Generalized quantum-classical correspondence for random walks on graphs

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We introduce a minimal set of physically motivated postulates that the Hamiltonian H of a continuous-time quantum walk should satisfy in order to properly represent the quantum counterpart of the classical random walk on a given graph. We found that these conditions are satisfied by infinitely many quantum Hamiltonians, which provide novel degrees of freedom for quantum enhanced protocols. In particular, the on-site energies, i.e., the diagonal elements of H, and the phases of the off-diagonal elements are unconstrained on the quantum side. The diagonal elements represent a potential-energy landscape for the quantum walk and may be controlled by the interaction with a classical scalar field, whereas, for regular lattices in generic dimension, the off-diagonal phases of H may be tuned by the interaction with a classical gauge field residing on the edges, e.g., the electromagnetic vector potential for a charged walker.

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Continuous-time quantum walks (CTQWs) on graphs are traditionally defined as the quantum analog of classical random walks (RWs) by promoting the classical transfer matrix, i.e., the RW graph Laplacian, to a Hamiltonian [1-3]. However, this association does not encompass all the possible quantum evolutions of a walker on a graph, thus strongly limiting the set of exploitable quantum Hamiltonians, with possible negative implications for the estimation of a quantum advantage of CTQWs vs RWs in specific tasks [4-14]. A question thus arises on whether it is possible to define more general quantum walks on a graph by considering all Hermitian Hamiltonians compatible with a given graph topology and how these generalized QWs compare with their classical analogs. Recently, a chiral quantum walk was introduced [15–18], showing that complex phases in the Hamiltonian generator of a CTQW may be exploited to introduce a directional bias in the dynamics. However, without further justification, the introduction of chiral CTQWs seems to be a departure from the original spirit of quantum walks. In particular, no clear and general connection with the classical RW has emerged for chiral CTQWs so far, and no interpretation of the new degrees of freedom entailed by Hermitian Hamiltonians for chiral CTQWs has been discussed, although partial common ground has been found through the definition of quantum stochastic walks [19] and a connection between classical and quantum random walks was found for the discrete-time case [20]. Nonetheless, such correspondence is a key requisite to compare the performance of chiral

quantum walks to classical ones and to establish when they do provide a speedup for given tasks.

In this work, we shall first put in a rigorous framework the concept of a continuous-time classical random walk on undirected simple graphs and show that the associated classical probabilities cannot arise from a unitary quantum evolution via the Born rule. Having excluded this simplest equivalence, we proceed by listing a number of reasonable minimal requests (of topological, algebraic, and probabilistic nature) for correspondence between a RW and a CTQW on the same graph. We show that these assumptions lead to a single equation that relates the classical generator L of bistochastic transformations (the graph Laplacian) to the Hermitian quantum generator H. As a special case, we recover the standard association H = L. However, such an equation admits infinitely many quantum Hamiltonians as solutions for a given legit classical generator L, consistent with the common intuition that any map from classical to quantum evolutions should be one to many. In particular, the on-site average energies and the complex phases of the off-diagonal elements are unconstrained on the quantum side. Therefore, any classical RW on a graph corresponds to infinitely many chiral CTQWs whose on-site energies are also arbitrary (an aspect that has been overlooked so far). It is important to stress that our correspondence is not meant to represent some form of classical limit for a quantum process (such as a CTQW), but rather we aim at identifying, given a chiral CTQW, which is the most natural classical RW to use as a classical benchmark when comparing the two evolutions to spot eventual quantum advantages.

We also provide a physical motivation for these additional degrees of freedom to appear: the diagonal elements can always be interpreted as a potential-energy landscape for the CTQW, in other words, as the interaction with a classical scalar field, whereas the off-diagonal phases of H arise from

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an interaction of the CTQW with a classical *gauge* field residing on the edges (for regular lattices in generic dimension). We are thus able to reinterpret chiral CTQW on lattices as the Schrödinger equation of the spatially discretized version for a nonrelativistic particle with minimal coupling to a vector gauge field.

