Microscopic derivation of open quantum walks

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Open quantum walks (OQWs) are exclusively driven by dissipation and are formulated as completely positive trace-preserving (CPTP) maps on underlying graphs. The microscopic derivation of discrete and continuous-in-time OQWs is presented. It is assumed that connected nodes are weakly interacting via a common bath. The resulting reduced master equation of the quantum walker on the lattice is in the generalized master equation form. The time discretization of the generalized master equation leads to the OQW formalism. The explicit form of the transition operators establishes a connection between dynamical properties of the OQWs and thermodynamical characteristics of the environment. The derivation is demonstrated for the examples of the OQW on a circle of nodes and on a finite chain of nodes. For both examples, a transition between diffusive and ballistic quantum trajectories is observed and found to be related to the temperature of the bath.

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I. INTRODUCTION

The mathematical concept of classical random walks (CRWs) finds wide applications in various areas of fundamental and applied science [1–5]. In the case of the classical random walk, the trajectory of the "walker" is a sequence of random steps fully determined by the stochastic matrix corresponding to the graph of the CRW. Unitary quantum walks were introduced more than two decades ago as the quantum analog of the CRW [6–8]. Unitary quantum walks are broadly used in quantum computing science, in the formulation of quantum algorithms, and in complexity theory [8]. The dynamical behaviors of the quantum walker and the classical random walker are very different. The probability distribution of the unitary quantum walker is the result of the interference between different positions of the walker, and it is determined not only by the underlying graph but also by the inner state of the quantum walker, e.g., spin or polarization [8].

In the description of the dynamics of any realistic quantum system, one needs to take into account the effect of dissipation and decoherence [9]. In the recently introduced open quantum walks (OQWs), these effects are naturally included in the description of the dynamics of the quantum "walker" [10–12]. Essentially, the dynamics of OQWs is driven by the dissipative interaction with environments. Mathematically, OQWs are formulated as completely positive trace-preserving maps (CPTP maps) on an appropriate Hilbert space [9,13]. OQWs and unitary quantum walks can be related via a "physical realization" procedure introduced in Ref. [11]. In a special scaling limit, OQWs become open quantum Brownian motion [14,15]. This is a new type of quantum Brownian motion where the position of the quantum Brownian particle is determined not only by the interaction with an environment but also by the state of the inner degree of freedom of the quantum Brownian particle.

The diverse dynamical behavior of OQWs has been studied extensively [10–12,16–21]. The asymptotic analysis of OQWs leads to a central limit theorem [22–24]. For large times, the position probability distribution of OQWs converges to Gaussian distributions [22,23]. For a special case of OQWs on $\mathbb{Z}$, it was shown that the probability distribution of the position of the quantum walker is given by the binomial distribution, and the number of different Gaussian distributions for large times is bound by the number of inner degrees of freedom of the OQWs [25].

OQWs can perform dissipative quantum computing (DQC) [26] and quantum state engineering [27]. It has been shown that the OQW implementation of DQC outperforms the conventional model of DQC. In particular, it has been found that OQWs can be designed to converge faster to the desired steady state and to increase the probability of detection of the outcome of the quantum computation [27].

A quantum optical implementation of simple OQWs has been suggested using a dissipative out-of-resonance cavity QED setup [28]. The Fock states of the cavity mode correspond to the nodes of the walk, and the state of the two-level system corresponds to an inner degree of freedom of the walker.

Recently, Bauer *et al.* found that the OQW quantum trajectories can switch between diffusive and ballistic behavior [14]. However, such switching was established for abstract CPTP maps without identifying the physics of the underlying system.

OWQs have been introduced formally, and the question of microscopic models leading to OQWs needs to be addressed. Due to the dissipative nature of the OQWs, it is natural to expect them to be obtained from an appropriate system-environment model as the reduced dynamics of a quantum walker on a graph. Indeed, for a simple case of an OQW on a two-node graph, a microscopic derivation has been described [29].

The aim of the present paper is to derive OQWs from a microscopic Hamiltonian on an arbitrary graph. The microscopic derivation includes the identification of an appropriate system environment model (the Hamiltonian of the system, the bath, and the system-bath interaction), the Born-Markov approximation, and tracing out the environmental degrees of freedom [9,30,31]. The resulting quantum master equation will be shown to have the form of a generalized master equation

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[32], and a discrete time version corresponds to the CPTP maps defining OQWs. The formalism is demonstrated for two examples of OQWs, namely an OQW on a circle of nodes and an OQW on a finite chain of nodes. The microscopic derivation allows us to connect the thermodynamic parameters of the environment and the dynamics of OQWs. It is shown that the temperature of the environment plays the role of the switch between diffusive and ballistic quantum trajectories corresponding to the OQWs.

The paper has the following structure. In Sec. II we briefly review the formalism of OQWs. In Sec. III we formulate the microscopic model and perform the microscopic derivation of the OQWs. In Sec. IV we demonstrate the microscopic derivation for two examples. In Sec. V we conclude.

II. FORMALISM OF OPEN QUANTUM WALKS

The open quantum walk is a quantum walk defined on a set of nodes, where the transitions between the nodes are exclusively driven by dissipation. Mathematically, open quantum walks are formulated in the language of completely positive trace-preserving (CPTP) maps. A CPTP map is defined on the graph $\mathcal{G} = (\mathcal{V}, E)$, where $\mathcal{V}$ is the set all nodes and $E = \{(i,j)|i,j \in \mathcal{V}\}$ is the set of all ordered edges denoting possible transitions between the nodes. The number of nodes can be finite ($P < \infty$) or infinitely countable ($P = \infty$), where P denotes cardinality of the set of nodes $\mathcal{V}$, i.e., $P = \mathrm{card}(\mathcal{V})$. The corresponding Hilbert space of the walk is defined as separable Hilbert space $\mathcal{K} = \mathbb{C}^P$ for the finite-dimensional case ($P < \infty$), and for the infinite-dimensional case ($P = \infty$) the Hilbert space is the space of square integrable functions $\mathcal{K} = l^2(\mathbb{C})$ with the orthonormal basis indexed by $|i\rangle$, where $i \in \mathcal{V}$. The internal degrees of freedom of the quantum walker, e.g., spin, polarization, or n-energy levels, are described by a separable Hilbert space $\mathcal{H}_N$ attached to each node. Any state of the walker will be described on the direct product of the Hilbert spaces $\mathcal{H}_N \otimes \mathcal{K}$.

To describe the dynamics of the internal degree of freedom of the walker for each edge (i,j), we introduce bounded operators B_j^i acting on $\mathcal{H}_N$. These operators describe the transformation of the internal degree of freedom of the quantum walker due to the "jump" from node j to node i (see Fig. 1). On each node j we define a CPTP map $\mathcal{M}_j$ in the Kraus representation on the space of operators on $\mathcal{H}_N$,

$$\mathcal{M}_j(\tau) = \sum_i B_j^i \tau B_j^{i\dagger}. \tag{1}$$

Complete positivity and trace preservation of the above map are guaranteed by the following normalization condition for each node j [13]:

$$\sum_i B_j^{i\dagger} B_j^i = I. \tag{2}$$

This condition is the generalization of the classical Markov chain condition.

From the physical point of view, the operators B_j^i affect only the internal degrees of freedom of the walker, and they do not perform transitions from node j to node i. We can extend the action of the operators B_j^i on the whole lattice with the help of the following dilation:

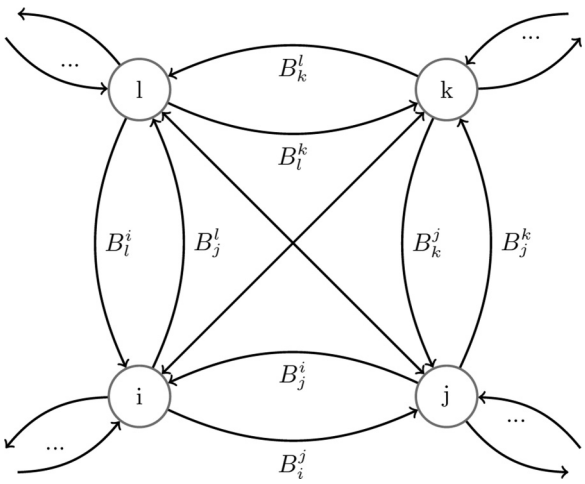

FIG. 1. Schematic illustration of the formalism of open quantum walks. The walk is realized on a graph with a set of vertices denoted by i,j,k,l. The operators B_i^j describe transformations in the internal degree of freedom of the "walker" during the transition from node (i) to node (j).

$$M_j^i = B_j^i \otimes |i\rangle\langle j|. \tag{3}$$

If the condition expressed in Eq. (2) is satisfied, then $\sum_{i,j} M_j^{i\dagger} M_j^i = 1$ [11]. This normalization condition allows us to define a CPTP map for density matrices on $\mathcal{H}_N \otimes \mathcal{K}$, i.e.,

$$\mathcal{M}(\rho) = \sum_i \sum_j M_j^i \, \rho \, M_j^{i\dagger}. \tag{4}$$

The CPTP map $\mathcal{M}$ defines the discrete-time *open quantum walk* [10,11]. It has been shown that for an arbitrary initial state, the density matrix $\sum_{i,j} \rho_{i,j} \otimes |i\rangle\langle j|$ will take a diagonal form in the position of Hilbert space $\mathcal{K}$ after just one step of the OQW [10,11]. For this reason, it is sufficient to assume that the initial state of the system is in the diagonal form in the "position" space $\rho = \sum_i \rho_i \otimes |i\rangle\langle i|$ with $\sum_i \mathrm{Tr}(\rho_i) = 1$.

