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Equivalent Markov processes under gauge group

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We have studied Markov processes on denumerable state space and continuous time. We found that all these processes are connected via gauge transformations. We have used this result before as a method to resolve equations, included the case in a previous work in which the sample space is time-dependent [Phys. Rev. E 90, 022125 (2014)]. We found a general solution through dilation of the state space, although the prior probability distribution of the states defined in this new space takes smaller values with respect to that in the initial problem. The gauge (local) group of dilations modifies the distribution on the dilated space to restore the original process. In this work, we show how the Markov process in general could be linked via gauge (local) transformations, and we present some illustrative examples for this result.

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I. INTRODUCTION

Continuous-time Markov processes are used to describe a variety of stochastic complex processes. They have been widely used in mathematical physics to describe the properties of important models in equilibrium and nonequilibrium, such as the Ising model [1].

Another important application is the use of continuous-time Markov chains in queueing theory [2]. In the field of biology, Markov chains are used to explain the properties of reaction networks, chemical systems involving multiple reactions and chemical species [3], and the kinetics of linear arrays of enzymes [4].

In this work, we demonstrate how to connect a given pair of Markov processes via gauge transformations. The link between different processes is a mathematical observation that enriches the description of the stochastic process. In addition, in some cases this observation could become a useful tool to study a particularly complex Markov problem using a simpler auxiliary Markov process, and we propose an adequate transformation to link both of them.

This approach was explored heuristically in our recent work [5] as an alternative method for the resolution of Markov process equations on denumerable state spaces and continuous time. Nevertheless, in order to obtain a phenomenological or approximate solution to a certain Markov process, some knowledge of the system parameters must be obtained. This is precisely the case in Ref. [5].

The structure of the paper is as follows: In Sec. II we present a mathematical description of a general stochastic system; Sec. III outlines the motivation of the problem; Sec. IV contains the formal aspects of the equivalence of the process; and finally the conclusions and final comments are presented in Sec. V.

II. MARKOVIAN PROCESS IN A DENUMERABLE STATE SPACE AND CONTINUOUS TIME

We start by reviewing the basics aspects of this class of stochastic processes. Let us consider a stochastic system described by a Markov process with a random variable x(t), which takes values from the state space at the *instant* t,

$$S = \{x_n : n \in \ell\},\tag{1}$$

where *t* represent a *time variable*, i.e., some parameter used to describe the evolution of the process, which takes values from a set $\mathcal{T} \subseteq \mathbb{R}$, and $\boldsymbol{\ell}$ is the countable set of *labels* for the states, such that $\boldsymbol{\ell} \subseteq \mathbb{Z}_0^+$.

We defined the conditional probability to find the system in the state x_l , at the instant t, given that at that instant s was in the state x_k , denoted by

$$\mathcal{P}_{lk}(t,s) = \mathbb{P}(x(t) = x_l | x(s) = x_k).$$
⁽²⁾

We understand this conditional probability as a transitional element between the states $x_k \mapsto x_l$ and with a temporal evolution $s \mapsto t$. These conditional probabilities describe the time evolution of the stochastic system in the sense that they allow us to connect any two ordered pairs (x_k, s) , (x_l, t) .

The time evolution of a Markov process is determined by the knowledge of a prior probability distribution for each t, denoted by

$$p_n(t) = \mathbb{P}(x(t) = x_n) \tag{3}$$

for all $(t,n) \in \mathcal{T} \times \boldsymbol{\ell}$.

An equivalent way to describe this process is through an initial value $p_n(0)$ and a conditional probability $\mathcal{P}_{nm}(t,s)$, which represents the transition matrix elements of the states $x_m \mapsto x_n$. For each *t* the events are mutually exclusive, thus

 $p_n(t) = \sum_{m \in \ell} \mathcal{P}_{nm}(t,s) \ p_m(s).$

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(4)



FIG. 1. Diagram associated with the finite pure birth process with the infinitesimal generator \mathbf{Q}_+ .

Consequently, at the time $t + \epsilon$ the probability to find the system in x_n is given by the transition from x_m at time t as

$$p_n(t+\epsilon) = \sum_{m \in \ell} \mathcal{P}_{nm}(t+\epsilon,t) \ p_m(t).$$
 (5)

After some elementary operations, we get

$$d_t p_n(t) = \sum_{m \in \ell} \mathbb{Q}_{nm}(t) \ p_m(t), \tag{6}$$

where d_t denotes the total time derivative, and $Q_{nm}(t)$ is given by

$$Q_{nm}(t) = \partial_t \mathcal{P}_{nm}(t,s)|_{s=t}, \qquad (7)$$

where $Q_{nm}(t)$ is called the *infinitesimal generator*.

Equation (6) is called the Kolmogorov equation, which is the foundational work of Ref. [6]. Other authors later referred to (6) as the forward Kolmogorov equation [7].

We define $\varphi(t)$ as an |S|-tuple of the probability distribution as $\varphi(t) = (p_0(t), p_1(t), \dots)^{\mathsf{T}}$. In addition, we use a notation for the cardinal number of a set **S** given by |S|, and $^{\mathsf{T}}$ represents the transposition operation.

