Equivalence between discrete quantum walk models in arbitrary topologies

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Coin and scattering are the two major formulations for discrete quantum walks models, each believed to have its own advantages in different applications. Although they are related in some cases, it was an open question their equivalence in arbitrary topologies. Here we present a general construction for the two models for any graph and also for position dependent transition amplitudes. We then prove constructively their unitary equivalence. Defining appropriate projector operators, we moreover show how to obtain the probabilities for one model from the evolution of the other.

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I. INTRODUCTION

In essence, there are three different possible implementations for quantum walks (QW), all taking place in discrete spaces (graphs). Two are quantum analogs of Markov chains [1,2]: generalizations of diffusionlike dynamics, where time is continuous (CTQW) [3], and discrete time unitary maps [1], known as coin QW (CQW). Recently, it has been shown to exist a direct relation between these two cases [4,5]. The third (SQW), also a discrete time formulation, is physically appealing since it is based on the idea of scattering in multiport interferometers [6,7].

Due to the importance of Markov chains in random algorithms, CQW and CTQW are extensively used in their quantum versions [8], often being more efficient because the exponentially faster hitting times of QW [3,9,10]. Relevant is also the finding that one can implement universal quantum computation through scattering processes in a CTQW model [11]. Regarding applications for SQW, they seem to be particularly suitable [12] to solve searching problems [13].

It is generally believed that CQW, CTQW, and SQW have distinct advantages in different contexts [7,14,15]. For instance, universal port gates in quantum computation such as Hadamard's [16] are easier to implemented with CQW, the most common formulation in the mathematical and computer science literature. On the other hand, the construction of SQW in graphs of arbitrary topologies is more direct, and thus conceivably simpler to realize experimentally. Furthermore, since it is based on an scattering approach, analytical techniques are far more developed for SQW than for coin models [14].

Hence; (i) to formulate in a constructive way both the CQW and SQW for graphs of any topology [17] and for position dependent quantum amplitudes [18]; (ii) to prove their unitary equivalence in the general case (previously established only for particular situations [6,19]); and finally (iii) to show how to obtain the probabilities for one model from the other; are fundamental because the following. First, a constructive rather than an abstract formulation makes easier concrete implementations of such systems, even for arbitrary topologies (e.g., by means of Bose-Einstein (BE) condensates in optical lattices [20]). Second, such results would bridge the gap between two apparent distinct quantization schemes for a same class of systems. Finally, they also would show that the usages for one model are equally possible for the other. The points (i)–(iii) are then the goals of the present paper.

II. GRAPH STRUCTURES AND BASIC DEFINITIONS

We assume an undirected simple arbitrary graph [17], whose nodes are labeled in $\mathbb{Z}$. Its topology is entirely determined by the sets $\mathcal{V}_j=\{j_1,j_2,\ldots,j_{N_j}\}$, which represent the N_j nodes connected to the node j. Thus, if j_i belongs to $\mathcal{V}_j$, then there exists exactly one edge between j and j_i. Also, to any node j we associate the set of integers $\Lambda_j=\{1,2,\ldots,N_j\}$. Each element σ of Λ_j corresponds to a different edge attached to j, in a one-to-one relation. Note that if j_r and j_s have a common edge, then there are two integers numbers, σ_r and σ_s, associated to such edge, one due to j_r and other to j_s.

A given mapping (function) on a graph is said locally adaptable if: (i) it can be constructed for any graph node j; (ii) for each j, it depends only on the edge structure of the nodes in $\mathcal{V}_j$; and (iii) it is always well-defined regardless the number of elements in $\Lambda_{\mathcal{V}_j}$. This is an important concept because if one can establish time evolution relaying only on locally adaptable mappings, then the resulting dynamics is valid for any graph topology.

