Continuous-Time Classical and Quantum Random Walk on Direct Product of Cayley Graphs

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Abstract

In this paper we define direct product of graphs and give a recipe for obtained prob-
ability of observing particle on vertices in the continuous-time classical and quantum 
random walk. In the recipe, the probability of observing particle on direct product of 
graph obtain by multiplication of probability on the corresponding to sub-graphs, where 
this method is useful to determine probability of walk on complicated graphs. Using this 
method, we calculate the probability of continuous-time classical and quantum random 
wells on many of finite direct product cayley graphs (complete cycle, complete $K_n$, 
charter and $n$-cube). Also, we inquire that the classical state the stationary uniform 
distribution is reached as $t \to \infty$ but for quantum state is not always satisfy.

Keywords: Continuous-time random walk, Classical random walk, Quantum 
random walk, Direct product of graphs, Cayley graphs.

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1 Introduction

The theory of Markov chains and random walks on graphs is fundamental to mathematics, physics, and computer science [1], [2], [3] as it provides a beautiful mathematical framework to study stochastic process and its applications. Among some of the known examples of these applications include Monte Carlo methods in statistics, the theory of diffusion in statistical physics, and algorithmic techniques for sampling and random generation of combinatorial structures in computer science (based on rapid mixing of certain Markov chains). Two pervasive algorithmic ideas in quantum computation are Quantum Fourier Transform (QFT) and amplitude amplification (see [4]). Most subsequent progress in quantum computing owed much to these two beautiful ideas. But there are many problems whose characteristics matches neither the QFT nor the amplitude amplification mold (e.g., the Graph Isomorphism problem). This begs for new additional tools to be discovered.

A natural way to discover new quantum algorithmic ideas is to adapt a classical one to the quantum model. An appealing well-studied classical idea in statistics and computer science is the method of random walks [5, 6]. Recently, the quantum analogue of classical random walks has been studied in a flurry of works [7, 8, 9, 10, 11, 12]. The works of Moore and Russell [11] and Kempe [12] showed faster bounds on instantaneous mixing and hitting times for discrete and continuous quantum walks on the hypercube (compared to the classical walk). A recent work by Childs et al. [13] gave an interesting and powerful algorithmic application of continuous-time quantum walks.

A study of quantum walks on simple lattice is well known in physics (see [14]). Recent studies of quantum walks on more general graphs were described in [8, 7, 10, 13, 15, 16, 17, 18, 19, 20, 21, 22]. Some of these works studies the problem in the important context of algorithmic problems on graphs and had suggested that quantum walks is a promising algorithmic technique for designing future quantum algorithms.
Several important classes of graphs studied in classical random walks include the binary $n$-cube, the circulant graphs, and the group-theoretic Cayley graphs. The binary $n$-cube and circulant graphs are important in the study of interconnection networks and complexity of Boolean function, and Cayley graphs capture strong group-theoretic ingredients of important problems, such as Graph Isomorphism. Since most of these graphs are regular, classical random walks on them are known to converge or to mix towards the uniform stationary distribution. The mixing properties of continuous-time quantum walks on the same graphs were found to exhibit non-classical behavior [11, 23, 24, 25].

In this paper we define direct product of graphs and give a recipe for obtained probability of observing particle on vertices in the continuous-time classical and quantum random walk. In the recipe the probability of observing particle on direct product of graph obtain by multiplication of probability on the corresponding to sub-graphs. This method is useful to determine probability of walk on complicated graphs. In the classical state the stationary uniform distribution is reached as $t \rightarrow \infty$ but for quantum state is not satisfy. Using this method, we calculate the probability of continuous-time classical and quantum walk on many of finite direct product cayley graphs (complete cycle, complete $K_n$, charter and $n$-cube).

The organization of this paper is as follow. In section 2, we give a brief outline of graphs and their adjacency matrix. In section 3, we present a concept of direct product of Cayley graphs. In the section 4, continuous-time classical random walks on graphs is studied, and we calculate some examples. In the section 5, we present continuous-time quantum walk on graphs, and calculate some examples. Finally, in section 6, the conclusions and future research are presented.
2 Graphs and its adjacency matrix

Any mathematical object involving point and connections between them may be called a graph. If all the connections are unidirectional, it is called a digraph. A graph $\Gamma = (V, E)$ consists of two sets $V$ and $E$. The elements of $V$ are called vertices (or nodes) and the elements of $E$ are called edges where $E$ is a subset of $\{\{x, y\} \mid x, y \in V, x \neq y\}$. Two vertices $x, y \in V$ are called adjacent if $\{x, y\} \in E$, and in this case we write $x \sim y$. We let $A$ be the $|V| \times |V|$ adjacency matrix of $\Gamma$, i.e., $A$ is indexed by elements of $V$ and is as follows:

$$A_{xy} = \begin{cases} 
1 & \text{if } x \sim y \\
0 & \text{otherwise}
\end{cases}$$

(1)

Obviously, (i) $A$ is symmetric; (ii) an element of $A$ takes a value in $\{0, 1\}$; (iii) a diagonal element of $A$ vanishes. Conversely, for a non-empty set $V$, a graph structure is uniquely determined by such a matrix indexed by $V$. The *degree* or *valency* of a vertex $x \in V$ is defined by

$$\kappa(x) = |\{y \in V; x \sim y\}|,$$

(2)

where $|\cdot|$ denotes the cardinality. A finite sequence $x_0; x_1; \ldots; x_n \in V$ is called a walk of length $n$ (or of $n$ steps) if $x_{k-1} \sim x_k$ for all $k = 1, 2, \ldots, n$. In a walk some vertices may occur repeatedly.

