Physical realizability of continuous-time quantum stochastic walks

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Quantum walks are a promising methodology that can be used to both understand and implement quantum information processing tasks. The quantum stochastic walk is a recently developed framework that combines the concept of a quantum walk with that of a classical random walk, through open system evolution of a quantum system. Quantum stochastic walks have been shown to have applications in as far reaching fields as artificial intelligence. However, there are significant constraints on the kind of open system evolutions that can be realized in a physical experiment. In this work, we discuss the restrictions on the allowed open system evolution and the physical assumptions underpinning them. We show that general direct implementations would require the complete solution of the underlying unitary dynamics and sophisticated reservoir engineering, thus weakening the benefits of experimental implementation.

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I. INTRODUCTION

With the ever increasing experimental control over single and complex quantum systems [1–4], harvesting the power of quantum physics for new technologies is no longer a far-fetched idea. For a clear example of the quantum world entering day-to-day life, one needs to look no further than quantum cryptography [5]. Quantum walks [6] are one of the most prominent frameworks in which to design and think about quantum algorithms. Both the continuous- [7] and discrete-time [8,9] versions have been shown to provide speedup over classical information processing tasks [10], and are universal for quantum computing [11,12]. Classical (probabilistic) and quantum unitary random walks yield different distributions due to interference effects between different paths the walker can take on the associated graph network. Combining the two, a stochastic, continuous-time quantum walk (QSW) can be defined in an axiomatic manner to include unitary and nonunitary effects, and include both classical and quantum walks as limiting cases [13].

While a general purpose quantum computer is still far over the horizon, intermediary technologies have been emerging with the promise to breach classical limitations. Within these, implementations of quantum neural networks, efficient quantum transport, and boson sampling [14] have appeared as some of the platforms displaying the power of quantum walks. In many cases, such as excitation transfer in photosynthetic complexes, or in neural networks, one of the key questions is the role of coherence in the process efficiency. Therefore, their description in a QSW formalism is natural [15,16]. More recently, exciting intermediary applications of quantum technologies have been proposed in artificial intelligence [17–19], which, at its core, involves an autonomous agent that can learn from environmental input and react to it, changing its behavior as more input is received. One such proposal uses quantum stochastic walks to speed up the learning of the agent [18].

As a standard quantum walk arises from unitary evolution, which is a special case of reversible evolution, the associated graphs are undirected. However, the stochastic processes present in QSWs can give some directionality to the graph network, at the price of introducing decoherence. Directionality, in turn, can enhance transport [20], or speed up memory access in artificial intelligence [18]. In order to preserve quantum speedup, the nature of the decoherence, i.e., its selectivity and rate, needs to be carefully designed.

In this work we investigate the implementation of QSWs with no active control of the environment or ancillary systems. We describe the limitations to physical implementations of such a QSW, and show that only a very restricted set of graphs can be implemented with quantum systems under the canonical nondegenerate weak-coupling assumptions. Our results suggest that a large class of master equations often found in literature cannot be directly engineered in real systems without either active environmental control, or solving the full system dynamics prior to its implementation. To our knowledge, this is the first rigorous demonstration of this claim. It should be noted that continuous-time, unitary quantum walks have recently been implemented in different systems, such as photonics (where efficient quantum circuits were used to implement a class of graphs [21] and determine vertex centrality [22]) and NMR (where time-reversal asymmetry lead to near-perfect transport [23]).

It is important to stress one key difference in our approach. We focus on the implementation of purpose-built quantum stochastic walks. It is well known and accepted that nature provides us with countless processes which can be described by QSWs. Understanding these can aid not only the understanding of nature, such as in transport problems, but also to find protocols to counter the effects of noise in quantum technologies. Our focus is on the opposite direction, i.e., one has the mathematical description of a QSW which performs a given task and wants to design the coherent and incoherent

processes that implement it. That is to say, our results do not affect models of physical processes based on QSWs, but only to algorithm and device designs, such as the implementations mentioned above [15,16,18].