So, consider two locally adaptable functions that direct reflect the specific structure of a given graph. The first, $e:\Lambda_j\to\mathcal{V}_j$, associates each σ from Λ_j to a single j_i from $\mathcal{V}_j$, such that $e(\sigma;j)$ gives the node connected to j through the edge labeled σ with respect to j. For the particular example schematically depicted in Fig. 1(a), we have $\mathcal{V}_j=\{j_1,j_2,j_3,j_4\}$ and $\Lambda_j=\{1,2,3,4\}$, thus $e(\sigma_1;j)=j_1$, $e(\sigma_2;j)=j_2$, $e(\sigma_3;j)=j_3$, and $e(\sigma_4;j)=j_4$, where each σ_i assumes one of the values in Λ_j. The second, $\gamma:\Lambda_j\to\Lambda_{\mathcal{V}_j}$, maps each σ_i from Λ_j to the single element σ of $\Lambda_{e(\sigma_i;j)}$ representing the edge joining j and $e(\sigma_i;j)$. Again in Fig. 1(a) we have $\gamma(\sigma_1;j)=\sigma_k$, $\gamma(\sigma_2;j)=\sigma_l$, $\gamma(\sigma_3;j)=\sigma_m$, and $\gamma(\sigma_4;j)=\sigma_n$. Here σ_k belongs to $\Lambda_{j_1}=\{1,2\}$, σ_l to $\Lambda_{j_2}=\{1,2,3\}$, and so forth. Note that in general $\gamma(\gamma(\sigma;j);e(\sigma;j))=\sigma$.

The above mappings are strictly related to the graph specific topology. However, more general locally adaptable

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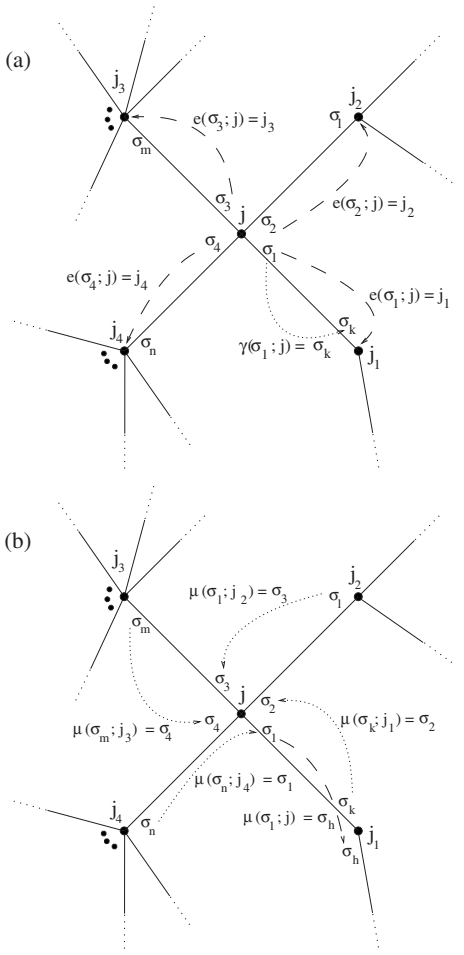

FIG. 1. Examples of locally adaptable mappings. (a) Mappings which are directly associated to the graph topology. (b) Arbitrary mappings, used to define the CQW evolution.

functions can also be defined. The next three will be very useful. $\mu:\Lambda_j\to\Lambda_{\mathcal{V}_j}$ extends γ since it associates each σ from Λ_j to an unique arbitrary element of $\Lambda_{e(\sigma;j)}$, e.g., in the particular case of Fig. 1(b), we have $\mu(\sigma_1;j)=\sigma_h$, where σ_h is in $\Lambda_{j_1}=\{1,2\}$. Although such function is locally adaptable, for an appropriate and consistent latter construction of the quantum evolution along the whole graph, we consider an extra restriction for μ. From its very definition, for any $\sigma\in\Lambda_j$ we have that $\mu(\gamma(\sigma;j);e(\sigma;j))$ is also an element of Λ_j. Then, we impose additionally that $\mu(\gamma(\sigma_r;j);e(\sigma_r;j))\neq\mu(\gamma(\sigma_s;j);e(\sigma_s;j))$ if $\sigma_r\neq\sigma_s$ $(\sigma_r;\sigma_s$ in $\Lambda_j)$, i.e., the set $\{\mu(\gamma(\sigma;j);e(\sigma;j))\}=\Lambda_j$. Observe that this restriction can always be fullfiled whatever the graph topology. For instance, in Fig. 1(b) we have $\{\mu(\sigma_n;j_4),\mu(\sigma_k;j_1),\mu(\sigma_l;j_2),\mu(\sigma_m;j_3)\}=\{\sigma_1,\sigma_2,\sigma_3,\sigma_4\}=\Lambda_j$. Naturally μ induces two other locally adaptable functions. Indeed, suppose σ_r running over Λ_j, so $\Omega_j=\{(\sigma_i,j_i)\}=\{(\mu(\sigma_r;j),e(\sigma_r;j))\}$ $[\sigma_i\in\Lambda_{j_i}$ and $j_i\in\mathcal{V}_j$, $(i=1,2,\ldots,N_j)]$ is a set where to each pair σ_i,j_i corresponds a distinct $\sigma\in\Lambda_j$. We have thus $\nu:\Omega_j\to\Lambda_j$ and $a:\Omega_j\to j$, such that $\nu(\sigma_i;j_i)=\sigma$ and $a(\sigma_i;j_i)=j$. By construction