3 The Direct product of cayley Graphs

In this section, we briefly discuss necessary background information on Cayley graphs of the group and will study their product.

Let $\Gamma_i, i = 1, 2, \ldots, d$ be graphs of finite vertices with the corresponding adjacency matrices $A_i, i = 1, 2, \ldots, d$. Then their direct product

$$\Gamma_1 \otimes \cdots \otimes \Gamma_d,$$

(3)
Continuous-time classical and quantum Random walk

is a graph with the following adjacency matrix $A$:

$$A = \sum_{j=1}^{d} I \otimes \cdots \otimes A_j \otimes \cdots \otimes I$$  \hspace{1cm} (4)

where the $j$th term in the sum has $A_j$ appearing in the $j-th$ place in the tensor product.

Let $G$ be a finite group and let $R \subseteq G$ be a set of generators for $G$ satisfying $g \in R \Leftrightarrow g^{-1} \in R$ for all $g \in G$ (in this case the Cayley graph will be equivalent to an undirected regular graph). Then the Cayley graph of $G$ with respect to $R$, which we denote by $\Gamma(G, R)$, is an undirected graph defined as follows. The set of vertices of $\Gamma(G, R)$ coincides with $G$, and for any $g, h \in G$, \{g, h\} is an edge in $\Gamma(G, R)$ if and only if $gh^{-1} \in R$.

Now let $\Gamma_i$ be Cayley graph of finite group $G_i$, with respect to $R_i$. Then the graph $\Gamma$ is generated by using Eq.(3) is the Cayley graph of finite group $G = G_1 \otimes \cdots \otimes G_n$, with respect to $R = \{(r^{(1)}_j, 1, \ldots, 1), (1, r^{(2)}_j, 1, \ldots, 1), \ldots, (1, 1, \ldots, r^{(n)}_j)\}$, where $r^{(i)}_j \in R_i$ and 1 as the neutral element of $G_i$. Thus, for any $g = (a_1, \ldots, a_n), h = (b_1, \ldots, b_n)$ where $a_i, b_i \in G$, the connected is defined if $gh^{-1} \in R$, i.e, $(a_1 b_1^{-1}, \ldots, a_n b_n^{-1}) \in R$, consequently, $a_i \neq b_i$ only in one element (the vertices $a_{i_1,i_2,i_3,\ldots,i_n}$ and $a_{j_1,j_2,j_3,\ldots,j_n}$ are connected provided that they differ only in one indices, i.e, $i_k = j_l$ for $k, l = 1, 2, \ldots, m - 1, m + 1, \ldots, n$ but $i_m \neq j_m$).

In the end we argue circulant graph which to deem necessary in the examples that we will investigate continuous-time classical and quantum random walk for them.

If $G$ is a cyclic group, then the Cayley graph is called a circulant graph. The adjacency matrix $A$ of circulant graph is given by

$$A = \sum_{k=0}^{n-1} a_k P^k,$$  \hspace{1cm} (5)
where $P$ is the $n \times n$ primary permutation matrix\textsuperscript{[26]} as follow:

\[ P = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}. \quad (6) \]

The adjacency matrix $A$ is belonging to $CG$-modules, that $C$ and $G = < P >$ are complex field and cyclic group with $ord(P) = n$, respectively. A well-known theorem states that any $CG$-modules can be expressed as a direct sum of irreducible $CG$-submodules. Also, the fact that the dimensional of every irreducible $CG$-modules is one for finite abelian group $G$, and the dual group of a cyclic group is isomorphic to the group itself, can be used Fourier transformation for diagonalizable of adjacency matrix $A$.

Thus the primary permutation matrix is that diagonalizable (unitarily) by the Fourier matrix

\[ F = \frac{1}{\sqrt{n}} V(\omega), \quad (7) \]

where $\omega = e^{2\pi i/n}$ and $V(\omega)$ is the Vandermonde matrix. Therefore, we have

\[ F^\dagger P F = \text{diag}(1, \omega, \omega^2, \omega^3, \omega^4, \ldots, \omega^{n-1}). \quad (8) \]

This Equation (8) shows that the eigenvalues of a circulant matrix can be obtained by using the Fourier transform $F$.

Some examples of circulant graphs that we study, they are the complete graphs(i.e, $a_1 = a_2 = \cdots a_{n-1} = 1$, $a_0 = 0$, $G = Z_N$ and $R = \{1, 2, \ldots, N-2\}$) and full-cycle(i.e, $a_1 = a_{n-1} = 1$ and otherwise 0, $G = Z_N$ and $R = \{1, N-2\} )$.