Let us start by defining the most general continuous-time quantum walk on a finite graph. We consider a finite-dimensional Hilbert space $\mathcal{H} \simeq \mathbb{C}^n$ with a preferred basis $\{|j\rangle\}_{j=1,\dots,n}$ formed by the localized states on the n distinct vertices of an *undirected*, *connected simple graph*. A Hermitian operator \hat{H} acting on \mathcal{H} is the Hamiltonian of a CTQW if and only if it respects the topology of the graph, that is to say, if for $j \neq k$ we have $[H]_{kj} = \langle k|\hat{H}|j\rangle \neq 0$ if and only if the vertices j and k are connected by an edge, where we introduced the matrix H that describes \hat{H} on the localized basis. Clearly, very little about the structure of \hat{H} is actually specified by the graph itself. If the starting state is a pure, localized state $\hat{\rho}_0 = |j\rangle\langle j|$, it will stay pure under the unitary evolution induced by \hat{H} :

$$\hat{\boldsymbol{\rho}}(t) = e^{-i\hat{H}t} |j\rangle\langle j|e^{i\hat{H}t} = |\psi_j(t)\rangle\langle\psi_j(t)|, \qquad (1)$$

where $|\psi_j(t)\rangle = \sum_{k=1}^n \alpha_{kj}(t)|k\rangle$ and

$$\alpha_{ki}(t) = \langle k|e^{-i\hat{H}t}|j\rangle = [e^{-iHt}]_{ki}. \tag{2}$$

We would like to find a classical counterpart to the dynamics described above. In particular, we are looking for a *classical* RW on the same graph. This is described by a continuous-time Markov chain, whose evolution satisfies a semigroup structure. In formulas, we seek a continuous family of stochastic $n \times n$ matrices P(t) with $t \ge 0$ acting on the vector $\underline{p} \in \mathbb{R}^n$ of probabilities associated with the sites of the graph, such that

$$P(t_2)P(t_1) = P(t_1 + t_2) \quad \forall t_1, t_2 \geqslant 0.$$
 (3)

Then there exists an $n \times n$ real matrix L that generates this evolution through

$$P(t) = e^{-tL} \quad \forall t \geqslant 0. \tag{4}$$

Again the graph topology will be imposed by the nonzero offdiagonal elements of the generator L. In Eq. (4), the request that P(t) is left stochastic $\forall t \ge 0$, which is necessary for a valid evolution of probabilities, implies that the sum of the entries in each column of L is zero. Moreover, it is natural to pick a symmetric L (thus P is bistochastic) to maintain a clear relation with the undirected, simple graph. Finally, one can check that positivity of P is satisfied $\forall t \ge 0$ if we impose that all the off-diagonal elements of L are negative, while the diagonal elements have to be positive to compensate for the vanishing sum of the columns (or rows). This entire construction will be assumed as the definition of a classical RW. In the special instance of unweighted graphs, L is uniquely specified by the topology, and it is the Laplacian matrix of the graph, i.e., L = D - A, where A is the adjancency matrix and D is the diagonal matrix encoding the connectivities of each vertex. Going back to quantum, the unitary evolution of the CTQW induces an evolution of the probabilities at each vertex of the graph according to Born's rule: $\pi_{kj}(t) = |\alpha_{kj}(t)|^2$, where $\pi_{kj}(t)$ stands for the probability of finding the particle on site k at time t if it is localized at site j at time zero, and it should *not* be interpreted, a priori, as a standard transition matrix in the sense of Eq. (3). Indeed, while it is true that if the initial state $\hat{\rho}_0$ is diagonal, $\hat{\rho}_0 = \sum_j \rho_j^0 |j\rangle\langle j|$, then \underline{p} evolves according to $p_k(t) = \sum_j \pi_{kj}(t)\rho_j^0$, this is no longer true at intermediate times or if the initial state is coherent in the localized basis. In fact, we shall now show that the semigroup structure of Eq. (3) can never be fulfilled by the quantum probabilities computed according to the Born rule. Indeed, we are looking for a real $n \times n$ matrix L fulfilling the equality

$$[e^{-tL}]_{kj} = |[e^{-iHt}]_{kj}|^2 \quad \forall t \geqslant 0.$$
 (5)

Expanding both sides to first order in t, we deduce

$$-tL_{kj} = -it(H_{jj} - H_{ij}^*)\delta_{jk}.$$

Since H is Hermitian, $H_{jj} - H_{jj}^* = 0$, and the equation above can be satisfied if and only if L = 0 as a matrix.

