Equivalence between discrete quantum walk models in arbitrary topologies

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(Dated: November 7, 2009)

In essence, there are three different possible implementations for quantum walks (QW), all taking place in discrete spaces (graphs). Two are quantum analogues of Markov chains [1,2]: generalizations of diffusion-like dynamics, where time is continuous (CTQW) [3], and discrete time unitary maps [4], known as coin QW (CQW). The third (SQW), also a discrete time formulation, is physically appealing since 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.

PACS numbers: 03.67.Lx, 05-40.Fb

I. INTRODUCTION

In essence, there are three different possible implementations for quantum walks (QW), all taking place in discrete spaces (graphs). Two are quantum analogues of Markov chains [1,2]: generalizations of diffusion-like dynamics, where time is continuous (CTQW) [3], and discrete time unitary maps [4], known as coin QW (CQW). The third (SQW), also a discrete time formulation, is physically appealing since 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.

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 \( V_j = \{ j_1, j_2, \ldots, j_{N_j} \} \), which represent the \( N_j \) nodes connected to the node \( j \). Thus, if \( j_i \) belongs to \( V_j \), 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 \( \sigma \) of \( \Lambda_j \) corresponds to a different edge attached to \( j \), in a one-to-one relation. Note that if \( j_i \) and \( j_j \) have a common edge, then there are two integers numbers, \( \sigma_i \) and \( \sigma_j \), associated to such edge, one due to \( j_i \) and other to \( j_j \).

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 \( V_j \); and (iii) it is always well-defined regardless the number of elements in \( \Lambda_{V_j} \). This is an important concept because if one can establish time evolution relying 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, \( e : \Lambda_j \rightarrow V_j \), associates each \( \sigma \) from \( \Lambda_j \) to a single \( j_i \) from \( V_j \), such that \( e(\sigma; j) \) gives the node connected to \( j \) through the edge labeled \( \sigma \) with respect to \( j \). For the particular example schematically depicted in Fig. 1 (a), we have \( V_j = \{ j_1, j_2, j_3, j_4 \} \) 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 \( \sigma_i \) assumes one of the values in \( \Lambda_j \). The second, \( \gamma : \Lambda_j \rightarrow \Lambda_{V_j} \), maps each \( \sigma_i \) from \( \Lambda_j \) to the

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Arbitrary mappings, used to define the CQW evolution.

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.

The above mappings are strictly related to the graph specific topology. However, more general locally-adaptable functions can also be defined. The next three will be very useful. $\mu : \Lambda_j \rightarrow \Lambda_{\nu_j}$ extends $\gamma$ since it associates each $\sigma$ from $\Lambda_j$ to an unique arbitrary element of $\Lambda_{\epsilon(\sigma;j)}$, e.g., in the particular case of Fig. 1 (b), we have $\mu(\sigma_1;j) = \sigma_h$, where $\sigma_h$ 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 $\mu$. 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 $\Lambda_j$. 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 fulfilled whatever the graph topology. For instance, in Fig. 1 (b) we have $\{\mu(\sigma_1;j_4), \mu(\sigma_2;j_4), \mu(\sigma_3;j_4), \mu(\sigma_4;j_4)\} = \{\sigma_1, \sigma_2, \sigma_3, \sigma_4\} = \Lambda_j$. Naturally $\mu$ induces two other locally-adaptable functions. Indeed, suppose $\sigma_r$ running over $\Lambda_j$, so $\Omega_j = \{\{\sigma_r;j\}\} = \{\{\mu(\sigma_r;j),e(\sigma_r;j)\}\}$ ($\sigma_r \in \Lambda_{j_1}$ and $j_i \in \nu_j$, $i = 1, 2, \ldots, N_j$) is a set where to each pair $(\sigma_r,j_i)$ corresponds a distinct $\sigma \in \Lambda_j$. We have thus $\nu : \Omega_j \rightarrow \Lambda_j$ and $\sigma : \Omega_j \rightarrow j$, such that $\nu(\sigma_r;j_i) = \sigma$ and $a(\sigma_r;j_i)$ = $j_i$. By construction

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

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

III. THE TWO DISCRETE TIME FORMULATIONS

For the coin version, the states are defined on the graph nodes $j$. Thus, the $\sigma$’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 $\{|j,\sigma\}_c$, 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 $\mathcal{H} = L^2(\mathbb{Z} \times \mathbb{Z}_{N_j})$. 