Also, two other examples, for direct product graphs that we study, are the hypercubes simple structure as a product simplex graph $K_2$, and charter graph(i.e, $G = Z_2 \otimes Z_n$ such that the corresponding product graph’s is $\Gamma = K_2 \otimes C_n$ ).
4 Continuous-time classical random walks on direct product of graphs

Let \( \Gamma = (V, E) \) be a simple (no self-loops), undirected, connected graph with adjacency matrix \( A \). Suppose that \( P : V(\Gamma) \rightarrow [0, 1] \) denotes a time-dependent probability distribution of a stochastic process on \( \Gamma \). The classical evolution of the discrete-time random walk is given by the equation

\[
P(t) = W^t P(0),
\]

(9)

where \( W \) is the stochastic transition matrix and \( t \in \mathbb{Z}^+ \). In a simple walk on a \( d \)-regular graph \( \Gamma \), we let \( W_d = \frac{1}{d} A \); this defines a random walk where, at each step, the particle moves to one of its \( d \) neighbors randomly. On the other hand, in a lazy walk on \( \Gamma \), the particle stays or moves to a random neighbor with equal probabilities; here we have \( W_l = \frac{1}{2} + \frac{1}{2} W_d \).

The Laplacian of \( \Gamma \) is defined as \( H = A - D \), where \( D \) is a diagonal matrix whose \( j \)-th entry is the degree of vertex \( j \) of \( G \). Suppose that \( P(t) \) is a probability distribution of continuous-time walk at time \( t \). The classical evolution of the continuous-time walk is given by the Kolmogorov equation

\[
\frac{d}{dt} P(t) = HP(0).
\]

(10)

The solution of this equation, modulo some conditions, is

\[
P(t) = e^{tH} P(0).
\]

(11)

Thus, the solution for the product of cayley graphs equation(3) with the normalized adjacency matrix equation(4) such that \( H_i = A_{d_i} - D_{d_i} \) is as follow:

\[
P(t) = \prod_{i=1}^{d} \otimes (e^{(A_{d_i} - D_{d_i})t} P(0),
\]

(12)

with initial probability \( P(0) = P_1(0) \otimes \cdots \otimes P_d(0) \). Then we obtain probability distribution of
continuous-time classical and quantum Random walk

9

continuous-time walk at time \( t \) as

\[
P(t) = \prod_{i=1}^{d} \otimes (e^{(A_{n_i} - D_{n_i})t}P_i(0)) = \prod_{i=1}^{d} \otimes (P_i(t)).
\] (13)

Therefore the probability for observing particle on direct product of graph obtain by multiplication of probability on the sub-graphs. This method is useful to determine probability of walk on complicated graphs.

4.1 The cycle graph \( C_n \)

Let \( \frac{1}{2}A_n \) be the normalized adjacency matrix of the full-cycle \( C_n \) on \( n \) vertices. According to [27], let \( H = \frac{1}{2}A_n - I_n \) be its Laplacian matrix of the full-cycle. Thus, the eigenvalues of \( H \) is given by, \( \lambda_j = \cos(\frac{2\pi j}{n}) - 1 \).

The direct product for cycle graphs is \( C_{n_1} \otimes \cdots \otimes C_{n_d} \), such that the corresponding Laplacian as follow :

\[
A = \sum_{i=1}^{d} I_{n_i} \otimes \cdots \otimes (\frac{1}{2}A_{n_i} - I_{n_i}) \otimes \cdots \otimes I_{n_d}
\] (14)

where the ith term in the sum has \( \frac{1}{2}A_{n_i} - I_{n_i} \) appearing in the ith place in the tensor product.

In order to, The solution of Kolmogorov equation for the direct product finite cycle is

\[
P(t) = \prod_{i=1}^{d} \otimes (e^{(\frac{1}{2}A_{n_i} - I_{n_i})}P(0)).
\] (15)

Using the orthonormal eigenvectors \( |F_j \rangle = \frac{1}{\sqrt{n}}|\omega_j \rangle \) (the columns of the Fourier matrix \( F \) (7)) and the initial probability vector \( P(0) = P_1(0) \otimes \cdots \otimes P_d(0) \), then for \( P(t) \), We have

\[
P(t) = \prod_{i=1}^{d} \otimes (\frac{1}{n_i} \sum_{j=0}^{n_i-1} e^{t(-1+\cos(2\pi j/n_i))}|\omega_j \rangle_i)
\] (16)

Thus for calculate the probability of particle, we use the probability of particle on single graph \( C_n \)(i.e, \( P_{s,k}(t) = \frac{1}{n} \sum_{j=0}^{n-1} e^{t(1-\cos(2\pi j/n))}|\omega_j \rangle^k \)). Therefore, the probability for observing the particle at the position \( \vec{K} \) is

\[
P_{\vec{K}}(t) = \prod_{i=1}^{d} P_{s,k_i}(t).
\] (17)
So, the stationary uniform distribution is reached as $t \to \infty$. The especially, if $n_1 = n_2 = \cdots = n_d = n$, we have

$$P(t) = (e^{(\frac{1}{2}A_n-I_n)})^{\otimes d}P(0) = \left(\frac{1}{n} \sum_{j=0}^{n-1} e^{t(-1+\cos(2\pi j/n))}\ket{\omega_j}\right)^{\otimes d}. \quad (18)$$

