Method to describe stochastic dynamics using an optimal coordinate

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A general method to describe the stochastic dynamics of Markov processes is suggested. The method aims to solve three related problems: the determination of an optimal coordinate for the description of stochastic dynamics; the reconstruction of time from an ensemble of stochastic trajectories; and the decomposition of stationary stochastic dynamics into eigenmodes which do not decay exponentially with time. The problems are solved by introducing additive eigenvectors which are transformed by a stochastic matrix in a simple way – every component is translated by a constant distance. Such solutions have peculiar properties. For example, an optimal coordinate for stochastic dynamics with detailed balance is a multivalued function. An optimal coordinate for a random walk on a line corresponds to the conventional eigenvector of the one-dimensional Dirac equation. The equation for the optimal coordinate in a slowly varying potential reduces to the Hamilton-Jacobi equation for the action function.

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I. INTRODUCTION

The description of a complex, multidimensional, stochastic process is often simplified by projecting it on one or a few variables [1–9]. During such dimensionality reduction one may lose some information; hence the variables should be optimally selected to preserve the information of interest. Here we are interested in the selection of variables that preserve the information about the dynamics. One aims to select a coordinate such that the dynamics projected on the coordinate is approximately Markovian, i.e., it is independent from the dynamics along other degrees of freedom. In other words, the current value of the coordinate alone determines the future dynamics of the coordinate. Such dynamics are often described as diffusion on a free-energy profile with a position-dependent diffusion coefficient, which can be determined from the coordinate time series [10].

The folding (splitting or committor) probability is considered to be an optimal coordinate [10–12] for the description of transition dynamics between any two chosen boundary states, i.e., a reaction. The name comes from the protein folding field, where this coordinate is equal to the probability of reaching the folded state before reaching the unfolded state starting from the current configuration [1]. The projection on the coordinate preserves some properties of the dynamics, in particular, the equilibrium flux between the boundary states, and the committor probability, by construction. These properties can be computed exactly by simulating diffusive dynamics with the determined free-energy landscape and diffusion coefficient [10].

The coordinate, however, is exact only for the description of the equilibrium transition dynamics between two boundary states. The dynamics inside the boundary states, or dynamics in general, without defining two end states, cannot be described. It may seem unlikely that a single coordinate, even though optimally selected, can give a complete description of multidimensional complex dynamics. Classical mechanics, however, provides an example. The action or the Hamilton principal function $S(x_i,t)$ gives a complete description of the dynamics of a system governed by the deterministic equations of classical mechanics. Here we suggest a class of optimal coordinates for the description of stochastic dynamics in general. We show that under some conditions the equations for the optimal coordinate, suggested here, are reduced to the Hamilton-Jacobi equation for the action function. In other words, the suggested optimal coordinate can be considered as a generalization of the action function to stochastic dynamics. The problem of the determination of such an optimal coordinate is closely related to two other problems.

A. The eigenmodes for stochastic dynamics

The decomposition of the dynamics of a multidimensional harmonic oscillator on normal modes is an example of a Markovian projection on coordinates. Each mode evolves independently. The phase of each normal mode can be considered as an optimal coordinate. A quantum mechanical wave function, which is a linear combination of basis eigenfunctions, is another example. Can one introduce analogous concepts for equilibrium stochastic dynamics? The conventional decomposition of the probability distribution on the eigenvectors of the master equation is not appropriate. Since all the eigenvalues (but the first) have negative real parts [13], the projections on each eigenvector exponentially decay with time. Thus after a finite amount of time only the equilibrium eigenvector survives. The latter does not describe dynamics. However, if one observes a particular dynamical trajectory of the process, the dynamics becomes stationary but never stops. Which leads us to the second problem. Can one define such eigenmodes that can be used to describe stationary stochastic dynamics?

The folding probability optimal coordinate which monitors the progress of the folding reaction, increases as the system comes closer to the folded state. It is natural to expect that an optimal coordinate that monitors the progress of the dynamics in general, without any relation to boundary states, steadily increases. In particular, it should increase whenever the system changes its state. A variable which always increases, whenever the system changes its state is time, which leads us to the third problem.

B. The reconstruction of time

Assume that we observe a stochastic process, generated by an unknown transition probability or transition rate matrix.

We have access to all the variables representing the state of the system apart from the time variable (which is external to the system). For example, one is given a trajectory of the system sampled with random unknown time intervals. Can one reconstruct the time variable? Such a reconstruction can be useful, for example, if one wants to determine the transition probability matrix.

Let $W(x)$ be such a function of coordinates that can be used to reconstruct the time interval as $t_2 - t_1 \sim W(x(t_2)) - W(x(t_1))$, where $x(t)$ is a trajectory. Since the dynamics is stochastic, such estimates fluctuate around the true value. Thus, to determine time accurately, one needs to average it over an ensemble of trajectories. The time interval can be estimated more precisely as $t_2 - t_1 \sim 1/N \sum_\alpha [W(x_\alpha(t_2)) - W(x_\alpha(t_1))]$, where the average is taken over an ensemble of trajectories $x_\alpha(t)$ $(\alpha = 1,N)$ leading from an initial distribution $x_\alpha(t_1)$ to a final distribution $x_\alpha(t_2)$ and $N \to \infty$.

Any such function that allows accurate time reconstruction can be considered as an optimal coordinate. The trajectory projected on such a coordinate has simple dynamics. There is no need to compute the free-energy profile and the diffusion coefficient. Starting from the current position t, its position after a time interval Δt is equal (on average) to $t + \Delta t$, i.e., it depends only on the current position.

While the optimal coordinate $W(x)$ describes the stochastic dynamics in a simple way, it might be useful to be able to map this description back to the original dynamics. In principle, one can invert the relationship. Given $x_\alpha(t_1)$ and $t_2 - t_1$, one may attempt to determine $x_\alpha(t_2)$. Since we have just a single equation to determine the final distribution $x_\alpha(t_2)$, the problem is ill defined. It can, however, be solved in the following cases. The first case, when one is interested in a single parameter of the distribution, for example, an average of some operator like the mean position. The time dependence of a single parameter can be determined from the single equation. The second case, if the initial distribution is an eigenmode of the dynamics, then (by construction) the distribution does not change with time. The only changing parameter is the "phase," which can be determined from the single equation. The general solution is then obtained as a superposition of all such eigenmodes. This case corresponds to the conventional way of solving a linear equation by decomposing it onto a sum of eigenmodes, i.e., it provides the solution to the second problem.

Here we introduce a general method to solve the three problems. Briefly, the main difference between the proposed method and the conventional one is to seek the solution of the master equation in the form $S = W - \nu t$, instead of the conventional $S = \psi e^{\lambda t}$. The proposed solution has a number of interesting, peculiar, and counterintuitive properties. For example, the optimal coordinate is a multivalued function. To familiarize the reader with these concepts we extensively use illustrative examples. We start by deriving the equations for the optimal coordinate by requiring it to be an ideal clock.

II. OPTIMAL COORDINATE AS AN IDEAL CLOCK

A. Equilibrium optimal coordinate

To illustrate counterintuitive properties of the optimal coordinate we first consider the more straightforward case of an equilibrium optimal coordinate. Consider an *ideal system* where a point performs a random walk along x with a constant diffusion coefficient and zero mean displacement. In this case the mean square displacement grows with time as $\langle \Delta x^2(\Delta t)\rangle = 2D\Delta t$. If one is given snapshots of the position of the point (trajectory) $x(t_i)$, one may estimate the time intervals between the snapshots (reconstruct the time) as $t_{i+1} - t_i = \Delta t \sim \Delta x^2/2D = [x(t_{i+1}) - x(t_i)]^2/2D$. Since the process is random such an estimate fluctuates around the true value. To improve the accuracy one may consider an ensemble of identical systems. Given an ensemble of trajectories $x_\alpha(t)$ $(\alpha = 1,N)$ sampled at the same (unknown) time points t_i, the time interval between the snapshots can be reconstructed with arbitrary accuracy as

$$t_{i+1} - t_i = \Delta t = \langle \Delta x^2\rangle_\alpha/2D = 1/(2DN)\sum_\alpha [x_\alpha(t_{i+1}) - x_\alpha(t_i)]^2.$$

For a *real system* where the diffusion coefficient or the potential energy surface depends on the coordinate, $\langle \Delta x^2\rangle$ does not grow strictly linearly with time. However, for any such system one can find a coordinate W (an optimal coordinate) such that the mean square displacement of the coordinate $\langle \Delta W^2\rangle$, computed for an equilibrium ensemble of trajectories, grows linearly with time [10].

Conversely, define the optimal coordinate as a coordinate whose mean square displacement grows linearly with time. Let us introduce some notation [10]. Consider a Markov process with transition matrix $\mathbf{P}$, where $P_{ji}(\Delta t)$ is the probability of transition from state i to j after time interval Δt:

$$P_i(t + \Delta t) = \sum_j P_{ij}(\Delta t) P_j(t). \tag{1}$$

The transition probability matrix for the time interval $n\Delta t$ is $\mathbf{P}(n\Delta t) = \mathbf{P}^n(\Delta t)$. Consider a stationary (steady-state) ensemble of trajectories $x_\alpha(t)$ $(\alpha = 1,N)$, generated by a Markov process [Eq. (1)]. We assume that the configuration space of the system is discrete and is represented by a (possibly infinite) set of integer numbers, i.e., indices. If the original system's dynamics is defined in a continuous configuration space, we assume that the space has been discretized. Thus, each trajectory $x_\alpha(t)$ is just a sequence of such indices denoting the current state. Such a representation is manifestly invariant with respect to the choice of the coordinate system. If trajectories are sampled with a constant time interval Δt one can determine the transition matrix $n_{ji}(\Delta t)$, which equals the number of transitions from state i to state j. $n_i = \sum_j n_{ji} = \sum_j n_{ij}$ is the number of times state i has been visited, which is proportional to P_i^{st}, the stationary (steady-state) probability distribution $P_i^{st} = \sum_j P_{ij}(\Delta t) P_j^{st}$. Based on n_i and $n_{ji}(\Delta t)$, the transition probability matrix can be estimated as $P_{ji}(\Delta t) = n_{ji}(\Delta t)/n_i$. Let the superscript T denote properties associated with the ensemble of time-reversed trajectories, i.e., trajectories that are read in the opposite direction, from the end to the start. These trajectories can be considered as a realization of a Markov process with $P_{ji}^T(\Delta t) = n_{ji}^T(\Delta t)/n_i$, where $n_{ji}^T(\Delta t) = n_{ij}(\Delta t)$ and $n_i^T = n_i$ [14].

If W is such that for every i

$$\sum_j P_{ji}(\Delta t)(W_j - W_i) = 0, \tag{2}$$

then

$$\langle \Delta W^2(n\Delta t)\rangle = n\langle \Delta W^2(\Delta t)\rangle = 2Dn\Delta t. \tag{3}$$

We prove this by induction. Assume that the statement is valid for n; then

$$\begin{aligned}
&\langle \Delta W^2[(n+1)\Delta t]\rangle \\
&= \sum_{ij} P_{ji}(n\Delta t + \Delta t)P_i^{st}(W_j - W_i)^2 \\
&= \sum_{ijk} P_{jk}(\Delta t)P_{ki}(n\Delta t)P_i^{st}(W_j - W_k + W_k - W_i)^2 \\
&= \sum_{ijk} P_{jk}(\Delta t)P_{ki}(n\Delta t)P_i^{st}[(W_j - W_k)^2 \\
&\quad + 2(W_j - W_k)(W_k - W_i) + (W_k - W_i)^2] \\
&= \sum_{jk} P_{jk}(\Delta t)P_k^{st}(W_j - W_k)^2 \\
&\quad + 2\sum_{ik} P_{ki}(n\Delta t)P_i^{st}(W_k - W_i)\sum_j P_{jk}(\Delta t)(W_j - W_k) \\
&\quad + \sum_{ik} P_{ki}(n\Delta t)P_i^{st}(W_k - W_i)^2 \\
&= \langle \Delta W^2(\Delta t)\rangle + n\langle \Delta W^2(\Delta t)\rangle.
\end{aligned}$$

Analogously, from Eq. (2) it follows that for all n

$$\sum_j P_{ji}(n\Delta t)(W_j - W_i) = 0, \tag{4}$$

i.e., the optimal coordinate is the same for the dynamics sampled with a different constant sampling interval. We prove this by induction. Assume that $\sum_j P_{ji}(n\Delta t)(W_j - W_i) = 0$; then

$$\begin{aligned}
&\sum_j P_{ji}(n\Delta t + \Delta t)(W_j - W_i) \\
&\quad = \sum_{jk} P_{jk}(\Delta t)P_{ki}(n\Delta t)(W_j - W_k + W_k - W_i) \\
&\quad = \sum_k P_{ki}(n\Delta t)\sum_j P_{jk}(\Delta t)(W_j - W_k) \\
&\qquad + \sum_k P_{ki}(n\Delta t)(W_k - W_i) = 0.
\end{aligned}$$

The transition matrix for a trajectory sampled with random intervals is the average $\langle P_{ij}\rangle = \sum_n \rho(n)P_{ij}(n\Delta t)$, where $\rho(n)$ is the probability of having an interval of $n\Delta t$. Averaging Eq. (4) with $\rho(n)$, one finds that the optimal coordinate can be found from

$$\sum_j \langle P_{ji}\rangle(W_j - W_i) = 0. \tag{5}$$

In summary, given a stationary ensemble of trajectories $x_\alpha(t)$ $(\alpha = 1, N)$, sampled at unknown time points t_i, one can determine the averaged transition matrix $\langle P_{ji}\rangle$ and thus the optimal coordinate W with Eq. (5). Using the optimal coordinate, the time interval between two time points can be reconstructed (up to a constant factor determined by D):

$$t_j - t_i = \langle \Delta W^2\rangle_\alpha/2D = 1/(N2D)\sum_{\alpha=1,N}\left[W_{x_\alpha(t_j)} - W_{x_\alpha(t_i)}\right]^2. \tag{6}$$

Here $W_{x_\alpha(t_j)}$ denotes the value of the optimal coordinate W_i at state $i = x_\alpha(t_j)$, which is attained by trajectory α at time instant t_j. Note that given both direct and time-reversed trajectories, Eq. (6) predicts only increase in time, which is in agreement with equilibrium statistical mechanics, where there is no difference between forward and time-reversed processes.