The evolution equation for the process can be expressed in *matrix form* as [8]

$$d_t \boldsymbol{\varphi}(t) = \mathbf{Q}(t) \, \boldsymbol{\varphi}(t). \tag{8}$$

In this way, we have a mathematical description of a Markov process in terms of a set of prior probabilities $\{p_0(t), p_1(t), ...\}$ and an infinitesimal generator $\mathbf{Q}(t)$.

III. MOTIVATION OF THE PROBLEM

In this section, we present a motivational example to show how a given pair of Markov processes could be linked via gauge transformations. Let us consider two particular stochastic processes, with their respective infinitesimal generators

$$\mathbf{Q}_{+} = \begin{pmatrix} -\nu & 0\\ \nu & 0 \end{pmatrix}, \quad \mathbf{Q}_{-} = \begin{pmatrix} 0 & \mu\\ 0 & -\mu \end{pmatrix}. \tag{9}$$

These matrices \mathbf{Q}_+ and \mathbf{Q}_- correspond to a *pure birth process* and a *pure death process*, where ν and μ are the birth and death rates, respectively. Note that $\mathbf{Q}_+ + \mathbf{Q}_-$, from (9), is equal to another infinitesimal generator that corresponds to a finite two-state birth-death process. Also, to be more explicit, we can represent each of these processes through the diagrams in Figs. 1 and 2.

The differential equation from (8) applied for each of these processes is summarized by

$$d_t \boldsymbol{\varphi}_+(t) = \mathbf{Q}_+(t) \, \boldsymbol{\varphi}_+(t),$$

$$d_t \boldsymbol{\varphi}_-(t) = \mathbf{Q}_-(t) \, \boldsymbol{\varphi}_-(t). \tag{10}$$



FIG. 2. Diagram associated with the finite pure death process with the infinitesimal generator \mathbf{Q}_{-} .

We demonstrate that there is a 2 × 2 matrix λ that connects the solutions φ_+ and φ_- in the following way:

$$\varphi_{+} = \lambda \varphi_{-}. \tag{11}$$

First of all, only for the particular case $\nu = \mu$ will we have a constant matrix λ ,

$$\boldsymbol{\lambda} = \begin{pmatrix} 0 & 1\\ 1 & 0 \end{pmatrix}, \tag{12}$$

which corresponds to an interchange of the states $(1) \leftrightarrow (2)$. In other words, (12) corresponds to a reflection that interchanges Fig. 1 with Fig. 2 and vice versa. Explicitly for the case $\nu = \mu$, using (12), we have

$$\mathbf{Q}_{+} = \mathbf{\lambda} \ \mathbf{Q}_{-} \ \mathbf{\lambda}^{-1}. \tag{13}$$

The preceding equation together with (10) involves (11). The matrix λ from (12) is a time-independent change of coordinates between Eqs. (10) for the case $\nu = \mu$.

We have noticed that λ is not a constant matrix for the case $\nu \neq \mu$. For the present case, we obtain the solutions with nontrivial initial conditions as

$$\boldsymbol{\varphi}_{+} = \begin{pmatrix} e^{-\nu t} \\ 1 - e^{-\nu t} \end{pmatrix}, \quad \boldsymbol{\varphi}_{-} = \begin{pmatrix} 1 - e^{-\mu t} \\ e^{-\mu t} \end{pmatrix}. \tag{14}$$

Using the explicit solutions (14), the proof that Eq. (11) is true is straightforward, since there is a matrix

$$\boldsymbol{\lambda} = \begin{pmatrix} 0 & e^{(\mu-\nu)t} \\ 1 & 1 - e^{(\mu-\nu)t} \end{pmatrix},\tag{15}$$

thus Eq. (11) is true.

This example shows, in pedagogical way, that it is possible to write the solution of a stochastic process starting from another process. The bridge between φ_+ and φ_- is built through a local transformation λ . In addition, the corresponding link between Q_+ and Q_- through a local transformation λ is given by

$$\mathbf{Q}_{+} = \mathbf{\lambda}\mathbf{Q}_{-}\mathbf{\lambda}^{-1} + d_{t}\mathbf{\lambda}\mathbf{\lambda}^{-1}$$
(16)

for all ν and μ . Expression (16) is almost equal to (13) but with an added term $d_t \lambda \lambda^{-1}$.