### 4.2 The complete graph $K_n$

Let $\frac{1}{n-1}A_n$ be the normalized adjacency matrix of the complete graph $K_n$ on $n$ vertices. Thus, $H = \frac{1}{n-1}A_n - I_n$ is the Laplacian matrix of the complete graph $K_n$. The eigenvalues of $H$ are $0$ (once) and $-\frac{n}{n-1}$ (n-1 times). The direct product of complete graphs is $K_{n_1} \otimes \cdots \otimes K_{n_d}$, such that the corresponding Laplacian as follow:

$$A = \sum_{i=1}^{d} I_{n_{i_1}} \otimes \cdots \otimes \left(\frac{1}{n_{i_1}-1}A_{n_{i_1}} - I_{n_{i_1}}\right) \otimes \cdots \otimes I_{n_{d}} \quad (19)$$

where the $i$th term in the sum has $(\frac{1}{n_{i_1}-1}A_{n_{i_1}} - I_{n_{i_1}})$ appearing in the $i$th place in the tensor product. The solution of Kolmogorov equation for direct product complete graphs is

$$P(t) = \prod_{i=1}^{d} \otimes (e^{(\frac{1}{n_{i_1}-1}A_{n_{i_1}} - I_{n_{i_1}})})P(0) = \begin{pmatrix}
\frac{1}{n_1}(1 + e^{-\frac{n_1 t}{n_1-1}}) \\
\frac{1}{n_2}(1 - e^{-\frac{n_1 t}{n_1-1}}) \\
\vdots \\
\frac{1}{n_1}(1 - e^{-\frac{n_1 t}{n_1-1}})
\end{pmatrix} \otimes \cdots \otimes 
\begin{pmatrix}
\frac{1}{n_d}(1 + e^{-\frac{n_d t}{n_d-1}}) \\
\frac{1}{n_d}(1 - e^{-\frac{n_d t}{n_d-1}}) \\
\vdots \\
\frac{1}{n_d}(1 - e^{-\frac{n_d t}{n_d-1}})
\end{pmatrix} \quad (20)$$

with initial probability $P(0) = P_1(0) \otimes \cdots \otimes P_d(0)$. Thus the probability of particle at the position $\ket{\vec{K}} = \ket{i_1, i_2, \ldots, i_d}$, is as follow:

$$P_{\vec{K}}(t) = \prod_{l=1}^{d} \frac{1}{n_l}[(1 + e^{-\frac{n_l t}{n_l-1}})\delta_{i_l,0} + (1 - e^{-\frac{n_l t}{n_l-1}})(1 - \delta_{i_l,0})]. \quad (21)$$

So, the stationary uniform distribution is reached as $t \to \infty$. 
The especially, if \( n_1 = n_2 = \cdots = n_d = n \), we have

\[
P(t) = (e^{t\frac{1}{n}A_n - I_n}) \otimes_d P(0) = \left( \begin{array}{c}
\frac{1}{n}(1 + e^{-\frac{nt}{n_1-1}}) \\
\frac{1}{n}(1 - e^{-\frac{nt}{n}}) \\
\vdots \\
\frac{1}{n}(1 - e^{-\frac{nt}{n}})
\end{array} \right)^{\otimes d}
\]

(22)

with initial probability \( P(0) = P_1(0) \otimes \cdots \otimes P_d(0) \). Thus for calculate the probability of particle, we use the probability of particle on single graph \( K_n \) (i.e, \( P_{s,0}(t) = \frac{1}{n}(1 + e^{-\frac{nt}{n}}) \), \( P_{s,j}(t) = \frac{1}{n}(1 - e^{-\frac{nt}{n}}) \) for \( j \neq 0 \)). Therefore, the probability for observing the particle at the position \( \vec{K} \) is

\[
P_{\vec{K}}(t) = (P_{s,0})^k(P_{s,j})^{d-k}
\]

(23)

where the \( k \) is the number of zeroes.

### 4.3 Charter

As an example axiomatic, direct product graphs for the continuous-time random walk, we can calculate the probability \( P(t) \) directly by exploiting the charters simple structure as a product simplex graph \( K_2 \) and cycle graph \( C_n \). Let \( G = Z_2 \otimes Z_n \) be a complete 2-partite graph where each partition has \( n > 2 \) vertices (the case \( n = 2 \) is the square graph). The direct product of complete graphs \( K_2 \) and cycle graph \( C_n \) is \( K_2 \otimes C_n \) such that the corresponding Laplacian as follows:

\[
A = I_2 \otimes \left( \frac{1}{2}A_n - I_n \right) + (\sigma_x - I_2) \otimes I_n.
\]

(24)

Thus, the solution of Kolmogorov equation for charter is

\[
P(t) = e^{tA} P(0) = (e^{t(\sigma_x - I_2)} \otimes e^{t(\frac{1}{2}A_n - I_n)}) P(0)
\]

\[
= \frac{1}{2n} \begin{pmatrix}
(1 + e^{-2t}) \sum_{j=0}^{n-1} e^{t(-1 + \cos(2\pi j/n))} |\omega_j\rangle \\
(1 - e^{-2t}) \sum_{j=0}^{n-1} e^{t(-1 + \cos(2\pi j/n))} |\omega_j\rangle
\end{pmatrix}
\]

(25)
Where, for calculate the probability of particle we use the probability of particle on single graphs $K_2$ and $C_n$, with the initial probability $P(0) = P_1(0) \otimes P_2(0)$. So, the stationary uniform distribution is reached as $t \to \infty$.