It is straightforward to give an explicit iteration formula for the OQW from step n to step $n+1$,

$$\rho^{[n+1]} = \mathcal{M}(\rho^{[n]}) = \sum_i \rho_i^{[n+1]} \otimes |i\rangle\langle i|, \tag{5}$$

where

$$\rho_i^{[n+1]} = \sum_j B_j^i \rho_j^{[n]} B_j^{i\dagger}. \tag{6}$$

This iteration formula gives a clear physical meaning to the CPTP mapping that we introduced: the state of the system on node i is determined by the conditional shift from all connected nodes j and the internal state of the walker on the node j. These conditional shifts are defined by the explicit form of the operators B_j^i. Also, it is straightforward to see that $\mathrm{Tr}[\rho^{[n+1]}] = \sum_i \mathrm{Tr}[\rho_i^{[n+1]}] = 1$.

As an example, let us consider a homogeneous OQW on the circle or on the line (see Fig. 2) with jump operators B_j^i defined as

$$B_i^{i+1} \equiv B, \quad B_i^i \equiv A, \quad B_i^{i-1} \equiv C \tag{7}$$

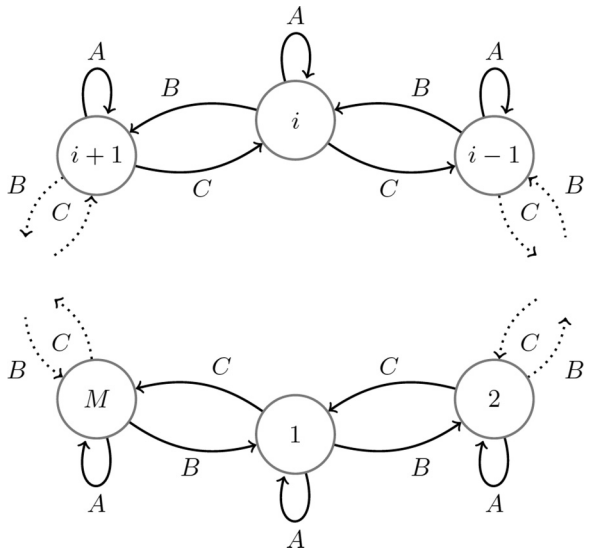

FIG. 2. Open quantum walk on a circle of nodes. A schematic representation of the OQW on the circle: all transitions to the right are induced by the operator B, while all transitions to the left are induced by the operator C and all steps without transitions are induced by the operator A.

and the normalization condition given by $A^\dagger A + B^\dagger B + C^\dagger C = 1$. The state of the walker $\rho^{[n]}$ after n steps reads

$$\rho^{[n]} = \sum_i \rho_i^{[n]} \otimes |i\rangle\langle i|, \tag{8}$$

where the form of $\rho_i^{[n]}$ ($i \in \mathbb{Z}$) is easily found by iteration,

$$\rho_i^{[n+1]} = A\rho_i^{[n]}A^\dagger + B\rho_{i-1}^{[n]}B^\dagger + C\rho_{i+1}^{[n]}C^\dagger. \tag{9}$$

Several examples of OQWs on $\mathbb{Z}$ can be found in [10–12,25].

III. MICROSCOPIC DERIVATION OF OQWs

As was stated before, OQWs are formulated as quantum walks on a set of nodes, where the transition between the nodes is driven by dissipation. This implies that it should be possible to derive OQWs using methods of the theory of open quantum systems [9]. From a microscopic point of view, the Hamiltonian of the total system is given by

$$H = H_S + H_B + H_{SB}, \tag{10}$$

where in the usual notation H_S, H_B, and H_{SB} stand for the Hamiltonian of the system, the bath, and the system-bath interaction, respectively. As a result of the microscopic derivation, we would like to obtain OQWs after tracing out the bath degrees of freedom. In the context of this work, the open system is not only the "quantum walker" but the quantum walker with the underlying lattice. Using the condition that the transitions between the nodes are driven by dissipation, it is easy to conclude that the system Hamiltonian by itself should describe only the local dynamics of the walker on each node, which implies the following form of the system Hamiltonian H_S for the M-node network:

$$H_S = \sum_{i=1}^{M} \Omega_i \otimes |i\rangle\langle i|. \tag{11}$$

The position of the walker is described by the set of orthogonal vectors $\{|i\rangle\}_{i=1}^M$, which form the basis in the position Hilbert space $\mathcal{C}^M$. The state of the inner degree of freedom of the walker is described by the operators $\Omega_i \in \mathcal{B}(\mathcal{H}_N)$, where $\mathcal{H}_N$ is an N-dimensional Hilbert space describing the inner degrees of freedom of the walker.

OQWs are designed such that the transitions between different sites are uncorrelated. This means that for each pair of nodes i and j between which transitions are possible, one needs to have at least one local environment that will drive the walker between the nodes. The direct consequence of this is the following form of the bath Hamiltonian H_B:

$$H_B = \sum_{i\neq j=1}^{M} \sum_n \omega_{i,j,n} a_{i,j,n}^\dagger a_{i,j,n}, \tag{12}$$

where $a_{i,j,n}^\dagger$ and $a_{i,j,n}$ are bosonic creation and annihilation operators of the modes (photonic or phononic) of the bath, with standard commutation relations.

The system-bath Hamiltonian H_{SB} describes environment-assisted transitions of the quantum walker between the nodes. This implies that for any two nodes i and j, this Hamiltonian has the following structure: $H_{SB}^{i\leftrightarrow j} = A_{i,j} \otimes X_{i,j} \otimes B_{i,j}$. As in a typical open quantum system, we assume a linear coupling between each component of the total system, but the crucial difference is that in the present work we have two different degrees of freedom of the system, namely the position and the internal degree of freedom, coupled simultaneously to the bath. The operator $A_{i,j} \in \mathcal{B}(\mathcal{H}_N)$ is an operator acting on the internal degree of freedom of the walker, and it plays the role of a "quantum coin" similar to the Hadamard matrix for the unitary quantum walks [7,8]. The operator A_{ij} is conditioning the probability of transition between the nodes to the internal state of the walker. If the operator A_{ij} is trivial, i.e., $A_{i,j} \equiv 1$, then the resulting open walk will be classical. The operator $X_{i,j} \in \mathcal{B}(\mathcal{C}^M)$ describes the transition between the nodes i and j. The simplest choice is the following: $X_{i,j} = |j\rangle\langle i| + |i\rangle\langle j|$. The coupling between the quantum walker and the corresponding environment is described by the operator $B_{i,j}$, and the simplest and typical choice is linear coupling of the system to the bath, i.e., $B_{i,j} = \sum_n g_{i,j,n}a_{i,j,n} + g_{i,j,n}^* a_{i,j,n}^\dagger$. It is clear that only the system-bath Hamiltonian containing the tensor product of these three operators $(A_{i,j}, X_{i,j}, B_{i,j})$ is minimally required to obtain OQWs. As was stated above, if A_{ij} is trivial, the walk will be classical; if $X_{i,j}$ is trivial, there will be no walk; and finally if B_{ij} is trivial, the quantum walk would not be environment-driven. The system-bath Hamiltonian H_{SB} describing environment-assisted transitions has the following form:

$$H_{SB} = \sum_{i,j} \sum_n A_{i,j} \otimes X_{i,j} \otimes (g_{i,j,n}a_{i,j,n} + g_{i,j,n}^* a_{i,j,n}^\dagger). \tag{13}$$

