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Quantum stochastic walks: A generalization of classical random walks and quantum walks

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We introduce the quantum stochastic walk (QSW), which determines the evolution of generalized quantum mechanical walk on a graph that obeys a quantum stochastic equation of motion. Using an axiomatic approach, we specify the rules for all possible quantum, classical and quantum-stochastic transitions from a vertex as defined by its connectivity. We show how the family of possible QSWs encompasses both the classical random walk (CRW) and the quantum walk (QW) as special cases, but also includes more general probability distributions. As an example, we study the QSW on a line, the QW to CRW transition and transitions to genearlized QSWs that go beyond the CRW and QW. QSWs provide a new framework to the study of quantum algorithms as well as of quantum walks with environmental effects.

Many classical algorithms, such as most Markov-chain Monte Carlo algorithms, are based on classical random walks (CRW), a probabilistic motion through the vertices of a graph. The quantum walk (QW) model is a unitary analogue of the CRW that is generally used to study and develop quantum algorithms [1, 2, 3]. The quantum mechanical nature of the QW yields different distributions for the position of the walker, as a QW allows for superposition and interference effects [4]. Algorithms based on QWs exhibit an exponential speedup over their classical counterparts have been developed [5, 6, 7]. QWs have inspired the development of an intuitive approach to quantum algorithm design [8], some based on scattering theory [9]. They have recently been shown to be capable of performing universal quantum computation [10].

The transition from the QW into the classical regime has been studied by introducing decoherence to specific models of the discrete-time QW [11, 12, 13, 14]. Decoherence has also been been studied as non-unitary effects on continuous-time QW in the context of quantum transport, such as environmentally-assisted energy transfer in photosynthetic complexes [15, 16, 17, 18, 19] and state transfer in superconducting qubits [20, 21]. For the purposes of experimental implementation, the vertices of the graph in a walk can be implemented using a qubit per vertex (an inefficient or unary mapping) or by employing a quantum state per vertex (the binary or efficient mapping). The choice of mapping impacts the simulation efficiency and their robustness under decoherence [22, 23, 24]. The previous proposed approaches for exploring decoherence in quantum walks have *added* environmental-effects to a QW based on computational or physical models such as pure dephasing [17] but have not considered walks where the environmental effects are constructed axiomatically from the underlying graph.

In this work, we define the quantum stochastic walk (QSW) using a set of axioms that incorporate unitary and non-unitary effects. A CRW is a type of classical stochastic processes. From the point of view of the theory of open quantum systems, the generalization of a classical stochastic process to the quantum regime is known to be a quantum stochastic process [16, 25, 26, 27, 28, 29] which is the most general type of evolution of a density matrix, not simply the Hamiltonian process proposed by the QW approach. The main goal of this paper is to introduce a set of axioms that allow for the construction of a quantum stochastic process constrained by a graph. We call all the walks that follow these axioms QSWs. We will show that the family of QSWs includes both the CRW and the QW as limiting cases. The QSW can yield new distributions that are not found either in the CRW or the QW. The connection between the three types of walks discussed in this manuscript is summarized in Fig. 1. For clarity, we focus on continuous-time walks, but
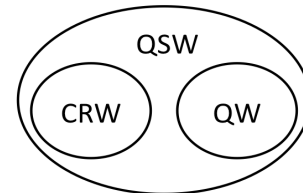
FIG. 1: The quantum stochastic walk (QSW) is a quantum stochastic process defined by a set of axioms that describe the connectivity of an underlying graph. The family of possible QSWs encompasses the classical random walk (CRW) and the quantum walk (QW) as limiting cases. QSWs can be used to generate walks that continuously interpolate between QW and CRW, and therefore can be employed to analyze algorithmic classical-to-quantum transitions. The family of QSWs also describes more general quantum stochastic processes with a behavior that cannot be recovered by the QW and CRW approaches.

also sketch the corresponding procedure for the discrete-time walks. The QSW provides the fundamental tools to study the quantum-to-classical transition of walks, as

well as new methods of control by the application of non-unitary operations on a quantum system.