### 4.4 n-cube

As another example, direct product graphs for the continuous-time random walk, we can calculate the probability $P(t)$ directly by exploiting the hypercubes simple structure as a product simplex graph. The binary $n$-cube is define over the set $(0,1)^n$ of $n$-cube binary sequence, where two sequence $x$ and $y$ are connected if they differ exactly in one bit position. As it turns out, the $n$-cube is also a complet graph.

Let $\sigma_x$ (Pauli matrix) be the normalized adjacency matrix of $K_2$, thus, $H = \sigma_x - I_2$ be its Laplacian. The direct product for hypercubes is $S_n = K_2 \otimes \cdots \otimes K_2$, such that the corresponding Laplacian as follow:

$$A = \sum_{i=1}^{n} I_2 \otimes \cdots \otimes (\sigma_x - I_2) \otimes \cdots I_2$$

where the $i$th term in the sum has $(\sigma_x - I_2)$ appearing in the $i$th place in the tensor product. The solution of Kolmogorov equation for hypercubes is

$$P(t) = (e^{(\sigma_x - I_2)})^\otimes d P(0) = \left( \begin{array}{c} \frac{1}{2} \left( 1 + e^{-2t} \right) \\ \frac{1}{2} \left( 1 - e^{-2t} \right) \end{array} \right)^\otimes d$$

with initial probability $P(0) = P_1(0) \otimes \cdots \otimes P_d(0)$. Thus for calculate the probability of particle, we use the probability of particle on single graph $Z_2$ (i.e, $P_{s,0}(t) = \frac{1}{2}(1+e^{-2t}), P_{s,1}(t) = \frac{1}{2}(1-e^{-2t})$). Therefore, the probability for observing the particle at the position $\vec{K}$ is

$$P_{\vec{K}}(t) = \prod_{i=1}^{2} P_{s,k_i}(t).$$

So, the stationary uniform distribution is reached as $t \to \infty$. 

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*Continuous-time classical and quantum Random walk*
5 Continuous-time quantum walks on direct product of graphs

A continuous-time quantum walk is defined by replacing Kolmogorov’s equation with Schrödinger’s equation. Continuous-time quantum walks was introduced by Farhi and Gutmann [7] (see also [8, 11]). Our treatment, though, follow closely the analysis of Moore and Russell [11] which we review next. Let $|\psi\rangle \colon V(\Gamma) \longrightarrow C$ be a time-dependent amplitude of the quantum process on $\Gamma$. The wave evolution of the quantum walk is

$$i\hbar \frac{d}{dt}|\psi_t\rangle = H|\psi_t\rangle,$$

(29)

where assume $\hbar = 1$, and $|\psi_0\rangle$ be the initial amplitude wave function of the particle, the solution is given by $|\psi_t\rangle = e^{-iHt}|\psi_0\rangle$.

But on $d$-regular graphs, $D = \frac{1}{d}I$, and since $A$ and $D$ commute, we get

$$e^{-itH} = e^{-it(A-\frac{1}{d}I)} = e^{-it/d}e^{-itA}$$

(30)

which introduces an irrelevant phase factor in the wave evolution.

The probability that the particle is at vertex $j$ at time $t$ is given by

$$P_t(j) = |\langle j|\psi_t\rangle|^2.$$

(31)

The average probability that the particle is at vertex $j$ is given by

$$P(j) = \lim_{T \to \infty} \frac{1}{T} \int_0^T P_t(j) dt.$$

(32)

Since $H$ is Hermitian, the matrix $U_t = e^{-iHt}$ is unitary. If $(\lambda_j, |z_j\rangle)_j$ are the eigenvalue and eigenvector pairs of $H$, then $(e^{-i\lambda_j t}, |z_j\rangle)_j$ are the eigenvalue and eigenvector pairs of $U_t$. Because $H$ is symmetric, there is an orthonormal set of eigenvectors, say $\{|z_j\rangle : j \in [n]\}$ (i.e., $H$ is unitarily diagonalizable). So, if $|\psi_0\rangle = \sum_j \alpha_j |z_j\rangle$ then

$$|\psi_t\rangle = \sum_j \alpha_j e^{-i\lambda_j t}|z_j\rangle.$$

(33)
Hence, in order to analyze the behavior of the quantum walk, we follow its wave-like patterns using the eigenvalues and eigenvectors of the unitary evolution $U_t$. To observe its classical behavior, we collapse the wave vector into a probability vector using Equation (31).