B. The optimal coordinate can have neither a maximum nor a minimum

The equation for the optimal coordinate [Eq. (2)] can be satisfied for every i, only if for every i there are such j that $W_j < W_i$ and such j that $W_i < W_j$ because $P_{ji} > 0$. For systems with infinite configuration space this does not seem to be a problem, e.g., for a random walk on the (infinite) line $W = x$, whereas systems with finite configuration space require special consideration, because they have a finite set of values of W_i and hence have maximum and minimum W_i. Consider a random walk on a ring, with probability $1/2$ to jump left or right. The transition matrix is $p_{i,i+1} = p_{i,i-1} = p_{1,N} = p_{N,1} = 1/2$. Consider the optimal coordinate as a function of the angle ϕ for $\phi = [0, 2\pi)$. Then the equation for the optimal coordinate is $W_i - W_{i-1} = W_{i+1} - W_i$, which means that points W_i are placed equidistantly on the ring $W_{i+1} - W_i = \text{const} = 2\pi/N$. If one starts from $W_1 = 0$ and uses the equation to consequently determine W_{i+1} from W_i along the ring, then when one completes the loop and returns to the first node one obtains $W_1 = 2\pi$. After the second loop $W_1 = 4\pi$ and so on. Thus, to satisfy Eq. (2) for all i, *the optimal coordinate has to be a multivalued function*. For the ring $W = \phi$, where $\phi = (-\infty, \infty)$ is the phase angle that covers the ring periodically. The inverse function, the mapping from the optimal coordinate to the states, is periodic.

Equation (2) can be rewritten for a single-valued function W_i restricted to any branch as

$$\sum_j P_{ji}(\Delta t)(W_j + d_{ji} - W_i) = 0, \tag{7}$$

where d_{ji} denotes the increment in the coordinate between two branches of the multivalued function. For a random walk on a ring $d_{1,N} = -d_{N,1} = 2\pi$ and otherwise $d_{ji} = 0$. Equation (7) is the conventional system of linear equations on a single-valued function, and can be solved by linear algebra methods. Note that, since the equation defines the solution up to a constant $W_i = W_i + c$, to solve it on a computer, one should supplement it with an equation which fixes the constant, for example, $W_1 = 0$.

A similar construction can be made for the dynamics on a segment between two boundary states A and B. Using the folding probability (p_{fold}) as an optimal coordinate the segment is mapped onto the $[0,1]$ segment, so that Eq. (2) is satisfied for all the points but A and B, which are mapped to 0 and 1, respectively [10]. To make the equation valid at points A and B,

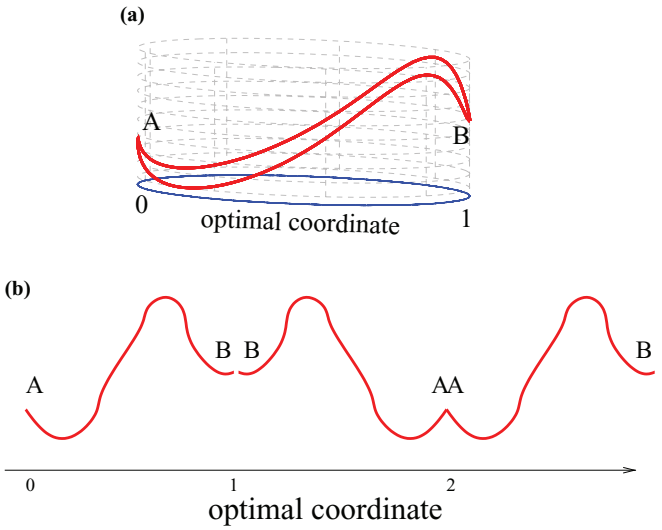

FIG. 1. (Color online) (a) Construction of an optimal coordinate with ring topology by joining the p_{fold} coordinate and its mirror image at the boundaries. (b) The resulting (periodic) profile along an infinite periodic coordinate of the ring. For such coordinate Eq. (3) is valid for all n. The red lines show a model free-energy profile.

the [0,1] segment and its mirror copy [1,0] are joined together to form a ring, the 0 ends are joined together and the 1 ends are joined together. Figure 1(a) visualizes the construction as a drawing on the surface of a cylinder; the joint profile wraps the cylinder. Equation (2) is satisfied for nodes A and B due to symmetry. Figure 1(b) shows a schematic realization of the mirroring construction along an infinite periodic optimal coordinate of the ring. For such a coordinate Eq. (3) is valid for all n. A practical realization of the procedure during an analysis of a reaction coordinate time series is as follows. Whenever the system reaches either A or B, a new current branch is selected out of the two with equal probabilities of 0.5. An alternative way to make Eq. (3) valid is to modify the counting scheme by considering the transition paths [10], which is not discussed here.

On this we finish the discussion of the equilibrium optimal coordinate and switch to a more powerful method which can be applied to nonequilibrium ensembles of trajectories and can estimate the change of time in both positive and negative directions.

C. Nonequilibrium optimal coordinate

Consider an *ideal system* where a point performs random jumps to the right with distance a and with rate r. In this case the average distance the system transits during time Δt is $\Delta x = ra\Delta t$. Accordingly, the time interval between two snapshots of the trajectory separated by distance Δx can be estimated as $\Delta t = \Delta x/(ra)$. For a realistic system, where the rate and jump distance can vary, $\Delta t = \Delta x/(ra)$ is no longer valid. Again, for any system an optimal coordinate W can be constructed so that time intervals can be determined as $\Delta t = \langle \Delta W\rangle/\nu$, where ν is a constant, with the dimension of frequency; W is dimensionless.

D. Left additive eigenvector

Let W^L and ν be a solution of

$$\sum_j n_{ji}(\Delta t)\big(W_j^L - W_i^L - \nu\Delta t\big) = 0 \tag{8}$$

or

$$\sum_j P_{ji}(\Delta t)\big(W_j^L - W_i^L - \nu\Delta t\big) = 0, \tag{9}$$

which can be considered as the definition of the left *additive* eigenvector

$$\sum_j P_{ji}(\Delta t)W_j^L = W_i^L + \nu\Delta t, \tag{10}$$

where $\nu\Delta t = \lambda$ is an *additive* eigenvalue. For a system with n states Eq. (8) consists of n equations, which together with the equation that fixes the origin of the eigenvector (e.g., $W_1^L = 0$) makes it $n+1$ equations for $n+1$ variables. The multiplication by (the transpose of) the matrix $\mathbf{P}$ changes the components of the vector $\mathbf{W}^L$ in a simple way by adding a constant. It is easy to see that

$$\sum_j P_{ji}(n\Delta t)W_j^L = \sum_j P_{ji}^n(\Delta t)W_j^L = W_i^L + n\nu\Delta t$$

or

$$\sum_j P_{ji}(n\Delta t)\big(W_j^L - W_i^L - n\nu\Delta t\big) = 0. \tag{11}$$

For example, for $n = 2$,

$$\begin{aligned}\sum_{jk} P_{jk}(\Delta t)P_{ki}(\Delta t)W_j^L &= \sum_k P_{ki}(\Delta t)\big(W_k^L + \nu\Delta t\big)\\ &= \sum_k P_{ki}(\Delta t)W_k^L + \sum_k P_{ki}(\Delta t)\nu\Delta t = W_i^L + 2\nu\Delta t.\end{aligned}$$

If the transition matrix $\langle P_{ji}\rangle = \sum_n \rho(n)P_{ji}(n\Delta t)$ is the average of the transition matrices with random distribution of steps $\rho(n)$ (a trajectory sampled with random intervals), then W^L is also the solution of

$$\sum_j \langle P_{ji}\rangle\big(W_j^L - W_i^L - \langle\Delta t\rangle\nu\big) = 0, \tag{12}$$

where $\langle\Delta t\rangle = \sum_n \rho(n)n\Delta t$ is the average sampling interval. Multiplying Eqs. (11) and (12) by n_i, one obtains

$$\sum_j n_{ji}(n\Delta t)\big(W_j^L - W_i^L - n\nu\Delta t\big) = 0 \tag{13}$$

and

$$\sum_j \langle n_{ji}\rangle\big(W_j^L - W_i^L - \langle\Delta t\rangle\nu\big) = 0. \tag{14}$$

Thus, given an ensemble of trajectories $x_\alpha(t)$ $(\alpha = 1,N)$, sampled at unknown time points t_i, one can determine the averaged transition matrix $\langle n_{ji}\rangle$ and thus the optimal coordinate W^L with Eq. (14).

E. Right additive eigenvector

It is useful to define the right *additive* eigenvector as a solution of the equation

$$\sum_j n_{ij}(\Delta t)\left(W_i^R - W_j^R - \nu\Delta t\right) = 0 \tag{15}$$

or, equivalently,

$$\sum_j \tilde{P}_{ij}(\Delta t)\left(W_i^R - W_j^R - \nu\Delta t\right) = 0 \tag{16}$$

and

$$\sum_j \tilde{P}_{ij}(\Delta t)W_j^R = W_i^R - \nu\Delta t,$$

where $\tilde{P}_{ij}(\Delta t) = n_{ij}(\Delta t)/n_i = P_{ij}(\Delta t)P_j^{st}/P_i^{st}$. It is easy to see that

$$\sum_j \tilde{P}_{ij}(n\Delta t)\left(W_i^R - W_j^R - n\nu\Delta t\right) = 0$$

and

$$\sum_j n_{ij}(n\Delta t)\left(W_i^R - W_j^R - n\nu\Delta t\right) = 0. \tag{17}$$

Note that $\tilde{P}_{ij}$ is not a stochastic matrix, i.e., $\sum_i \tilde{P}_{ij} \neq 1$; however, $\sum_j \tilde{P}_{ij} = 1$. If detailed balance holds, i.e., $n_{ji}(\Delta t) = P_{ji}(\Delta t)n_i = P_{ij}(\Delta t)n_j = n_{ij}(\Delta t)$, then $\tilde{P}_{ij} = P_{ji}$.

Given an ensemble of trajectories $x_\alpha(t)$ ($\alpha = 1,N$), which describes the stationary dynamics of the system, one can define the following averages to measure time intervals. Averaging over the entire ensemble of trajectories,

$$1/N\sum_\alpha \left[W_{x_\alpha(t_2)} - W_{x_\alpha(t_1)}\right]. \tag{18}$$

Averaging over the subset of trajectories starting from a particular state at time t_1 (or a subset of states),

$$\frac{\sum_\alpha \left[W_{x_\alpha(t_2)} - W_{x_\alpha(t_1)}\right]A_{x_\alpha(t_1)}}{\sum_\alpha A_{x_\alpha(t_1)}}, \tag{19}$$

where A is the indicator function of the subset of states, i.e., $A_x = 1$ if x is in the chosen subset of states and zero otherwise. For a single state i, $A_x = \delta_{xi}$, the Kronecker symbol. Averaging over the subset of trajectories ending in a particular state at time t_2 (or a subset of states),

$$\frac{\sum_\alpha \left[W_{x_\alpha(t_2)} - W_{x_\alpha(t_1)}\right]A_{x_\alpha(t_2)}}{\sum_\alpha A_{x_\alpha(t_2)}}. \tag{20}$$

Equations (19) and (20) reduce to Eq. (18) for $A_x = 1$ for all x.

Multiplying Eq. (13) by A_i and summing over i, one finds that *the left eigenvector can be used to measure time for trajectories starting from a set of states*

$$t_2 - t_1 = 1/\nu\frac{\sum_\alpha \left[W^L_{x_\alpha(t_2)} - W^L_{x_\alpha(t_1)}\right]A_{x_\alpha(t_1)}}{\sum_\alpha A_{x_\alpha(t_1)}}. \tag{21}$$

Multiplying Eq. (17) by A_i and summing over i one finds that *the right eigenvector can be used to measure time for trajectories ending in a set of states*

$$t_2 - t_1 = 1/\nu\frac{\sum_\alpha \left[W^R_{x_\alpha(t_2)} - W^R_{x_\alpha(t_1)}\right]A_{x_\alpha(t_2)}}{\sum_\alpha A_{x_\alpha(t_2)}}. \tag{22}$$

For stationary processes, the averaging in Eqs. (18)–(22) may include averaging over time, e.g., for Eq. (21) one has

$$\Delta t = 1/\nu\frac{\sum_{\alpha,t} \left[W^L_{x_\alpha(t+\Delta t)} - W^L_{x_\alpha(t)}\right]A_{x_\alpha(t)}}{\sum_{\alpha,t} A_{x_\alpha(t)}}. \tag{23}$$

F. Time-reversed trajectories

The equation for the left eigenvector of time-reversed trajectories is

$$\sum_j n^T_{ji}(\Delta t)\left(W_j^{TL} - W_i^{TL} - \nu\Delta t\right) = 0,$$

which can be transformed to Eq. (15) with negative Δt,

$$\sum_j n_{ij}(\Delta t)\left[W_i^{TL} - W_j^{TL} - \nu(-\Delta t)\right] = 0,$$

i.e., the right eigenvector for forward trajectories can be taken as the left eigenvector for time-reversed trajectories, and vice versa.