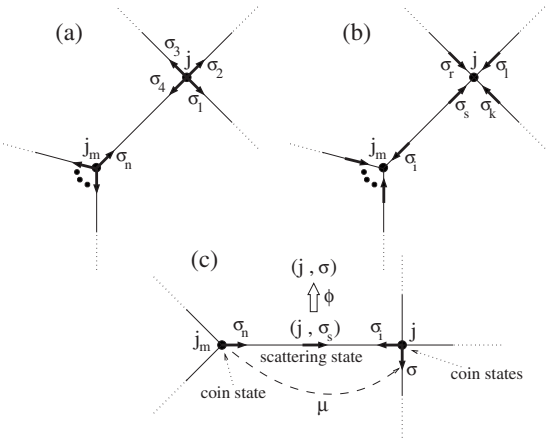

FIG. 2. In the coin (a) and scattering (b) QW formulations, σ is associated, respectively, to nodes and edge states. (c) An example of relabeling for scattering states, Eq. (7).

$$j=a(\mu(\sigma;j);e(\sigma;j))=e(\nu(\sigma;j);a(\sigma;j)),$$

$$\sigma=\nu(\mu(\sigma;j);e(\sigma;j))=\mu(\nu(\sigma;j);a(\sigma;j)). \tag{1}$$

III. THE TWO DISCRETE TIME FORMULATIONS

For the coin version, the states are defined on the graph nodes j [21]. Thus, the σ's labeling the edges attached to j can be associated to the quantum numbers representing the different "outgoing" directions leaving j, as schematically shown in Fig. 2(a). Hence, we have as the base states $\{|j,\sigma\rangle_c\}$, where for each j, $\sigma=1,2,\ldots,N_j$ and $\langle\sigma',j'|j'',\sigma''\rangle_c=\delta_{j'j''}\delta_{\sigma'\sigma''}$, which spans the Hilbert space $\mathcal{H}=L^2(\mathbb{Z}\times\mathbb{Z}_{N_{\mathbb{Z}}})$.

To establish the system dynamics, we first consider the shift operator S (and its adjoint $S^\dagger$ [22]), such that

$$S|j,\sigma\rangle_c=|e(\sigma;j),\mu(\sigma;j)\rangle_c,$$

$$S^\dagger|j,\sigma\rangle_c=|a(\sigma;j),\nu(\sigma;j)\rangle_c. \tag{2}$$

From Eq. (1), it follows that $S^\dagger S=SS^\dagger=\mathbb{I}$ in $\mathcal{H}$. Then, for each j, let $C^{(j)}$ to be a "coin" operator, represented by a $N_j\times N_j$ unitary matrix, whose action over a basis state (of quantum number j) is $C^{(j)}|j,\sigma\rangle_c=\Sigma_{\sigma'=1}^{N_j}c_{\sigma'\sigma}^{(j)}|j,\sigma'\rangle_c$. Finally, we set the unitary one step time evolution as [23]

$$U_c=S\sum_j\sum_{\sigma=1}^{N_j}C^{(j)}|j,\sigma\rangle\langle\sigma,j|_c, \tag{3}$$

which is valid for any topology (encoded in the functions e and γ) and defines a very general time evolution for the problem through the functions μ, ν and a.

For the scattering version, note first that even for a same graph, the σ labeling [24] for the scattering [6,7] can be completely distinct than that for the coin formulation [see Figs. 2(a) and 2(b)]. Thus, in principle the functions e and γ can assume different values in the two cases (and they will be distinguished when necessary).