We will see that the group of this kind of transformation is structured as a gauge group. We formalize and generalize this idea in the following sections, and we prove that it is possible to connect any pair of infinitesimal generators (\mathbf{Q}, \mathbf{Q}') and any pair of prior distributions of probability ($\boldsymbol{\varphi}, \boldsymbol{\varphi}'$) associated with these infinitesimal generators in a similar way to (16) and (11), respectively,

$$\mathbf{Q}' = \mathbf{\lambda} \mathbf{Q} \mathbf{\lambda}^{-1} + d_t \mathbf{\lambda} \mathbf{\lambda}^{-1},$$

$$\boldsymbol{\varphi}' = \mathbf{\lambda} \boldsymbol{\varphi}.$$
 (17)

IV. FORMAL ASPECTS OF EQUIVALENT MARKOV PROCESSES

We considered a map Γ_{λ} , given a nonsingular matrix λ , which transforms a matrix **Q** as

$$\Gamma_{\lambda}(\mathbf{Q}) = \lambda \mathbf{Q} \lambda^{-1} + d_t \lambda \lambda^{-1}, \qquad (18)$$

where λ , $\mathbf{Q} \in \mathbb{R}^{|\boldsymbol{\ell}| \times |\boldsymbol{\ell}|}$ are *t*-dependent differentiable matrices. Thereby, λ is a local transformation, and we will prove that Γ_{λ} forms a group of local (gauge) transformations. In particular, $\Gamma_{\lambda} \in \mathbb{R}^{|\boldsymbol{\ell}| \times |\boldsymbol{\ell}|}$.

In addition, in this section we study the possibility that for all pairs of matrices **Q** and **Q**', *t*-dependent and differentiable, there is a nonsingular matrix λ , *t*-dependent and differentiable, that connects **Q** and **Q**' as

$$\mathbf{Q}' = \mathbf{\Gamma}_{\boldsymbol{\lambda}}(\mathbf{Q}). \tag{19}$$

If we compose two transformations $\Gamma_{\lambda} \circ \Gamma_{\lambda'}$ with λ and λ' nonsingular, we see that

$$\Gamma_{\lambda} \circ \Gamma_{\lambda'}(\mathbf{Q}) = \Gamma_{\lambda\lambda'}(\mathbf{Q}). \tag{20}$$

From (20) we see that

$$[\boldsymbol{\lambda},\boldsymbol{\lambda}'] = \mathbf{0} \Longrightarrow \boldsymbol{\Gamma}_{\boldsymbol{\lambda}} \circ \boldsymbol{\Gamma}_{\boldsymbol{\lambda}'}(\mathbf{Q}) = \boldsymbol{\Gamma}_{\boldsymbol{\lambda}'} \circ \boldsymbol{\Gamma}_{\boldsymbol{\lambda}}(\mathbf{Q}).$$
(21)

Using this properties of composition (20) and (21), we give an expression for the inverse map Γ_{λ}^{-1} . First of all, we have trivially

$$\Gamma_1(\mathbf{Q}) = \mathbf{Q},\tag{22}$$

where 1 is the identity matrix. If we consider the composed transform $\lambda'' = \lambda \lambda'$ such that $\lambda \lambda' = 1 = \lambda' \lambda$, then from (21) we have

$$\Gamma_{\lambda} \circ \Gamma_{\lambda'} = 1 = \Gamma_{\lambda'} \circ \Gamma_{\lambda}. \tag{23}$$

Finally from (23) the inverse of Γ_{λ} is *unique* and is given by

$$\Gamma_{\lambda}^{-1} = \Gamma_{\lambda^{-1}}.$$
 (24)

For more details on the properties of composition (20) and the inverse transformation (24), see Appendix A 1.

We will demonstrate that for any pair of *t*-dependent differentiable matrices **Q** and **Q**', for both $|\boldsymbol{\ell}| \times |\boldsymbol{\ell}|$ there exist nonsingular *t*-dependent differentiable matrices $\boldsymbol{\lambda}$ of $|\boldsymbol{\ell}| \times |\boldsymbol{\ell}|$ that connect them. For that we can define the following *equivalence relation*:

$$\mathbf{Q}' \sim \mathbf{Q} \Longleftrightarrow \exists \boldsymbol{\lambda} : \mathbf{Q}' = \boldsymbol{\Gamma}_{\boldsymbol{\lambda}}(\mathbf{Q}). \tag{25}$$

For more evidence that \sim is a well-defined *equivalence relation*, see Appendix A 1. From the equivalence relation (25), λ satisfies the differential equation

$$d_t \mathbf{\lambda} = \mathbf{Q}' \mathbf{\lambda} - \mathbf{\lambda} \mathbf{Q}. \tag{26}$$

First of all, the solution of (26) exists for the trivial cases $\mathbf{Q} = \mathbf{0}$ and $\mathbf{Q}' = \mathbf{0}$, i.e., we denote by λ_1 and λ_2 the respective solutions for each case,

$$d_t \boldsymbol{\lambda}_1 = \mathbf{Q}' \boldsymbol{\lambda}_1, \tag{27}$$

$$d_t \boldsymbol{\lambda}_2 = -\boldsymbol{\lambda}_2 \mathbf{Q}. \tag{28}$$

We can obtain (λ_1, λ_2) as an iterative nonsingular solution. For more details of this solution, see Appendix A 2. The existence of solutions for (27) and (28) implies that λ_1 and λ_2 connect $\mathbf{Q}' \sim \mathbf{0}$ and $\mathbf{0} \sim \mathbf{Q}$, respectively. This implication is true from the definition of the equivalence relation. From the existence of solutions for (27) and (28), we have