G. Time-dependent reaction coordinate

By introducing $S_i^L(t) = W_i^L - \nu t$ and $S_i^R(t) = W_i^R - \nu t$, Eqs. (8) and (15) can be written as

$$\begin{aligned}\sum_j n_{ji}\left[S_j^L(t+\Delta t) - S_i^L(t)\right] = 0,\\ \sum_j n_{ij}\left[S_i^R(t+\Delta t) - S_j^R(t)\right] = 0.\end{aligned} \tag{24}$$

These equations can be considered as a generalization of the equation for the p_{fold} reaction coordinate [Eq. (2)] to time-dependent reaction coordinates S^L and S^R. For $\nu = 0$, when the coordinates do not change with time and $n_{ij} = n_{ji}$ the single-valued solutions equal $S^L = S^R = p_{\text{fold}}$. The equations, as well as Eq. (2), mean that the average change of the (time-dependent) optimal coordinates along a trajectory is zero.

So far we have assumed that the optimal coordinate is a function of the state index i. Such a description is invariant with respect to the choice of the coordinate system. As shown in the illustrative examples below, it might be useful to embed the index in spatial coordinates, so that the optimal coordinate becomes a function of position $W(x)$. For example, in the one-dimensional case, one assigns position x_i to state i and assumes that $W_{i+1} - W_i = \hbar\Delta x$, where $\hbar = k/2\pi = 1/\lambda$ has the meaning of the wave number and λ is the wavelength; the dimension of k is the inverse of x to keep W dimensionless. In this case the change of the optimal coordinate can be written in a form where space and time are on an equal footing:

$$S_{x+\Delta x}(t+\Delta t) - S_x(t) = \hbar\Delta x - \nu\Delta t.$$

H. Symmetric or relativistic coordinate

According to Eqs. (21) and (22) one needs to use two different optimal coordinates S^R and S^L (or two additive eigenvectors) to describe incoming and outgoing or forward and time-reversed subsets of trajectories. It might be useful to introduce a single coordinate to describe all the subsets. The procedure is analogous to the symmetrization of the transition probability matrix $P_{ij} \to P_{ij}\sqrt{P_j^{st}/P_i^{st}}$ in the conventional case, which leads to the left and right eigenvectors being equal. Let

$$\sum_j P_{ji}(\Delta t)\left[S_j^L(t+\Delta t) - S_i^L(t)\right] = 0,$$
$$\sum_j P_{ij}(\Delta t)P_j/P_i\left[S_i^R(t+\Delta t) - S_j^R(t)\right] = 0$$

be two optimal coordinates that describe a stationary solution. Let $R_i = \sqrt{P_i}$; then

$$\sum_j P_{ji}(\Delta t)(R_i/R_j)(R_j/R_i)\left(S_j^L(t+\Delta t) - S_i^L(t)\right) = 0,$$
$$\sum_j P_{ij}(\Delta t)(R_j/R_i)(R_j/R_i)\left(S_i^R(t+\Delta t) - S_j^R(t)\right) = 0.$$

Introduce

$$\begin{aligned} S_j^L(t+\Delta t) - S_i^L &= R_i/R_j\left[S_j^s(t+\Delta t) - S_i^s(t)\right], \\ S_j^R(t+\Delta t) - S_i^R &= R_j/R_i\left[S_j^s(t+\Delta t) - S_i^s(t)\right], \end{aligned} \tag{25}$$

i.e., the change of S^s is the geometric mean of the changes of S^L and S^R. Then

$$\sum_j P_{ji}(\Delta t)R_i/R_j\left[S_j^s(t+\Delta t) - S_i^s(t)\right] = 0,$$
$$\sum_j P_{ij}(\Delta t)R_j/R_i\left[S_i^s(t+\Delta t) - S_j^s(t)\right] = 0,$$

or, if $\tilde{P}_{ij}$ is known,

$$\sum_j P_{ji}(\Delta t)R_i/R_j\left[S_j^s(t+\Delta t) - S_i^s(t)\right] = 0,$$
$$\sum_j \tilde{P}_{ij}(\Delta t)R_i/R_j\left[S_i^s(t+\Delta t) - S_j^s(t)\right] = 0,$$

or

$$\sum_j \tilde{P}_{ji}(\Delta t)R_j/R_i\left[S_j^s(t+\Delta t) - S_i^s(t)\right] = 0,$$
$$\sum_j P_{ij}(\Delta t)R_j/R_i\left[S_i^s(t+\Delta t) - S_j^s(t)\right] = 0.$$

Introducing $W_i^s - v^s t = S_i^s(t)$ one obtains

$$\sum_j P_{ji}(\Delta t)R_i/R_j\left(W_j^s - W_i^s - v^s\Delta t\right) = 0,$$
$$\sum_j P_{ij}(\Delta t)R_j/R_i\left(W_i^s - W_j^s - v^s\Delta t\right) = 0, \tag{26}$$

or

$$\sum_j P_{ji}(\Delta t)R_i/R_j\left(W_j^s - W_i^s - v^s\Delta t\right) = 0,$$
$$\sum_j \tilde{P}_{ij}(\Delta t)R_i/R_j\left(W_i^s - W_j^s - v^s\Delta t\right) = 0, \tag{27}$$

or

$$\sum_j \tilde{P}_{ji}(\Delta t)R_j/R_i\left(W_j^s - W_i^s - v^s\Delta t\right) = 0,$$
$$\sum_j P_{ij}(\Delta t)R_j/R_i\left(W_i^s - W_j^s - v^s\Delta t\right) = 0. \tag{28}$$

W^s is not an additive eigenvector, meaning that Eqs. (25)–(28) are valid only in the limit of $\Delta t \to 0$. They are not valid for an arbitrarily large Δt, as we show later, since the symmetrized matrix is not a stochastic matrix. However, such a coordinate can be used in the limit of small Δt to measure time for both starting and ending subsets of trajectories as

$$t_2 - t_1 = \frac{\sum_\alpha \left[W^s_{x_\alpha(t_2)} - W^s_{x_\alpha(t_1)}\right] A_{x_\alpha(t_1)} R^{-1}_{x_\alpha(t_2)} R^{-1}_{x_\alpha(t_1)}}{\sum_\alpha A_{x_\alpha(t_1)} R^{-1}_{x_\alpha(t_2)} R^{-1}_{x_\alpha(t_1)}} \Big/ v^s \tag{29}$$

and

$$t_2 - t_1 = \frac{\sum_\alpha \left[W^s_{x_\alpha(t_2)} - W^s_{x_\alpha(t_1)}\right] A_{x_\alpha(t_2)} R^{-1}_{x_\alpha(t_2)} R^{-1}_{x_\alpha(t_1)}}{\sum_\alpha A_{x_\alpha(t_2)} R^{-1}_{x_\alpha(t_2)} R^{-1}_{x_\alpha(t_1)}} \Big/ v^s. \tag{30}$$

Equation (25) can be used to determine S^s and R from S^L and S^R.

I. Equations for the rate matrix

To derive the equations for the rate matrix we let $P_{ji}(\Delta t) = e^{\Delta t K_{ji}} \approx \delta_{ji} + \Delta t K_{ji}$, where K_{ji} is the rate of going from state i to state j and $\sum_j K_{ji} = 0$; then

$$\begin{aligned} \sum_j (\delta_{ji} + K_{ji}\Delta t)\left(W_j^L - W_i^L - v\Delta t\right) &= 0, \\ \sum_j K_{ji}\Delta t\left(W_j^L - W_i^L\right) - v\Delta t &= 0, \\ \sum_j K_{ji}\left(W_j^L - W_i^L\right) - v &= 0. \end{aligned} \tag{31}$$

Similarly one obtains

$$\sum_j \tilde{K}_{ij}\left(W_i^R - W_j^R\right) - v = 0, \tag{32}$$

where $\tilde{K}_{ij} = K_{ij}(\Delta t)P_j^{st}/P_i^{st}$. For the symmetric coordinate one obtains

$$\sum_j (\delta_{ji} + K_{ji}\Delta t)R_i/R_j\left(W_j^s - W_i^s - v^s\Delta t\right) = 0,$$
$$\sum_j K_{ji}R_i/R_j\left(W_j^s - W_i^s\right) - v^s\left(1 + \Delta t\sum_j K_{ji}R_i/R_j\right) = 0,$$

which shows that W^s and v^s become independent of Δt in the limit of $\Delta t \to 0$, where Eq. (26) reads

$$\begin{aligned} \sum_j K_{ji} R_i / R_j \left(W_j^s - W_i^s\right) - v^s &= 0, \\ \sum_j K_{ij} R_j / R_i \left(W_i^s - W_j^s\right) - v^s &= 0, \end{aligned} \tag{33}$$

or, if $\tilde{K}_{ij}$ is known,

$$\begin{aligned} \sum_j K_{ji} R_i / R_j \left(W_j^s - W_i^s\right) - v^s &= 0, \\ \sum_j \tilde{K}_{ij} R_i / R_j \left(W_i^s - W_j^s\right) - v^s &= 0. \end{aligned} \tag{34}$$

J. Illustrative Example 1

To illustrate the introduced concepts, consider the following example. Consider a system that moves to the right with rate $K_{i+1,i} = r_i$. For a small Δt only $n_{i,i}$ and $n_{i+1,i}$ are nonzero. For such a system the number of transitions from i to $i+1$ is constant: $n_{i+1,i} = \text{const} = J\Delta t = r_i \Delta t n_i$, and $n_i = J/r_i$, where J is the flux. For the number of transitions from i to i one has $n_{i,i} = (1 - r_i \Delta t) n_i = J(1 - r_i \Delta t)/r_i$. For the left eigenvector optimal coordinate one finds [Eq. (8)]

$$\begin{aligned} n_{i,i}\left(W_i^L - W_i^L - v\Delta t\right) + n_{i+1,i}\left(W_{i+1}^L - W_i^L - v\Delta t\right) &= 0, \\ -v + r_i\left(W_{i+1}^L - W_i^L\right) &= 0, \\ W_{i+1}^L - W_i^L &= v/r_i. \end{aligned} \tag{35}$$

For the right eigenvector optimal coordinate one obtains [Eq. (15)]

$$\begin{aligned} n_{i,i}\left(W_i^R - W_i^R - v\Delta t\right) + n_{i,i-1}\left(W_i^R - W_{i-1}^R - v\Delta t\right) &= 0, \\ -v/r_i + W_i^R - W_{i-1}^R &= 0, \\ W_i^R - W_{i-1}^R &= v/r_i, \\ W_{i+1}^R - W_i^R &= v/r_{i+1}, \end{aligned}$$

i.e., it is different from that of the left eigenvector.

The same result can be found using Eq. (32). $\tilde{K}_{i+1,i} = K_{i+1,i} P_i^{st}/P_{i+1}^{st} = r_i (J/r_i)/(J/r_{i+1}) = r_{i+1}$. Hence,

$$\begin{aligned} r_{i+1}\left(W_{i+1}^R - W_i^R\right) - v &= 0, \\ W_{i+1}^R - W_i^R &= v/r_{i+1}. \end{aligned}$$

For the symmetrized (relativistic) optimal coordinate one finds using Eqs. (33) ($R_i = \sqrt{J/r_i}$)

$$\begin{aligned} r_i R_i / R_{i+1}\left(W_{i+1}^s - W_i^s\right) - v^s &= 0, \\ r_i R_i / R_{i+1}\left(W_{i+1}^s - W_i^s\right) - v^s &= 0, \\ \sqrt{r_i r_{i+1}}\left(W_{i+1}^s - W_i^s\right) - v^s &= 0, \\ W_{i+1}^s - W_i^s &= v^s/\sqrt{r_i r_{i+1}}, \end{aligned}$$

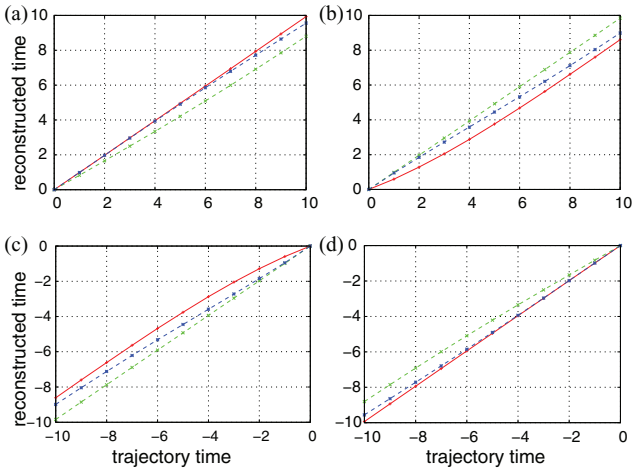

FIG. 2. (Color online) Reconstruction of time from system snapshots (configurations) of an ensemble of (a) forward trajectories starting from $x = 50$, (b) forward trajectories ending at $x = 50$, (c) time-reversed trajectories starting from $x = 50$, and (d) time-reversed trajectories ending at $x = 50$. Reconstructions using W^L, W^R, and W^s are shown by red, green, and blue lines, respectively. The plots show the reconstructed time vs the actual time.

or, if one knows $\tilde{K}_{ji}$, then Eq. (34) can be used to find both R_i and W_i^s:

$$\begin{aligned} r_i R_i / R_{i+1}\left(W_{i+1}^s - W_i^s\right) - v^s &= 0, \\ r_{i+1} R_{i+1} / R_i \left(W_{i+1}^s - W_i^s\right) - v^s &= 0, \\ r_i R_i / R_{i+1} &= r_{i+1} R_{i+1} / R_i, \\ R_i &= \sqrt{J/r_i}, \\ \sqrt{r_i r_{i+1}}\left(W_{i+1}^s - W_i^s\right) - v^s &= 0, \\ W_{i+1}^s - W_i^s &= v^s/\sqrt{r_i r_{i+1}}. \end{aligned}$$

Equation (35) defines the optimal coordinate as a function of the index i. The index i can be embedded into a spatial coordinate, i.e., each state (i) can be given a position x_i, so that the optimal coordinate is a function of the position. For example, if x_i are selected as $x_{i+1} - x_i = c/r_i$, where c is a constant with the dimension of velocity, then $W^L = \bar{k}\, x$, $v = c\bar{k}$, and $S = W - vt = \text{const}$ describes a wave moving to the right with constant velocity of c. For the right coordinate one has $x_{i+1} - x_i = c/r_{i+1}$, i.e., both coordinates cannot be simultaneously embedded to keep c constant.