Now, two quantum states are defined along each edge, e.g., for the edge connecting the nodes j and j_m in Fig. 2(b), we denote the state "incoming" to the node j (j_m) by $|j,\sigma_s\rangle_s$ ($|j_m,\sigma_i\rangle_s$), which can be written also as $|e(\sigma_i;j_m),\gamma(\sigma_i;j_m)\rangle_s$ ($|e(\sigma_s;j),\gamma(\sigma_s;j)\rangle_s$). Actually, for any edge, if one state is $|j,\sigma\rangle_s$, the other is given by $|e(\sigma;j),\gamma(\sigma;j)\rangle_s$. So, the basis set is $\{|j,\sigma\rangle\}_s$, spanning the Hilbert space $\mathcal{H}=L^2(\mathbb{Z}\times\mathbb{Z}_{N_\mathbb{Z}})$, as in the coin case.

For the dynamics, we set $U_s=R+T$ [23], where the action of the operators R and T are given by [22]

$$R|j,\sigma\rangle_s = r^{(j)}_{\sigma,\sigma}|e(\sigma;j),\gamma(\sigma;j)\rangle_s,$$

$$T|j,\sigma\rangle_s = \sum_{\alpha\in\Lambda_j,\alpha\neq\sigma} t^{(j)}_{\alpha,\sigma}|e(\alpha;j),\gamma(\alpha;j)\rangle_s,$$

$$R^\dagger|j,\sigma\rangle_s = r^{(e(\sigma;j))*}_{\gamma(\sigma;j),\gamma(\sigma;j)}|e(\sigma;j),\gamma(\sigma;j)\rangle_s,$$

$$T^\dagger|j,\sigma\rangle_s = \sum_{\alpha\in\Lambda_{e(\sigma;j)},\alpha\neq\gamma(\sigma;j)} t^{(e(\sigma;j))*}_{\gamma(\sigma;j),\alpha}|e(\sigma;j),\alpha\rangle_s. \quad (4)$$

We also define $N_j\times N_j$ scattering matrices $\Gamma^{(j)}$, such that $\Gamma^{(j)}_{\sigma\sigma}=r^{(j)}_{\sigma,\sigma}$ and $\Gamma^{(j)}_{\sigma'\sigma}=t^{(j)}_{\sigma',\sigma}$ (for both $\sigma'\neq\sigma$ in Λ_j). If for all j we impose that $\Gamma^{(j)}$ is unitary, then the coefficients r and t satisfy the usual relations in scattering theory [25,26]. So, U_s is unitary.

IV. OBTAINING THE PROBABILITIES

For QW, stochasticity—in the classical sense—comes into play only through measurements, when one calculates the probabilities for the walker to be found in different locations along the graph [27]. Suppose we shall know at time n what is the probability $p_j(n)$ to be in the position state j [which means a node (edge) in the coin (scattering) model], regardless the value of the coin (direction) quantum number σ. So, we define the scattering and coin projector operators as

$$P^{(j,\sigma)}_{\rm s} = |j,\sigma\rangle\langle\sigma,j|_s + |e(\sigma;j),\gamma(\sigma;j)\rangle\langle\gamma(\sigma;j),e(\sigma;j)|_s,$$

$$P^{(j)}_{\rm c} = \sum_{\sigma=1}^{N_j} |j,\sigma\rangle\langle\sigma,j|_c. \quad (5)$$

The desired probability is thus the expected value

$$p^{(j)}(n) = \langle\Psi(n)|P|\Psi(n)\rangle, \quad |\Psi(n)\rangle = U^n|\Psi(0)\rangle \quad (6)$$

for P one of the expressions in Eq. (5).

V. PROVING THE EQUIVALENCE OF THE TWO FORMULATIONS

For so, three steps are necessary: (a) to establish a correspondence between the different walks states; (b) to properly associate their time evolutions; and (c) to construct projector operators to obtain the probabilities of one in terms of the other.

Regarding (a), note that we always can define a locally adaptable function $\varphi:\Lambda_j\to\Lambda_j$, which for each node j, maps the quantum number σ associated to a specific edge in the scattering formulation to the quantum number σ' labeling the same edge, but in the coin formulation. For example, for the situation in Fig. 2, we have $\varphi(\sigma_k;j)=\sigma_1$, $\varphi(\sigma_l;j)=\sigma_2$, $\varphi(\sigma_r;j)=\sigma_3$, and $\varphi(\sigma_s;j)=\sigma_4$. Also, the actual σ's values are not relevant. They are just a way to label nodes and edges states. Thus, without loss of generality, for any j we always can rename one of the model states by $|j,\sigma\rangle\Rightarrow|j,\phi(\sigma;j)\rangle$ for ϕ a bijection $\Lambda_j\to\Lambda_j$. Choosing to retag the scattering case, we consider the following particular ϕ:

$$\phi(\sigma;j) = \mu(\gamma_c(\varphi(\sigma;j);j);e_c(\varphi(\sigma;j);j)), \quad (7)$$

whose "action" is pictorially represented in Fig. 2(c).