$$\exists \boldsymbol{\lambda}_1 : \boldsymbol{\mathsf{Q}}' = \boldsymbol{\Gamma}_{\boldsymbol{\lambda}_1}(\boldsymbol{\mathsf{0}}) \Longleftrightarrow \boldsymbol{\mathsf{Q}}' \sim \boldsymbol{\mathsf{0}}, \tag{29}$$

$$\exists \boldsymbol{\lambda}_2 : \boldsymbol{0} = \boldsymbol{\Gamma}_{\boldsymbol{\lambda}_2}(\boldsymbol{Q}) \Longleftrightarrow \boldsymbol{0} \sim \boldsymbol{Q}, \tag{30}$$

and from the transitivity of the equivalence relation (25) we have $\mathbf{Q}' \sim \mathbf{Q}$, which means that there is a given λ that $\mathbf{Q}' = \Gamma_{\lambda}(\mathbf{Q})$.

We express the solution λ as a function of the solutions of (27) and (28), (λ_1, λ_2) , respectively. We say that a solution λ built in this way is a *transitive solution*, or a *composite solution*. The name will become clear in the construction procedure of the solution λ . From (29) and (30) we see that the *transitivity solution* is constructed from the composition of transformations $\mathbf{Q}' = \Gamma_{\lambda_1}(\mathbf{0})$ and $\mathbf{0} = \Gamma_{\lambda_2}(\mathbf{Q})$ as follows:

$$\mathbf{Q}' = \mathbf{\Gamma}_{\boldsymbol{\lambda}_1}(\mathbf{\Gamma}_{\boldsymbol{\lambda}_2}(\mathbf{Q})) \tag{31}$$

from the composition rule (20) applied to (31),

$$\mathbf{Q}' = \mathbf{\Gamma}_{\boldsymbol{\lambda}_1 \boldsymbol{\lambda}_2}(\mathbf{Q}), \tag{32}$$

where the transitive solution is given by

$$\boldsymbol{\lambda} = \boldsymbol{\lambda}_1 \boldsymbol{\lambda}_2. \tag{33}$$

We have demonstrated that for any pair of matrices $(\mathbf{Q}, \mathbf{Q}')$, *t*-dependent and differentiable, there is a nonsingular matrix λ , *t*-dependent and differentiable, that connect \mathbf{Q} and \mathbf{Q}' through the map Γ_{λ} , given by the expression (18),

$$\mathbf{Q}' = \mathbf{\Gamma}_{\boldsymbol{\lambda}}(\mathbf{Q}). \tag{34}$$

Suppose now that **Q** and **Q'** are the infinitesimal generators, *t*-dependent and differentiable, of the following differential equations:

$$d_t \boldsymbol{\varphi} = \mathbf{Q} \, \boldsymbol{\varphi},$$

$$d_t \boldsymbol{\varphi}' = \mathbf{Q}' \boldsymbol{\varphi}'. \tag{35}$$

Finally, from (34) and (35) we have

$$\boldsymbol{\varphi}' = \boldsymbol{\lambda} \boldsymbol{\varphi}. \tag{36}$$

We found that for any pair of infinitesimal generators, *t*-dependent and differentiable, with $(\mathbf{Q}, \mathbf{Q}')$ associated to (35), there exists another *t*-dependent and differentiable matrix λ that connects the distribution of probability $\boldsymbol{\varphi}$ and $\boldsymbol{\varphi}'$.

Up to now we have considered the equivalence of Markov processes of the same dimension, i.e., the state spaces of every couple of processes have the same cardinality. We will go one step further now and prove the equivalence of all continuoustime Markov processes on a denumerable state space.

Without loss of generality, we define (\mathbf{Q}, S) and (\mathbf{Q}', S') as the respective infinitesimal generators and state spaces, such that n = |S| < |S'| = n'. We can construct another process associated with \mathbf{Q} , such that the infinitesimal generator, \mathbf{Q} , is



FIG. 3. (Color online) This diagram shows the composed process on the state space $\mathbf{S} \approx S'$, in the sense that $|\mathbf{S}| = |S'|$, with the infinitesimal generator \mathbf{Q} .

given by

$$\mathbf{Q}_{ij} = \begin{cases} \mathsf{Q}_{ij}, & \forall \, i, j \in [1,n] \subseteq \mathbb{N}, \\ 0, & \forall \, i, j \in [n+1,n'] \subseteq \mathbb{N} \end{cases}$$
(37)

or in block form

$$\mathbf{Q} = \begin{pmatrix} \mathbf{Q} & 0 & \cdots \\ 0 & 0 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}.$$
(38)

The matrix **Q** corresponds to a new process on a state space **S** that has the same cardinality of S'. We have completed the process on S with a number of *redundant* states, such that the resulting state space **S** satisfies $|\mathbf{S}| = n' = |S'|$. For illustrative purposes, Fig. 3 shows the composed state space **S** from S and a set of isolated and absorbing states {&: $k \in [n + 1, n'] \subseteq \mathbb{N}$ }:

All the states of $\{\widehat{\mathbb{C}}: k \in [n + 1, n'] \subseteq \mathbb{N}\}\$ are isolated or mutually disconnected and are also from each state of \mathcal{S} ; they are all absorbing states. If the process starts in some $\widehat{\mathbb{C}}$ of this redundant set, it stays there forever.