1. Numerical example

Consider a system with $r_i = [\text{mod}(i,5) + 5]/25$. 10 000 trajectories have been simulated by the Monte Carlo method (with time step of $dt = 0.1$) starting from $i = 1$ until the system reached $i = 100$. Figure 2 shows time reconstructed from the trajectories using left, right, and symmetric optimal coordinates for $n\Delta t = 1, \ldots, 10$ by applying corresponding variants of Eq. (23). Figure 2(a) shows that time reconstructed for trajectories starting from $i = 50$ agrees with the actual time if reconstruction is performed with the left coordinate and disagrees significantly if performed with the right coordinate. Figure 2(b) shows that time reconstructed for a subset of trajectories ending in $i = 50$ is accurate if the right coordinate is used and not if the left one is used. The relativistic coordinate

reconstructs time accurately for both sets of trajectories but only for relatively short time intervals. At longer time intervals the reconstructed time deviates from the actual one. To accurately reconstruct time for long time intervals using the relativistic coordinate, the trajectory needs to be divided into short segments, the times for which can be accurately reconstructed, and then the total time can be found as their sum. The left and right coordinates reconstruct times accurately for their corresponding sets of trajectories for arbitrary long trajectory segments. Figures 2(c) and 2(d) show results for time-reversed trajectories, where the left and right coordinates exchange their functions.

III. DYNAMICS WITH DETAILED BALANCE

From now on we consider only systems with stationary dynamics where detailed balance holds, $n_{ij} = n_{ji}$, and where, correspondingly, $\tilde{P}_{ji}(\Delta t) = P_{ij}(\Delta t)$ and $\tilde{K}_{ji} = K_{ij}$. For such systems, as can be easily seen, straightforward computation of right or left additive eigenvectors leads to $\nu = 0$. For example, by summing up over i, Eqs. (8), one obtains

$$\sum_{ij} n_{ij}\left(W_i^L - W_j^L - \nu\Delta t\right) = 0,$$
$$\nu\Delta t \sum_{ij} n_{ij} = \sum_{ij} n_{ij}\left(W_i^L - W_j^L\right) = 0.$$

Thus, solutions with nonzero ν, necessary for the estimation of time intervals, are not possible (in the space of single-valued functions).

Solutions with $\nu \neq 0$ become possible, however, if one assumes that W_i is not a single-valued function, i.e., that the next time the system visits the same state i, W_i can be different. One can suggest multiple reasons for that. For example, if a system moves on a line, it has to move in the reverse direction to return to the same point. The optimal coordinates that describe the motion in the backward and forward directions should not necessarily be the same. So each time the system changes direction, it may be described by a new coordinate. For systems moving on a ring the situation is more familiar. For example, for a random walk on a ring, considered above, the optimal coordinate equals ϕ, the angular position (phase) on the ring, which covers the ring periodically. When the system returns to the same point by completing a cycle around the ring, the change in W_i is analogous to the increase in ϕ by 2π. The classical action function is yet another example.

Note that the multivaluedness may lead to the following counterintuitive property:

$$\begin{aligned}(W_i - W_j) + (W_j - W_i) &\neq 0,\\ (W_i - W_j) &\neq -(W_j - W_i),\end{aligned} \tag{36}$$

if the W_i in different parentheses belong to different branches. It seems that (to the best of my knowledge) the theory of such multivalued solutions for left and right additive eigenvectors has not been developed. I will present below some examples where particular solutions can be found in a straightforward manner.

A. Reducing equations to a particular branch of a multivalued function

While the equations for optimal coordinates are just simple systems of linear equations, they cannot be solved with conventional linear algebra methods because the coordinates are multivalued functions. Assume that, for example, based on physical intuition, one knows where the transition between different branches of the multivalued function happens and that the difference between the branches is always the same (the solution is periodic). For example, if a new branch is reached at the transition from i to j and the value on the new branch is related to the value of an old branch as $W_j^{\text{new}} = W_j + d_{ji}$, then Eqs. (9) and (16) can be rewritten for values at one (old) branch as

$$\sum_j P_{ji}(\Delta t)\left(W_j^L + d_{ji} - W_i^L - \nu\Delta t\right) = 0, \tag{37}$$
$$\sum_j \tilde{P}_{ij}(\Delta t)\left(W_i^R + d_{ij} - W_j^R - \nu\Delta t\right) = 0, \tag{38}$$

where d_{ij} are the differences (in phase) between different branches of the multivalued functions. The values at any branch can be taken since the solution is invariant to a constant shift $W_i = W_i + c$. Assume further that any solution with many nonzero d_{ij} can be represented as a linear combination of basis solutions with few or even a single nonzero d_{ij}. Since the solution is defined up to a factor, for the latter case we can set the nonzero $d_{ij} = 1$.

For the rate matrix one obtains

$$\sum_j K_{ji}\left(W_j^L + d_{ji} - W_i^L\right) - \nu = 0, \tag{39}$$
$$\sum_j \tilde{K}_{ij}\left(W_i^R + d_{ij} - W_j^R\right) - \nu = 0. \tag{40}$$

For a relativistic optimal coordinate, for example, Eq. (34), one obtains

$$\begin{aligned}\sum_j K_{ij}R_i/R_j\left(W_j^s + d_{ji} - W_i^s\right) - \nu^s &= 0,\\ \sum_j \tilde{K}_{ij}R_i/R_j\left(W_i^s + d_{ij} - W_j^s\right) - \nu^s &= 0.\end{aligned} \tag{41}$$

Alternatively, one can explicitly introduce multivaluedness by introducing a variable l that describes the current branch. The optimal coordinate becomes a function of two variables $W_{l,i}$, where one further assumes $W_{l,i} = ld + W_i$. For such defined optimal coordinates Eq. (36) is no longer counterintuitive:

$$\begin{aligned}(W_{l,i} - W_{l,j}) + (W_{l+1,j} - W_{l,i}) &\neq 0,\\ (W_{l,i} - W_{l,j}) + (W_{l,j} - W_{l,i}) &= 0.\end{aligned}$$

B. Illustrative example 2: Transitions between two states with different rates

Consider a system with dynamics described by the following master equation:

$$\partial p_1/\partial t = -r_1 p_1 + r_2 p_2,$$
$$\partial p_2/\partial t = -r_2 p_2 + r_1 p_1.$$

We assume that an optimal coordinate changes branches when the system makes the transition $2 \to 1$. The coordinate is taken in the form $W_{l,i} = l + W_i$. For the left additive eigenvector one obtains [Eq. (31)]

$$\begin{aligned} r_1\left(W^L_{l,2} - W^L_{l,1}\right) - \nu &= 0,\\ r_2\left(W^L_{l+1,1} - W^L_{l,2}\right) - \nu &= 0,\\ \left[W^L_2 - W^L_1\right] - \nu/r_1 &= 0,\\ \left[W^L_1 + 1 - W^L_2\right] - \nu/r_2 &= 0,\\ \nu &= 1/(1/r_1 + 1/r_2),\\ W^L_1 &= 0,\\ W^L_2 &= \nu/r_1. \end{aligned}$$

Thus, one has $W^L_2 - W^L_1 = \nu/r_1$, $W^L_1 - W^L_2 = \nu/r_2$, and $(W^L_2 - W^L_1) + (W^L_1 - W^L_2) = 1 \neq 0$ because W^L_1 in the second set of parentheses belongs to the next branch.

For stationary (equilibrium) populations one has $P^{st}_1 = 1/r_1$ and $P^{st}_2 = 1/r_2$, and $\tilde{K}_{12} = K_{21} = r_1$, $\tilde{K}_{21} = r_2$. For the right additive eigenvector one finds [Eq. (32)]

$$\begin{aligned} r_2\left(W^R_{l,2} - W^R_{l,1}\right) - \nu &= 0,\\ r_1\left(W^R_{l+1,1} - W^R_{l,2}\right) - \nu &= 0,\\ \nu &= 1/(1/r_1 + 1/r_2),\\ W^R_1 &= 0,\\ W^R_2 &= \nu/r_2. \end{aligned}$$

Thus while ν for both coordinates is the same, $W^L \neq W^R$.

1. Explicit symmetrization

For the symmetric rate matrix one obtains $K^s_{21} = K_{21}\sqrt{P^{st}_1/P^{st}_2} = r_1\sqrt{r_2/r_1} = \sqrt{r_1 r_2} = K^s_{12}$. W^s can be found as a left or right eigenvector of the symmetric rate matrix

$$\begin{aligned} \sqrt{r_1 r_2}\left(W^s_{l,2} - W^s_{l,1}\right) - \nu^s &= 0,\\ \sqrt{r_1 r_2}\left(W^s_{l+1,1} - W^s_{l,2}\right) - \nu^s &= 0,\\ \nu^s &= \sqrt{r_1 r_2}/2,\\ W^s_1 &= 0,\\ W^s_2 &= 1/2. \end{aligned}$$

2. Implicit symmetrization

The equation for the relativistic coordinate, Eq. (34), reads

$$\begin{aligned} r_1 R_1/R_2\left(W^s_{l,2} - W^s_{l,1}\right) - \nu^s &= 0,\\ r_2 R_2/R_1\left(W^s_{l+1,1} - W^s_{l,2}\right) - \nu^s &= 0,\\ r_2 R_2/R_1\left(W^s_{l,2} - W^s_{l,1}\right) - \nu^s &= 0,\\ r_1 R_1/R_2\left(W^s_{l+1,1} - W^s_{l,2}\right) - \nu^s &= 0. \end{aligned}$$

After the substitution $W^s_{l,i} = l + W^s_i$ one finds both W^s_i and R_i:

$$\begin{aligned} r_1 R_1/R_2\left(W^s_2 - W^s_1\right) - \nu^s &= 0,\\ r_2 R_2/R_1\left(W^s_1 + 1 - W^s_2\right) - \nu^s &= 0,\\ r_2 R_2/R_1\left(W^s_2 - W^s_1\right) - \nu^s &= 0, \end{aligned}$$

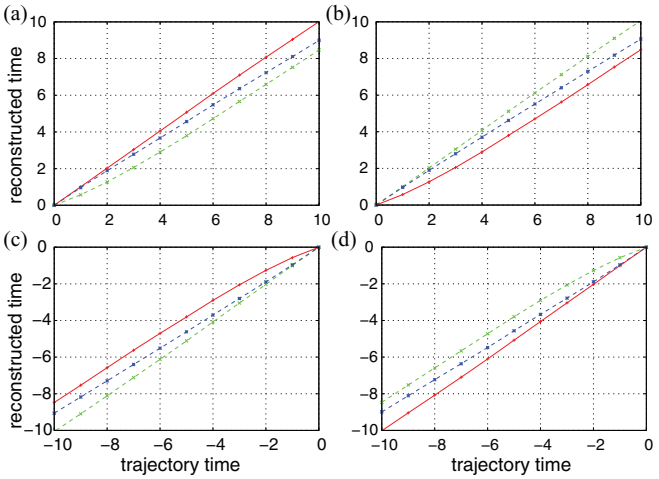

FIG. 3. (Color online) Reconstruction of time from system snapshots (configurations) from ensembles of (a) forward trajectories starting from $x = (10,1)$, (b) forward trajectories ending at $x = (10,1)$, (c) time-reversed trajectories starting from $x = (10,1)$, and (d) time-reversed trajectories ending at $x = (10,1)$. Reconstructions using W^L, W^R, and W^s are shown by red, green, and blue lines, respectively. The plots show the reconstructed time vs the actual time.

$$\begin{aligned} r_1 R_1/R_2\left(W^s_1 + 1 - W^s_2\right) - \nu^s &= 0,\\ r_2 R_2/R_1 &= r_1 R_1/R_2,\\ R_1 = 1/\sqrt{r_1}, \quad R_2 &= 1/\sqrt{r_2},\\ \sqrt{r_1 r_2}\left(W^s_2 - W^s_1\right) - \nu^s &= 0,\\ \sqrt{r_1 r_2}\left(W^s_1 + 1 - W^s_2\right) - \nu^s &= 0,\\ \nu^s &= \sqrt{r_1 r_2}/2,\\ W^s_1 &= 0,\\ W^s_2 &= 1/2. \end{aligned}$$

3. Numerical example

1000 trajectories (time series of l,i) each of length $10^5 dt$ were simulated by the Monte Carlo (MC) method with time steps of $dt = 0.01$ and saved with time intervals of $\Delta t = 1$. The transition rates are $r_1 = 0.1$ and $r_2 = 0.2$. Figure 3 shows the reconstructed time vs the actual time. For forward trajectories, starting from $x = (10,1)$, time can be reconstructed only by the left coordinate and conversely for forward trajectories ending in the state, time can be reconstructed only by the right coordinate. The relativistic coordinate can be used to reconstruct time in both cases but only for short time intervals.