On the other hand, we do know a way to associate a RW to a CTQW: just take L = H and forget about the Born rule. Classical probabilities will evolve according to Eqs. (3) and (4), while the quantum dynamics is independently specified by Eqs. (1) and (2).

However, there are a few objections to this simpler approach. First, imposing L = H forces H to be real, not a natural request for a Hamiltonian: this points to the fact that a classical-to-quantum correspondence should be one to many; therefore, some further structure is required to specify *all* the *Hermitian* Hamiltonians associated with the given classical generator L. Second, it is a rather arbitrary and artificial way to define the quantum-classical correspondence, with no physical motivation, and many other correspondences could exist (although we have just excluded that based on the Born rule).

We shall address these issues and find a generalized quantum-classical correspondence for continuous-time random walks. We start by stating reasonable requests to be fulfilled by any equation linking a Laplacian matrix $L \in \operatorname{Mat}(n, \mathbb{R})$ and a generic Hermitian Hamiltonian $H \in \operatorname{Mat}(n, \mathbb{C})$ that describe a RW and a CTQW, respectively, on the same undirected, simple graph with n vertices (T denotes topological requests, A is for algebraic, and P is for probabilistic):

Condition T0. By definition of continuous-time quantum and classical random walks, both H and L should preserve the topology of the underlying physical system; therefore the equation must enforce that $L_{ik} \neq 0$ iff $H_{ik} \neq 0$ ($j \neq k$).

Condition A1. Given H, the equation must admit a unique solution for L with $\sum_{j} L_{kj} = 0 \ \forall k$, so that it is a valid Laplacian matrix of a (possibly weighted) graph.

Condition A2. The correspondence should reproduce the simple association L = H whenever H is already a Laplacian matrix of an unweighted graph. This is necessary to be consistent with the existing literature on nonchiral CTQWs, and it is also a consequence of T0.

Condition P3. In compliance with the probabilistic interpretations of quantum mechanics and classical stochastic processes, respectively, the off-diagonal terms of H should be interpreted as transition amplitude rates, while (the negative

of) those of L should be the corresponding transition probability rates.

Condition P4. Given H, the diagonal term of the solution L of the equation should maintain the meaning of total probabilities of leaving the corresponding sites.

In general, for $j \neq k$, $H_{jk} \in \mathbb{C}$, and $L_{jk} \in \mathbb{R}$. Then Condition T0 suggests

$$L_{ik} = -|H_{ik}|^2, (6)$$

which also satisfies P3 for the off-diagonal terms. Conditions P4 and A1 for the diagonal terms may be jointly enforced by

$$L_{jj} = \sum_{s \neq j}^{n} |H_{js}|^2 = \langle j|\hat{H}^2|j\rangle - \langle j|\hat{H}|j\rangle^2. \tag{7}$$

Condition A2 is also satisfied since one can immediately check that $[L^2]_{jj}\delta_{jk}-(L_{kj})^2=L_{kj}$ (to be read as a self-consistency equation for the matrix elements of L) whenever H is a Laplacian and the simple identification L=H is recovered. Alternative definitions, e.g., $L_{kj}=-|H_{jk}|^n$ with $n\neq 2$, would satisfy T0 and A2 and possibly A1, but they would unavoidably violate P3 and P4. Indeed, the choice n=2 is naturally suggested by the Born rule at the level of transition rates: the classical rate of transition should be the square modulus of the corresponding transition amplitude. In compact form the sought equation is

$$[L]_{kj} = [H^2]_{ij}\delta_{jk} - H_{jk}H_{kj}. \tag{8}$$

As stated by this expression, there are many CTQWs corresponding to the same RW: the moduli of the off-diagonal entries of H are fixed to the square root of the moduli of the corresponding off-diagonal elements of L, whereas the phases are completely free. The diagonal elements of H, i.e., the on-site energies of the vertices, are also unconstrained: from a physical point of view, they do not possess a classical analog because the corresponding classical system is open and energy is not conserved. Conversely, by Eq. (8) the diagonal elements of L are fixed to be the quantum fluctuations of the energy of each site, which are also equal to the total probability of escaping each site, analogous to the connectivity for a Laplacian. We have thus found all possible quantum walks associated with an arbitrary classical random walk on a given graph, assuming the minimal and reasonable requests detailed above. As shown in the Supplemental Material [21], Eq. (8) may be also derived by adding a decoherence term with respect to the energy eigenbasis to the von Neumann evolution equation of a chiral CTQW on a graph, thus adding physical intuition to the formal consistency implied by Conditions T0–P4.