A final comment is related to the case in which the state space is a time-dependent Markov process. In this sense, its cardinality is a function of time n_t , meaning that for a given generation time t (i.e., $t \in \mathbb{N}$), the state space S_t : $|S_t| = n_t$. Explicitly, we have

$$\mathcal{S}_t = \{x_1, x_2, \dots, x_{n_t}\}\tag{39}$$

for a given t. If \mathbf{Q}_t is the infinitesimal generator for each t, we can construct another process associated with \mathbf{Q}_t such that the infinitesimal generator, \mathbf{Q} , is constructed in a similar way to (37),

$$\mathbf{Q}_{ij} = \begin{cases} (\mathbb{Q}_t)_{ij}, & \forall i, j \in [1, n_t] \subseteq \mathbb{N}, \\ 0, & \forall i, j \in [n_t + 1, N] \subseteq \mathbb{N} \end{cases}$$
(40)

for a sufficiently big number $N \in \mathbb{Z}_0^+$. In other terms, we can write

$$\mathbf{Q}_{ij} = (\mathbf{Q}_t)_{ij} \ u(n_t - i)u(n_t - j), \tag{41}$$

where u(x) is a Heaviside step function,

$$u(x) := \begin{cases} 0 : & x < 0, \\ 1 : & x \ge 0. \end{cases}$$
(42)

In matrix form we express the dilution of S_t inside $S = \{x_1, x_2, \dots, x_N\}$ for a finite value of N or $N \to \infty$:

$$\mathbf{Q} = \begin{pmatrix} \mathbf{Q}_t & 0 & \cdots \\ 0 & 0 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}.$$
(43)

The matrix \mathbf{Q} corresponds to a new process on a state space \mathbf{S} , which is equivalent to any other.

V. CONCLUSION AND FINAL OBSERVATIONS

The aim of present work is to demonstrate that there is a way to modify the solution for a simple or known process, which is represented by the infinitesimal generator \mathbf{Q} , in order to get another process partially known, or at least with a very profound difficulty to be resolved, and represented by \mathbf{Q}' . We have shown how for a given pair of Markov processes (\mathbf{Q}, S) and (\mathbf{Q}', S') they could be linked via gauge (local) transformations λ that allow us obtain \mathbf{Q}' from \mathbf{Q} via Γ_{λ} . Even when the state space of each process has different cardinality, it is still possible to establish a link via a local transformation. This connection also could be explored when the state space is time-dependent, in the sense that the number of states changes with time, which was used intuitively in [5].

In addition, we can address a new problem through a nonlocal modulation of the well-known solution following the expression (36). We have not only shown that this is feasible to do through a formal and constructive proof of existence of λ , but also we indicated that it should be done across a linear and local (time-dependent) operation.

Future research from the standpoint of a Lagrangian description (working process) may reveal novel applications of the present proposal. In this approach, the role of this kind of transformation λ will be a symmetry of the Lagrangian. A gauge theory of stochastic processes can be improved formally through a variational principle.

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APPENDIX

We considered the study of an evolution over a timedependent and denumerable state space S with a random variable x(t) and probability distribution $p_n(t) = \mathbb{P}[X(t) = x_n]$. This evolution is governed by the conditional probability given by

$$\mathcal{P}_{nm}(t,s) = \mathbb{P}[x(t) = x_n | x(s) = x_m].$$
(A1)

The matrix $\mathcal{P}(t,s)$ satisfies the Chapman-Kolmogorov identity [7,8]

$$\mathcal{P}(t,s) = \mathcal{P}(t,u)\mathcal{P}(u,s) \tag{A2}$$

for $0 \leq s \leq u \leq t$. It is a matrix form of each identity,

$$\mathcal{P}_{lj}(t,s) = \sum_{k \in \ell} \mathcal{P}_{lk}(t,u) \mathcal{P}_{kj}(u,s).$$
(A3)

Also, the sum of each element of every column is

$$\sum_{n \in \ell} \mathcal{P}_{nm}(t,s) = 1.$$
 (A4)

For the general case, we can develop a power series of the matrix $\mathcal{P}(t + \epsilon, s)$ for a fixed value of *s*. Then we have

$$\mathcal{P}_{nm}(t+\epsilon,s) = \mathcal{P}_{nm}(t,s) + \epsilon \ \partial_t \mathcal{P}_{nm}(t,s) + \cdots,$$
 (A5)

where ∂_t is a simplified notation of the partial time derivative $\frac{\partial}{\partial t}$.