II. PROBLEM DESCRIPTION

The classical random walk is an important and well studied model in statistical physics [24] describing the probabilistic movement of a walker along a graph. System evolution in a classical random walk is described by the transition probabilities from one node of the graph to all other nodes connected to it. In a quantum walk the evolution is instead described by transition probability amplitudes, that is, by unitary evolution of the quantum state describing the walker. Therefore, the main difference between classical and quantum walks is coherence.

The generalization encompassing both concepts is the so-called quantum stochastic walk [13]. Each quantum stochastic walk is defined by its Lindblad master equation, which can be generally written as

$$\dot{\rho} = -i[\hat{H},\rho] + \sum_k \gamma_k \left(\hat{L}_k \rho \hat{L}_k^\dagger - \frac{1}{2}\{\hat{L}_k^\dagger \hat{L}_k, \rho\} \right), \quad (1)$$

where ρ denotes the density operator of the walker, $\hat{L}_k$ are the Lindblad operators and γ_k the associated rates (transition probabilities) responsible for the incoherent part of the time evolution, and $\hat{H}$ is the Hamiltonian describing the coherent part of the time evolution. The structure of the graph is encoded by the associated matrices—nonzero elements of $\hat{H}$ encode coherent edges and those of the Lindblad operators encode incoherent edges. Equation (1) incorporates both the classical random walk and the quantum walk as special cases, and also allows for the study of more general walks that exhibit both coherent quantum and random classical behavior.

The quantum stochastic walk has been used to develop quantum algorithms, such as the machine learning algorithms of Refs. [18,19], and to model transport phenomena in photosynthetic complexes [20] and quantum neural networks [15]. In these, the incoherent evolution conserves the excitation number of the graph, so that evolution remains in the fixed excitation subspace when a given number of walkers is present, and the walkers cannot be lost. If we consider the situation where each node of the graph is represented by a qubit, then the Lindblad operator describing incoherent excitation exchange from node n to node m of the graph is given by $\hat{L}_k = \hat{\sigma}_n^- \hat{\sigma}_m^+$. The full Lindblad equation is therefore given by

$$\dot{\rho} = -i[\hat{H},\rho] + \sum_{nm} \gamma_{nm} \left(\hat{\sigma}_m^+ \hat{\sigma}_n^- \rho \hat{\sigma}_n^+ \hat{\sigma}_m^- - \frac{1}{2}\{\hat{\sigma}_n^+ \hat{\sigma}_m^- \hat{\sigma}_m^+ \hat{\sigma}_n^-, \rho\} \right), \quad (2)$$

and it is the physical implementation of this walk that will be the focus of this work. Note that for a general, potentially directed walk, we must allow $\gamma_{nm} \neq \gamma_{mn}$.

It is important to notice that Eq. (2) and the following analysis apply to walks with any number of walkers, as long as this is a conserved quantity. Let us consider a single-excitation QSW. In this case only N basis states are required to describe a walk on N nodes. Therefore, a quantum computer would require only $\log_2 N$ qubits, and this can in principle be efficiently (in memory) simulated on a classical computer (but not in terms of run time). However, QSWs with more than one excitation have faster scaling (in number of qubits), albeit subexponential, and need not have an efficient classical implementation. Moreover, Eq. (2) is not a specific example of one QSW, but is a generic description, and in general the evolution of any particle number conserving fixed-excitation system can be written in the form of Eq. (2). Therefore, the results presented here apply to a large class of open quantum systems, including most QSW-based algorithms found in the literature. Later in the paper we will also briefly comment on relaxing the assumption of particle number conservation, further broadening the applicability of our results.

While approaches to achieve open-system dynamics exist for few qubits, the physical implementation of the quantum stochastic walk of Eq. (2) is challenging, as incoherent excitation exchange between many nodes is required, while at the same time the excitation must be protected from decaying into the environment. In the following we will show explicitly that the incoherent evolution of Eq. (2) cannot be built without active control of the system and environment, or the solution of the complete unitary dynamics. While it is well known that master equations built from phenomenological models can lead to unphysical results [25,26], our work, on the other hand, focuses on whether a microscopic implementation can be created to mimic the desired dynamics.