The possibility of choosing *complex* off-diagonal entries in the Hamiltonian H accounts for chirality [15,18], i.e., asymmetry under the time-reversal transformation $t \to -t$. We shall then keep calling *chiral quantum walks* all the generalized CTQWs compatible with a given L through Eq. (8), even if they are more general than the original definition, since the diagonal terms are also unconstrained. Concerning classical RWs, instead, time reversal is not meaningful because e^{-tL} is guaranteed to be a stochastic matrix only if $t \ge 0$, and this is directly related to the irreversible dynamics of classical RWs. We deduce that, whenever H is real, the quantum-classical comparison is unambiguous under time reversal: there is just

one possible choice of time direction for the classical walk, and both choices for the quantum walk are equivalent. In contrast, when H is complex the quantities $|\langle k|e^{-iHt}|j\rangle|^2$ are not, in general, symmetric under $t \to -t$, and a possible ambiguity in the quantum-classical comparison arises. This is resolved when considering all possible Hamiltonians H that are compatible with a given L according to our rule, Eq. (8). Indeed, if we choose freely the phases of the off-diagonal entries of H, we can accommodate both time directions, while the diagonal entries can always be taken to be positive by shifting H by a multiple of the identity.

Overall, given an undirected unweighted simple graph with N vertices and E edges, L is completely fixed by the topology, and the number of free real parameters of Hamiltonians H compatible with L is N+E-1, of which N-1 are positive but unbounded real numbers d_j for $j=1,\ldots,N-1$ and E are phases $e^{i\phi_k}$ with $\phi_k \in [0,2\pi)$ and $k=1,\ldots,E$. Despite the fact that all these parameters will contribute nontrivially to the unitary quantum evolution operator $e^{-i\hat{H}t}$, not all of them affect the evolution of transition probabilities between sites. This is best understood by considering a change in basis that sends localized states to localized states, without changing their labels:

$$|j\rangle \mapsto |\tilde{j}\rangle := e^{i\alpha_j}|j\rangle$$
 (9)

$$\langle j|\hat{H}|k\rangle = [H]_{jk} \mapsto [\tilde{H}]_{\tilde{i}\tilde{k}} = e^{i(\alpha_k - \alpha_j)}[H]_{jk}, \quad (10)$$

where \tilde{H} is the Hamiltonian matrix in the transformed basis. Physical quantities will not be affected: we can profit from this change in basis to cancel some of the phases in H at the cost of changing relative phases in superposition states to keep all basis-independent quantities unaltered. However, if we restrict ourselves to transition probabilities between sites such as $\pi_{kj}(t) = |\langle k|e^{-i\hat{H}t}|j\rangle|^2$ and functions thereof, we can neglect the overall phases of the transformed initial and final states. This means that, as far as $\pi_{kj}(t)$ are concerned, N-1 phases of H will be redundant. Indeed, consider the unitary transformation $U_{\varrho}(\alpha) = \operatorname{diag}(e^{i\alpha_1}, \dots, e^{i\alpha_N})$, where α is an N-dimensional real vector that encodes the phases which describe the transformation. The Hamiltonian will change according to $\tilde{H} = U_g^{\dagger}(\underline{\alpha}) \cdot H \cdot U_g(\underline{\alpha})$; therefore, only N-1 of the components of $\underline{\alpha}$ actually change H, while an overall phase can always be factored out. Consequently, the number of free parameters in H that actually affect the evolution of on-site probabilities is N + (E - N + 1) - 1 = E, which is just the number of edges. A fuller description of gauge degrees of freedom for chiral CTQW can be found in [22].