C. Illustrative example 3: Stochastic model of the telegrapher's equation

Consider a particle that jumps in a constant direction, and changes direction with rate r. The model can be considered as a discrete version of the stochastic model of the telegrapher's equation [15]. We assume that every time the direction is changed the dynamics is described by a new coordinate. The dynamics in the positive direction is described by coordinates $W_{2l+1,i}$, while that in the negative direction is described by coordinates $W_{2l+2,i}$. Thus we have the following set of

transitions: $W_{2l+1,i} \to$ to $W_{2l+1,i+1}$ with probability $1 - r\Delta t$ or to $W_{2l+2,i-1}$ with probability $r\Delta t$; $W_{2l+2,i} \to$ to $W_{2l+2,i-1}$ with probability $1 - r\Delta t$ or to $W_{2l+3,i+1}$ with probability $r\Delta t$. For the left additive eigenvector one has [Eq. (9)]

$$\begin{aligned}(1 - r\Delta t)\left[W^L_{2l+1,i+1} - W^L_{2l+1,i} - \nu\Delta t\right] \\ + r\Delta t\left[W^L_{2l+2,i-1} - W^L_{2l+1,i} - \nu\Delta t\right] = 0, \\ (1 - r\Delta t)\left[W^L_{2l+2,i-1} - W^L_{2l+2,i} - \nu\Delta t\right] \\ + r\Delta t\left[W^L_{2l+3,i+1} - W^L_{2l+2,i} - \nu\Delta t\right] = 0.\end{aligned}$$

We assume that the (basis) solutions are periodic, i.e., $W^L_{l+m,i} = W^L_{l,i} + md$; in particular, we consider the case where $m = 2$. Let $W^L_{2l+1,i} = 2l + 1 + i\Delta x\,\hbar + w_1$, $W^L_{2l+2,i} = 2l + 2 + (i + 1)\Delta x\,\hbar + w_2$, i.e., the index i is considered to be embedded into coordinate x as $i\Delta x \sim x$ and $W \sim \hbar\, x$. After substitution one finds

$$\begin{aligned}(1 - r\Delta t)\hbar\Delta x + r\Delta t[w_2 + 1 - w_1] - \nu\Delta t = 0, \\ -(1 - r\Delta t)\hbar\Delta x + r\Delta t[w_1 + 1 - w_2] - \nu\Delta t = 0, \\ \nu = r.\end{aligned}$$

We assume that $\Delta x = c\Delta t$, where c is a constant, so that the limit $\Delta t \to 0$ exists. We let $w_1 = 0$ and find

$$\begin{aligned}w_2 &= -(1 - r\Delta t)c\hbar\,/\nu, \\ W^L_{2l+1,i} &= 2l + 1 + \hbar\, i\Delta x, \\ W^L_{2l+2,i} &= 2l + 2 + \hbar\,(i + 1)\Delta x - (1 - r\Delta t)c\hbar\,/\nu.\end{aligned}$$

In the limit $\Delta t \to 0$ and, correspondingly, $\Delta x \to 0$,

$$\begin{aligned}W^L_{2l+1,x} &= 2l + 1 + \hbar\, x, \\ W^L_{2l+2,x} &= 2l + 2 + \hbar\, x - c\hbar\,/\nu.\end{aligned}$$

For the right additive eigenvector

$$\begin{aligned}(1 - r\Delta t)\left[W^R_{2l+1,i} - W^R_{2l+1,i-1} - \nu\Delta t\right] \\ + r\Delta t\left[W^R_{2l+1,i} - W^R_{2l,i-1} - \nu\Delta t\right] = 0, \\ (1 - r\Delta t)\left[W^R_{2l+2,i} - W^R_{2l+2,i+1} - \nu\Delta t\right] \\ + r\Delta t\left[W^R_{2l+2,i} - W^R_{2l+1,i+1} - \nu\Delta t\right] = 0,\end{aligned}$$

one analogously finds

$$\begin{aligned}(1 - r\Delta t)\hbar\Delta x + r\Delta t[w_1 + 1 - w_2] - \nu\Delta t = 0, \\ -(1 - r\Delta t)\hbar\Delta x + r\Delta t[w_2 + 1 - w_1] - \nu\Delta t = 0, \\ \nu = r, \\ w_1 = 0, \\ w_2 = (1 - r\Delta t)c\hbar\,/\nu, \\ W^R_{2l+1,i} = 2l + 1 + \hbar\, i\Delta x, \\ W^R_{2l+2,i} = 2l + 2 + \hbar\,(i + 1)\Delta x + (1 - r\Delta t)c\hbar\,/\nu, \\ W^R_{2l+1,x} = 2l + 1 + \hbar\, x, \\ W^R_{2l+2,x} = 2l + 2 + \hbar\, x + c\hbar\,/\nu,\end{aligned}$$

i.e., $W^L \neq W^R$. Note that the equations for the left and right additive eigenvectors allow more complex solutions with quadratic dependence on x, but we do not consider them here.

1. The relativistic coordinate

Since the left and right additive eigenvectors are different, it is useful to find the relativistic coordinate. Note, however, that the situation is slightly different from the one considered before. Here the transition matrix is symmetric and the left and right additive eigenvectors at $\hbar = 0$ (in the rest frame) are equal. They differ in a moving frame. We proceed analogously.

Let the left and right optimal coordinates be

$$\begin{aligned}\sum_j P_{ji}(\Delta t)\left[S^L_j(t + \Delta t) - S^L_i(t)\right] = 0, \\ \sum_j P_{ij}(\Delta t)\left[S^R_i(t + \Delta t) - S^R_j(t)\right] = 0,\end{aligned}$$

where $P_{ij} = P_{ji}$. We introduce the symmetric (relativistic) reaction coordinate as

$$\begin{aligned}S^L_j(t + \Delta t) - S^L_i(t) = R_j/R_i\left[S^s_j(t + \Delta t) - S^s_i(t)\right], \\ S^R_i(t + \Delta t) - S^R_j(t) = R_j/R_i\left[S^s_i(t + \Delta t) - S^s_j(t)\right].\end{aligned} \tag{42}$$

Such a definition makes the comparison with the conventional relativistic equations of physics more straightforward. The equation is identical to Eq. (25) if one makes the substitution $R_i \to 1/R_i$ (or exchanges S^L and S^R). One obtains

$$\begin{aligned}\sum_j P_{ji}(\Delta t)R_j/R_i\left[S^s_j(t + \Delta t) - S^s_i(t)\right] = 0, \\ \sum_j P_{ij}(\Delta t)R_j/R_i\left[S^s_i(t + \Delta t) - S^s_j(t)\right] = 0,\end{aligned} \tag{43}$$

or

$$\begin{aligned}\sum_j P_{ji}(\Delta t)R_j/R_i\left(W^s_j - W^s_i - \nu^s\Delta t\right) = 0, \\ \sum_j P_{ij}(\Delta t)R_j/R_i\left(W^s_i - W^s_j - \nu^s\Delta t\right) = 0.\end{aligned} \tag{44}$$

The time intervals can be estimated as [substitute $R_i \to 1/R_i$ in Eqs. (29) and (30)]

$$t_2 - t_1 = \frac{\sum_\alpha \left[W^s_{x_\alpha(t_2)} - W^s_{x_\alpha(t_1)}\right]A_{x_\alpha(t_1)}R_{x_\alpha(t_2)}R_{x_\alpha(t_1)}}{\sum_\alpha A_{x_\alpha(t_1)}R_{x_\alpha(t_2)}R_{x_\alpha(t_1)}} \Big/ \nu^s, \tag{45}$$

and

$$t_2 - t_1 = \frac{\sum_\alpha \left[W^s_{x_\alpha(t_2)} - W^s_{x_\alpha(t_1)}\right]A_{x_\alpha(t_2)}R_{x_\alpha(t_2)}R_{x_\alpha(t_1)}}{\sum_\alpha A_{x_\alpha(t_2)}R_{x_\alpha(t_2)}R_{x_\alpha(t_1)}} \Big/ \nu^s. \tag{46}$$

From Eq. (43)

$$\begin{aligned}(1 - r\Delta t)\frac{R_{2l+1,i+1}}{R_{2l+1,i}}\left[W^s_{2l+1,i+1} - W^s_{2l+1,i} - \nu^s\Delta t\right] \\ + r\Delta t\frac{R_{2l+2,i-1}}{R_{2l+1,i}}\left[W^s_{2l+2,i-1} - W^s_{2l+1,i} - \nu^s\Delta t\right] = 0, \\ (1 - r\Delta t)\frac{R_{2l+2,i-1}}{R_{2l+2,i}}\left[W^s_{2l+2,i-1} - W^s_{2l+2,i} - \nu^s\Delta t\right] \\ + r\Delta t\frac{R_{2l+3,i+1}}{R_{2l+2,i}}\left[W^s_{2l+3,i+1} - W^s_{2l+2,i} - \nu^s\Delta t\right] = 0,\end{aligned}$$

$$
\begin{aligned}
&(1-r\Delta t)\frac{R_{2l+1,i-1}}{R_{2l+1,i}}\left[W^s_{2l+1,i}-W^s_{2l+1,i-1}-v^s\Delta t\right]\\
&\quad+r\Delta t\frac{R_{2l,i-1}}{R_{2l+1,i}}\left[W^s_{2l+1,i}-W^s_{2l,i-1}-v^s\Delta t\right]=0,\\
&(1-r\Delta t)\frac{R_{2l+2,i+1}}{R_{2l+2,i}}\left[W^s_{2l+2,i}-W^s_{2l+2,i+1}-v^s\Delta t\right]\\
&\quad+r\Delta t\frac{R_{2l+1,i+1}}{R_{2l+2,i}}\left[W^s_{2l+2,i}-W^s_{2l+1,i+1}-v^s\Delta t\right]=0.
\end{aligned}
$$

Assume that optimal coordinates are periodic for index l with period 2, meaning $R_{2l+1,i}=R_{1,i}$, $R_{2l+2,i}=R_{2,i}$. Since the system is translationally invariant $R_{1,i}=R_1$, $R_{2,i}=R_2$. We assume, again, that $W^s_{2l+1,i}=2l+1+i\Delta x\,\hbar+w_1$, $W^s_{2l+2,i}=2l+2+(i+1)\Delta x\,\hbar+w_2$, and $\Delta x=c\Delta t$. After substitution and taking the limit $\Delta t\to 0$ (the equation for the relativistic coordinate is valid only in this limit),

$$
\begin{aligned}
\hbar\,c+rR_2/R_1(w_2+1-w_1)-v&=0,\\
-\hbar\,c+rR_1/R_2(w_1+1-w_2)-v&=0,\\
\hbar\,c+rR_2/R_1(w_1+1-w_2)-v&=0,\\
-\hbar\,c+rR_1/R_2(w_2+1-w_1)-v&=0.
\end{aligned}
$$

We dropped the superscript s to simplify the notation. By subtracting the third equation from the first, one finds that $w_2=w_1$, which we can set to 0, since the coordinate is defined up to a constant. Then one finds

$$
\begin{aligned}
\hbar\,c+rR_2/R_1-v&=0,\\
-\hbar\,c+rR_1/R_2-v&=0,\\
v^2&=r^2+c^2\hbar^2,\\
R_2/R_1&=\sqrt{(v-c\hbar)/(v+c\hbar)},\\
R_1=\sqrt{1+c\hbar/v},&\quad R_2=\sqrt{1-c\hbar/v},
\end{aligned}
\tag{47}
$$

i.e., the infinite set of solutions, parametrized by $\hbar$ with the relativistic relation between v and $\hbar$, which is the reason behind naming the coordinate relativistic.

The stochastic dynamics projected on the optimal relativistic coordinate is described by $S=W-vt=\text{const}$, which describes a plane wave running in (l,x) space with the phase velocity along x of $v/\hbar$. To compute the group velocity, we consider a "wave packet"—two solutions with close but different values of $\hbar$ [16]. Let their phases be equal at some point, $\hbar_1x+l-v_1t=\hbar_2x+l-v_2t$. The equation for the phase agreement at the new position $(x+dx)$ at the next time instant $(t+dt)$ is $\hbar_1(x+dx)+l-v_1(t+dt)=\hbar_2(x+dx)+l-v_2(t+dt)$. Hence $(\hbar_1-\hbar_2)dx=(v_1-v_2)dt$, or $v=dx/dt=(v_1-v_2)/(\hbar_1-\hbar_2)=\partial v/\partial\hbar=\hbar\,c^2/v$. Thus, one obtains $v=r/\sqrt{1-(v/c)^2}$, $\hbar=(vr/c^2)/\sqrt{1-(v/c)^2}$, and $R_1=\sqrt{1+v/c}$, $R_2=\sqrt{1-v/c}$. By introducing $E=hv$, $p=h\hbar$, $mc^2=hr$, where h has the meaning of the Planck constant, one obtains the more familiar $E^2=m^2c^4+p^2c^2$, $v=pc^2/E$, $E=mc^2/\sqrt{1-(v/c)^2}$, and $p=mv/\sqrt{1-(v/c)^2}$.

Interpreting $R_i=\sqrt{P_i}$, where P_i are the stationary probabilities, one can compute the mean velocity $v=(cP_1-cP_2)/(P_1+P_2)=\hbar\,c^2/v$, which equals the group velocity.