Having specified the Hamiltonian of the total system, we can proceed and derive the reduced master equation describing the dynamics of the system, which consists of the quantum walker

and the lattice. Here we assume that the system is weakly interacting with the reservoirs, so that the Born-Markov approximation is valid [9]. Under these assumptions, the reduced dynamics of the system in the interaction picture is given by the following equation:

$$\frac{d}{dt}\rho_s(t) = -\int_0^\infty d\tau\, \mathrm{Tr}_B[H_{SB}(t),[H_{SB}(t-\tau),\rho_s(t)\otimes\rho_B]], \quad (14)$$

where $\rho_s(t)$ is the reduced density matrix of the system (walker on the network) and ρ_B is the state of the reservoir. In general, Eq. (14) does not guarantee that the resulting master equation will be in the Gorini-Kossakowski-Sudarshan-Lindblad form (GKSL form) [9,33–35]. To obtain the master equation in the form of the generator of the dynamical semigroup, one needs to perform an additional rotating-wave approximation [9]. This rotating-wave approximation can be straightforwardly performed if we decompose the system-bath Hamiltonian in the basis of eigenoperators of the system Hamiltonian H_S. Toward that end, on each node $|i\rangle$ we introduce the set of orthonormal projection operators $\{\Pi_i(\lambda^{(i)})\}$ onto the eigenvalues $\lambda^{(i)}$ of each Hamiltonian Ω_i such that

$$\Omega_i = \sum_{\lambda^{(i)}} \lambda^{(i)}\Pi_i(\lambda^{(i)}). \quad (15)$$

It is easy to see that in the interaction picture, the system-bath Hamiltonian H_{SB} takes now the following form:

$$H_{SB}(t) = \sum_{i,j}\sum_{\lambda^{(i)},\lambda^{(j)}} e^{it(\lambda^{(i)}-\lambda^{(j)})}\Pi_i(\lambda^{(i)})A_{i,j}\Pi_j(\lambda^{(j)}) \otimes |i\rangle\langle j| \otimes B_{i,j}(t) + \mathrm{H.c.}, \quad (16)$$

where the operator $B_{i,j}(t)$ is given by

$$B_{i,j}(t) = e^{itH_B}\left(\sum_n g_{i,j,n}a_{i,j,n} + g^*_{i,j,n}a^\dagger_{i,j,n}\right)e^{-itH_B} = \sum_n g_{i,j,n}a_{i,j,n}e^{-it\omega_{i,j,n}} + \mathrm{H.c.} \quad (17)$$

Equation (16) can be rewritten as

$$H_{SB}(t) = \sum_{i,j}\sum_\omega e^{it\omega}A^\dagger_{i,j}(\omega)\otimes|i\rangle\langle j|\otimes B_{i,j}(t) + \mathrm{H.c.} + \sum_{i,j}\sum_{\omega'} e^{-it\omega'}A_{i,j}(\omega')\otimes|i\rangle\langle j|\otimes B_{i,j}(t) + \mathrm{H.c.}, \quad (18)$$

where the operators $A^\dagger_{i,j}(\omega)$ and $A_{i,j}(\omega')$ are defined as

$$A_{i,j}(\omega) = \sum_{\lambda^{(i)}-\lambda^{(j)}=\omega<0}\Pi_i(\lambda^{(i)})A_{i,j}\Pi_j(\lambda^{(j)}),$$
$$A^\dagger_{i,j}(\omega') = A_{i,j}(-\omega'). \quad (19)$$

It is straightforward to see that the summation over all frequencies ω and ω' gives the original operators $A_{i,j}$,

$$\sum_\omega A_{i,j}(\omega) + \sum_{\omega'} A^\dagger_{i,j}(\omega') = A_{i,j}. \quad (20)$$

Having defined the system-bath Hamiltonian H_{SB}, we can put the explicit expression for the Hamiltonian Eq. (16) into the generic equation for the reduced density matrix Eq. (14) and obtain the master equation for the system. In Eq. (14), we will need to trace out the bath degrees of freedom. Here, we assume that the environment is in a thermal equilibrium state, i.e., the state of the reservoir is given by the canonical distribution $\rho_B = \exp(-\beta H_B)/\mathrm{Tr}[\exp(-\beta H_B)]$, where β is the inverse temperature of the bath, $\beta = (k_B T)^{-1}$. Using the explicit form of the system-bath interaction Hamiltonian in the interaction picture $H_{SB}(t)$ [Eq. (16)], and utilizing the rotating-wave approximation for the transition frequencies ω and ω' [9,35], it follows that

$$\frac{d}{dt}\rho_s(t) = \sum_{i,j}\sum_\omega \gamma_{i,j}(-\omega)\mathcal{L}[A_{i,j}(\omega)\otimes|j\rangle\langle i|]\rho_s(t) + \gamma_{i,j}(\omega)\mathcal{L}(A^\dagger_{i,j}(\omega)\otimes|i\rangle\langle j|)\rho_s(t) + \sum_{i,j}\sum_{\omega'}\gamma_{i,j}(-\omega')\mathcal{L}[A_{i,j}(\omega')\otimes|i\rangle\langle j|]\rho_s(t) + \gamma_{i,j}(\omega')\mathcal{L}(A^\dagger_{i,j}(\omega')\otimes|j\rangle\langle i|)\rho_s(t), \quad (21)$$

where $\mathcal{L}(A)\rho$ denotes the dissipative superoperator in diagonal GKSL form [9,33,34],

$$\mathcal{L}(A)\rho = A\rho A^\dagger - \tfrac{1}{2}\{A^\dagger A,\rho\}, \quad (22)$$

and $\gamma_{i,j}(\omega)$ is the real part of the Fourier transform of the reservoir correlation functions $\langle B^\dagger_{i,j}(\tau)B_{i,j}(0)\rangle$,

$$\gamma_{i,j}(\pm\omega) = \frac{\gamma^{\mathrm{se}}_{i,j}}{2}\left[\coth\left(\frac{\beta\omega}{2}\right)\mp 1\right], \quad (23)$$

where $\gamma^{\mathrm{se}}_{i,j}$ is the coefficient of the spontaneous emission in the corresponding local reservoir. In Eq. (21), the Lamb-type shift terms are neglected. These terms describe shifts in energy levels of the system due to the interaction with the heat bath, and typically they do not influence the dissipative dynamics of the system. The value of the Lamb-type shift is much smaller than other characteristic parameters in the system Hamiltonian, and traditionally these terms are dropped. For the cases in which the dimension of the reduced system is large enough, these Lamb-type shifts might affect the dissipative dynamic of the reduced system [36,37]. However, for simplicity in the present paper, we assume that one can neglect these contributions.

It is interesting to note that the quantum master equation (21) has the form of the generalized master equation introduced by Breuer [32]. For the generalized master equation, it is assumed that the total density matrix of the reduced system can be written as $\rho = \sum_i \rho_i \otimes |i\rangle\langle i|$, where each operator ρ_i satisfies the following differential equation:

$$\frac{d}{dt}\rho_i = \mathcal{K}_i(\rho_1,\ldots,\rho_n), \quad (24)$$

where the general form of the generators $\mathcal{K}_i$ is given by

$$\mathcal{K}_i(\rho_1,\ldots,\rho_n) = -i[H_i,\rho_i] + \sum_{j,\lambda}\left(R_\lambda^{ji}\rho_j R_\lambda^{ji\dagger} - \frac{1}{2}\{R_\lambda^{ji\dagger}R_\lambda^{ji},\rho_i\}\right), \tag{25}$$

with Hermitian operators H_i and non-Hermitian operators R_λ^{ji}.

It is straightforward to see that by writing the density matrix of the reduced system from Eq. (21) as $\rho_s(t) = \sum_{i=1}^M \rho_i(t)\otimes|i\rangle\langle i|$, where $|i\rangle\langle i|$ is a projection on the node i, the quantum master equation (21) reduces to the system of differential equations for $\rho_i(t)$:

$$\frac{d}{dt}\rho_i(t) = \mathcal{K}_i(\rho_1,\ldots,\rho_M), \tag{26}$$

where $\mathcal{K}_i(\rho_1,\ldots,\rho_M)$ is now explicitly given by

$$\begin{aligned}\mathcal{K}_i(\rho_1,\ldots,\rho_M) = &\sum_{j,\omega}\gamma_{j,i}(-\omega)A_{j,i}(\omega)\rho_j A_{j,i}^\dagger(\omega) - \frac{\gamma_{i,j}(-\omega)}{2}\{A_{i,j}^\dagger(\omega)A_{i,j}(\omega),\rho_i\}\\ &+\sum_{j,\omega}\gamma_{i,j}(\omega)A_{i,j}^\dagger(\omega)\rho_j A_{i,j}(\omega) - \frac{\gamma_{j,i}(\omega)}{2}\{A_{j,i}(\omega)A_{j,i}^\dagger(\omega),\rho_i\}\\ &+\sum_{j,\omega'}\gamma_{i,j}(-\omega')A_{i,j}(\omega')\rho_j A_{i,j}^\dagger(\omega') - \frac{\gamma_{j,i}(-\omega')}{2}\{A_{j,i}^\dagger(\omega')A_{j,i}(\omega'),\rho_i\}\\ &+\sum_{j,\omega'}\gamma_{j,i}(\omega')A_{j,i}^\dagger(\omega')\rho_j A_{j,i}(\omega') - \frac{\gamma_{i,j}(\omega')}{2}\{A_{i,j}(\omega')A_{i,j}(\omega')^\dagger,\rho_i\}.\end{aligned} \tag{27}$$

The system of differential equations (26) and (27) defines the *continuous-time open quantum walk*. Continuous-time OQWs have been introduced recently as the continuous-in-time limit of the discrete-time OQWs [Eq. (5)] [21].