To provide physical intuition for the phase degrees of freedom, we remark that the idea of compensating for a local change in phase in the wave function by changing some parameters in the Hamiltonian reminds us of local gauge invariance with gauge group U(1), i.e., of a coupling between a charged particle described by the wave function and a classical Abelian gauge field. Indeed, we will now argue that the most general unweighted chiral CTQW on a regular lattice and in any dimension may be interpreted as the discretization of the nonrelativistic Schrödinger equation for a scalar charged particle coupled to a classical electromagnetic field. Let us consider a *lattice*, i.e., an infinite graph which

tiles periodically a *d*-dimensional Euclidean space. If the graph is regular (each vertex has the same connectivity), then the lattice is called regular too. Since we are interested in linking quantum walks on lattices to discretized Schrödinger equations in a *d*-dimensional space, we require that all the edges have the same weight, reflecting the idea that, apart for the effect of potentials, the transition amplitudes between nearby points in an empty Euclidean space should just depend upon the absolute distance between them. We will refer to a chiral, unweighted QW on a regular lattice as a *homogeneous* (continuous-time) *quantum walk*, and they are our natural candidates to interpret as spatial discretizations of quantum theories in Euclidean spaces.

Let us start by considering the simple scenario of an infinite two-dimensional (2D) square lattice. Referring to some arbitrary vertex, we can label each point with a pair of integers $(n, m) \in \mathbb{Z}^2$, and the corresponding localized state will be $|n, m\rangle$. We will denote by $\Psi_{n,m}(t) = \langle n, m | \Psi(t) \rangle$ the amplitude of the walker at time t to be found at site (n, m) and by $\Psi(t)$ the vector of the amplitudes over all the sites of the lattice. It is also convenient to explicitly write the rate γ that governs the time evolution, so that the Schrödinger equation is symbolically written as $(\hbar = 1)$ $i\partial_t \Psi = \gamma H \cdot \Psi$. The most general Hamiltonian matrix H for a CTQW on this lattice will be an infinite, sparse matrix specified by the following entries [23]: $\frac{1}{\nu}\langle p, q|H|n, m\rangle = [4 + d(n, m)]\delta_{p,n}\delta_{q,m} - \exp[if_x(p-1, q)]$ $\delta_{p,n+1}\delta_{q,m} - \exp[-if_x(p,q)]\delta_{p,n-1}\delta_{q,m} - \exp[if_y(p,q-1)]$ $\delta_{p,n}\delta_{q,m+1} - \exp[-if_y(p,q)]\delta_{p,n}\delta_{q,m-1}$, where $\delta_{p,n}$ is the Kronecker delta and $f_x(n, m)$, $f_y(n, m)$, and d(n, m) are real-valued functions of the site positions. Now let a be the lattice spacing, which can be assumed to be the same in all directions without loss of generality. By exploring all possible scaling laws of the functions f_x , f_y , and d with a, a slight variation of an argument by Feynman [24] shows that the only nontrivial continuous limit $(a \rightarrow 0)$ of this model leads to a Hamiltonian operator $\hat{H}_c(x)$ of the following form (see the Supplemental Material):

$$\hat{H}_c(\underline{x})\Psi(\underline{x}) = -K[\nabla - i\underline{F}(\underline{x})]^2\Psi(\underline{x}) + U(\underline{x})\Psi(\underline{x}), \quad (11)$$

where now $\underline{x} \in \mathbb{R}^2$, $U(\underline{x}) = \gamma d(\underline{x})$, $K = \lim_{a \to 0} a^2 \gamma$, $\underline{F}(\underline{x}) = \lim_{a \to 0} \frac{1}{a} (f_x(\underline{x}), f_y(\underline{x}))$, and $d(\underline{x})$, $f_x(\underline{x})$, $f_y(\underline{x})$ are the continuum generalizations of d(n, m), $f_x(n, m)$, and $f_y(n, m)$, respectively. The existence of all these limits is a prerequisite to find a nontrivial theory as $a \to 0$. We can now restore \hbar and write U(x) = qV(x), F(x) = qA(x), and $K = \frac{\hbar^2}{2m}$ in order to arrive at the standard nonrelativistic Schrödinger equation for a scalar particle with mass m and charge q in the presence of an electromagnetic field:

