPS KAKENHI Grant Number 26400385. MO was supported by JSPS KAKENHI Grant Number 15H03699 and the Kayamori Foundation of Informational Science Advancement. The authors are grateful for financial support from the JSPS Core-to-Core program, Non-equilibrium Dynamics of Soft Matter and Information.

Appendix A: Derivation of the brachistochrone equation

The purpose of this Appendix is to present the explicit form of Eq. (72). For this purpose, we need eigenstates of $W$ with nonzero eigenvalues:

$$\langle L_\pm | = (\begin{pmatrix} \alpha_\pm & \beta_\pm & \gamma_\pm \end{pmatrix} ,$$

$$| R_\pm \rangle = (\begin{pmatrix} \alpha_\pm \\ \beta_\pm \\ \gamma_\pm \end{pmatrix} .$$

Using $\langle \pi | L_\pm \rangle = 0$ and $\langle R_\pm | \pi \rangle = 0$, we have

$$\gamma = -\sqrt{\frac{\pi_1}{\pi_3}} \alpha - \sqrt{\frac{\pi_2}{\pi_3}} \beta,$$

$$\gamma' = -\sqrt{\frac{\pi_1}{\pi_3}} \alpha' - \sqrt{\frac{\pi_2}{\pi_3}} \beta'.$$

The eigenvalue equations $W | R_\pm \rangle = \Lambda | R_\pm \rangle$ and $\langle L_\pm | W = \langle L_\pm | \Lambda$ give

$$\beta = -C \alpha = -\left( \frac{W_{11} - \sqrt{\frac{\pi_1}{\pi_3}} W_{13} - \Lambda}{W_{12} - \sqrt{\frac{\pi_1}{\pi_3}} W_{13}} \right) \alpha,$$

$$\beta' = -C' \alpha' = -\left( \frac{W_{11} - \sqrt{\frac{\pi_1}{\pi_3}} W_{13} - \Lambda}{W_{21} - \sqrt{\frac{\pi_1}{\pi_3}} W_{31}} \right) \alpha'.$$

These conditions determine the relations between components of the eigenstate vectors. The left and right eigenstates are related by the normalization condition $\langle L_\pm | R_\pm \rangle = 1$. We obtain

$$\frac{1}{\pi_3} \left[ 1 - \pi_2 - \sqrt{\pi_1 \pi_2} (C + C') + (1 - \pi_1) CC' \right] \alpha \alpha' = 1.$$

(A7)
We have omitted the subscript \( \pm \) in the above equations. The normalization condition does not fully determine \( \alpha \) and \( \alpha' \). The substitutions \( \alpha \rightarrow k \alpha \) and \( \alpha' \rightarrow \alpha'/k \) do not change the condition.

Now, we return to Eq. (A12). Using the obtained relations of the eigenstate vectors, we can write

\[
\langle L_+ | X | R_+ \rangle = - (C_+ + C'_+) \alpha_+ \alpha'_+. \tag{A9}
\]

Then, the ratio is written as

\[
\frac{C_- + C'_+}{C_+ + C'_-} \left[ 1 - \frac{\pi_3 - \pi_2}{\sqrt{\pi_1 \pi_2}} (C_+ + C'_+) + (1 - \pi_1)C_+ C'_+ \right] \left( \frac{\alpha'_+}{\alpha_-} \right)^2 = \frac{p_+ \phi_-}{p_- \phi_+} \exp \Delta \tau. \tag{A10}
\]

Next, we consider the relations between \( p_\pm \) and \( \alpha'_\pm \). They are determined by \( p_\pm = \langle L_\pm | P(0) \rangle \). We obtain

\[
p_\pm = \frac{1}{\pi_3} \left[ \frac{1}{\sqrt{\pi_1}} (p_1 \pi_3 - p_3 \pi_1) - \frac{1}{\sqrt{\pi_2}} (p_2 \pi_3 - p_3 \pi_2) \right] \alpha'_\pm. \tag{A11}
\]

These are inserted to Eq. (A10) to obtain

\[
\frac{C_- + C'_+}{C_+ + C'_-} \left[ 1 - \frac{\pi_3 - \pi_2}{\sqrt{\pi_1 \pi_2}} (C_+ + C'_+) + (1 - \pi_1)C_+ C'_+ \right] \left[ \frac{1}{\sqrt{\pi_1}} (p_1 \pi_3 - p_3 \pi_1) - \frac{1}{\sqrt{\pi_2}} (p_2 \pi_3 - p_3 \pi_2) \right]^2 = \exp \Delta \tau. \tag{A12}
\]

We see that the arbitrariness of the choice of eigenfunctions does not appear in this expression, as expected. The last equation is deformed as

\[
\delta = - \frac{D_{+} \exp \Delta \tau \left( \frac{D_{2}^{2} + \delta^{2}}{2D_{-}} \right) - D_{-} \exp \Delta \tau \left( \frac{D_{2}^{2} + \delta^{2}}{2D_{+}} \right)}{D_{+} \exp \Delta \tau \left( D - \frac{D_{2}^{2} + \delta^{2}}{2D_{-}} \right) - D_{-} \exp \Delta \tau \left( D + \frac{D_{2}^{2} + \delta^{2}}{2D_{+}} \right)}, \tag{A13}
\]

where

\[
D = \frac{2}{\Delta} \sqrt{\frac{\pi_1 \pi_2}{\pi_3}} \left[ \frac{\pi_3 (a-b)}{2(1-\pi_1)} \left( 2(1-\pi_2)(a-b) + A - 2a \right) - \delta^2 \right], \tag{A14}
\]

\[
D_{\pm} = \frac{1}{\sqrt{\pi_1}} (p_1 \pi_3 - p_3 \pi_1) \sqrt{\pi_1 \pi_2} (a-b) - \frac{1}{\sqrt{\pi_2}} (p_2 \pi_3 - p_3 \pi_2) \left( (1-\pi_2)(a-b) - \Lambda_\pm + a \right), \tag{A15}
\]

\[
D_{C} = \frac{1 - \pi_2 - \sqrt{\pi_1 \pi_2} (C_+ + C'_+) + (1 - \pi_1)C_+ C'_+}{1 - \pi_2 - \sqrt{\pi_1 \pi_2} (C_- + C'_-) + (1 - \pi_1)C_- C'_-}. \tag{A16}
\]

We conclude that the explicit form of Eq. (A10) is given by Eq. (A13). We note that the right-hand side of (A13) depends on \( \delta^2 \), rather than on \( \delta \). This fact is shown by using the property \( D_{C}(-\delta) = D_{C}(\delta) \).

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