To obtain Eq. (6), we study the time evolution $t \mapsto t + \epsilon$ for a small value of ϵ . We need to know $\mathcal{P}_{nm}(t + \epsilon, t)$. Expression (A.5) then becomes

$$\mathcal{P}_{nm}(t+\epsilon,t) = \delta_{nm} + \epsilon \; \partial_t \mathcal{P}_{nm}(t,s)|_{s=t} + \cdots . \tag{A6}$$

We can recognize the second term of A.7 as the infinitesimal generator $Q_{nm}(t)$,

$$Q_{nm}(t) = \lim_{\epsilon \to 0} \frac{\mathcal{P}_{nm}(t+\epsilon,t) - \delta_{nm}}{\epsilon}.$$
 (A7)

We express $\mathcal{P}_{nm}(t + \epsilon, t)$ from A.7,

$$\mathcal{P}_{nm}(t+\epsilon,t) = \delta_{nm} + \mathbb{Q}_{nm}(t)\epsilon + O_t(\epsilon), \qquad (A8)$$

where $O_t(x)$ represents a type of function that goes to zero with x faster than x for a given t, that is,

$$\lim_{x \to 0} \frac{O_t(x)}{x} = 0.$$
 (A9)

Replacing (A8) in expression (5) from Sec. II, we have

$$p_n(t+\epsilon) = \sum_{m \in \ell} [\delta_{nm} + \mathbb{Q}_{nm}(t)\epsilon + O_t(\epsilon)] p_m(t).$$

Then

$$\frac{p_n(t+\epsilon)-p_n(t)}{\epsilon} = \sum_{m\in\ell} \left[\mathsf{Q}_{nm}(t) + \frac{O_t(\epsilon)}{\epsilon} \right] p_m(t),$$

taking the limit $\epsilon \to 0$,

$$d_t p_n(t) = \sum_{m \in \ell} \mathbb{Q}_{nm}(t) \ p_m(t). \tag{A10}$$

The stochastic process described by Eq. (A10) corresponds to the general class of stochastic dynamics of the Markov process on a denumerable state space.

We can write (A10) in matrix form as

$$d_t \boldsymbol{\varphi}(t) = \mathbf{Q}(t) \boldsymbol{\varphi}(t), \qquad (A11)$$

where $\varphi(t) = (p_0(t), p_1(t), ...)^{\mathsf{T}}$ and $Q(t) = \{Q_{nm}(t)\}.$

1. Some relevant properties of map Γ_{λ}

a Composite maps

We compose two transformations $\Gamma_{\lambda} \circ \Gamma'_{\lambda}$ with λ and λ' nonsingular, and then we prove that

$$\boldsymbol{\Gamma}_{\boldsymbol{\lambda}} \circ \boldsymbol{\Gamma}_{\boldsymbol{\lambda}'}(\boldsymbol{\mathsf{Q}}) = \boldsymbol{\Gamma}_{\boldsymbol{\lambda}\boldsymbol{\lambda}'}(\boldsymbol{\mathsf{Q}}). \tag{A12}$$

We calculate directly

$$\begin{split} \mathbf{\Gamma}_{\boldsymbol{\lambda}} \circ \mathbf{\Gamma}_{\boldsymbol{\lambda}'}(\mathbf{Q}) &= \mathbf{\Gamma}_{\boldsymbol{\lambda}}(\boldsymbol{\lambda}'\mathbf{Q}\boldsymbol{\lambda}'^{-1} + d_t\boldsymbol{\lambda}'\boldsymbol{\lambda}'^{-1}) \\ &= \boldsymbol{\lambda}[\boldsymbol{\lambda}'\mathbf{Q}\boldsymbol{\lambda}'^{-1} + d_t\boldsymbol{\lambda}'\boldsymbol{\lambda}'^{-1}]\boldsymbol{\lambda}^{-1} + d_t\boldsymbol{\lambda}\boldsymbol{\lambda}^{-1} \\ &= \boldsymbol{\lambda}\boldsymbol{\lambda}'\mathbf{Q}(\boldsymbol{\lambda}\boldsymbol{\lambda}')^{-1} + \boldsymbol{\lambda}d_t\boldsymbol{\lambda}'(\boldsymbol{\lambda}\boldsymbol{\lambda}')^{-1} + d_t\boldsymbol{\lambda}\boldsymbol{\lambda}'(\boldsymbol{\lambda}\boldsymbol{\lambda}')^{-1} \\ &= \boldsymbol{\lambda}\boldsymbol{\lambda}'\mathbf{Q}(\boldsymbol{\lambda}\boldsymbol{\lambda}')^{-1} + d_t(\boldsymbol{\lambda}\boldsymbol{\lambda}')(\boldsymbol{\lambda}\boldsymbol{\lambda}')^{-1} \\ &= \mathbf{\Gamma}_{\boldsymbol{\lambda}\boldsymbol{\lambda}'}(\mathbf{Q}), \end{split}$$

where in the second line the term $d_t \lambda' \lambda'^{-1}$ is written as $d_t \lambda' (\lambda \lambda^{-1}) \lambda'^{-1}$. This completes the demonstration that satisfies expression (20).