To obtain a discrete-time OQW in the form (4), one needs to introduce discretized time steps. There are at least two ways of achieving this. The first way is to discretize the solution of the system of equations (26), however it cannot be done in a generic setting. The second way, which is the one way to do a discretization in general, is to discretize the system of the differential equations (26). To do this, one needs to replace the time derivative by the finite difference with a small time step Δ,

$$\frac{d}{dt}\rho_i(t) \to \frac{\rho_i(t+\Delta)-\rho_i(t)}{\Delta}. \tag{28}$$

The above substitution leads to the following transition operators:

$$\begin{aligned}B_j^{i(1)}(\omega) &= \sqrt{\Delta\gamma_{j,i}(-\omega)}A_{j,i}(\omega), \quad B_j^{i(2)}(\omega) = \sqrt{\Delta\gamma_{i,j}(\omega)}A_{i,j}^\dagger(\omega),\\ B_j^{i(1)}(\omega') &= \sqrt{\Delta\gamma_{i,j}(-\omega')}A_{i,j}(\omega'), \quad B_j^{i(2)}(\omega') = \sqrt{\Delta\gamma_{j,i}(\omega')}A_{j,i}^\dagger(\omega'),\\ B_i^i &= I_N - \frac{\Delta}{2}\sum_{j,\omega}(\gamma_{i,j}(-\omega)A_{i,j}^\dagger(\omega)A_{i,j}(\omega) + \gamma_{j,i}(\omega)A_{j,i}(\omega)A_{j,i}^\dagger(\omega))\\ &\quad - \frac{\Delta}{2}\sum_{j,\omega'}(\gamma_{j,i}(-\omega')A_{j,i}^\dagger(\omega')A_{j,i}(\omega') + \gamma_{i,j}(\omega')A_{i,j}(\omega')A_{i,j}(\omega')),\end{aligned} \tag{29}$$

where I_N is an N-dimensional identity operator on the Hilbert space $\mathcal{H}_N$. One can see that the set of transition operators introduced above satisfies standard normalization conditions up to $O(\Delta^2)$,

$$B_j^{j\dagger}B_j^j + \sum_{k=1}^2\sum_{j,i,\omega}B_j^{i(k)\dagger}(\omega)B_j^{i(k)}(\omega) + \sum_{k=1}^2\sum_{j,i,\omega}B_j^{i(k)\dagger}(\omega')B_j^{i(k)}(\omega') = I_N. \tag{30}$$

Hence, the iteration formula for the discrete-time OQW reads

$$\rho_i^{[n+1]} = B_i^i\rho_i^{[n]}B_i^{i\dagger} + \sum_{k=1}^2\sum_{j,\omega}B_j^{i(k)}(\omega)\rho_j^{[n]}B_j^{i(k)\dagger}(\omega) + \sum_{k=1}^2\sum_{j,\omega'}B_j^{i(k)}(\omega')\rho_j^{[n]}B_j^{i(k)\dagger}(\omega'). \tag{31}$$

The explicit expression for the transition operators Eq. (29) establishes a connection between the dynamical properties of the OQWs and the thermodynamic parameters of the environment.

IV. EXAMPLES OF OPEN QUANTUM WALKS

A. First example

As an example of the above microscopic derivation of OQWs, we consider a two-level system (two-level atom or electron with spin) as a quantum walker on a circle with M nodes (Fig. 2). In this case, the system Hamiltonian H_S of the two-level system ("quantum walker") on the circle reads

$$H_S = \sum_{i=1}^{M} \frac{\omega_0}{2}\sigma_z \otimes |i\rangle\langle i| + \lambda(\vec{n}_\lambda \vec{\sigma}) \otimes |i\rangle\langle i|, \tag{32}$$

where σ_i are the Pauli matrices, and the term $\lambda(\vec{n}_\lambda\vec{\sigma})$ describes a weak external field $\lambda \ll \omega_0$ in the direction of the unit vector $\vec{n}_\lambda$. We consider a system-bath Hamiltonian H_{SB} of the following form:

$$H_{SB} = \sum_{i=1}^{M} g_{i,n}\sigma_- \otimes |i+1\rangle\langle i| \otimes a_{i,n}^\dagger + g_{i,n}^*\sigma_+ \otimes |i\rangle\langle i+1| \otimes a_{i,n}, \tag{33}$$

where $|M+1\rangle \equiv |1\rangle$. Taking into account that the external field in the Hamiltonian H_S is weak, $\lambda \ll \omega_0$, the system-bath Hamiltonian in the interaction picture reads

$$H_{SB} = \sum_{i=1}^{M} g_{i,n}\sigma_- \otimes |i+1\rangle\langle i| \otimes a_{i,n}^\dagger e^{-i(\omega_0-\omega_{i,n})t} + \text{H.c.} \tag{34}$$

The corresponding quantum master equation for the reduced density matrix takes the following form:

$$\frac{d}{dt}\rho_s(t) = \sum_{i=1}^{M} \big(-i[\lambda(\vec{n}_\lambda\vec{\sigma}) \otimes |i\rangle\langle i|, \rho_s(t)] + \gamma_i(-\omega_0)\mathcal{L}(\sigma_- \otimes |i+1\rangle\langle i|)\rho_s(t) + \gamma_i(\omega_0)\mathcal{L}(\sigma_+ \otimes |i\rangle\langle i+1|)\rho_s(t)\big). \tag{35}$$

The superoperator defined by Eq. (35) preserves the block-diagonal structure of the density matrix $\rho_s(t) = \sum_{i=1}^{M} \rho_i(t) \otimes |i\rangle\langle i|$. The continuous-time OQW has the same structure as Eq. (26),

$$\frac{d}{dt}\rho_i(t) = -\imath\lambda[\vec{n}_\lambda\vec{\sigma}, \rho_i(t)] + \gamma_i(-\omega_0)\left(\sigma_-\rho_{i-1}(t)\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho_i(t)\}_+\right) + \gamma_i(\omega_0)\left(\sigma_+\rho_{i+1}(t)\sigma_- - \frac{1}{2}\{\sigma_-\sigma_+, \rho_i(t)\}_+\right). \tag{36}$$

Finally, it is easy to obtain the explicit form of the operators B_i^j following the time-dicretization procedure introduced in Eq. (36),

$$B = \sqrt{\Delta\gamma(\langle n\rangle + 1)}\sigma_-, \quad C = \sqrt{\Delta\gamma\langle n\rangle}\sigma_+,$$
$$A = I_2 - \frac{\Delta}{2}[\gamma(\langle n\rangle + 1)\sigma_+\sigma_- + \gamma\langle n\rangle\sigma_-\sigma_+] - \imath\lambda\Delta\vec{n}_\lambda\vec{\sigma}. \tag{37}$$

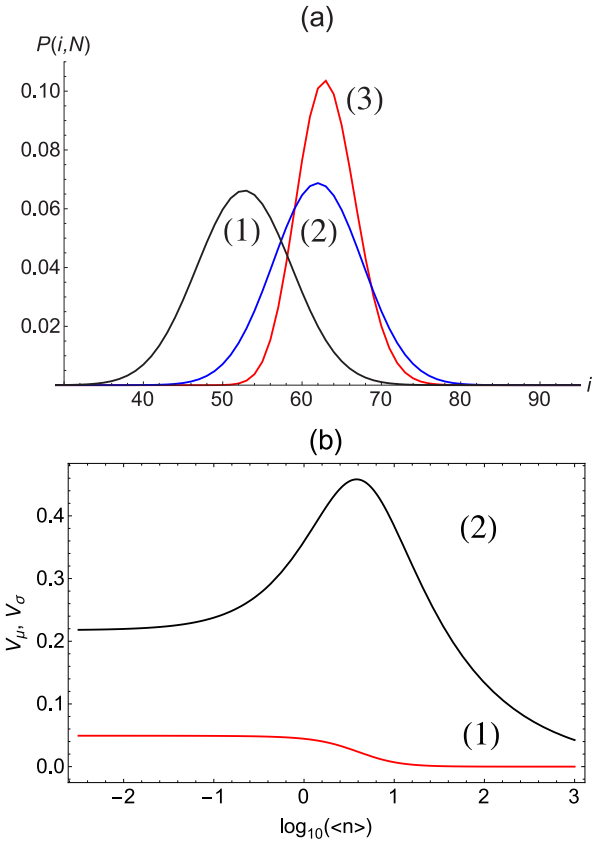

FIG. 3. (Color online) Open quantum walk on a circle of nodes. Operators A, B, and C are given by Eq. (37). Part (a) shows the occupation probability of the "walker" $P(i,N) = \text{Tr}[\rho_i^{[N]}]$ after 5000 steps. The initial state of the "walker" is given by $\rho^{[0]} = \frac{1}{2}I_2 \otimes |51\rangle\langle 51|$ and curves (1)–(3) correspond to the different temperatures of the environment $\langle n\rangle = 10$, 1, and 0.1, respectively; the parameters are $\gamma = 0.1$, $\lambda = 0.3$, and $\Delta = 0.05$. Part (b) shows the dependence of the "speed" of the Gaussian V_μ (curve 1) and "spread" of the Gaussian V_σ (curve 2) given by Eqs. (38) and (39) as a function of the temperature of the environment; the parameters are $\gamma = 0.1$ and $\lambda = 0.3$.