The CRW describes probabilistic motion over a graph. The dynamics of the probability distribution function is given by the master equation for a classical stochastic process,

$$\frac{d}{dt}p_a = \sum_b M_b^a \, p_b,\tag{1}$$

where the vector element p_b is the probability of being found at the vertex b of the graph. The matrix M is the generator for the evolution; its structure is constrained by axioms derived from the connectivity of the graph. For example, if vertices a and b are connected, $M_b^a = -\gamma$, if they are not, $M_b^a = 0$, and $M_a^a = d_a \gamma$ where d_a is the degree of vertex a.

In analogy to the CRW, the QW [1] has been defined so that the probability vector element p_a is replaced with $\langle a|\psi\rangle$, which evolves according to the Schrödinger equation,

$$\frac{d}{dt}\langle a|\psi\rangle = -i\sum_b \langle a|H|b\rangle\langle b|\psi\rangle,\tag{2}$$

where H is a Hamiltonian to be defined based on axioms coming from the graph. A choice of this definition is $\langle a|H|b\rangle = M_b^a$. This unitary evolution effectively rotates populations into coherences and back [32]. The QW fails to completely capture the stochastic nature of CRW. The random aspect of the QW comes solely from the probabilistic nature of measurements performed on the wavefunction.

Since a classical stochastic process can be generalized to the quantum regime by means of a quantum stochastic process, a CRW should be generalized to a QSW derived from the graph [33]. For the generalization, we identify the probability vector with elements p_a with a density matrix with elements $\rho_{a\alpha}$, and generalize the evolution to a quantum stochastic process, $\frac{d}{dt}\rho = \mathcal{M}[\rho]$, where $\mathcal{M}$ is a superoperator [25, 26, 28]. To make this evolution look similar to Eq. (1), we write the density matrix in terms of its indices, $\rho = \sum_{a,\alpha}\rho_{a\alpha}|a\rangle\langle\alpha|$, and the quantum stochastic master equation becomes,

$$\frac{d}{dt}\rho_{a\alpha} = \sum_{b,\beta}\mathcal{M}_{b\beta}^{a\alpha}\,\rho_{b\beta},\tag{3}$$

with the tensor $\mathcal{M}_{b\beta}^{a\alpha} = \langle a|\,\mathcal{M}\big[\,|b\rangle\langle\beta|\,\big]\,|\alpha\rangle$. This correspondence was pointed out by Mohseni *et al.* in the context of energy transfer [16].

For a quantum stochastic process to be related to a walk, the superoperator $\mathcal{M}$ must reflect the graph. The connectivity of the vertices will impose conditions on the transition rates of $\mathcal{M}$. Since the quantum stochastic process is more general than both the classical stochastic process and the Schrödinger equation, the correspon-

dence of the connectivity of the graph to the rules imposed on $\mathcal{M}$ should include and go beyond the connectivity axioms for each of those. For a vertex m connected to vertices that include vertex n, we define a processes $|m\rangle \leftrightarrows |n\rangle$ which occurs at some rate that can evolve $|m\rangle$ to and from $|n\rangle$. Transition rates for vertices that are not connected are defined to be zero. We employ these connectivity rules as the main principle for defining valid QSWs from a given graph. To further explore the connection from the QSW to the CRW and QW as well as more general behaviors, we discuss the different limiting cases.

For the classical case, the allowed transitions come from incoherent population hopping of the form $|m\rangle\langle m| \leftrightarrows |n\rangle\langle n|$, and, for completeness, $|m\rangle\langle m| \leftrightarrows |m\rangle\langle m|$. These conditions constrain $\mathcal{M}$ to operate only on the diagonal elements of ρ, like Eq. (1). In other words, the QSW transition tensor must have the property $\sum_{\alpha,\beta}\delta_{a\alpha}\mathcal{M}_{b\beta}^{a\alpha}\delta_{b\beta} = M_b^a$.