FIG. 2: In the coin (a) and scattering (b) QW formulations, $\sigma$ is associated, respectively, to nodes and edge states. (c) An example of relabeling for scattering states, Eq. 7.
To establish the system dynamics, we first consider the shift operator $S$ (and its adjoint $S^\dagger$) [22], such that

$$S[j, \sigma]_c = |e(\sigma; j), \mu(\sigma; j)|_c$$

and

$$S^\dagger[j, \sigma]_c = |o(\sigma; j), \nu(\sigma; j)|_c.$$  \(\tag{2}\)

From Eq. \(\text{(1)}\), it follows that $S^\dagger S = SS^\dagger = \mathbb{1}$ 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 $C^{(j)}|j, \sigma\rangle_c = \sum_{\sigma' = 1}^{N_j} C^{(j)}_{\sigma' \sigma}|j, \sigma'\rangle_c$. 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 $\gamma$) and defines a very general time evolution for the problem through the functions $\mu$, $\nu$ and $\alpha$.

For the scattering version, note first that even for a same graph, the $\sigma$ labeling [24] for the scattering [4, 7] can be completely distinct than that for the coin formulation (see Figs. 2 (a) and (b)). Thus, in principle the functions $e$ and $\gamma$ can define 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 $j_0$ in Fig. 2 (b), we denote the state “incoming” to the node $j$ ($j_0$) by $|j, \sigma,s\rangle_s$ ($|j_0, \sigma, c\rangle_c$), which can be written also as $|e(\sigma; j_0), \gamma(\sigma; j_0)|_{s} \langle e(\sigma; j), \gamma(\sigma; j)|_{c}$. Actually, for any edge, if one state is $|j, \sigma, s\rangle$ then the other is given by $|e(\sigma; j), \gamma(\sigma; j)|_s$. So, the basis set is $\{|j, \sigma\rangle\}_s$, spanning the Hilbert space $\mathcal{H} = L^2(\mathbb{Z} \times \mathbb{N})$, 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]

$$R[j, \sigma]|s\rangle_s = \sum_{\alpha \in \Lambda_j(\sigma), \alpha \neq \gamma(\sigma; j)} t^{(j)}_{\alpha \sigma e(\alpha; j), \gamma(\sigma; j)}|e(\alpha; j), \gamma(\sigma; j)|_s,$$

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

$$R^\dagger[j, \sigma]|s\rangle_s = \sum_{\alpha \in \Lambda_j(\sigma), \alpha \neq \gamma(\sigma; j)} t^{\dagger(j)}_{\alpha \sigma} e(\alpha; j), \gamma(\sigma; j)|_s,$$

$$T^\dagger[j, \sigma]|s\rangle_s = \sum_{\alpha \in \Lambda_j(\sigma), \alpha \neq \gamma(\sigma; j)} t^{\dagger(j)}_{\alpha \sigma} e(\alpha; j), \gamma(\sigma; j)|_s.$$ \(\tag{4}\)

We also define $N_j \times N_j$ scattering matrices $\Gamma^{(j)}$, such that $\Gamma^{(j)}_{\sigma \sigma'} = \Gamma^{(j)}_{\sigma \sigma'}$ and $\Gamma^{(j)}_{\sigma \sigma'} = \Gamma^{(j)}_{\sigma \sigma'},$ (for both $\sigma' \neq \sigma$ in $\Lambda_j$). 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 of the value of the coin (direction) quantum number $\sigma$. So, we define the scattering and coin projector operators as

$$P^{(j)}_c = |j, \sigma\rangle\langle\sigma, j|_c + |e(\sigma; j), \gamma(\sigma; j)f(\gamma(\sigma; j), e(\sigma; j)|_c,$$

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

The desired probability is thus the expected value

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

for $P$ one of the expressions in Eq. \(\text{(5)}\).