The relativistic coordinate can be found from the left and right additive eigenvectors using Eqs. (41). From

$$
\begin{aligned}
v&=r,\\
W^L_{2l+1,i}&=2l+1+\hbar\,i\,\Delta x,\\
W^L_{2l+2,i}&=2l+2+\hbar\,(i+1)\Delta x-(1-r\Delta t)c\hbar/v,\\
W^R_{2l+1,i}&=2l+1+\hbar\,i\,\Delta x,\\
W^R_{2l+2,i}&=2l+2+\hbar\,(i+1)\Delta x+(1-r\Delta t)c\hbar/v,
\end{aligned}
$$

one computes

$$
\begin{aligned}
S^L_{2l+1,i+1}-S^L_{2l+1,i}&=\hbar\,\Delta x-v\Delta t=-(v-\hbar\,c)\Delta t,\\
S^L_{2l+2,i-1}-S^L_{2l+1,i}&=1-(1-r\Delta t)c\hbar/v-v\Delta t\\
&=(1-r\Delta t)(1-c\hbar/v),\\
S^L_{2l,i-1}-S^L_{2l,i}&=-(v+\hbar\,c)\Delta t,\\
S^L_{2l+1,i+1}-S^L_{2l,i}&=(1-r\Delta t)(1+c\hbar/v),\\
S^R_{2l+1,i+1}-S^R_{2l+1,i}&=-(v-\hbar\,c)\Delta t,\\
S^R_{2l,i-1}-S^R_{2l,i}&=-(v+\hbar\,c)\Delta t,\\
S^R_{2l+2,i-1}-S^R_{2l+1,i}&=(1-r\Delta t)(1+c\hbar/v),\\
S^R_{2l+1,i+1}-S^R_{2l,i}&=(1-r\Delta t)(1-c\hbar/v),
\end{aligned}
$$

where we used the shorthand notation $S_j-S_i=S_j(t+\Delta t)-S_i(t)$. $P_{1,i}=P_1$, since $(S^L_{2l+1,i+1}-S^L_{2l+1,i})/(S^R_{2l+1,i+1}-S^R_{2l+1,i})=P_{1,i+1}/P_{1,i}=1$, and hence $S^s_{2l+1,i+1}-S^s_{2l+1,i}=S^L_{2l+1,i+1}-S^L_{2l+1,i}=-(v-\hbar\,c)\Delta t$, where $v=r$. Analogously, $P_{2,i}=P_2$ and $S^s_{2l,i-1}-S^s_{2l,i}=S^L_{2l,i-1}-S^L_{2l,i}=-(v+\hbar\,c)\Delta t$. For transitions with reversal of direction

$$
\begin{aligned}
P_2/P_1&=\left(S^L_{2l+2,i-1}-S^L_{2l+1,i}\right)/\left(S^R_{2l+2,i-1}-S^R_{2l+1,i}\right)\\
&=(1-c\hbar/v)/(1+c\hbar/v),\\
S^s_{2l+2,i-1}-S^s_{2l+1,i}&=(1-r\Delta t)\sqrt{1-(c\hbar/v)^2},\\
S^s_{2l+1,i+1}-S^s_{2l,i}&=(1-r\Delta t)\sqrt{1-(c\hbar/v)^2}.
\end{aligned}
$$

The coordinate obtained differs from the relativistic coordinate found before by an overall factor of $d=\sqrt{1-(c\hbar/v)^2}$, as can be seen by, e.g., computing $S^s_{2l+2,i}-S^s_{2l,i}$. By rescaling the coordinates $S^s\to S^s/d$, $\hbar\to\hbar/d$, and $v\to v/d$ one finds that

$$
\begin{aligned}
v&=r/\sqrt{1-(c\hbar/v)^2},\\
r^2&=v^2[1-(c\hbar/v)^2]=v^2-(c\hbar)^2.
\end{aligned}
$$

2. *Numerical example*

1000 trajectories (time series of l,i) each of length 10^5dt were simulated by the MC method with time steps of $dt=0.01$ and saved with time intervals of $\Delta t=1$. The reversal rate is $r=0.1$. Figure 4 shows times reconstructed with the optimal coordinates with $\hbar=0.05$. Relativistic coordinates with larger values of $\hbar$ correctly reconstruct the time at shorter time intervals. Figure 5 shows the dynamics of a wave packet.

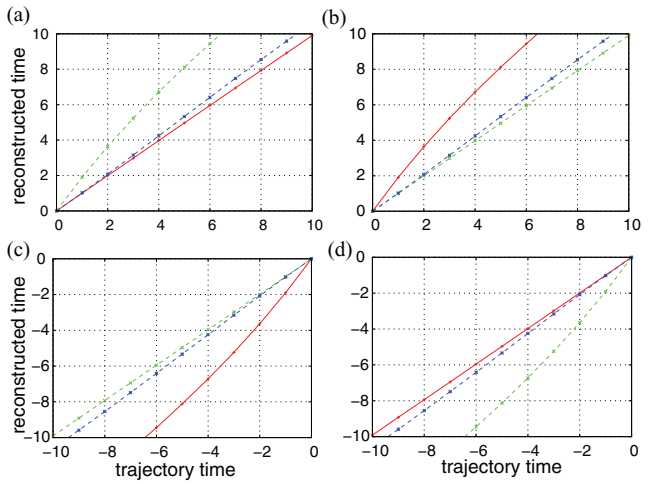

FIG. 4. (Color online) Reconstruction of time from system snapshots (configurations) from ensembles of (a) forward trajectories starting from the positive direction, (b) forward trajectories ending in the positive direction, (c) time-reversed trajectories starting from the positive direction, and (d) time-reversed trajectories ending in the positive direction. Reconstructions using W^L, W^R, and W^s are shown by red, green, and blue lines, respectively. The plots show the reconstructed time vs the actual time.

IV. THE RELATION BETWEEN THE ADDITIVE AND CONVENTIONAL (MULTIPLICATIVE) EIGENVECTORS

An additive eigenvector is modified by matrix multiplication as $\mathbf{A}\mathbf{W}^R = \mathbf{W}^R + \boldsymbol{\lambda}$, where $\boldsymbol{\lambda} = \{\lambda, \ldots, \lambda\}$ is a vector where all components equal λ. An additive eigenvector is a multivalued function of position, meaning that j as a function of W_j is a periodic function similar to $\exp(i2\pi W_j)$. A conventional eigenvector is modified by matrix multiplication as $\mathbf{A}\psi^R = \lambda\psi^R$. Eigenvectors of the master equation are often periodic functions. All this suggests that there might be a relation between an additive eigenvector and a phase (or logarithm) of a conventional eigenvector. Indeed, as we show below, under certain conditions it is possible to establish the correspondence. It requires, however, a certain modification of the acting operator and correspondingly the underlying dynamics. The correspondence is similar to that between the classical action function and the wave function in quantum mechanics.

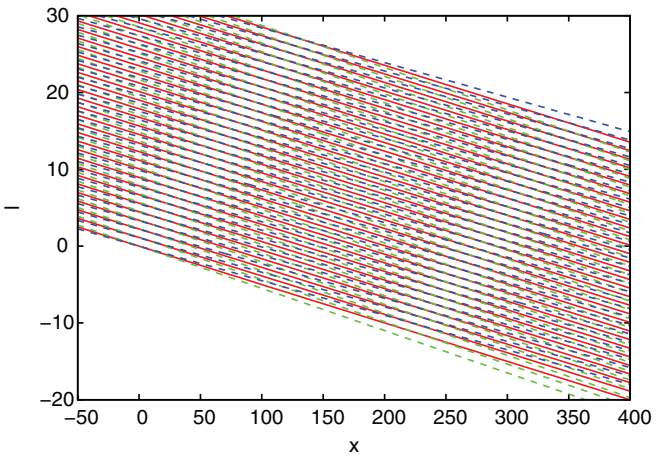

FIG. 5. (Color online) The dynamics of a wave packet. Surfaces of (relativistic) $S(l,x,t_i) = l + \hbar k\, x - v t_i = \text{const}$ for $t_i = 0,10,20,\ldots,300$ are shown for three solutions with $\hbar k = \hbar k_0$, $\hbar k = 1.1\hbar k_0$, and $\hbar k = 0.9\hbar k_0$ for $\hbar k_0 = 0.05$. The region where the phases are in agreement starts at $(l = 0, x = 0, t = 0)$ and moves with time along x with the group velocity $v = \hbar k / v$.

Let ψ^R and ψ^L be the solutions of the equations

$$\psi_i^R(t+\Delta t) = \sum_j P_{ij}(\Delta t)\psi_j^R(t),$$
$$\psi_i^L(t) = \sum_j P_{ji}(\Delta t)\psi_j^L(t+\Delta t), \tag{48}$$

where $\sum_j P_{ji}(\Delta t) = 1$, or the corresponding continuous-time equations. If $\psi_i^L(t) = e^{i2\pi S_i^L(t)} = e^{i2\pi(W_i^L - vt)}$, where $\lambda = e^{-i2\pi v\Delta t}$ is the corresponding eigenvalue, then

$$\exp\left[i2\pi S_i^L(t)\right] = \sum_j P_{ji}(\Delta t)\exp\left[i2\pi S_j^L(t+\Delta t)\right],$$
$$1 = \sum_j P_{ji}(\Delta t)\exp\left\{i2\pi\left[S_j^L(t+\Delta t) - S_i^L(t)\right]\right\}.$$

Assume that $S_j^L(t+\Delta t) - S_i^L(t)$ are always close to 0 or some other integer number, i.e., $|S_j^L(t+\Delta t) - S_i^L(t) + d_{ji}| \ll 1$, where d_{ji} is an integer; then one can expand the exponent and obtain Eq. (37):

$$1 \approx \sum_j P_{ji}(\Delta t)\left\{1 + i2\pi\left[S_j^L(t+\Delta t) - S_i^L(t) + d_{ji}\right]\right\},$$
$$0 \approx \sum_j P_{ji}(\Delta t)\left[S_j^L(t+\Delta t) - S_i^L(t) + d_{ji}\right],$$
$$\sum_j P_{ji}(\Delta t)\left(W_j^L - W_i^L + d_{ji} - v\Delta t\right) \approx 0.$$

For the right eigenvector $\psi_j^R(t) = P_j e^{i2\pi S_j^R(t)}$ one obtains Eq. (38):

$$P_i \exp\left[i2\pi S_i^R(t+\Delta t)\right] = \sum_j P_{ij}(\Delta t)P_j \exp\left[i2\pi S_j^R(t)\right],$$
$$1 = \sum_j P_{ij}(\Delta t)P_j/P_i \exp\left\{-i2\pi\left[S_i^R(t+\Delta t) - S_j^R(t)\right]\right\},$$
$$\sum_j P_{ij}(\Delta t)P_j/P_i\left[S_i^R(t+\Delta t) - S_j^R(t) - d_{ij}\right] \approx 0,$$
$$\sum_j P_{ij}(\Delta t)P_j/P_i\left(W_i^R - W_j^R - d_{ij} - v\Delta t\right) \approx 0.$$

Numerical analysis of the eigenvectors and eigenvalues of the system from illustrative example 1 shows that the relation is accurate for small eigenvalues and becomes inaccurate for large eigenvalues. To investigate the reason we consider the

case $r_i = r$ analytically:

$$\begin{aligned}
&\exp\{i2\pi[W_j - \nu(t+\Delta t)]\}\\
&\quad = (1 - r\Delta t)\exp[i2\pi\left(W_j - \nu t\right)]\\
&\qquad + r\Delta t\exp[i2\pi\left(W_{j-1} - \nu t\right)],\\
&\exp(-i2\pi\nu\Delta t)\\
&\quad = (1 - r\Delta t) + r\Delta t\exp[i2\pi(W_{j-1} - W_j)],\\
&\qquad -i2\pi\nu = r\{\exp[i2\pi(W_{j-1} - W_j)] - 1\}.
\end{aligned}$$

The equation reduces to $W_j - W_{j-1} = \nu/r$ only in the limit of $W_{j-1} - W_j \to 0$ or $\nu \to 0$. One way to make it work for finite ν is to make the transition from $j-1$ to j gradual by introducing intermediate states $j + k/n$, where $k = 0, \ldots, n-1$, so that the corresponding $W_{j+(k+1)/n} - W_{j+k/n} \to 0$ for $n \to \infty$, while W_j and ν stay the same. Let the time interval Δt be further divided into n subintervals. Instead of making a single jump from $j-1$ to j with rate r during Δt, the system makes n jumps from $j + (k-1)/n$ to $j + k/n$ with (a yet unknown) rate a each during $\Delta t/n$. The equations for the additive eigenvector are

$$a\Delta t/n(W_{j+(k+1)/n} - W_{j+k/n}) - \nu\Delta t/n = 0.$$

Summing the equations for $k = 0, \ldots, n-1$, one finds that $a = rn$. The master equation is

$$\begin{aligned}
p_{j+k/n}(t + \Delta t/n) = (1 - rn\Delta t/n)p_{j+k/n}(t)\\
+rn\Delta t/np_{j+(k-1)/n}(t)
\end{aligned}$$

for $k = 0, \ldots, n-1$. Let $x = \Delta x(j + k/n)$; then in the limit $n \to \infty$ one can approximate the finite differences by derivatives and obtain

$$\begin{aligned}
&p_{j+k/n} + (\Delta t/n)\partial p_{j+k/n}/\partial t\\
&\quad = (1 - r\Delta t)p_{j+k/n} + r\Delta t[p_{j+k/n} - (1/n)\partial p_{j+k/n}/\partial j],\\
&\qquad (\Delta t/n)\partial p_{j+k/n}/\partial t + r(\Delta t/n)\partial p_{j+k/n}/\partial j = 0, \quad (49)\\
&\qquad\qquad \partial p_{j+k/n}/\partial t + r\partial p_{j+k/n}/\partial j = 0,\\
&\qquad\qquad \partial p(x,t)/\partial t + c\partial p(x,t)/\partial x = 0,
\end{aligned}$$

where $c = r\Delta x$. The eigenfunction of the equation is $\exp[i2\pi(\nu x/c + \nu t)) = \exp(i2\pi(W_x - \nu t)]$. Thus, we have found an equation with (multiplicative) eigenfunctions and eigenvalues, which correspond exactly to *additive* eigenvectors and eigenvalues. However, in order to do that it was necessary to modify the underlying dynamics of the system. First, the dynamics is no longer stochastic. The differential operator describes a deterministic running wave. Second, the configuration space of the system has been extended. Instead of being integer, $j \in Z$, it became real, $x \in R$. It seems reasonable to name operators like those in Eq. (49) virtual operators, since they describe virtual dynamics, not the actual dynamics of the system, and are just a mathematical tool to obtain (multiplicative) eigenfunctions and eigenvalues, which correspond exactly to *additive* ones.