For simplicity, in Eq. (37) we assume that all damping rates are the same, i.e., $\forall\, i, \gamma_i(-\omega_0) \equiv \gamma(-\omega_0) = \gamma(\langle n\rangle + 1)$ and $\forall\, i, \gamma_i(\omega_0) \equiv \gamma(\omega_0) = \gamma\langle n\rangle$, where γ is the coefficient of spontaneous emission and $\langle n\rangle = [\exp(\frac{\hbar\omega_0}{k_B T}) - 1]^{-1}$ is the mean number of thermal photons on the frequency ω_0 for a bath at temperature T. The iteration formula for OQWs with jump operators A, B, and C [Eq. (37)] is given by Eq. (9).

Figure 3 shows the dynamics of different observables for the OQW on the circle with $M = 101$ nodes and the jump operators given by Eq. (37). The occupation probability of the "walker" $P(i,N) = \text{Tr}[\rho_i^{[N]}]$ after $N_{\text{steps}} = 5000$ steps for different temperatures of environment is shown in Fig. 3(a). It is clear that when decreasing the temperature of the bath [from Fig. 3(a1) to Fig. 3(a3)], the Gaussian distribution describing the occupation probability of the position of the "walker" moves faster to the right, and in the case of higher temperatures of the environment [Fig. 3(a1)] the average position of the "walker" essentially remains near the initial node 51. However, the width of the Gaussian distributions corresponding to the

temperatures $\langle n\rangle = 1$ and 10 seems to be the same. To explain this, one needs to analyze the average and variance of the position of the "walker." Using Eq. (36), one can derive a system of equations for the mean $\mu(t) = \sum_{i=1}^{M} i\mathrm{Tr}[\rho_i(t)]$ and the variance $\sigma^2(t) = \sum_{i=1}^{M}\{i^2\mathrm{Tr}[\rho_i(t)] - \mu(t)^2\}$ of the "walker" in position space (see the Appendix for details). Using analytical expressions for $\mu(t)$ and $\sigma^2(t)$, it is possible to calculate the asymptotic velocity of these quantities,

$$V_\mu = \lim_{t\to\infty}\frac{\mu(t)}{t} = \frac{4\gamma\lambda^2}{\Omega^2}, \tag{38}$$

where $\Omega = \sqrt{8\lambda^2 + \gamma^2(2\langle n\rangle + 1)^2}$, and

$$V_\sigma^2 = \lim_{t\to\infty}\frac{\sigma^2(t)}{t} = \frac{\gamma}{2}(2\langle n\rangle + 1) - \frac{3}{2}\frac{\gamma^7(2\langle n\rangle + 1)^5}{\Omega^6} + \frac{3\gamma^5(2\langle n\rangle + 1)^3}{\Omega^4} - \frac{\gamma^3(2\langle n\rangle + 1)(\langle n\rangle^2 + \langle n\rangle + 1)}{\Omega^2}. \tag{39}$$

Figure 3(b) shows the dependence of the "speed" (V_μ, curve 1) and "spread" (V_σ, curve 2) of the Gaussian distributions as a function of the temperature of the environment on a logarithmic scale. This figure perfectly explains the dynamics of the Gaussians shown in Fig. 3(a). Figure 3(b) shows that the "speed" of the Gaussian is a monotonically decreasing function of the temperature of the environment. However, the biggest change in the velocity is happening for the temperature corresponding to the average number of photons in the bath between 1 ($\log_{10}\langle n\rangle = 0$) and 10 ($\log_{10}\langle n\rangle = 1$). Figure 3(a) demonstrates that dependence: a Gaussian distribution curve Fig. 3(a1) ($\log_{10}\langle n\rangle = 1$) is much slower than Figs. 3(a2) and 3(a3) corresponding to $\log_{10}\langle n\rangle = 0$ and $\log_{10}\langle n\rangle = -1$, respectively. The "speed" (V_μ) corresponding to Figs. 3(a2) and 3(a3) is approximately the same. The dependence of the "spread" of the Gaussians as a function of the temperature of the environment [Fig. 3(b2)] is nonmonotonic. Upon increasing the temperature of the environment, the "spread" grows to a certain point and decreases afterward. This nonmonotonic dependence explains the same width of the Gaussians corresponding to different temperatures of the bath in Fig. 3(a1) ($\log_{10}\langle n\rangle = 1$) and Fig. 3(a2) ($\log_{10}\langle n\rangle = 0$).

Figure 4 shows the dynamics of the total coherence,

$$\sigma_x(t) = \sum_{i=1}^{M}\mathrm{Tr}\left[\rho_i^{[t]}\sigma_x\right], \tag{40}$$

of the "walker." The time in Fig. 4 is in the number of steps of the walk multiplied by the time-discretization step Δ, so each unit of time corresponds to 20 steps of the walk. One can see that for all considered temperatures of the environment, there is some nonzero level of coherence present in the system. The presence of the steady-state coherence in the OQWs demonstrates that even if the steady-state position of the walker is a classically distributed degree of freedom, the inner state of the walker remains quantum. Obviously, for lower temperatures [Fig. 4(3)] the amount of coherence is higher, and it takes more steps to achieve a steady-state coherence. Figure 5 shows examples of quantum trajectories of the "walker" for

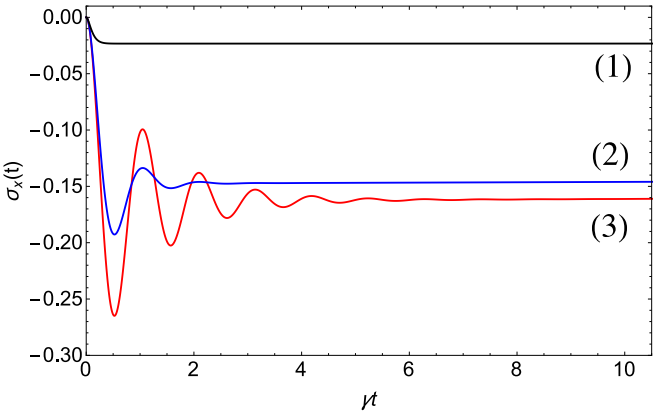

FIG. 4. (Color online) Open quantum walk on a circle of nodes. Operators A, B, and C are given by Eq. (37). The figure shows the dynamics of the total coherence of the "walker" $\sigma_x(t) = \sum_{i=1}^{M}\mathrm{Tr}[\rho_i^{[t]}\sigma_x]$. The initial state of the "walker" is given by $\rho^{[0]} = \frac{1}{2}I_2 \otimes |51\rangle\langle 51|$ and the curves (1)–(3) correspond to the different temperatures of the environment $\langle n\rangle = 10$, 1, and 0.1, respectively; the parameters are $\gamma = 0.1$, $\lambda = 0.3$, and $\Delta = 0.05$.

nonzero and zero temperature of the environment, respectively. The quantum trajectories of the "walker" were obtained using the unraveling of the OQWs [10–12]. In the zero-temperature case, the jump operator C vanishes ($C \equiv 0$), which implies that there will be only two options for the walker, namely to stay on the same node or to move to the right. The temperature of the bath plays the role of a switch between diffusive and ballistic trajectories of the "walker."

Similar behavior of the OQWs was described by Bauer *et al.* [14] using parametrized generic CPTP maps. Only the microscopic derivation presented here allows us to identify the physical conditions necessary to observe the transition in the behavior of quantum trajectories.