The QSW should also recover the QW, where evolution among vertices happens through coherences developed by a Hamiltonian. These transitions include terms of the form, $|m\rangle\langle m| \leftrightarrows |m\rangle\langle n|$, that exchange populations to coherences with the connected vertices. For completeness, we also consider transitions of the form $|m\rangle\langle n| \leftrightarrows |m\rangle\langle n|$. If m is also connected to another vertex l, additional transitions can happen. One transition exchanges populations into coherences among the two vertices connected to m, $|m\rangle\langle m| \leftrightarrows |l\rangle\langle n|$; the other exchanges coherences between m and a connected vertex into coherence among two vertices connected to m, $|m\rangle\langle n| \leftrightarrows |l\rangle\langle n|$. These conditions allow for the recovery of Eq. (2). By including the conjugates of these, we have now exhausted all the possibilities of the transitions that can happen following the connectivity of vertex m. These rules can be applied to vertices with any number of connections, and serve as the basis for the correspondence of the graph to the QSW.

To complete the generalization, we need an equation of motion for a quantum stochastic process. We choose the Kossakowski-Lindblad master equation [26, 27, 28], $\frac{d}{dt}\rho = \mathcal{L}[\rho] = \sum_k -i\,[H,\rho] - \frac{1}{2}L_k^\dagger L_k\rho - \frac{1}{2}\rho L_k^\dagger L_k + L_k\rho L_k^\dagger$, which evolves the density matrix as a quantum stochastic process inspired by environmental effects under the Markov approximation. The Hamiltonian term describes the coherent evolution (Schrödinger equation) while the rest describe a stochastic evolution. We now set $\mathcal{M} \to \mathcal{L}$ in Eq. (3), where,

$$\mathcal{L}_{b\beta}^{a\alpha} = \sum_k \delta_{\alpha\beta}\langle a|\left(-iH - \frac{1}{2}L_k^\dagger L_k\right)|b\rangle\tag{4}$$

$$+ \delta_{ab}\langle\beta|\left(iH - \frac{1}{2}L_k^\dagger L_k\right)|\alpha\rangle + \langle a|L_k|b\rangle\langle\beta|L_k^\dagger|\alpha\rangle.$$

The connectivity conditions between a vertex m and some connected vertices n and l and the corresponding

Axiom	Matrix elements' connectivity	Transition rate
1	$|m\rangle\langle m| \leftrightarrows |m\rangle\langle m|$	$\mathcal{L}_{mm}^{mm} = \langle m|L_k|m\rangle\langle m|L_k^\dagger|m\rangle - \langle m|L_k^\dagger L_k|m\rangle$
2	$|m\rangle\langle m| \leftrightarrows |n\rangle\langle n|$	$\mathcal{L}_{mm}^{nn} = \langle n|L_k|m\rangle\langle m|L_k^\dagger|n\rangle$
3	$|m\rangle\langle m| \leftrightarrows |m\rangle\langle n|$	$\mathcal{L}_{mm}^{mn} = \langle m|L_k|m\rangle\langle m|L_k^\dagger|n\rangle + i\langle m|H|n\rangle - \frac{1}{2}\langle m|L_k^\dagger L_k|n\rangle$
4	$|m\rangle\langle n| \leftrightarrows |m\rangle\langle n|$	$\mathcal{L}_{mn}^{mn} = \langle m|L_k|m\rangle\langle n|L_k^\dagger|n\rangle - i\langle m|H|m\rangle + i\langle n|H|n\rangle - \frac{1}{2}\langle m|L_k^\dagger L_k|m\rangle - \frac{1}{2}\langle n|L_k^\dagger L_k|n\rangle$
5	$|m\rangle\langle n| \leftrightarrows |l\rangle\langle n|$	$\mathcal{L}_{mn}^{ln} = \langle l|L_k|m\rangle\langle n|L_k^\dagger|n\rangle - i\langle l|H|m\rangle - \frac{1}{2}\langle l|L_k^\dagger L_k|m\rangle$
6	$|m\rangle\langle m| \leftrightarrows |l\rangle\langle n|$	$\mathcal{L}_{mm}^{ln} = \langle l|L_k|m\rangle\langle m|L_k^\dagger|n\rangle$

TABLE I: Axioms for the quantum stochastic walk for processes that connect vertex $|m\rangle$ to its neighbors. Sum over k, and conjugate elements are implied. Axioms (1) and (2) correspond to the classical random walk. Axioms (3), (4) and (5) contain the quantum walk using H and additional evolution due to $\{L_k\}$ terms. Axiom (6) comes only from the quantum stochastic walk, having no equivalent in the classical random walk or quantum walk.

non-zero transition rates according to Eq. (4) can be summarized in Table I [34].