For the relativistic coordinate the correspondence is established analogously. Let $P_{ij}(\Delta t)$ be such that the solutions of Eqs. (48) can be expressed as

$$\psi_j^R = \psi_j^L = R_j e^{i2\pi S_j^s(t)} = R_j e^{i2\pi(W_j^s - \nu t)}.$$

Then

$$\begin{aligned}
&e^{-i2\pi\nu^s\Delta t}R_i e^{i2\pi W_i^s} = \sum_j P_{ij}(\Delta t)R_j e^{i2\pi W_j^s},\\
&e^{-i2\pi\nu^s\Delta t} = \sum_j P_{ij}(\Delta t)R_j/R_i e^{-i2\pi(W_i^s - W_j^s)},\\
&1 - i2\pi\nu^s\Delta t\\
&\quad \approx \sum_j(\delta_{ij} + \Delta t K_{ij})R_j/R_i\left[1 - i2\pi\left(W_i^s - W_j^s + d_{ij}\right)\right],\\
&\sum_j K_{ij}R_j/R_i\left(W_i^s - W_j^s + d_{ij}\right) - \nu^s \approx 0,
\end{aligned}$$

where, in the last line, we took the imaginary part (K_{ji} is real). For the left eigenvector one obtains

$$\sum_j K_{ji}R_j/R_i\left(W_j^s - W_i^s + d_{ji}\right) - \nu \approx 0.$$

The two equations are the multivalued rate matrix versions of Eq. (44).

Consider a system with dynamics described by the following master equation:

$$\begin{aligned}
p_1(t + \Delta t) = (1 - r\Delta t)p_1 + r\Delta t p_2,\\
p_2(t + \Delta t) = (1 - r\Delta t)p_2 + r\Delta t p_1,
\end{aligned}$$

where p_1 and p_2 are the probabilities of being in states 1 and 2, respectively, which is equivalent to the system considered in illustrative example 2 if one sets $r_1 = r_2 = r$. For this system, the left, right, and relativistic coordinates are the same, $W_{l,1} = l$, $W_{l,2} = l + 1/2$, and $\nu = r/2$.

The equation has two eigenvalues $\lambda = 1$ and $\lambda = 1 - 2r\Delta t$, which correspond to $[\lambda = \exp(i2\pi\nu\Delta t)]$ $\nu = 0$ and $\nu = ir/\pi$. The eigenvector of the second eigenvalue is $\psi_1 = 1 = e^{2\pi i0} = e^{2\pi i W_1}$ and $\psi_2 = -1 = e^{2\pi i 1/2} = e^{2\pi i W_2}$, in agreement with the additive eigenvectors.

The second eigenvalue is not in correspondence because $W_1 - W_2$ is not small and the exponent cannot be expanded just to linear terms. Since after two steps the systems returns to itself, each step corresponds to rotation through π rad. To make the linear exponent expansion accurate, for the correspondence to be valid, each step should be made infinitesimally small. Analogously to the above, one way to do this is to make the rotation gradual, i.e., instead of rotation about π rad with rate r, make n rotations through π/n rad with rate nr where $n \to \infty$. Let the time interval Δt be further divided into n subintervals and let $p_{1+j/n}$ represent the intermediate values, representing rotation by an angle of π/n. The equation for the additive eigenvector is

$$rn\Delta t/n\left(W_{1+(j+1)/n} - W_{1+j/n}\right) - \nu\Delta t/n = 0$$

for $j = 1, \ldots, 2n$. The master equation is

$$\begin{aligned}
p_{1+j/n}(t + \Delta t/n) = (1 - rn\Delta t/n)p_{1+j/n}(t)\\
+rn\Delta t/np_{1+(j-1)/n}(t).
\end{aligned}$$

If n is large, one can expand the finite-difference equation and obtain

$$\begin{aligned}
(\Delta t/n)\partial p_{1+j/n}/\partial t = -rn(\Delta t/n)\partial p_{1+j/n}/\partial j,\\
\partial p_\phi/\partial t = -r\pi\,\partial p_\phi/\partial\phi,
\end{aligned}$$

where $\phi = 2\pi j/2n$ is the rotation angle. The equation has the solution $p = e^{i\phi - ir\pi t}$ with eigenvalue $\mu = ir\pi$ corresponding

to $\nu = r/2$. The eigenfunction $e^{i\phi}$ at the points $\phi = 0$ and $\phi = \pi$ corresponds to W_1 and W_2. Thus, in order to obtain the correct correspondence between the additive and multiplicative eigenvectors and eigenvalues the stochastic process had to be modified. The process now consists of infinitesimal jumps instead of finite jumps and it describes deterministic rotation instead of the original stochastic dynamics. In this process the system can have any ϕ, while in the original process only $\phi = 0$ and $\phi = \pi$ are possible.

In the previous construction many intermediate $p_{1+j/n}$ were introduced to explicitly represent the rotation by a small angle of π/n. The rotation can also be represented by a rotation matrix in some (e_x,e_y) basis. As e_x and e_y one can take unit vectors associated with p_1 and $p_{1+1/2}$. p_2 corresponds to $-e_x$ and cannot be taken as basis vector because a rotation cannot be represented as a linear sum of e_x and $-e_x$. Each $p_{1+j/n} = xe_x + ye_y$ is a linear combination of the basis vectors with coefficients x, y. Since x and y are coordinates and not probabilities, they can be negative. When the system makes the transition from $p_{1+(j-1)/n}$ to $p_{1+j/n}$, the x, y coordinates are changed by the rotation matrix

$$\begin{pmatrix} \cos\pi/n & -\sin\pi/n \\ \sin\pi/n & \cos\pi/n \end{pmatrix}.$$

So the master equation is

$$\begin{aligned} \begin{matrix} x(t+\Delta t/n) \\ y(t+\Delta t/n) \end{matrix} &= (1 - rn\Delta t/n) \begin{matrix} x(t) \\ y(t) \end{matrix} \\ &\quad + rn\Delta t/n \begin{pmatrix} \cos\pi/n & \sin\pi/n \\ -\sin\pi/n & \cos\pi/n \end{pmatrix} \begin{matrix} x(t) \\ y(t) \end{matrix}; \end{aligned}$$

the rotation matrix for the angle $-\pi/n$ is taken to express $p_{1+(j-1)/n}$ from $p_{1+j/n}$. Expanding the equation one obtains

$$\begin{aligned} x + (\Delta t/n)\partial x/\partial t &= x - rn(\Delta t/n)x \\ &\quad + rn(\Delta t/n)x + rn\pi(\Delta t/n^2)y, \\ y + (\Delta t/n)\partial y/\partial t &= y - rn(\Delta t/n)y \\ &\quad + rn(\Delta t/n)y - rn\pi(\Delta t/n^2)x, \\ \partial x/\partial t &= r\pi y, \\ \partial y/\partial t &= -r\pi x. \end{aligned}$$

The equation is similar to the one-dimensional relativistic Dirac equation for an electron in its rest frame. However, the original system operates only with p_1 and p_2; $p_{1+1/2}$ cannot be observed. To alleviate this, the original cycle $(1 \to 2 \to 1)$ can be extended to the cycle $1 \to 2 \to 3 \to 4 \to 1$, where state 3 is identical to 1 and 4 to 2. The additive eigenvalue and eigenvector are $\nu = r/4$, and $W_{l,1} = l$, $W_{l,2} = l + 1/4$, $W_{l,3} = l + 1/2$, and $W_{l,4} = l + 3/4$. In this system e_1 and e_2 are associated with p_1 and p_2, and the virtual operator is [the rotation rate now is $rn(\pi/2)/n = r\pi/2$]

$$\begin{aligned} da_1/dt &= r\pi/2a_2, \\ da_2/dt &= -r\pi/2a_1, \\ a_3 &= -a_1, \\ a_4 &= -a_2. \end{aligned} \tag{50}$$

The eigenvalue $\mu = i\pi r/2$ corresponds to the additive eigenvalue of $\nu = r/4$, and the eigenfunction is $\psi_1 = 1/2 = e^0/2$, $\psi_2 = i/2 = e^{i\pi/2}/2$, $\psi_3 = -1/2$, and $\psi_4 = -i/2$, which is in correspondence with the additive eigenvector.

The dynamics described by the stochastic telegrapher's equations is the superposition of constant motion to the left or to the right and change with rate r between the two motions (directions). Hence the virtual operator for this equation is the superposition of Eqs. (49) and (50):

$$\begin{aligned} \partial a_1/\partial t + c\partial a_1/\partial x &= r\pi/2a_2, \\ \partial a_2/\partial t - c\partial a_2/\partial x &= -r\pi/2a_1, \\ a_3 &= -a_1, \\ a_4 &= -a_2, \end{aligned}$$

which is equivalent to the one-dimensional Dirac equation, if one denotes $r\pi/2$ as $mc^2/\hbar$ or $mc^2 = hr/4$. The eigenvector of the virtual operator

$$\begin{aligned} a_1 &= \sqrt{1 + c\bar{k}/\nu}\, e^{i2\pi(\bar{k}x - \nu t)}, \\ a_2 &= \sqrt{1 - c\bar{k}/\nu}\, e^{i2\pi(\bar{k}x - \nu t + 1/4)}, \\ a_3 &= \sqrt{1 + c\bar{k}/\nu}\, e^{i2\pi(\bar{k}x - \nu t + 2/4)}, \\ a_4 &= \sqrt{1 - c\bar{k}/\nu}\, e^{i2\pi(\bar{k}x - \nu t + 3/4)}, \end{aligned}$$

where $\nu^2 = (r/4)^2 + \bar{k}^2c^2$, is in agreement with the optimal coordinate [Eq. (47)]. The factor of 4, compare to the solution given by Eq. (47), is due to different normalization of the optimal coordinates $W_{l+4,i} = W_{l,i} + 1$ vs $W_{l+2,i} = W_{l,i} + 2$.

Note that two reversals of the direction, $1 \to 2 \to 3$ (which result in the original direction), lead to the change of sign $a_1 \to a_3 = -a_1$. It requires four reversals of the direction to return to the original sign, analogous to the transformation of a spinor under 2π or 4π rotation.

Thus, the change of direction during a random walk can be transformed to the virtual continuous operator representing rotation (in internal space). Every equilibrium stochastic dynamics, by definition, contains movements in opposite directions, meaning that virtual operators representing rotations are ubiquitous.

The strategy of finding the virtual operator can be summarized as follows. The correspondence holds if $P(\Delta t)$ is such that $W_i - W_j \approx 0$ and ν is real. If it is not the case, then the configuration space is expanded with intermediate states (denoted by the fractional index $i + k/n$) on which virtual dynamics described by a virtual operator $A(\Delta t/n)$ is introduced, such that $W_{i+(k+1)/n} - W_{i+k/n} \to 0$ with $n \to \infty$, while W_i and ν do not change. For such an operator the correspondence between the additive and multiplicative eigenvectors and eigenvalues is exact. Hence, the correspondence is exact between the additive eigenvectors and eigenvalues of the original P and the conventional eigenvectors and eigenvalues of the virtual operator A on the original configuration space (integer index).

A. Illustrative example 4: The telegrapher's equation in a slowly varying potential

Let the reversal rate now be a function of the position (r_i), corresponding to a random walk in a potential:

$$\begin{aligned} &(1 - r_i\Delta t)\frac{R_{2l+1,i+1}}{R_{2l+1,i}}\left[W^s_{2l+1,i+1} - W^s_{2l+1,i} - \nu^s\Delta t\right] \\ &\quad + r_i\Delta t\frac{R_{2l+2,i-1}}{R_{2l+1,i}}\left[W^s_{2l+2,i-1} - W^s_{2l+1,i} - \nu^s\Delta t\right] = 0, \end{aligned}$$

$$(1-r_i\Delta t)\frac{R_{2l+2,i-1}}{R_{2l+2,i}}\left[W^s_{2l+2,i-1}-W^s_{2l+2,i}-\nu^s\Delta t\right]$$
$$+r_i\Delta t\frac{R_{2l+3,i+1}}{R_{2l+2,i}}\left[W^s_{2l+3,i+1}-W^s_{2l+2,i}-\nu^s\Delta t\right]=0,$$
$$(1-r_i\Delta t)\frac{R_{2l+1,i-1}}{R_{2l+1,i}}\left[W^s_{2l+1,i}-W^s_{2l+1,i-1}-\nu^s\Delta t\right]$$
$$+r_i\Delta t\frac{R_{2l,i-1}}{R_{2l+1,i}}\left[W^s_{2l+1,i}-W^s_{2l,i-1}-\nu^s\Delta t\right]=0,$$
$$(1-r_i\Delta t)\frac{R_{2l+2,i+1}}{R_{2l+2,i}}\left[W^s_{2l+2,i}-W^s_{2l+2,i+1}-\nu^s\Delta t\right]$$
$$+r_i\Delta t\frac{R_{2l+1,i+1}}{R_{2l+2,i}}\left[W^s_{2l+2,i}-W^s_{2l+1,i+1}-\nu^s\Delta t\right]=0.$$

Let $R_{2l+1,i}=R_{1,i}$, $R_{2l+2,i}=R_{2,i}$, $W^s_{l,i+1}-W^s_{l,i}=\hbar_i\Delta x$, $W^s_{2l+3,i}=2+W^s_{2l+1,i}$, and $W^s_{2l+2,i}=2+W^s_{2l,i}$. Assume that r_i changes slowly with i (fine discretization), meaning $\hbar_i\approx\hbar_{i+1}$ and $R_{1,i+1}/R_{1,i}\approx R_{2,i+1}/R_{2,i}\approx 1$; then one arrives at (we dropped the superscript s)

$$\hbar_i c+r_i\frac{R_{2,i-1}}{R_{1,i}}[W_{2l+2,i-1}-W_{2l+1,i}]-\nu=0,$$
$$-\hbar_i c+r_i\frac{R_{1,i+1}}{R_{2,i}}[W_{2l+3,i+1}-W_{2l+2,i}]-\nu=0,$$
$$\hbar_i c+r_i\frac{R_{2,i-1}}{R_{1,i}}[W_{2l+1,i}-W_{2l,i-1}]-\nu=0,$$
$$-\hbar_i c+r_i\frac{R_{1,i+1}}{R_{2,i}}[W_{2l+2,i}-W_{2l+1,i+1}]-\nu=0,$$
$$\hbar_i c+r_i\frac{R_{2,i-1}}{R_{1,i}}-\nu=0,$$
$$-\hbar_i c+r_i\frac{R_{1,i+1}}{R_{2,i}}-\nu=0,$$
$$r_i^2=\nu^2-(\hbar_i c)^2.$$

Since $\hbar_i$ changes slowly with i one can use the continuous representation, where $\hbar(x)=\partial W(x)/\partial x$ and the last equation becomes

$$r^2(x)+c^2[\partial W(x)/\partial x]^2-\nu^2=0.$$

Alternatively, for $S=W(x)-\nu t$

$$r^2(x)+c^2(\partial S/\partial x)^2-(\partial S/\partial t)^2=0,$$

the (dimensionless) relativistic Hamilton-Jacobi equation with mass that is a function of the coordinate.