Thus, the wave function $|\psi_t\rangle$ for the product Cayley graphs Eq.(3) with the normalized adjacency matrix Eq.(4) such that $H_j = A_{n_j} - \frac{1}{n_j} I_{n_j}$ (regular graph) as follow:

$$|\psi_t\rangle = \exp(-iAt)|\psi_0\rangle = e^{-itA_1}|0\rangle_1 \otimes \cdots \otimes e^{-itA_d}|0\rangle_d = \prod_{j=1}^{d} e^{-itA_{n_j}}|0\rangle_j$$

with initial state $|\psi_0\rangle = |0\rangle_1 \cdots |0\rangle_d$. Also, the above equation show that the amplitude wave function of the particle on direct product of graph obtain by multiplication of amplitudes at the sub-graphs. This method is useful to determine amplitudes of walk on complicated graphs.

**Definition 1** (instantaneous and average mixing [8, 11])

Let $\epsilon \geq 0$. A graph $G = (V, E)$ has the instantaneous $\epsilon$-uniform mixing property if there exists $t \in R^+$, such that the continuous-time quantum walk on $G$ satisfies $\| P_t - U \| \leq \epsilon$, where $\| Q_1 - Q_2 \| = \sum_x |Q_1(x) - Q_2(x)|$ is the total variation distance between two probability distribution $Q_1, Q_2$, and $U$ us the uniform distribution on the vertices of $G$. Whenever $\epsilon = 0$ is achievable, $G$ is said to have instantaneous exactly uniform mixing.

The graph $G = (V, E)$ has the average uniform mixing property if the average probability distribution satisfies $P(t) = 1/|V|$ for all $j \in V$.

**5.1 The cycle graph $C_n$**

Since the finite cycle is a regular graph, instead of the Laplacian, we use the adjacency matrix directly. Let $\frac{1}{2}A_n$ be the normalized adjacency matrix of the full-cycle $C_n$ on $n$ vertices. Using the properties of circulant matrices, the eigenvalues of $\frac{1}{2}A_n$ is given by

$$\lambda_j = \frac{1}{2}(\omega_j - \omega_j^{n-1}) = \cos(2\pi j/n).$$
The direct product for cycle graphs as $C_{n_1} \otimes \cdots \otimes C_{n_d}$, then the corresponding normalized adjacency matrix as follow:

$$A = \frac{1}{d} \sum_{i=1}^{d} I_{n_i} \otimes \cdots \otimes \frac{1}{2} A_{n_i} \otimes \cdots \otimes I_{n_d}$$  \hspace{1cm} (36)$$

where the $i$th term in the sum has $\frac{1}{2} A_{n_i}$ appearing in the $i$th place in the tensor product.

Then, we have

$$U_t = \exp(-iAt) = \prod_{i=1}^{d} I_{n_i} \otimes \cdots \otimes e^{-it\frac{1}{2d} A_{n_i}} \otimes \cdots \otimes I_{n_d}$$

$$= e^{-it\frac{1}{2d} A_{n_1}} \otimes \cdots \otimes e^{-it\frac{1}{2d} A_{n_d}}.$$ \hspace{1cm} (37)$$

Using the eigenvalues (35) and orthonormal eigenvectors $|F_j\rangle = \frac{1}{\sqrt{n}} |\omega_j\rangle$ (the columns of the Fourier matrix $F$ (7)) and the initial amplitude vector $|\psi_0\rangle = |0\rangle_1|0\rangle_2 \cdots |0\rangle_d$, then for $|\psi_t\rangle$, We have

$$|\psi_t\rangle = U_t|\psi_0\rangle = \prod_{i=1}^{d} \left( \frac{1}{n_i} \sum_{j=0}^{n_i-1} e^{-it\frac{1}{d} \cos(2\pi j/n_i)} |\omega_j\rangle_i \right)$$ \hspace{1cm} (38)$$

the especially, if $n_1 = n_2 = \cdots = n_d$, we have

$$|\psi_t\rangle = U_t|\psi_0\rangle = (e^{-it\frac{1}{2d} A_n}|0\rangle)^\otimes d = \left( \frac{1}{n} \sum_{j=0}^{n-1} e^{-it\frac{1}{d} \cos(2\pi j/n)} |\omega_j\rangle \right)^\otimes d = \left( \frac{1}{n} \sum_{j=0}^{n-1} e^{-it\frac{1}{d} \cos(2\pi j/n)} |\omega_j\rangle \right)^\otimes d$$ \hspace{1cm} (39)$$

Thus, for calculate the amplitude of particle, we using the amplitude the particle on the graph $G = C_n$ (i.e, $P_k(t) = \langle k|\psi_t\rangle = \frac{1}{n} \sum_{j=0}^{n-1} e^{-it\cos(2\pi j/n)\omega_j^k}$ with $t \rightarrow t/d$). Then, the amplitude for observing particle at the position $\vec{R}$ is

$$\langle \vec{R}|\psi_t\rangle = \prod_{i=1}^{d} P_{k_i}(t).$$ \hspace{1cm} (40)$$

One can show only for $d = 1$ with $n_1 = 3$ (i.e., $C_3$) and $d = 2$ with $n_1 = n_2 = 2$ (i.e., $C_4 = C_2 \otimes C_2$) have the instantaneous exactly uniform mixing property the continuous-time quantum walk model.