$$i\hbar \frac{\partial}{\partial t} \Psi(\underline{x}) = -\frac{\hbar^2}{2m} [\nabla - iq\underline{A}(\underline{x})]^2 \Psi(\underline{x}) + qV(\underline{x})\Psi(\underline{x}), \quad (12)$$

where $\underline{A}(\underline{x})$ is the vector potential and $V(\underline{x})$ is the scalar potential. The derivation can be readily generalized to cubic lattices by introducing the appropriate vector potential $\underline{A}(x)$ with suitable discretizations of the Laplacian [25], and it shows that chiral CTQWs on regular lattices, despite being the most general of their kind, are, in fact, always equivalent to discretizations of the Schrödinger equation for a scalar parti-

cle in the presence of an electromagnetic field, also suggesting a practical implementation for chiral QWs. The reasoning can also be inverted to deduce the form of the phases f(n,m) from a given vector potential. The result is known as Peierls substitution [26–30], and in our case for a d-dimensional cubic lattice it reduces to $f_j(\underline{x}) = q \int_{\gamma} \underline{A}(\mathbf{r}(t)) dt$, where γ : $t \in [0,1] \to \mathbb{R}^d$ is a path from $\underline{x} \in \mathbb{Z}^d$ to $\underline{x} + a\underline{e}_j$ and \underline{e}_j is the versor in the jth direction. Note that this is consistent with $F(\underline{x}) = qA(\underline{x}) = \lim_{a \to 0} \frac{1}{a} f(\underline{x})$ via the integral mean value theorem.

Finally, let us return to gauge invariance. For the 2D square lattice, for each vertex we can cancel the phase of one link attached to it by a phase rotation of the corresponding localized state; therefore, we can always set $f_x(n, m) = 0 \ \forall n, m \in \mathbb{Z}^2$, for example. The discretized magnetic field is then given by $B(n,m) = [f_v(n+1,m) - f_v(n-1,m)]/2a$ [31], assuming a symmetric discrete derivative. B(n, m) should be understood as the component of the magnetic field at position (n, m) in the orthogonal direction to the plane. As an example, assuming a constant B such that $f_v(n, m) = nB$, the spectrum of the corresponding H as a function of the parameter B is the Hofstadter butterfly [30]. However, our result is much more general since it can be stated in any dimension and for any choice of the gauge field and, correspondingly, of the magnetic field. It also offers a nice interpretation of the chiral behavior of chiral CTQWs: in the presence of magnetic fields, the dynamics of a charged particle can be directional and asymmetric under time reversal. Going beyond regular lattices, consider now a planar graph, which has an unambiguously defined number of faces [32] F. By Euler's formula V - E + F = 2. Since the number of loops is just L = F - 1, we deduce that the number of gauge-invariant phases on a planar graph is E - V + 1 =L. This has a clear physical interpretation in terms of magnetic fields: up to gauge transformations, the chiral Hamiltonian of a CTQW on a planar graph is fully specified by the scalar potential and the fluxes of the magnetic field through all its loops.

In conclusion, we have put forward a minimal set of physically motivated postulates that a CTQW Hamiltonian should satisfy to properly describe the quantum counterpart of a classical RW on a graph. We found that these conditions are satisfied by infinitely many quantum Hamiltonians and that any classical RW on a graph corresponds to infinitely many chiral CTQWs whose on-site energies are also arbitrary. Our results provide a full characterization of the additional quantum degrees of freedom, available to achieve a quantum advantage of CTQWs vs RWs in specific tasks. We also found how to control and manipulate these additional degrees of freedom for a charged walker. The diagonal elements may be determined by the interaction with a classical scalar field, whereas, for regular lattices in generic dimension, the offdiagonal phases may be tuned with a classical gauge field residing on the edges.

As an outlook on future developments, it could be rewarding to investigate how the additional degrees of freedom described in the present work could affect the quantum advantage of CTQWs over their classical counterparts (see [33]) and also to better identify the limits of the magnetic field model for chiral CTQW on nonplanar graphs, where the number of independent loops is not so well defined, in general.

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