It is important to note that in this work we consider the quantum stochastic walk as defined in Ref. [13], and not the open quantum walk of Refs. [27,28], which, despite the similar nomenclature, is an entirely different framework of open system evolution involving both internal and positional degrees of freedom of the walker. The QSW investigated here follows the paradigm of Ref. [7], where the continuous-time evolution takes place exclusively on the position space of the walker, with no internal (coin) space needed.

III. BUILDING A QSW FROM STANDARD DECOHERENCE MODELS

We consider the standard microscopic derivation of a Lindblad form master equation in the weak-coupling limit [29] using the secular approximation. While in principle the Lindblad equation can also be derived in the singular coupling limit [29], this situation only plays a minor role in quantum computing platforms as it requires either strong damping or high bath temperature for the Markov approximation to be valid. Even though in the case of a QSW this would only apply to *some* degrees of freedom, it is more than challenging to engineer a quantum system where some degrees of freedom are coherent and others are strongly damped in a controlled way.

We assume from here on a system with nondegenerate transition frequencies. We begin with a Hamiltonian of the form

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{H}_{SB}, \quad (3)$$

where $\hat{H}_S$ is the self-Hamiltonian of the system, which in our case describes the graph, and $\hat{H}_B$ is the self-Hamiltonian of the environmental bath, possibly consisting of many distinct

baths. The term $\hat{H}_{\rm SB}$ describes the system-bath interaction, and without loss of generality has the form

$$\hat{H}_{\rm SB} = \sum_{k,j} \widetilde{\eta}_k^{(j)} \hat{S}_k^{(j)} \otimes \hat{B}_k, \tag{4}$$

where $\hat{S}_k^{(j)}$ and $\hat{B}_k$ are system and bath operators, respectively, and each bath k can interact with many local nodes j with a coupling strength given by $\widetilde{\eta}_k^{(j)}$. Starting from these, our goal is to obtain a Lindblad master equation of the form of Eq. (2). In the following, Latin letters are used for the system local basis states, $\{|m\rangle\}$, and Greek letters for the system eigenbasis, $\{|\alpha\rangle\}$. In the local basis, the master equation takes the form [30]

$$\frac{d}{dt}\rho_{mn} = -\frac{i}{\hbar}\sum_{m'} H_{s,mm'}\rho_{m'n} + \frac{i}{\hbar}\sum_{n'} \rho_{mn'}H_{s,n'n} + \sum_{m'n'} R_{mn,m'n'}\rho_{m'n'}, \tag{5}$$

where $H_{s,mm'} \equiv \langle m|\hat{H}_s|m'\rangle$ describes coherent dynamics and $R_{mn,m'n'}$ the incoherent transition rates in the local basis.

Within the secular approximation, fast oscillating terms are neglected and the transition rates between diagonal elements, i.e., $R_{mm,nn} \equiv \Gamma_{mn}$, can be written as

$$\Gamma_{mn} = \sum_{\alpha\neq\alpha'} T_{mn;\alpha\alpha'}\Gamma_{\alpha\alpha'} - \sum_{\alpha\beta} \widetilde{T}_{mn;\alpha\beta}\widetilde{\Gamma}_{\alpha\beta}. \tag{6}$$

Here $\Gamma_{\alpha\alpha'}$ represents the transition rate between eigenstates, $\widetilde{\Gamma}_{\alpha\beta}$ their total dephasing rate, and we have defined $\widetilde{T}_{mn;\alpha\beta} \equiv \langle m|\alpha\rangle\langle\beta|m\rangle\langle\alpha|n\rangle\langle n|\beta\rangle$ and $T_{mn;\alpha\alpha'} \equiv |\langle m|\alpha\rangle|^2|\langle\alpha'|n\rangle|^2$. All other contributions are suppressed under the secular approximation, as we have assumed all transition frequencies are nondegenerate. The interested reader is encouraged to see Sec. II G of Ref. [30] for a detailed presentation of the calculations leading to Eq. (6). Let us define

$$\Xi_1 = \sum_{\alpha\neq\alpha'} T_{mn;\alpha\alpha'}\Gamma_{\alpha\alpha'}, \tag{7}$$

$$\Xi_2 = \sum_{\alpha\beta} \widetilde{T}_{mn;\alpha\beta}\widetilde{\Gamma}_{\alpha\beta}, \tag{8}$$

so that $\Gamma_{mn} = \Xi_1 - \Xi_2$.