### 5.2 The Complete Graphs $K_n$

Let $\frac{1}{n-1} A_n$ be the normalized adjacency matrix of complete graph $K_n$. Thus, eigenvalues of $\frac{1}{n-1} A_n$ are 1 (once) and $-\frac{1}{n-1}$ (n-1 times). The corresponding normalized adjacency matrix of
Continuous-time classical and quantum Random walk

direct product complete graphs (i.e., $K_{n_1} \otimes \cdots \otimes K_{n_d}$) as follow:

$$A = \frac{1}{d} \sum_{i=1}^{d} I_{n_1} \otimes \cdots \otimes \frac{1}{n_i - 1} A_{n_i} \otimes \cdots \otimes I_{n_d} \quad (41)$$

where the $i$th term in the sum has $\frac{1}{n_i - 1} A_{n_i}$ appearing in the $i$th place in the tensor product. Then, we have

$$U_t = \exp(-iAt) = \prod_{i=1}^{d} I_{n_1} \otimes \cdots \otimes e^{-it\frac{1}{(n_i - 1)d} A_{n_i}} \otimes \cdots \otimes I_{n_d}$$

Using the orthonormal eigenvectors $|F_j\rangle = \frac{1}{\sqrt{n}} |\omega_j\rangle$ (the columns of the Fourier matrix $F$ (7)) and the initial amplitude vector $|\psi_0\rangle = |0\rangle_1 \cdots |0\rangle_d$, then for $|\psi_t\rangle$, We have

$$|\psi_t\rangle = U_t |\psi_0\rangle = \prod_{i=1}^{d} \left[ \frac{1}{n_i} (e^{-it\frac{1}{d}}) + (n_i - 1) e^{it\frac{1}{(n_i - 1)d}} \right] |0\rangle_i + \frac{1}{n_i} (e^{it\frac{1}{d}} - e^{it\frac{1}{(n_i - 1)d}}) \sum_{l=1}^{n_i-1} |l\rangle_i \quad (43)$$

Thus the probability of particle at the position $|\vec{K}\rangle = |i_1, i_2 \ldots i_d\rangle$, is as follow:

$$P_{\vec{K}}(t) = \prod_{l=1}^{d} \frac{1}{n_l} \left[ (e^{-it\frac{1}{d}}) + (n_l - 1) e^{it\frac{1}{(n_l - 1)d}} \right] \delta_{i_1,0} + \left( e^{it\frac{1}{d}} - e^{it\frac{1}{(n_l - 1)d}} \right) (1 - \delta_{i_1,0}) \quad (44)$$

The especially, if $n_1 = n_2 = \cdots = n_d = n$ we have

$$|\psi_t\rangle = \left[ \frac{1}{n} (e^{-it\frac{1}{d}}) + (n - 1) e^{it\frac{1}{(n - 1)d}} \right] |0\rangle + \frac{1}{n} (e^{it\frac{1}{d}} - e^{it\frac{1}{(n - 1)d}}) \left( |1\rangle + |2\rangle + \cdots + |n - 1\rangle \right) \quad (45)$$

and we see that the continuous-time quantum walk is equivalent to $d$ non-interacting $n$-state systems. Thus the amplitude for observing the particle at a position $\vec{k}$ is

$$\langle \vec{k} | \psi_t \rangle = \left[ \frac{1}{n} (e^{-it\frac{1}{d}}) + (n - 1) e^{it\frac{1}{(n - 1)d}} \right]^k \left[ \frac{1}{n} (e^{it\frac{1}{d}} - e^{it\frac{1}{(n - 1)d}}) \right]^{d-k} \quad (46)$$
where the $k$ is the number of zeroes. We can rewrite equation (46) with using the amplitude for observing the particle on the graph $K_n$ [23], i.e., if $\langle l|\phi_t \rangle$ and $\langle j|\phi_t \rangle$, amplitude of observing the particle at the site $|l\rangle = |0\rangle$ and $|j\rangle$ for $j \neq 0$ in the time-$t$, respectively, then

$$\langle \vec{k}|\psi_t \rangle = (\langle l|\phi_{t/d}\rangle)^k(\langle j|\phi_{t/d}\rangle)^{n-k}. \quad (47)$$

One can show only for $d = 1$ with $n = 2, 3, 4$ (i.e., $K_2, K_3$ and $K_4$) has the instantaneous exactly uniform mixing property the continuous-time quantum walk model.