B. Second example

The second example of the microscopic derivation is an OQW on a finite chain of nodes. As in the previous example, the quantum walker will be a two-level system. The Hamiltonian of the walker on the finite chain of nodes is given by

$$H_S = \sum_{i=1}^{M}\frac{\epsilon_i}{2}\sigma_z \otimes |i\rangle\langle i|, \tag{41}$$

where the constants ϵ_k read

$$\epsilon_k = \epsilon_0 + k\Delta_0, \tag{42}$$

where ϵ_0 and Δ_0 are some positive constants. In this example, we will assume a pure dephasing system-bath interaction,

$$H_{SB} = \sum_{i=1}^{M-1}\sum_{n}(\alpha\sigma_z + \beta I)X_{i,i+1} \otimes (g_{i,n}a_{i,n} + \mathrm{H.c.}), \tag{43}$$

where $X_{i,i+1} = |i+1\rangle\langle i| + |i\rangle\langle i+1|$ and $\alpha,\beta \in \mathbb{R}$. The free parameters α and β allow us to address different types of dephasing coupling. For $\alpha = 1$ and $\beta = 0$, we obtain σ_z coupling, and for $\alpha = \pm\beta = 1/2$, we couple excited

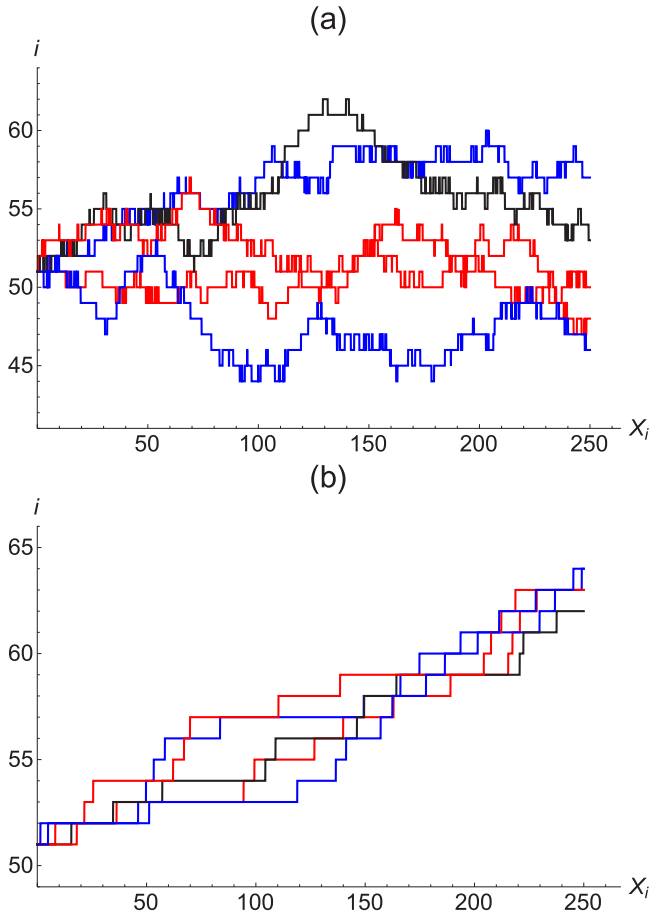

FIG. 5. (Color online) Open quantum walk on a circle of nodes. Operators A, B, and C are given by Eq. (37). Parts (a) and (b) show examples of quantum trajectories of the "walker" in the diffusive and the ballistic case, respectively. The axis labels i and X_i denote the node of the position of the walk and the number of steps of the OQW. The diffusive behavior of the quantum trajectories of the "walker" shown in (a) corresponds to the nonzero temperature of the environment ($\langle n\rangle = 5$), while the ballistic behavior of the quantum trajectories of the "walker" shown in (b) corresponds to an environment at zero temperature ($\langle n\rangle = 0$). The initial state of the "walker" is given by $\rho^{[0]} = \frac{1}{2} I_2 \otimes |51\rangle\langle 51|$; the parameters are $\gamma = 0.1$, $\lambda = 0.3$, and $\Delta = 0.05$.

and ground levels of the two-level system, respectively. In the interaction picture, the Hamiltonian of the system bath interaction $H_{SB}(t)$ reads

$$H_{SB}(t) = \sum_{i=1}^{M-1}\sum_{n}(\alpha\sigma_z + \beta I)\otimes(|i+1\rangle\langle i|e^{i\Delta_0 t} + |i\rangle\langle i+1|e^{-i\Delta_0 t})\otimes(g_{i,n}a_{i,n}e^{-i\omega_{i,n}t} + \text{H.c.}). \tag{44}$$

After application of the rotating-wave approximation (RWA), we obtain the Hamiltonian of the system-bath interaction,

$$H_{SB}^{\text{RWA}}(t) = \sum_{i=1}^{M-1}\sum_{n}(\alpha\sigma_z + \beta I)\otimes(g_{i,n}|i\rangle\langle i+1|a_{i,n}e^{i(\omega_{i,n}-\Delta_0)t} + \text{H.c.}). \tag{45}$$

It is straightforward to obtain the corresponding master equation in the Born-Markov approximation:

$$\frac{d}{dt}\rho = \sum_{i=1}^{M-1}\gamma(\langle n\rangle + 1)\mathcal{L}((\alpha\sigma_z + \beta I)\otimes|i\rangle\langle i+1|)\rho + \sum_{i=1}^{M-1}\gamma\langle n\rangle\mathcal{L}((\alpha\sigma_z + \beta I)\otimes|i+1\rangle\langle i|)\rho, \tag{46}$$

where γ is the coefficient of spontaneous emission and $\langle n\rangle = [\exp(\frac{\hbar\Delta_0}{k_B T}) - 1]^{-1}$ is the number of thermal photons on the frequency Δ_0 of the bath at temperature T. As in the generic case Eq. (21) and in the example Eq. (35), the above master equation preserves the block-diagonal structure of the density matrix. By direct substitution of $\rho_s(t) = \sum_{i=1}^{M}\rho_i(t)\otimes|i\rangle\langle i|$, one obtains the following generalized master equations:

$$\begin{aligned}
\frac{d}{dt}\rho_1(t) &= \gamma(\langle n\rangle + 1)S\rho_2(t)S - \frac{\gamma\langle n\rangle}{2}\{S^2,\rho_1(t)\}_+,\\
\frac{d}{dt}\rho_i(t) &= \gamma(\langle n\rangle + 1)\left(S\rho_{i-1}(t)S - \frac{1}{2}\{S^2,\rho_i(t)\}_+\right)\\
&\quad + \gamma\langle n\rangle\left(S\rho_{i+1}(t)S - \frac{1}{2}\{S^2,\rho_i(t)\}_+\right)\\
&\quad (i = 2,\ldots,M-1),\\
\frac{d}{dt}\rho_M(t) &= \gamma\langle n\rangle S\rho_{M-1}(t)S - \frac{\gamma(\langle n\rangle + 1)}{2}\{S^2,\rho_M(t)\}_+,
\end{aligned} \tag{47}$$

where the operator S is defined as $S = S^\dagger = \alpha\sigma_z + \beta I$. Performing the discretization procedure in Eq. (47), we obtain the following jump operators:

$$\begin{aligned}
B_{i+1}^i &= \sqrt{\gamma(\langle n\rangle + 1)\Delta}S,\\
B_i^{i+1} &= \sqrt{\gamma\langle n\rangle\Delta}S \quad (i = 1,\ldots,M-1),\\
B_j^j &= I - \frac{\gamma(2\langle n\rangle + 1)\Delta}{2}S^2 \quad (j = 2,\ldots,M-1),\\
B_1^1 &= I - \frac{\gamma(\langle n\rangle + 1)\Delta}{2}S^2, \quad B_M^M = I - \frac{\gamma\langle n\rangle\Delta}{2}S^2.
\end{aligned} \tag{48}$$

The interaction formula takes the following form:

$$\begin{aligned}
\rho_1^{[n+1]} &= B_1^1\rho_1^{[n]}B_1^{1\dagger} + B_2^1\rho_2^{[n]}B_2^{1\dagger},\\
\rho_M^{[n+1]} &= B_M^M\rho_M^{[n]}B_M^{M\dagger} + B_{M-1}^M\rho_{M-1}^{[n]}B_{M-1}^{M\dagger},\\
\rho_i^{[n+1]} &= B_i^i\rho_i^{[n]}B_i^{i\dagger} + B_{i-1}^i\rho_{i-1}^{[n]}B_{i-1}^{i\dagger} + B_{i+1}^i\rho_{i+1}^{[n]}B_{i+1}^{i\dagger}\\
&\quad (i = 2,\ldots,M-1).
\end{aligned} \tag{49}$$

Figure 6 shows the dynamics of different observables of the OQW on the line with $M = 101$ nodes and the jump operators given by Eq. (48). The occupation probability of the "walker" $P(i,N) = \text{Tr}[\rho_i^{[N]}]$ after $N_{\text{steps}} = 5000$ steps for different temperatures of the environment is shown in Fig. 6(a). As in the previous example, upon decreasing the temperature of the bath [from Fig. 6(a1) to 6(a3)], the dispersion of the distribution grows. However, in contrast to the previous example, the average speed of the "walker" is independent of the temperature of the bath. In this special example, the jump operators (A, B, and C) are diagonal, which implies that each operator $\rho_i^{[n]}$ ($\rho_{i(k)}^{[n]} = \langle k|\rho_i^{[n]}|k\rangle$) evolves independently from