Then, using this new notation for the scattering states, one has the isomorphic unitary operator $E:\mathcal{H}\to\mathcal{H}$ [6]

$$E|j,\sigma\rangle_s = |j,\sigma\rangle_c \quad (8)$$

associating the scattering state σ incoming to j to the coin state σ outgoing from j [see Fig. 2(c)].

For point (b), from the explicit form of U_c and U_s, one finds that by setting one of the two akin relations

$$\Gamma^{(j)}_{\sigma_b\sigma_a} = c^{(j)}_{\gamma_c(\nu(\sigma_b;j);a(\sigma_b;j))\sigma_a},$$

$$c^{(j)}_{\sigma_b\sigma_a} = \Gamma^{(j)}_{\mu(\gamma_c(\sigma_b;j);e_c(\sigma_b;j))\sigma_a}, \quad (9)$$

then, in both models the time evolution transition probability amplitudes are exactly the same. In this case, the resulting dynamics are unitary equivalent since

$$U_{\rm s} = E^\dagger U_{\rm c} E. \quad (10)$$

Finally, for (c) even if the two formulations are unitarily related, the resulting probabilities—through projections—are not [6]. This is so because each description assumes distinct spatial configurations, nodes or edges, to characterize the system, thus not leading to same probabilities. In fact, in each edge the two scattering states are mapped by E to coin states in different nodes. Thus, the probability, Eq. (6), to be in a unique node is not equal to the probability to be in a unique edge.

However, there is a very direct way to obtain the walk probabilities for the coin (scattering) model from the scattering (coin) model. We just define

$$P^{(j)}_{\rm s}|_{\rm c} = E^\dagger P^{(j)}_{\rm c} E, \quad P^{(j)}_{\rm c}|_{\rm s} = E P^{(j)}_{\rm s} E^\dagger. \quad (11)$$

Then, suppose we construct a SQW with arbitrary r's and t's. By using $P^{(j,\sigma)}_{\rm s}$ of Eq. (5) into Eq. (6), we get the scattering walker probabilities at the step n. But now if we use $P^{(j)}_{\rm s}|_{\rm c}$ for this system, the resulting probabilities are exactly those from a coin model, for which the coin matrices elements are given by such r's and t's values according to the correspondence in Eqs. (9). The other way around, to get the scattering model results from the CQW, follows in the same fashion.

VI. REMARKS AND CONCLUSION

Although there are some few discussions in the literature on how to formulate discrete random walks in general terms

[14,17,19], here we have developed a explicit procedure that allows one to write, in a constructive way, the time evolution operator directly from the system topology and local dynamics. It also includes the case of position dependent quantum amplitudes (through the $C^{(j)}$'s and $\Gamma^{(j)}$'s). Moreover, in the CQW case, it is not necessary all the matrices $C^{(j)}$ to have the dimensions equal to the largest coordination number of the graph, as in certain formulations [14].

In the present framework, a regular graph can be defined in terms of the Λ_j's sizes (e.g., all equal to N) and the features of e, γ and μ (e.g., independent on the j's and having specific patterns along the graph). For instance, for all nodes with the same number of edges, we know that for the coin, $\mathcal{H}$ can be written as the direct product of two subspaces, thus $|j,\sigma\rangle \to |\sigma\rangle \otimes |j\rangle$. So, we naturally find from Eq. (3) that $\Sigma_j \Sigma_{\sigma=1}^{N_j} C^{(j)} |j,\sigma\rangle\langle\sigma,j| = \Sigma_j C^{(j)} \otimes |j\rangle\langle j|$, as in [28].

Usually, it is believed that analytical methods are easier to implement for the SQW than for CQW [14,29]. Since in fact they can be mapped each other, the existing methods for the former should be extendable to the latter. Our constructive approach may serve as a guide to implement such extensions [30].

Lastly, by using the cross operators in Eq. (11), we have been able to calculate—for different examples—the probabilities for SQW and CQW from a single implementation. This will be communicated elsewhere [30].

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