b Inverse map

We calculate explicitly $\Gamma_{\lambda^{-1}}(\mathbf{Q})$ and then prove that

$$\boldsymbol{\Gamma}_{\boldsymbol{\lambda}^{-1}}(\mathbf{Q}) = \boldsymbol{\Gamma}_{\boldsymbol{\lambda}}^{-1}(\mathbf{Q}) \tag{A13}$$

for all **Q**. Let us calculate the left-hand side of (A13),

$$\begin{split} \mathbf{\Gamma}_{\boldsymbol{\lambda}^{-1}}(\mathbf{Q}) &= \boldsymbol{\lambda}^{-1}\mathbf{Q}\boldsymbol{\lambda} + d_t(\boldsymbol{\lambda}^{-1})\boldsymbol{\lambda} \\ &= \boldsymbol{\lambda}^{-1}\mathbf{Q}\boldsymbol{\lambda} + d_t(\boldsymbol{\lambda}^{-1})\boldsymbol{\lambda} \\ &= \boldsymbol{\lambda}^{-1}\mathbf{Q}\boldsymbol{\lambda} - \boldsymbol{\lambda}^{-1}d_t\boldsymbol{\lambda}. \end{split}$$

Finally, we check directly that $\Gamma_{\lambda^{-1}}$ is equal to Γ_{λ}^{-1} ,

$$\begin{split} \Gamma_{\lambda} \circ \Gamma_{\lambda^{-1}}(\mathbf{Q}) &= \Gamma_{\lambda}(\lambda^{-1}\mathbf{Q}\lambda - \lambda^{-1}d_{t}\lambda) \\ &= \lambda(\lambda^{-1}\mathbf{Q}\lambda - \lambda^{-1}d_{t}\lambda)\lambda^{-1} + d_{t}\lambda\lambda^{-1} \\ &= \lambda\lambda^{-1}\mathbf{Q}\lambda\lambda^{-1} - \lambda\lambda^{-1}d_{t}\lambda\lambda^{-1} + d_{t}\lambda\lambda^{-1} \\ &= \mathbf{Q} - d_{t}\lambda\lambda^{-1} + d_{t}\lambda\lambda^{-1} \\ &= \mathbf{Q}, \end{split}$$

where we used $d_t(\lambda^{-1}\lambda) = \mathbf{0} \Longrightarrow d_t(\lambda^{-1})\lambda = -\lambda^{-1}d_t\lambda$. This completes the demonstration that (24) is true, i.e., $\Gamma_{\lambda^{-1}} = \Gamma_{\lambda}^{-1}$.

$c \ \Gamma_{\lambda}$ as an equivalence relation

We say that the map Γ_{λ} defines an equivalence relation between the vector space of matrices of the same dimension. For a given two matrices (\mathbf{Q}, \mathbf{Q}'), we can define a relation between them,

$$\mathbf{Q}' \sim \mathbf{Q} \Longleftrightarrow \exists \mathbf{\lambda} : \mathbf{Q}' = \mathbf{\Gamma}_{\mathbf{\lambda}}(\mathbf{Q}),$$
 (A14)

where $\Gamma_{\lambda}(\mathbf{Q}) := \lambda \mathbf{Q} \lambda^{-1} + d_t \lambda \lambda^{-1}$, and λ is a nonsingular matrix. This relation \sim is an equivalence in the sense that for all $\mathbf{Q}, \mathbf{Q}', \mathbf{Q}''$ the following properties are true:

- (**R**) $\mathbf{Q} \sim \mathbf{Q}$ (reflexivity),
- (S) $\mathbf{Q} \sim \mathbf{Q}' \Rightarrow \mathbf{Q}' \sim \mathbf{Q}$ (symmetry),
- $(\boldsymbol{T}) \quad \boldsymbol{\mathsf{Q}}'' \sim \boldsymbol{\mathsf{Q}}' \wedge \boldsymbol{\mathsf{Q}}' \sim \boldsymbol{\mathsf{Q}} \Rightarrow \boldsymbol{\mathsf{Q}}'' \sim \boldsymbol{\mathsf{Q}} \quad \text{(transitivity)}.$

The first assertion (**R**) is true from the identity matrix $\lambda = 1$ and by definition $\Gamma_1(\mathbf{Q}) = \mathbf{Q}$. The assertion (**S**) is also true from the existence of the inverse matrix λ^{-1} , and through (A13) the *inverse* connection $\mathbf{Q}' \sim \mathbf{Q}$ is constructed. The last assertion (**T**) is true from the composed transformation of nonsingular matrices $\lambda = \lambda''\lambda'$ and (A12), such that $\mathbf{Q}'' = \Gamma_{\lambda''}(\mathbf{Q}')$ and $\mathbf{Q}' =$ $\Gamma_{\lambda'}(\mathbf{Q})$. Then $\mathbf{Q}'' = \Gamma_{\lambda''}(\Gamma_{\lambda'}(\mathbf{Q})) = \Gamma_{\lambda''\lambda'}(\mathbf{Q}) = \Gamma_{\lambda}(\mathbf{Q})$. Finally, we arrive at $\mathbf{Q}'' \sim \mathbf{Q}$.