The Axioms from Table I capture the behavior sketched in Fig. (1). To recover the CRW, it suffices to consider Axioms (1) and (2). These Axioms are a classical subset of the transition rates of the QSW. On the other hand, the QW is obtained by making all the rates of each element of $\{L_k\}$ zero. In this case, only the subset of Axioms (3), (4) and (5) from Table I are relevant, corresponding to the Hamiltonian, and the QW is recovered. If the rates of $\{L_k\}$ are nonzero, these Axioms contain behavior beyond the QW. Finally, Axiom (6) has properties that have no equivalent in either the CRW or the QW; it is a type of transition that appears exclusively in the QSW and leads to different distributions. The choice of H or $\{L_k\}$ is not uniquely determined by the Axioms.

For example, a CRW is equivalent to a QSW with the choice of each element of $\{L_k\}$ to be associated to M in the following manner. First, since connections are defined between two vertices, it is easier to write the index k in terms of two indices $k \equiv (\kappa, \kappa')$. Using this notation, we enforce the graph by choosing $L_{(\kappa,\kappa')} = M_\kappa^{\kappa'}|\kappa\rangle\langle\kappa'|$. The Hamiltonian rates of H are set to zero. This choice ensures all the transition rates to be zero except Axiom (2) from Table I, thereby recovering the CRW. An interpolation between the CRW and the QW conditions can be used to obtain the classical-to-quantum transition of any graph by changing the relative rates of the unitary and non-unitary processes.

Other sets of $\{L_k\}$ can yield behavior different from both the classical and quantum walks. To illustrate the difference between these choices, we study a simple example: the walk on an infinite line, where a vertex j is only connected to its nearest neighbors. The conditions for the dynamics of the walk on the line can be obtained from Table I by making $j = m$, $j - 1 = l$ and $j + 1 = n$. To obtain behavior that is different from both the CRW and the QW, we specify a set $\{L_k\}$ with only one member that is $L = \sum_{\kappa,\kappa'} M_\kappa^{\kappa'}|\kappa\rangle\langle\kappa'|$. This choice makes Axiom (6) nonzero, a type of transition that cannot be inter-

preted either as the CRW or the QW. We illustrate the resulting distribution, and compare it to CRW and the QW, in Fig. 2.

The QSW provides a general framework to study the transition between the CRW and the QW. In Fig. 2a, we use the parameter $\omega = [0, 1]$ to interpolate between the QW and the CRW: $\mathcal{L}_\omega[\rho] = -(1 - \omega)i[H, \rho] + \omega \sum_k \left(-\frac{1}{2}L_k^\dagger L_k\rho - \frac{1}{2}\rho L_k^\dagger L_k + L_k\rho L_k^\dagger\right)$. By combining the unitary evolution and the evolution due to the $\{L_{(\kappa,\kappa')}\}$ terms, the transition from the QW to the CRW can be studied as one quantum stochastic walk. This procedure can be done in general to study the transition from any QW to a CRW for any graph [35]. To highlight the difference between the QSW and the QW, we show the transition between them with $L = \sum_{\kappa,\kappa'} M_\kappa^{\kappa'}|\kappa\rangle\langle\kappa'|$ on Fig. 2b.

Although in this paper we focused on continuous-time walks, a parallel argument holds for discrete-time walks. A discrete-time CRW evolves each time step by a Markov chain with a stochastic matrix $\mathcal{S}$ following $p_a = \sum_b \mathcal{S}_b^a\, p_b$. The quantum analogue is to use a quantum stochastic map $\mathcal{B}$ [25] by means of $\rho'_{a\alpha} = \sum_{b\beta} \mathcal{B}_{b\beta}^{a\alpha}\, \rho_{b\beta}$, or equivalently as a superoperator, $\rho' = \mathcal{B}[\rho] \equiv \sum_k \mathcal{C}_k\rho\mathcal{C}_k^\dagger$. A similar set of Axioms to Table I can be computed by using $\mathcal{B}_{b\beta}^{a\alpha} = \sum_k \langle a|\mathcal{C}_k|b\rangle\langle\beta|\mathcal{C}_k^\dagger|\alpha\rangle$ [36]. The connection between the discrete-time QW and the continuous-time QW has been studied by Strauch [30].