As discussed before, Eq. (2) does not allow for incoherent annihilation of local excitations and so we require that $\Gamma_{mn} = 0$ whenever $|m\rangle$ and $|n\rangle$ contain a different number of excitations, while allowing other Γ_{mn} to be fashioned in accordance with the desired dynamics. However, as $\Gamma_{\alpha\alpha'}, \widetilde{\Gamma}_{\alpha\beta}, T_{mn;\alpha\alpha'} \geqslant 0$ the first sum in Eq. (6), Ξ_1, will be non-negative. Vanishing transition rates then mean that either both Ξ_1 and Ξ_2 vanish or that $\Xi_1 = \Xi_2$. We will now consider these scenarios.

IV. EIGENSTATE TRANSITION RATES

To determine the conditions required to set $\Gamma_{mn} = 0$ we start by looking at $\Xi_1 = \Xi_2 \neq 0$. Nonzero terms in the sum in Ξ_2 would require the existence of pairs of eigenstates $\{|\alpha\rangle,|\beta\rangle\}$ with nonzero overlap with both $|m\rangle$ and $|n\rangle$; otherwise $\widetilde{T}_{mn;\alpha\beta} = 0$. Thus, avoiding transitions between local states with different excitation numbers, by canceling the two sums of Eq. (6), would demand eigenstates of the system Hamiltonian spanning states with different numbers of walkers. However, as discussed previously, applications of quantum walks usually rely on number-conserving graphs. As such, $\widetilde{T}_{mn;\alpha\beta} = 0$ for all $|m\rangle$ and $|n\rangle$ with a different number of excitations, and $\Xi_2 = 0$. Therefore, Ξ_1 must also vanish so that $\Gamma_{mn} = 0$. We will now examine the requirements to set $\Xi_1 = 0$.

The transition rates between eigenstates are given by [30]

$$\Gamma_{\alpha\alpha'} = \frac{2\pi}{\hbar Z_b}\sum_{\omega\omega'} e^{-E_{\omega'}/(k_BT)}\delta(\epsilon_\alpha - \epsilon_{\alpha'} + E_\omega - E_{\omega'})|V_{\alpha\omega,\alpha'\omega'}|^2, \tag{9}$$

where Z_b is the bath partition function, k_B the Boltzmann constant, and T the bath temperature. Here ϵ_α and $|\alpha\rangle$ [E_ω and $|\phi_B(\omega)\rangle$] are the system (bath) eigenenergies and eigenvectors, and

$$V_{\alpha\omega,\alpha'\omega'} \equiv \langle\alpha,\phi_B(\omega)|\hat{H}_{SB}|\alpha',\phi_B(\omega')\rangle. \tag{10}$$

For the interaction Hamiltonian of Eq. (4) we have

$$V_{\alpha\omega,\alpha'\omega'} = \langle\alpha,\phi_B(\omega)|\sum_{k,j}\widetilde{\eta}_k^{(j)}\hat{S}_k^{(j)}\otimes\hat{B}_k|\alpha',\phi_B(\omega')\rangle = \sum_{k,j}\eta_k^{(j)}\langle\alpha|\hat{S}_k^{(j)}|\alpha'\rangle \equiv \langle\alpha|\overline{V}(\omega,\omega')|\alpha'\rangle, \tag{11}$$

where $\eta_k^{(j)} = \widetilde{\eta}_k^{(j)}\langle\phi_B(\omega)|\hat{B}_k|\phi_B(\omega')\rangle$.