2. Alternative expression for gauge transformation λ

In the present work, in order to provide an expression for the solution of (26), the *transitivity solution* is constructed from the composed transformation $\lambda = \lambda_1 \lambda_2$ and (A12),

$$\boldsymbol{\Gamma}_{\boldsymbol{\lambda}_1 \boldsymbol{\lambda}_2}(\boldsymbol{\mathsf{Q}}) = \boldsymbol{\Gamma}_{\boldsymbol{\lambda}_1} \circ \boldsymbol{\Gamma}_{\boldsymbol{\lambda}_2}(\boldsymbol{\mathsf{Q}}) = \boldsymbol{\mathsf{Q}}', \qquad (A15)$$

where λ_1 and λ_2 are solution of (27) and (28), respectively,

$$\mathbf{Q}' \sim \mathbf{0} \Longleftrightarrow d_t \, \mathbf{\lambda}_1 = \mathbf{Q}' \mathbf{\lambda}_1,$$
$$\mathbf{0} \sim \mathbf{Q} \Longleftrightarrow d_t \, \mathbf{\lambda}_2 = -\mathbf{\lambda}_2 \mathbf{Q}.$$
(A16)

We express the solutions of (A16) as a formal iterative solution,

$$\boldsymbol{\lambda}_{1}(t) = \left[1 + \int_{0}^{t} \mathbf{Q}(t_{1}) dt_{1} + \int_{0}^{t} \int_{0}^{t_{1}} \mathbf{Q}(t_{1}) \mathbf{Q}(t_{2}) dt_{1} dt_{2} + \cdots \right] \boldsymbol{\lambda}_{1}(0),$$

- E. Ising, Contribution to the theory of ferromagnetism, Z. Phys. 31, 253 (1925).
- [2] L. Kleinrock, *Queueing Theory*, Vol. I (Wiley-Interscience, New York, 1975).
- [3] D. Anderson and T. Kurtz, Design and Analysis of Biomolecular Circuits, Continuous Time Markov Chain Models for Chemical Reaction Networks (Springer, New York, 2011), Chap. 1.
- [4] L. Shapiro and D. Zeilberger, A Markov chain occurring in enzyme kinetics, J. Math. Biol. 15, 351 (1982).
- [5] M. Caruso and C. Jarne, Markov chain approach to the distribution of ancestors in species of biparental reproduction, Phys. Rev. E 90, 022125 (2014).

$$\boldsymbol{\lambda}_{2}(t) = \boldsymbol{\lambda}_{2}(0) \bigg[1 - \int_{0}^{t} \mathbf{Q}'(t_{1}) dt_{1} + \int_{0}^{t} \int_{0}^{t_{1}} \mathbf{Q}'(t_{1}) \mathbf{Q}'(t_{2}) dt_{1} dt_{2} + \cdots \bigg].$$
(A17)

We obtain a general expression of the iterative solution (A17) through a Magnus series [9],

$$\boldsymbol{\lambda}_{1}(t) = \sum_{n \in \mathbb{N}} \frac{1}{n!} \boldsymbol{\Lambda}_{n}(t),$$
$$\boldsymbol{\lambda}_{2}(t) = \sum_{n \in \mathbb{N}} \frac{(-1)^{n}}{n!} \boldsymbol{\Lambda}_{n}'(t),$$
(A18)

where $\mathbf{\Lambda}_n(t)$ and $\mathbf{\Lambda}'_n(t)$ are given by

$$\mathbf{\Lambda}_{n}(t) = \int_{0}^{t} \mathbf{Q}(t_{1}) dt_{1} \int_{0}^{t_{1}} \mathbf{Q}(t_{2}) dt_{2} \cdots \int_{0}^{t_{n-1}} \mathbf{Q}(t_{n-1}) dt_{n},$$

$$\mathbf{\Lambda}_{n}'(t) = \int_{0}^{t} \mathbf{Q}'(t_{1}) dt_{1} \int_{0}^{t_{1}} \mathbf{Q}'(t_{2}) dt_{2} \cdots \int_{0}^{t_{n-1}} \mathbf{Q}'(t_{n-1}) dt_{n}.$$

(A19)

- [6] A. Kolmogorov, Ber die analytischen methoden in der wahrscheinlichkeitsrechnung, Math. Ann. 104, 415 (1931) [English version: On Analytical Methods in Probability Theory, Selected Works of A. N. Kolmogorov (Springer, Dordrecht, the Netherlands, 1992), Vol. II].
- [7] W. Feller, An Introduction to Probability Theory and Its Applications (Wiley, New York, 1968), Vols. 1 and 2.
- [8] M. Kijima, Markov Processes for Stochastic Modeling (Chapman & Hall, New York, 1997).
- [9] W. Magnus, On the exponential solution of differential equations for a linear operator, Commun. Pure Appl. Math. VII 7, 649 (1954).