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 $\varphi : \Lambda_j \rightarrow \Lambda_j$, which for each node $j$, maps the quantum number $\sigma$ associated to a specific edge in the scattering formulation to the quantum number $\sigma'$ labeling the same edge, but in the coin formulation. For example, for the situation in Fig. 2, we have $\varphi(\sigma; j) = \sigma_1$, $\varphi(\sigma; j) = \sigma_2$, $\varphi(\sigma; j) = \sigma_3$, and $\varphi(\sigma; j) = \sigma_4$. Also, the actual $\sigma$’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 $|j, \sigma\rangle \Rightarrow |j, \varphi(\sigma; j)\rangle$ for $\phi$ a bijection $\Lambda_j \rightarrow \Lambda_j$. Choosing to retag the scattering case, we consider the following particular $\phi$

$$\phi(\sigma; j) = \mu(\gamma_c(\varphi(\sigma; j); j); \varphi(\sigma; j); j)),$$ \(\tag{7}\)

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

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

$$E[j, \sigma] = |j, \sigma\rangle_c.$$ \(\tag{8}\)

associating the scattering state $\sigma$ incoming to $j$ to the coin state $\sigma$ 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

$$\Gamma^{(j)}_{\sigma \sigma'} = \sum_{\nu(\sigma; j), (\sigma; j)} \Gamma^{(j)}_{\sigma \sigma'},$$

$$\Gamma^{(j)}_{\sigma \sigma'} = \sum_{\nu(\sigma; j), (\sigma; j)} \Gamma^{(j)}_{\sigma \sigma'},$$ \(\tag{9}\)

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

$$U_s = E^\dagger U_c E.$$ \(\tag{10}\)
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. (10), 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

\[
P_s^{(j)}|_c = E^\dagger P_c^{(j)} E, \quad P_c^{(j)}|_s = E P_s^{(j)} E^\dagger. \tag{11}
\]

Then, suppose we construct a SQW with arbitrary \( r \)'s and \( t \)'s. By using \( P_s^{(j)} \sigma \) of Eq. (3) into Eq. (b), we get the scattering walker probabilities at the step \( n \). But now if we use \( P_s^{(j)}|_c \) 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. (3). 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 \( \Lambda_j \)'s sizes (e.g., all equal to \( N \)) and the features of \( c, \gamma \) and \( \mu \) (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 \( |j, \sigma \rangle \rightarrow |\sigma \rangle \otimes |j\rangle \). So, we naturally find from Eq. (6) that \( \sum_j \sum_{\sigma=1}^{N_j} C^{(j)} |j, \sigma \rangle \langle \sigma, j| \). This will be communicated elsewhere [30].

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].

**VII. ACKNOWLEDGEMENT**

Research grants are provided by Capes and CNPq.