In conclusion, we introduced an axiomatic approach to define the quantum stochastic walk, which behaves according to a quantum stochastic process as constrained by a particular graph. This walk recovers the classical random walk and the quantum walk as special cases, as well as the transition between them. The quantum stochastic walk allows for the construction of new types of walks that result in different probability distributions. As an example, we studied the walk on a line. The quantum stochastic walk provides a framework to study quantum walks under decoherence. Reexamination of previous work that considered environmental effects from physical motivations might suggest that, if interpreted
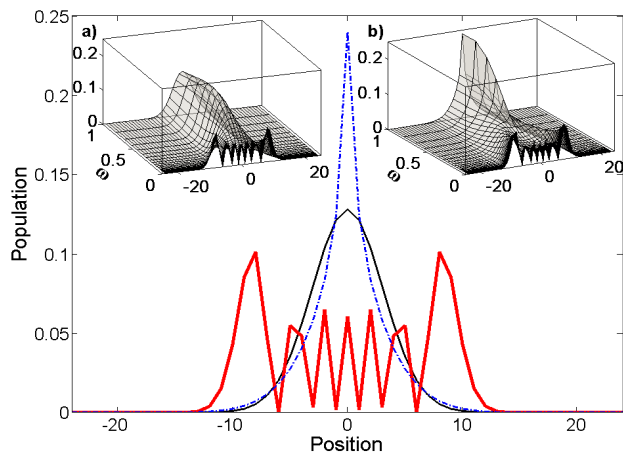
FIG. 2: Probability distributions of a walker starting at position 0 of an infinite line defined by M are shown at time $t = 5$. The heavy line represents the quantum walk, the thin line represents the classical random walk and the dotted line represents a choice of a quantum stochastic walk due to a single operator $L = \sum_{\kappa,\kappa'} M_\kappa^{\kappa'} |\kappa\rangle\langle\kappa'|$ whose distribution cannot be obtained from the classical or quantum walks. **a)** The transition of the quantum walk to the classical random walk is shown. The diagonal elements of the density matrix (Population) are plotted as a function of the vertex of the walker (Position) and a coupling parameter ω. When $\omega = 0$ the evolution is due only to the Hamiltonian, and when $\omega = 1$ the Hamiltonian dynamics are not present with the environmental dynamics taking over. **b)** The transition of the quantum walk to the quantum stochastic walk is shown.

as a quantum stochastic walk, the environment is changing the effective graph. Since the quantum stochastic walk is more general than the quantum walk, it is therefore universal for quantum computation. Its quantum to classical transiton can also be used to examine decoherence phenomena in quantum computation and classical-to-quantum phase transitions. New quantum stochastic distributions might suggest new kinds of quantum algorithms or even new classes of quantum algorithms based on this model.

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[32] The Hermitian form of the Hamiltonian eliminates directed graphs from consideration, motivating work on pseudo-Hermitian Hamiltonians [31].
[33] Just like a classical stochastic process includes, but is not limited, to bistochastic processes, a quantum stochastic processes includes but is not limited to unitary processes [25].
[34] For compactness, we assume that all connections are equally weighted; the general case can be obtained by having coefficients that depend on the vertices.
[35] Our decoherence model comes from the graph, while the

ones discussed in Ref. [11] were inspired by a physical model that localizes the position and thus give different distributions. We propose studies like Ref. [11] could be reinterpreted as a QSW, where the environmental part, as interpreted from Table I, affects the connectivity of the graph and thus generates different distributions.

[36] There is no need for an explicit coin, as the stochastic map is the most general evolution of a density matrix, including random processes. However, if desired, a coin could be implemented as an environment from the open quantum system interpretation of the map.