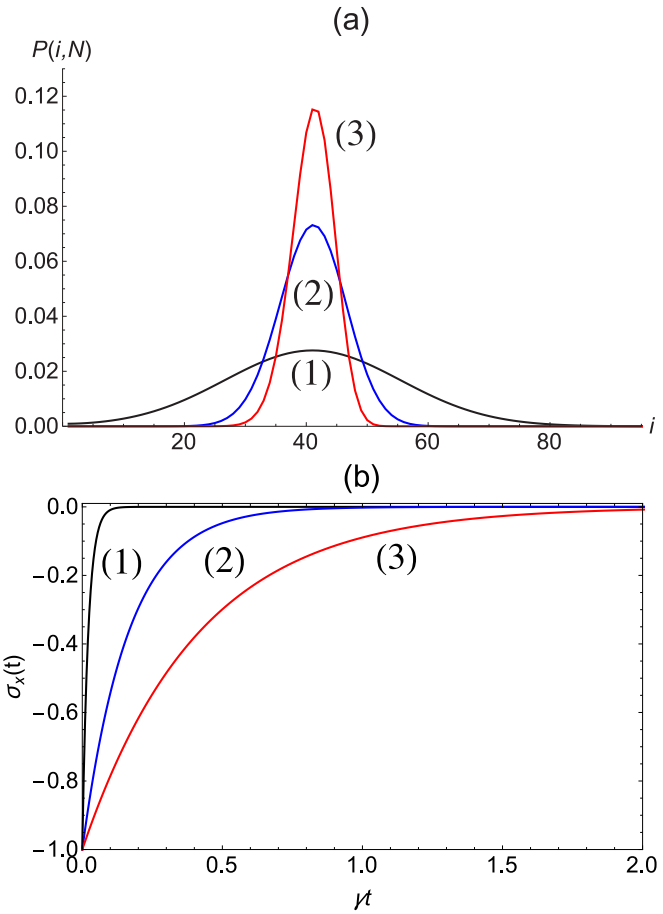

FIG. 6. (Color online) Open quantum walk on a finite chain of nodes. Parts (a) and (b) show the occupation probability of the "walker" $P(i,N) = \mathrm{Tr}[\rho_i^{[N]}]$ after 5000 steps and the dynamics of the total coherence of the "walker" $\sigma_x(t) = \sum_{i=1}^{M} \mathrm{Tr}[\rho_i^{[t]}\sigma_x]$. The initial state of the "walker" is given by $\rho^{[0]} = |-\rangle\langle -| \otimes |51\rangle\langle 51|$, and curves (1)–(3) correspond to the different temperatures of the environment $\langle n\rangle = 10$, 1, and 0.1, respectively; the parameters are $\gamma = 0.1, \lambda = 0.3, \Delta = 0.05, \alpha = 1, \beta = 0$, and $|-\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |0\rangle)$.

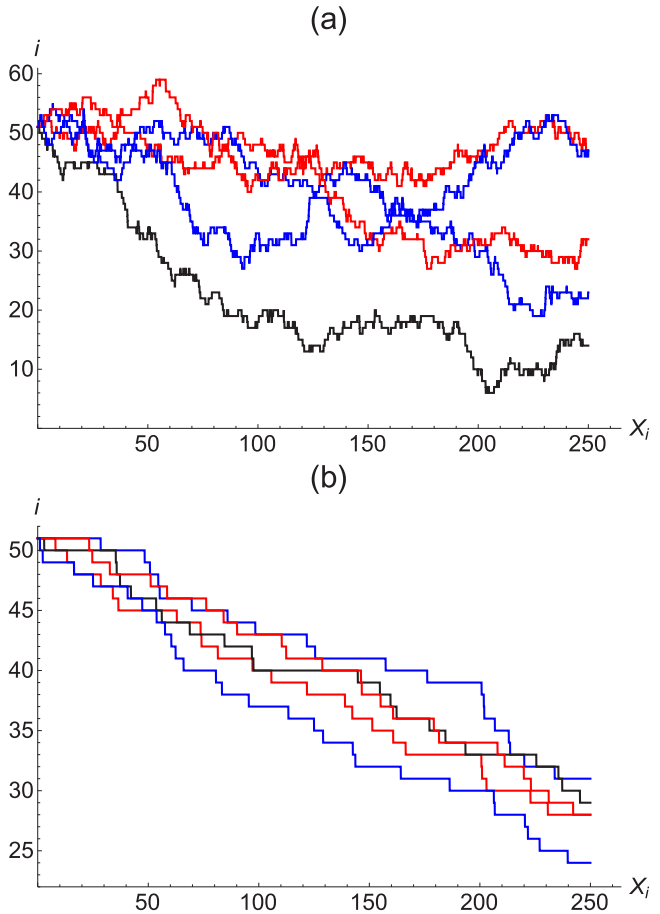

FIG. 7. (Color online) Open quantum walk on a finite chain of nodes. Parts (a) and (b) show examples of quantum trajectories of the "walker" in the diffusive and the ballistic case, respectively. The axis labels i and X_i denote the node of the position of the walk and the number of steps of the OQW. The diffusive behavior of the quantum trajectories of the "walker" shown in (a) corresponds to nonzero temperature of the environment ($\langle n\rangle = 5$), while the ballistic behavior of the quantum trajectories of the "walker" shown in (b) corresponds to an environment at zero temperature ($\langle n\rangle = 0$). The initial state of the "walker" is given by $\rho^{[0]} = |-\rangle\langle -| \otimes |51\rangle\langle 51|$; the parameters are $\gamma = 0.1$, $\lambda = 0.3$, $\Delta = 0.05$, $\alpha = 1$, $\beta = 0$, and $|-\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |0\rangle)$.

other elements of the operator $\rho_i^{[n]}$. The iteration formula for the diagonal elements $\rho_{i(k)}^{[n]}$ reads

$$\rho_{i(k)}^{[n+1]} = [1 - \gamma(2\langle n\rangle + 1)\Delta]\rho_{i(k)}^{[n]} + \gamma(\langle n\rangle + 1)\Delta\rho_{i+1(k)}^{[n]} + \gamma\langle n\rangle\Delta\rho_{i-1(k)}^{[n]}. \quad (50)$$

This means that on average, the "walker" is always moving to the left with drift velocity $\gamma\Delta$ [Fig. 6(a)]. Figure 6(b) shows the dynamics of the total coherence of the "walker" $\sigma_x(t) = \sum_{i=1}^{M} \mathrm{Tr}[\rho_i^{[t]}\sigma_x]$. Due to the pure decoherent interaction with the heat bath, one can see that for all temperatures the coherence is vanishing. As is expected for higher temperatures [Fig. 6(b1)], the coherence vanishes faster than for lower ones [Fig. 6(b3)]. Figure 7 shows samples of the quantum trajectories of the "walker" for nonzero and zero temperature of the environment, respectively. For the zero temperature of the bath, the jump operator B_i^{i+1} vanishes ($B_i^{i+1} \equiv 0$), which implies that the "walker" can stay on the same node or move to the left. The continuous-time limit ($\Delta \to 0$) of the iteration equation (50) is a differential equation for the Poisson process, i.e., $d\rho_{i(k)}/dt = \gamma(\rho_{i+1(k)} - \rho_{i(k)})$. As in the previous example, the temperature of the bath plays the role of a switch between diffusive and ballistic trajectories of the "walker."

V. CONCLUSION

In this paper, we presented the generic case of the microscopic derivation of open quantum walks. We started by identifying the Hamiltonian of the "walker" and the nodes as the system Hamiltonian, the Hamiltonian of the reservoirs, and the Hamiltonian of the system-bath interaction. The Hamiltonian of the system-bath interaction was chosen such that only dissipative interaction drove transitions between the nodes of the OQW. We applied the Born-Markov approximation to obtain the reduced master equation of the density matrix of the system ("walker" and nodes of the walk). The resulting

master equation has the generalized master equation form, and it defined a continuous-time open quantum walk. The generalized master equation conserves the diagonal in position form of the reduced density matrix. The time discretization of the generalized master equation leads to the discrete-time OQW formalism.

The formalism was demonstrated for the examples of the OQW on a circle of nodes and a finite chain of nodes. The presented microscopic derivation allows us to connect the different dynamic behaviors of the OQWs with the thermodynamic parameters of the total system. For both examples, a transition between the diffusive and ballistic quantum trajectories was observed. The temperature of the bath was identified as a switching parameter between these different types of quantum trajectories. As was shown in the example of the OQWs on a circle of nodes, there is a persistent coherence in the OQWs even after the system reaches steady Gaussian distribution.

It was shown that OQWs can efficiently performs dissipative quantum computing [27] and efficiently transport excitations [10]. However, only with the help of a microscopic derivation is it possible to identify the Hamiltonians that are necessary to implement these walks in a realistic physical system. This will be the subject of future research in this field.