### 5.3 Charter

As an example, direct product graphs for the continuous-time quantum walks, we can calculate the wave function $|\psi_t\rangle$ directly by exploiting the charters simple structure as a product simplex graph $K_2$ and cycle graph $C_n$. Let $G = Z_2 \otimes Z_n$ be a complete 2-partite graph where each partition has $n > 2$ vertices (the case $n = 2$ is the square graph). The direct product of complete graphs $K_2$ and cycle graph $C_n$ is $K_2 \otimes C_n$ such that the corresponding Laplacian as follow:

$$A = \frac{1}{2}(I_2 \otimes \frac{1}{2}A_n + \sigma_x \otimes I_n). \quad (48)$$

If $|\psi_0\rangle = |0_1\rangle|0_n\rangle$, then, for wave amplitude function $|\psi_t\rangle = e^{-it\sigma_x/2}|0_1\rangle \otimes e^{-it\sigma_y/2}|0_n\rangle$, we have

$$\langle k|\psi_t \rangle = \begin{cases} \frac{1}{n} \cos\left(\frac{t}{2}\right) \sum_{j=0}^{n-1} e^{-it(\cos(2\pi j/n))} \omega^{jk} & \text{for } k = 0, \ldots, n-1 \\ -\frac{i}{n} \sin\left(\frac{t}{2}\right) \sum_{j=0}^{n-1} e^{-it(\cos(2\pi j/n))} \omega^{jk} & \text{for } k = n, \ldots, 2n \end{cases} \quad (49)$$

Thus

$$P_k(t) = \begin{cases} \frac{1}{n^2} \cos^2\left(\frac{t}{2}\right) \sum_{l,j=0}^{n-1} e^{-it(\cos(2\pi j/n) - \cos(2\pi l/n))} \omega^{k(j-l)} & \text{for } k = 0, \ldots, n-1 \\ \frac{1}{n^2} \sin^2\left(\frac{t}{2}\right) \sum_{l,j=0}^{n-1} e^{-it(\cos(2\pi j/n) - \cos(2\pi l/n))} \omega^{k(j-l)} & \text{for } k = n, \ldots, 2n \end{cases} \quad (50)$$

Also, for above graph’s there isn’t exactly uniform mixing property under the continuous-time quantum walk model; but, for $n = 3$ and $n = 4$, there is property balanced (i.e., as example for $n = 3$ at $t = \frac{16l\pi}{3} \pm \frac{8l\pi}{3}$, $l \in Z$ the half of probabilities are constant and for other half there
is another constant amount). Furthermore, there isn’t average uniform mixing property under the continuous-time quantum walk model.

5.4 n-Cube

As an example direct product simplex graph for the continuous-time quantum walks, we can calculate the wave function $|\psi_t\rangle$ directly by exploiting the hypercubes simple structure as a product graph. The binary $n$-cube is defined over the set $(0,1)^n$ of $n$-cube binary sequence, where two sequence $x$ and $y$ are connected if they differ exactly in one bit position. As it turns out, the $n$-cube is also a complete graph.

The corresponding normalized adjacency matrix of hypercubes as direct product of $K_2$ as follow:

$$A = \frac{1}{n} \sum_{i=1}^{n} I_2 \otimes \cdots \otimes \sigma_x \otimes \cdots \otimes I_2$$ (51)

where the $i$th term in the sum has $\sigma_x$ (Pauli matrix) appearing in the $i$th place in the tensor product. Then, we have

$$U_t = \exp(-iAt) = \prod_{i=1}^{n} I_2 \otimes \cdots \otimes e^{i\sigma_x/n} \otimes \cdots \otimes I_2$$

$$= e^{i\sigma_x/n} \otimes \cdots \otimes e^{i\sigma_x/n} = (e^{i\sigma_x/n})^n$$

$$= \left( \begin{array}{cc} \cos(t/n) & isin(t/n) \\ isin(t/n) & \cos(t/n) \end{array} \right)^n$$ (52)

where $B^n$ is the tensor product of $n$ copies of $B$. If $|\psi_0\rangle = |0\rangle^n$, then

$$|\psi_t\rangle = U_t|\psi_0\rangle = [\cos(t/n)|0\rangle + isin(t/n)|1\rangle]^n$$ (53)

and we see that the continuous-time quantum walk is equivalent to $n$ non-interacting one-qubit systems. Then the amplitude for observing the particle at a position $\vec{k}$ with Hamming weight $k$ is

$$\langle \vec{k}|\psi_t\rangle = (\cos\frac{t}{n})^{n-k}(isin\frac{t}{n})^k.$$ (54)
We can rewrite equation (54) with using the amplitude for observing the particle on the graph $G = Z_2$, i.e., if $\langle 0 | \phi_t \rangle$ and $\langle 1 | \phi_t \rangle$, amplitude of observing for particle, respectively at the site $|0\rangle$ and $|1\rangle$ in the time-$t$, then

$$\langle \vec{k} | \psi_t \rangle = (\langle 0 | \phi_{t/n} \rangle)^{n-k} (\langle 1 | \phi_{t/n} \rangle)^k.$$  

(55)

This implies that for $t = (2k - 1)\frac{1}{\pi} n$, where $k \in Z^+$, we have $P_k(t) = 2^{-n}$, the uniform distribution.

6 Conclusion

We have defined direct product of graphs and have given a recipe for obtained probability of observing particle on vertices in the continuous-time classical and quantum random walk. In the recipe the probability of observing particle on direct product of graphs are obtained by multiplication of probability on the corresponding to sub-graphs. Also, we have shown in the classical state the stationary uniform distribution is reached as $t \longrightarrow \infty$ but for quantum state is not satisfy. This recipe is useful to determine probability of walk on complicated graphs. Using this method, we have calculated the probability of continuous-time classical and quantum walk on many of finite direct product cayley graphs (complete cycle, complete $K_n$, charter and $n$-cube).

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