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[1] Y. Aharonov, L. Davidovich, and N. Zagury, Phys. Rev. A **48**, 1687 (1993); D. A. Meyer, J. Stat. Phys. **85**, 551 (1996).
[2] A. Ambainis, E. Bach, A. Nayak, A. Vishwanath, and J. Watrous, in *STOC’01: Proceedings of the 33rd Annual ACM Symposium on Theory of Computing*, (ACM, New York, 2001), pp. 50-59; D. Aharonov, A. Ambainis, J. Kempe, and U. Vazirani, *ibid*, pp. 37-49.
[3] E. Farhi and S. Gutmann, Phys. Rev. A **58**, 915 (1998). A. M. Childs, E. Farhi, and S. Gutmann, Quantum Information Processing **1**, 35 (2002).
[4] F. W. Strauch, Phys. Rev. A **74**, 030301(R) (2006).
[5] A. M. Childs, arXiv: 0810.0312.
[6] M. Hillery, J. Bergou, and E. Feldman, Phsy. Rev. A **68**, 032314 (2003).
[7] E. Feldman and M. Hillery, J. Phys. A **40**, 11343 (2007).
[8] A. Ambainis, in *SOFSEM 2008: Theory and Practice of Computer Science*, Eds. V. Geffert, J. Karhumaki, A. Bertoni, B. Preneel, P. Navrat, M. Bielikova, (Springer, Berlin, 2008), pp. 1-4.
[9] A. M. Childs, R. Cleve, E. Deotto, E. Farhi, S. Gutmann, and D. A. Spielman, in *STOC’03: Proceedings of the 35th annual ACM symposium on theory of Computing* (ACM Press, New York, 2003), pp. 59-68.
[10] J. Kempe, Probab. Theory Relat. Fields **133**, 215 (2005).
[11] A. M. Childs, Phys. Rev. Lett. **102**, 180501 (2009).
[12] A. Gabris, T. Kiss, and I. Jex, Phys. Rev. A **76**, 062315 (2007); D. Reitzent, M. Hillery, E. Feldman, and V. Buzek, Phys. Rev. A **79**, 012309 (2009).
[13] T. A. Brun, H. A. Carteret, and A. Ambainis, Phys. Rev. A **75**, 082314 (2007); P. Ribeiro, P. Milman, and R. Mosseri, Phys. Rev. Lett. **93**, 190503 (2004).
[14] M. A. Nielsen and I. S. Chuang, *Quantum Computation and Quantum Information* (Cambridge Univ. Press, Cambridge, 2000).
[15] V. Kendon, Int. J. Quantum Inf. **4**, 791 (2006).
[16] T. A. Brun, H. A. Carteret, and A. Ambainis, Phys. Rev. A **72**, 052307 (2006); A. M. Childs and J. Goldstone, Phys. Rev. A **70**, 022314 (2004).
[17] V. Kendon, Math. Struct. Comp. Sci. **17**, 1169 (2007).
[18] B. Tregenna, W. Flanagan, R. Maile, and V. Kendon, N. J. Phys. **5**, 83 (2003).
[19] R. Mosseri, Phys. Rev. Lett. **87**, 211601 (2001).
[20] K. Manouchehri and E. B. Wang, arXiv: 0809.0034.
[21] J. Watrous, in *STOC’01: Proceedings of the 33rd Annual ACM Symposium on Theory of Computing* (ACM Press, New York, 2001), pp. 60-67.
[22] In agreement with the general definition of the adjoint \( O^\dagger \) of a bounded linear operator \( O \): for any \( \varphi \) and \( \psi \) in \( \mathcal{H} \), it holds that \( (\varphi, O\psi) = (O^\dagger \varphi, \psi) \).
One also may consider $U \rightarrow \exp[i\theta] U$, associating $\theta$ with translations between nodes, as for stationary scattering solutions discussed, e.g., in E. Feldman and M. Hillery, Phys. Lett. A 324, 277 (2004).

Without loss of generality we assume a same $j$ labeling.

K. Chadam and P. C. Sabatier Inverse Problems in Quantum Scattering Theory (Springer, Berlin, 1989).

A. G. M. Schmidt, B. K. Cheng, and M. G. E. da Luz, J. Phys. A 36, (2003) L545.

J. Kempe, Contemp. Phys. 44, 307 (2003).

N. Linden and J. Sharam, arXiv: 0906.3692

E. Feldman and M. Hillery, in Coding Theory and Quantum Computing, Contemporary Mathematics Vol. 381, edited by E. Evans, J. Holt, C. Jones, K. Klintworth, B. Parshall, O. Pfister, and H. Ward (American Mathematical Society, Providence-RI, 2005) pp.71-98.

F. M. Andrade and M. G. E. da Luz, unpublished.