Let us focus on transitions between local basis states $|m\rangle$ and $|n\rangle$ with

$$|m\rangle = \sum_\alpha c_\alpha|\alpha\rangle, \quad |n\rangle = \sum_{\alpha'} c'_{\alpha'}|\alpha'\rangle. \tag{12}$$

As $\Gamma_{\alpha\alpha'}, T_{mn;\alpha\alpha'} \geqslant 0$, Ξ_1 will vanish only if $\Gamma_{\alpha\alpha'} = 0$ for all $\{\alpha,\alpha'\}$ with $c_\alpha, c'_{\alpha'} \neq 0$. From Eq. (9) we see that $\Gamma_{\alpha\alpha'} = 0$ only if $V_{\alpha\omega,\alpha'\omega'}$ vanishes for all bath states for which the Dirac Delta is nonzero. Let us assume that the bath spectrum is dense, as is already implied by the Markov approximation being applicable, such that the energy-conservation condition $\epsilon_\alpha - \epsilon_{\alpha'} + E_\omega - E_{\omega'} = 0$ can always be fulfilled. This means that, to prevent transitions $|m\rangle \leftrightarrow |n\rangle$, we require that for all $\{\alpha,\alpha'\}$ with $c_\alpha, c'_{\alpha'} \neq 0$, the following statements can be inferred from one another

$$\langle\alpha|\overline{V}(\omega,\omega')|\alpha'\rangle = 0 \tag{13}$$

$$\Longrightarrow c_\alpha c'_{\alpha'}\langle\alpha|\overline{V}(\omega,\omega')|\alpha'\rangle = 0 \tag{14}$$

$$\Longrightarrow \sum_{\alpha,\alpha'} c_\alpha c'_{\alpha'}\langle\alpha|\overline{V}(\omega,\omega')|\alpha'\rangle = 0 \tag{15}$$

$$\Longrightarrow \langle m|\overline{V}(\omega,\omega')|n\rangle = 0. \tag{16}$$

Of course, the validity of this last equality does not imply $\Gamma_{\alpha\alpha'} = 0$, but if it does not hold, then $\Gamma_{\alpha\alpha'} \neq 0$ for at least one pair $\{\alpha,\alpha'\}$.

The naturally occurring coupling of qubit nodes to their environments can be described by the usual decoherence maps: qubit decay, dephasing, and depolarization. Below we investigate these maps as a means to fulfill Eqs. (13)–(16).

V. SEMILOCAL DECAY INTO THE RESERVOIR

Let us start with qubit decay into their environments, where $\hat{S}_k^{(j)} = \hat{\sigma}_x^{(j)}$, and work out the above condition, Eq. (16), for $|n\rangle = |1\rangle_n$ (one walker at node n) and $|m\rangle = |0\rangle$ (vacuum state). For this,

$$\langle m|\overline{V}(\omega,\omega')|n\rangle = \sum_{k,j} \eta_k^{(j)} \langle 0|\hat{\sigma}_x^{(j)}|1\rangle_n = \sum_k \eta_k^{(n)} = 0. \quad (17)$$

As all transitions $|1\rangle_n \leftrightarrow |0\rangle$ have to be avoided, this must hold for all n, and so

$$\overline{V}(\omega,\omega') = \sum_{k,j} \eta_k^{(j)} \hat{\sigma}_x^{(j)} = \sum_j \hat{\sigma}_x^{(j)} \sum_k \eta_k^{(j)} = 0. \quad (18)$$

This is an effective system-bath decoupling, as $\langle\alpha|\overline{V}(\omega,\omega')|\alpha'\rangle = 0$, which implies $\Gamma_{\alpha\alpha'} = 0$ for all eigenstates $|\alpha\rangle$, $|\alpha'\rangle$. Therefore, if we require that Ξ_1 vanish for all transitions $|1\rangle_n \leftrightarrow |0\rangle$, it must vanish for all transitions, regardless of the nodes and number of excitations involved.

As Ξ_2 vanishes for excitation conserving QSWs, and as we have just shown, so too must Ξ_1, we argue that local decay cannot be used to generate any relevant dynamics of the form of Eq. (2). We note that it is clear that the calculations shown above can be directly generalized to $\hat{S}_k^{(j)} = \hat{\sigma}_y^{(j)}$.

While transitions from a single-excitation subspace to the vacuum were used to draw the above conclusion, Eq. (18) shows that the entire Hilbert space of the qubits is decoupled from the environment, and not only a specific subspace. Moreover, the calculations can be readily generalized for any pair of local states with different number of walkers. Thus $\hat{S}_k^{(j)} = \hat{\sigma}_x^{(j)}$ and $\hat{S}_k^{(j)} = \hat{\sigma}_y^{(j)}$ cannot be used to generate QSWs of the form of Eq. (2) with any number of walkers.