ACKNOWLEDGMENTS

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APPENDIX: DERIVATION OF THE COEFFICIENTS V_μ AND V_σ^2

To derive an equation for the coefficient V_μ, one needs to obtain the equation for $\mu(t) = \sum_{i=1}^{N} i\,\mathrm{Tr}[\rho_i(t)]$. The generalized master equation (36) can be rewritten as

$$\begin{aligned}
\dot{Y}_i &= -\frac{\gamma(2\langle n\rangle+1)}{2}Y_i,\\
\dot{X}_i &= 2\lambda Z_i - \frac{\gamma(2\langle n\rangle+1)}{2}X_i,\\
\dot{Z}_i &= -2\lambda X_i - \frac{\gamma}{2}P_i - \frac{\gamma(2\langle n\rangle+1)}{2}Z_i\\
&\quad + \frac{\gamma\langle n\rangle}{2}(P_{i+1}-Z_{i+1}) - \frac{\gamma(\langle n\rangle+1)}{2}(P_{i-1}+Z_{i-1}),\\
\dot{P}_i &= -\frac{\gamma(2\langle n\rangle+1)}{2}P_i - \frac{\gamma}{2}Z_i\\
&\quad + \frac{\gamma(\langle n\rangle+1)}{2}(P_{i-1}+Z_{i-1}) + \frac{\gamma\langle n\rangle}{2}(P_{i+1}-Z_{i+1}),
\end{aligned} \tag{A1}$$

where the index i runs from 1 to M with periodic boundary conditions ($M+1\equiv 1$). The functions $Y_i,\dots,P_i$ are defined as $P_i = \mathrm{Tr}[\rho_i(t)]$ and $A_i = \mathrm{Tr}[\sigma_A\rho_i(t)]$ (σ_A is corresponding Pauli matrix). Using this system of differential equations for $Y_i,\dots,P_i$, one can find a corresponding system of differential equations for the following collective functions: $A_s = \sum_{i=1}^{M} A_i$, $\langle A\rangle = \sum_{i=1}^{M} i\,A_i$, and $\langle\langle A\rangle\rangle = \sum_{i=1}^{M} i^2 A_i$, where $A_i \in (P_i, X_i, Y_i, Z_i)$. By definition, the coefficients V_μ and V_σ^2 are asymptotic linear parts of the functions $\mu(t) = \langle P\rangle$ and $\sigma^2(t) = \langle\langle P\rangle\rangle - \langle P\rangle^2$, respectively.

Using the definition of the collective variable $A_s = \sum_{i=1}^{M} A_i$ and periodic boundary conditions, it is easy to obtain a system of differential equations for P_s, X_s, and Z_s,

$$\begin{aligned}
\frac{d}{dt}P_s &= 0,\\
\frac{d}{dt}\begin{pmatrix}Z_s\\X_s\end{pmatrix} &= G_2\begin{pmatrix}Z_s\\X_s\end{pmatrix} - \begin{pmatrix}\gamma P_s\\0\end{pmatrix},
\end{aligned} \tag{A2}$$

where $G_2 = \begin{pmatrix}-\gamma(2\langle n\rangle+1) & -2\lambda\\ 2\lambda & -\gamma\frac{2\langle n\rangle+1}{2}\end{pmatrix}$. The first equation of this system has a very simple physical meaning, knowing that $P_S = \sum_{i=1}^{M} P_i$, where P_i is the probability to find the walker on the node i, and $\sum_{i=1}^{M} P_i$ is just the trace of the total reduced density matrix of the walker on the ring of nodes. This implies that P_s is the total probability to find the walker on one of the nodes, so $P_s = P_s(0) = 1$. The equation for X_s and Z_s can be integrated as

$$\begin{pmatrix}Z_s\\X_s\end{pmatrix} = e^{tG_2}\begin{pmatrix}Z_s(0)\\X_s(0)\end{pmatrix} - \gamma\int_0^t d\tau\, e^{(t-\tau)G_2}\begin{pmatrix}1\\0\end{pmatrix}. \tag{A3}$$

Now, we can write down the equation for $\langle A\rangle = \sum_{i=1}^{M} i\,A_i$,

$$\begin{aligned}
\frac{d}{dt}\langle P\rangle &= \gamma\frac{2\langle n\rangle+1}{2}Z_s + \frac{\gamma}{2}P_s,\\
\frac{d}{dt}\begin{pmatrix}\langle Z\rangle\\\langle X\rangle\end{pmatrix} &= G_2\begin{pmatrix}\langle Z\rangle\\\langle X\rangle\end{pmatrix}\\
&\quad - \left(\gamma\langle P\rangle + \frac{\gamma}{2}Z_s + \frac{\gamma(2\langle n\rangle+1)}{2}P_s\right)\begin{pmatrix}1\\0\end{pmatrix}.
\end{aligned} \tag{A4}$$

The formal solution for the function $\langle P\rangle$ has the form

$$\langle P\rangle(t) = \langle P\rangle(0) + \frac{\gamma t}{2} + \gamma\frac{2\langle n\rangle+1}{2}\int_0^t d\tau\, Z_s(\tau). \tag{A5}$$

Using the spectral decomposition theorem for the matrix G_2, it is easy to obtain

$$\begin{aligned}
G_2 &= \lambda_+\Pi_+ + \lambda_-\Pi_-,\\
\lambda_\pm &= -\frac{3}{4}\gamma(2\langle n\rangle+1) \pm \frac{\omega}{4},\\
\Pi_\pm &= \pm\frac{2}{\omega}(G_2 - \lambda_\mp 1_2),
\end{aligned} \tag{A6}$$

where $\lambda_\pm$ and $\Pi_\pm$ are eigenvalues and corresponding orthogonal projectors on the eigenspaces of the matrix G_2, 1_2 denotes the 2×2 identity matrix, and the constant ω is given by $\omega = \sqrt{\gamma^2(2\langle n\rangle+1)^2 - 64\lambda^2}$. Using the decomposition of the matrix G_2, the expression for the collective variable $\langle P\rangle$ reads

$$\begin{aligned}
\langle P\rangle(t) &= \langle P\rangle(0) + \frac{\gamma t}{2}\\
&\quad + \gamma\frac{2\langle n\rangle+1}{2}\sum_{k=+,-}\left\{\frac{e^{\lambda_k t}-1}{\lambda_k}(1\quad 0)\Pi_k\begin{pmatrix}Z_s(0)\\X_s(0)\end{pmatrix}\right.\\
&\quad \left. - \frac{\gamma}{\lambda_k^2}(e^{\lambda_k t} - 1 - \lambda_k t)(1\quad 0)\Pi_k\begin{pmatrix}1\\0\end{pmatrix}\right\}.
\end{aligned} \tag{A7}$$

With the help of Eq. (A7), the coefficient V_μ is given by

$$V_\mu = \lim_{t\to\infty}\frac{\langle P\rangle(t)}{t} = \frac{\gamma}{2} + \gamma^2\frac{2\langle n\rangle+1}{2}\sum_{k=+,-}\frac{1}{\lambda_k}(1 \quad 0)\Pi_k\begin{pmatrix}1\\0\end{pmatrix} = \frac{4\gamma\lambda^2}{8\lambda^2+\gamma^2(2\langle n\rangle+1)^2}. \tag{A8}$$

The differential equation for the collective variable $\langle\langle P\rangle\rangle$ has the form

$$\frac{d}{dt}\langle\langle P\rangle\rangle = \gamma\langle P\rangle + \gamma(2\langle n\rangle+1)\langle Z\rangle + \frac{\gamma}{2}Z_s + \frac{\gamma(2\langle n\rangle+1)}{2}. \tag{A9}$$

The solution of the function $\langle Z\rangle$ is obtained from the system (A4) as

$$\begin{pmatrix}\langle Z\rangle\\ \langle X\rangle\end{pmatrix} = e^{tG_2}\begin{pmatrix}\langle Z\rangle(0)\\ \langle X\rangle(0)\end{pmatrix} - \gamma\int_0^t d\tau\left\{\langle P\rangle(\tau) + \frac{1}{2}Z_s(\tau) + \frac{2\langle n\rangle+1}{2}\right\}e^{(t-\tau)G_2}\begin{pmatrix}1\\0\end{pmatrix}. \tag{A10}$$

Using the explicit solutions for the functions $\langle Z\rangle$, $\langle P\rangle$, and Z_s, it is straightforward to obtain the solution for the function $\langle\langle P\rangle\rangle$. The coefficient V_σ^2 can be obtained as

$$V_\sigma^2 = \lim_{t\to\infty}\frac{\langle\langle P\rangle\rangle - \langle P\rangle^2}{t} = \frac{\gamma}{2}(2\langle n\rangle+1) - \frac{3}{2}\frac{\gamma^7(2\langle n\rangle+1)^5}{\Omega^6} + \frac{3\gamma^5(2\langle n\rangle+1)^3}{\Omega^4} - \frac{\gamma^3(2\langle n\rangle+1)(\langle n\rangle^2+\langle n\rangle+1)}{\Omega^2}, \tag{A11}$$

where $\Omega = \sqrt{8\lambda^2+\gamma^2(2\langle n\rangle+1)^2}$.

The expressions (A8) and (A11) conclude the derivation of Eqs. (38) and (39), respectively.

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