In the derivation it was, again, assumed that $\Delta x=c\Delta t$, which can be considered as a property of the stochastic model. If, however, one assumes that the stochastic model is a microscopic model of (one-dimensional) general relativity, then the speed of light is the universal constant only in local inertial frames of reference. For small velocities, i.e., small potential $U_i\ll r$, where $r_i=r+U_i$, the relativistic effects are negligible. In this case $\nu=r+e$, where $e\ll r$, and one obtains for $S=W(x)-et$

$$c^2[\partial S(x)/\partial x]^2/2r+U(x)+\partial S/\partial t=0,$$

the classical (dimensionless) Hamilton-Jacobi equation. The dimensionality can be restored by multiplying W and S by h and replacing $h\nu=E$, $hr=mc^2$, and $\hbar h=p$.

B. Illustrative example 5: Random walk with rate r

Consider a random walk on a line, where a system jumps to a nearby left or right state with rate r. The coordinate $W^s_{2l+1,i}$ describes movement to the right or when the system stays in the same state, and $W^s_{2l+2,i}$ describes movement to the left or when the system stays in the same state. In other words the optimal coordinate changes together with the direction. The equations for the relativistic coordinate are (the superscript s is omitted)

$$r\Delta t\frac{R_{2l+1,i+1}}{R_{2l+1,i}}[W_{2l+1,i+1}-W_{2l+1,i}-\nu\Delta t]+(1-2r\Delta t)$$
$$\times[-\nu\Delta t]+r\Delta t\frac{R_{2l+2,i-1}}{R_{2l+1,i}}[W_{2l+2,i-1}-W_{2l+1,i}-\nu\Delta t]=0,$$
$$r\Delta t\frac{R_{2l,i-1}}{R_{2l,i}}[W_{2l,i-1}-W_{2l,i}-\nu\Delta t]+(1-2r\Delta t)$$
$$\times[-\nu\Delta t]+r\Delta t\frac{R_{2l+1,i+1}}{R_{2l,i}}[W_{2l+1,i+1}-W_{2l,i}-\nu\Delta t]=0,$$
$$r\Delta t\frac{R_{2l+1,i-1}}{R_{2l+1,i}}[W_{2l+1,i}-W_{2l+1,i-1}-\nu\Delta t]+(1-2r\Delta t)$$
$$\times[-\nu\Delta t]+r\Delta t\frac{R_{2l,i-1}}{R_{2l+1,i}}[W_{2l+1,i}-W_{2l,i-1}-\nu\Delta t]=0,$$
$$r\Delta t\frac{R_{2l+2,i+1}}{R_{2l+2,i}}[W_{2l+2,i}-W_{2l+2,i+1}-\nu\Delta t]+(1-2r\Delta t)$$
$$\times[-\nu\Delta t]+r\Delta t\frac{R_{2l+1,i+1}}{R_{2l+2,i}}[W_{2l+2,i}-W_{2l+1,i+1}-\nu\Delta t]=0.$$

Analogously with the above, we assume $R_{2l+1,i}=R_1$, $R_{2l+2,i}=R_2$, $W_{2l+1,i}=w_1+i\hbar\Delta x+2l+1$, and $W_{2l+2,i}=w_2+(i+1)\hbar\Delta x+2l+2$:

$$r\hbar\Delta x+rR_2/R_1[w_2+1-w_1]-\nu=0,$$
$$-r\hbar\Delta x+rR_1/R_2[w_1+1-w_2]-\nu=0,$$
$$r\hbar\Delta x+rR_2/R_1[w_1+1-w_2]-\nu=0,$$
$$-r\hbar\Delta x+rR_1/R_2[w_2+1-w_1]-\nu=0.$$

Solving, one finds $(\nu/r)^2=1+(\hbar\Delta x)^2$, i.e., the relativistic spectrum of a particle with mass 1, where r and Δx define the temporal and spatial scales. Or, analogously to the above, $\nu^2=r^2+\hbar^2c^2$ if one denotes $c=r\Delta x$. Thus, the obtained results are not a peculiarity of the telegrapher's model.

V. DISCUSSION

The problem of determining an optimal coordinate that describes dynamics in general has been considered. It has been shown that the problem is closely related to the problem of reconstructing time from a trajectory and to the problem of defining the eigenmodes for stochastic dynamics. They are solved by introducing additive eigenvectors. The eigenvectors are modified under the action of a stochastic matrix in a simple way, $\mathbf{W^L P}=\mathbf{W^L}+\boldsymbol{\lambda}$. Such left and right additive eigenvectors can be used to reconstruct time from ensembles

of trajectories starting or ending, respectively, in a set of states. A symmetric or relativistic coordinate can be introduced. It allows one to reconstruct time for both ensembles of trajectories, but only for relatively small time intervals. For dynamics with detailed balance the additive eigenvectors are multivalued functions. It was shown that it is possible to establish a correspondence between an additive eigenvector and an eigenvalue and a conventional eigenvector and an eigenvalue of a virtual operator. The virtual operator, however, describes different dynamics in an extended configuration space. In particular, the virtual operator for a random walk on the line corresponds to the one-dimensional Dirac equation.

The close relation between the equations describing stochastic dynamics and that of quantum mechanics is well known [17,18]. In particular, analytical continuation, e.g., $t \to it$, is a straightforward way to obtain the Schrödinger equation from the diffusion equation or the one-dimensional Dirac equation from the telegrapher's equation [18]. The presented results differ in the following ways. First, no analytic continuation is performed. Second, the resulting Dirac equation is a virtual operator, i.e., it does not describe the actual dynamics, it is just a mathematical tool to match the eigenvectors and eigenvalues. Third, the results are valid for generic one-dimensional random walks; no specific stochastic process is selected. Interestingly, the l coordinate that explicitly keeps track of the branches of the multivalued functions (or rather its continuous analog) seems analogous to the action coordinate in the five-optics of Rumer [19]. In five-optics all physical quantities are periodic along the action coordinate and the period equals the Planck constant (or 1 in dimensionless units).

Equations with detailed balance have no additive eigenvectors with $\nu \neq 0$ in the space of single-valued functions. In order to obtain solutions with $\nu \neq 0$ we postulate that additive eigenvectors are multivalued functions, i.e., we have enlarged the configuration space of the solutions, in particular, by introducing an additional variable which explicitly describes the branches of the multivalued function. The whole construction may seem artificial at first. However, it could be viewed as being analogous to the introduction of complex numbers. Complex numbers have real and imaginary parts and are necessary to describe all the solutions of a polynomial equation just with real coefficients. As illustrated above, W_i and R_i can be considered as the polar representation of a complex number.

The purpose of an optimal coordinate being multivalued and the difference from the conventional description can be illustrated as follows. Consider a system that stochastically transits between two states 1 and 2 (illustrative example 2). Let an ensemble of such systems be initially in state 1. With time some systems will transit to state 2 and then some of them will return to state 1. State 1 now contains two sets of systems: the systems which came back there from state 2 and the systems which never left state 1. The future dynamics of the two sets are described by the same set of equations and, conventionally, one considers them identical and counts them together. However, after such mixing, the information about the past dynamics (which was different) is lost; one cannot reconstruct dynamics back in time. The multivaluedness (of an optimal coordinate) is used to distinguish the two sets. The systems which came back from state 2 now belong to a different branch and thus the two sets can be distinguished.

The branches of the optimal coordinate can be straightforwardly computed from the system trajectory if it is known with sufficiently fine temporal resolution. That is how it was done in the numerical examples and how it can be done in a real-life experiment. If an experimental system does not allow the observation of a trajectory with sufficient temporal resolution, then, in principle, one may attempt to infer the branches from auxiliary variables. For example, the dynamics of a molecular motor or an enzyme might be described by an optimal coordinate with ring topology. The auxiliary variables for such systems could be the position of the motor along a track or the number of ATP, substrate, or product molecules.

The transition to the next branch of an optimal coordinate when a system returns to a state visited before can be compared to the phenomenon of the geometric phase, i.e., the increment of the phase acquired when a quantum mechanical [20] or stochastic system [21–23] is undergoing adiabatic cyclic evolution in parameter space. In the case of stochastic systems one considers the dynamics to be described by the master equation with detailed balance. The equilibrium net flux between any two states is therefore zero. If the parameters (rates) of the master equation are changing in a periodic manner (while detailed balance is still satisfied at any time moment) a system may exhibit a nonzero net flux. If the change is adiabatic (slow), then the net flux does not depend on the speed with which the parameters are changed and is determined only by the trajectory in parameter space. While the analogy is clear, there are the following differences. In order to have a nonzero additive eigenvalue we postulate that the phase increment may happen whenever the system returns to a previously visited state. The parameters are kept constant. An optimal coordinate is a multivalued function *per se*, not due to a periodic evolution of parameters. The geometric phase and the net flux are completely determined by the trajectory in the parameter space. The equations for the optimal coordinate are more flexible; they just specify that the optimal coordinate is a multivalued function, without specifying the exact details; any solution with nonzero ν can be used.

The solutions presented in the illustrative examples represent a subset of all possible solutions for very simple systems. For example, the equation for the optimal coordinate for a random walk on a line allows other solutions, e.g., solutions with longer periodicity $W_{l+m,i} = W_{l,i}$ for $m > 2$, which were not considered. To fully appreciate the properties of the derived equations, it is necessary to completely develop a mathematical formalism similar to the conventional eigenvector decomposition, which would allow one to obtain all the solutions of the equations and to answer general questions as to the completeness and properties of the basis of additive eigenvectors and the definition of orthogonality or of a scalar product. The correspondence between the additive and multiplicative eigenvectors could be useful as a guiding principle. Two other generic questions for the method are obvious. What are the microscopic models for other relativistic equations of physics and which virtual operators correspond to various stochastic master equations?

It seems that while the solutions using relativistic or symmetric optimal coordinates are closer to the conventional physical picture, the solutions using left and right eigenvectors are more flexible. Consider for example a random walk in many dimensions. To describe it one can partition the configuration space and compute a transition matrix. One can expect that while at very short time intervals the description by the transition matrix may deviate from the actual dynamics, it will closely approximate it at longer time intervals, when the fine-grained structure of the partitioning can be neglected. The partitioning can be done in many ways, provided that it is sufficiently fine grained. Thus if one can use sufficiently long time intervals the description of the dynamics should be independent of the chosen partition. In particular, if a system performs a random walk along the edges of a cubic lattice, one should be able to accurately describe the dynamics by using any other lattice, i.e., at longer time intervals the space becomes isotropic. The description with the relativistic coordinates, however, is exact only in the limit of $\Delta t \to 0$, when the original anisotropy of space partitioning is evident.

The fact that we were able to derive model relativistic equations can be explained as follows. The description of dynamics using Markov state models with master equations is manifestly invariant with respect to the choice of spatial coordinates, since the states are defined only by an index. The method described here allows one to reconstruct time, meaning now the temporal coordinate can also be represented just by an index and the description becomes invariant with respect to the choice of spatial-temporal coordinates. Such a description can be used to describe the dynamics of an arbitrary system using an arbitrary moving frame of reference in an invariant way. By observing a system's trajectory, one can reconstruct time. Having the trajectory as a function of time, one can reconstruct the transition probability (or rate) matrix and thus obtain a complete description of the system dynamics. Alternatively, the dynamics can be described by an optimal coordinate, which can be determined directly from the averaged matrix [Eq. (12) or (14)]. To predict a future state of the system as a function of time, one can use an auxiliary system as a clock. Note that the equivalent description which uses two coordinates – the left and right additive eigenvectors – does not exhibit any explicit relativistic effects; in particular, v is independent of $\hbar$.

Since the method is capable of reconstructing time intervals from a trajectory without time stamps, it can be applied to "reconstruct time" from inherently timeless objects.

In conclusion, we have suggested a general method for the description of stochastic dynamics. The dynamics is described by using optimal coordinates or additive eigenvectors. While the mathematical formalism is not yet developed to completely characterize the solution space, we believe that we have demonstrated the self-consistency of the method and its potential.

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