VI. SEMILOCAL RESERVOIR INDUCED DEPHASING

We now look at qubit dephasing, described by coupling operators $\hat{S}_k^{(j)} = \hat{\sigma}_z^{(j)}$. From the arguments above, we immediately see that this can in principle be used to generate $\Gamma_{\alpha\alpha'} = 0$, as

$$\sum_{k,j} \eta_k^{(j)} \langle m|\hat{\sigma}_z^{(j)}|n\rangle = 0 \quad (19)$$

is trivially fulfilled if $|m\rangle$ and $|n\rangle$ have different local excitation numbers. By the same token, in the one-walker subspace, this is also fulfilled by any two states $|1\rangle_m$ and $|1\rangle_n$, with $m \neq n$, which could suggest another effective system-bath decoupling.

However, this does not imply $\Gamma_{mn} = 0$ for such states. As mentioned before, the validity of Eq. (16) does not imply Eq. (13), and we require that Eq. (13) be valid for the correct set of eigenstates to guarantee that $\Gamma_{mn} = 0$ when we want it to be. If, for example, two eigenstates span both $|1\rangle_m$ and $|1\rangle_n$, then it is possible to have $\Gamma_{mn} \neq 0$, even though Eq. (16) holds.

Setting Γ_{mn} to a given value would thus require one to know all eigenstates with nonzero overlap with states $|m\rangle$ and $|n\rangle$, and engineer a reservoir that fulfills Eq. (6) for the desired Γ_{mn}. We will further discuss the implication of this conclusion below, but for now note that while we used single-excitation states above, the preceding analysis can be straightforwardly generalized to subspaces of any fixed number of excitations.

The next point is to see if we can cancel local pure dephasing, which will unequivocally occur in this setting, while maintaining $\Gamma_{mn} \neq 0$ between fixed excitation states of the nodes. Local pure dephasing is described by the rate

$$\widetilde{\Gamma}_{mn} \equiv R_{mn,mn} = \sum_{\alpha\neq\alpha'} \widetilde{T}_{mn;\alpha\alpha'} \Gamma_{\alpha\alpha'} - \sum_{\alpha\beta} T_{mn;\alpha\beta} \widetilde{\Gamma}_{\alpha\beta}, \quad (20)$$

and we desire that this vanish. As we require that $\Gamma_{mn}\neq 0$, there must be eigenstates for which $\widetilde{T}_{mn;\alpha\alpha'}$, $\Gamma_{\alpha\alpha'}$, $T_{mn;\alpha\beta}$, and $\widetilde{\Gamma}_{\alpha\beta} \neq 0$. Therefore, in general, we need to cancel the two sums in Eq. (20) to obtain $\widetilde{\Gamma}_{mn} = 0$, which requires an environment tailored to the graph. While engineering an environment that is locally compatible with the graph Hamiltonian is in principle doable, adapting the environment to the global eigenstates of the graph is equivalent to first solving the problem the quantum computer is supposed to solve.

The conclusions drawn above show that if the Hamiltonian of the graph preserves excitation number, then local dephasing can be used to obtain $\Gamma_{mn} \neq 0$ only for transitions that conserve excitation number, as desired. However, to do so we must first calculate the eigensystem of H_S, then solve a set of coupled equations that give the appropriate system-bath couplings for the desired incoherent transition rates and zero local pure dephasing. This is effectively reservoir engineering, and can be a considerable undertaking when the graph is of sufficient size. However, it must be noted that as both dephasing and H_S preserve excitation number, only one block of the Hamiltonian must be diagonalized, corresponding to the appropriate number of walkers. This is not true for local decay, which does not conserve excitation number. As discussed earlier, in the single-walker case on an N-dimensional graph, this is equivalent to diagonalizing an N-dimensional effective Hamiltonian, which can be efficiently done on a classical computer, so the main challenge would lie on the experimental implementation of the engineered reservoir.

VII. DEPOLARIZING CHANNEL

A common decoherence model is the depolarizing channel, described by a coupling of the reservoir to all qubit operators, $\hat{\sigma}_x^{(j)}$, $\hat{\sigma}_y^{(j)}$, and $\hat{\sigma}_z^{(j)}$. The calculations above can be easily generalized to show that such coupling to the bath leads to all the restrictions found for both decay and dephasing. As expected, this model cannot lead to the desired master equation.

In both the decay and dephasing cases, it is in principle possible to solve the full set of equations, Eq. (6), and find parameters for which all the unwanted transitions vanish. However, this would involve full diagonalization of both $\hat{H}_S$ and $\hat{H}_B$, and possibly (definitely in the case of local decay) require very intricate bath engineering. In addition, such techniques would intricately link the coherent and incoherent transition rates.

One possibility would be to design reservoirs such that for certain pairs of states, the energy-conservation condition of Eq. (9) cannot be fulfilled, and thus Eq. (16) would not be valid. In doing so, one would cancel unwanted transitions by a carefully designed reservoir spectrum. While such strategies for reservoir engineering can be useful [31–35], for the applications usually envisioned for quantum walks their use would

again rely on the laborious solution of the complete unitary problem.

We note that other types of Lindblad equations can be conceived, where local excitation decay plays an important role, e.g., in an energy transfer process [16]. However, as these models do not usually include incoherent creation of excitations, implementations of such dynamics would be plagued by the same issues discussed here, even at zero temperature, as transitions between system eigenstates that lower the energy of the system are not guaranteed to conserve excitation number in the node basis when the coupling between nodes is strong. More concretely, as a consequence of the secular approximation the rates Γ_{mn} and Γ_{nm} cannot be independently set, so preventing one such transition while allowing the other would pose the same requirements as for Eq. (2). By the same token, the secular approximation prevents the direct implementation of any directed graph.

VIII. DISCUSSION AND CONCLUSIONS

Master equations in Lindblad form describe the most general quantum state evolution that is guaranteed to be completely positive and trace preserving. However, the set of Lindblad operators allowed for a given physical system is limited by the physical interactions naturally occurring. In other words, often the mathematical formulation of a dynamical system cannot be realizable in real world applications. We have studied such limitations for an arbitrary, number-conserving, stochastic master equation, under the usual secular and Markov approximations. We have discussed the problems of creating such an evolution using ubiquitous decoherence models, such as pure dephasing, amplitude damping, and depolarizing channels.

Our results show that microscopic implementation of general open system evolution can only be realized if the full unitary dynamics have been solved and control of the reservoir is available. For interesting cases, actual experimental implementations of quantum stochastic walks are intended to tackle classically hard problems, which makes solving the full unitary dynamics of the system infeasible. Moreover, as all two-body system-bath interactions can be described by the interaction Hamiltonians studied above, carefully designed interactions can only circumvent the restrictions found by properly engineered local reservoir spectra, or for systems for which the secular approximation does not apply. In the latter case, this could be done by suitable use of degenerate transitions; however, engineering these would again require complete knowledge of the unitary dynamics. Our results affect any direct implementation of continuous-time, excitation conserving QSWs. Algorithmic applications of QSWs must either work within the constraints presented here or use indirect implementations of the required dynamics. As investigated in Ref. [36], an alternative approach to circumvent some of these issues could be to simulate the quantum stochastic walk on a quantum computer using an adapted quantum trajectories technique; however, this can only be used for a restricted class of QSWs.

Although the difficulties in implementing stochastic processes and/or reservoir engineering are sometimes recognized, we present here a careful analysis of the underlying reasons for these difficulties. However, we note that our results are only valid within the model described by Eq. (2), and it is not obvious how they would impact ancilla-based implementations of continuous-time QSWs [37] or QSWs with time-dependent, active control [38]. As such, it is likely that in nature there exist many processes accurately described by QSWs, but any direct laboratory implementation will require overcoming the obstacles described here, which can only be practically achieved by violating one of the assumptions in Sec. III (two-body interactions, the Born-Markov approximation, or no ancillary systems).

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