Investigation of continuous-time quantum walk by using Krylov subspace-Lanczos algorithm

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Abstract

In papers[1, 2], the amplitudes of continuous-time quantum walk on graphs possessing quantum decomposition (QD graphs) have been calculated by a new method based on spectral distribution associated to their adjacency matrix. Here in this paper, it is shown that the continuous-time quantum walk on any arbitrary graph can be investigated by spectral distribution method, simply by using Krylov subspace-Lanczos algorithm to generate orthonormal bases of Hilbert space of quantum walk isomorphic to orthogonal polynomials. Also new type of graphs possessing generalized quantum decomposition have been introduced, where this is achieved simply by relaxing some of the constrains imposed on QD graphs and it is shown that both in QD and GQD graphs, the unit vectors of strata are identical with the orthonormal basis produced by Lanczos algorithm. Moreover, it is shown that probability amplitude of observing walk at a given vertex is proportional to its coefficient in the corresponding unit vector of its stratum, and it can be written in terms of the amplitude of its stratum. Finally the capability of Lanczos-based algorithm for evaluation of walk on arbitrary graphs (GQD or non-QD types), has been tested by calculating the probability amplitudes of quantum walk on some interesting finite (infinite) graph of GQD type and finite (infinite) path graph of non-GQD type, where the asymptotic behavior of the probability amplitudes at infinite limit of number of vertices, are in agreement with those of central limit theorem of Ref.[3].

Keywords: Continuous-time quantum walk, Spectral distribution, Graph, Krylov subspace, Lanczos algorithm.

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1 Introduction

Random walks on graphs are the basis of a number of classical algorithms. Examples include 2-SAT (satisfiability for certain types of Boolean formulas), graph connectivity, and finding satisfying assignments for Boolean formulas. It is this success of random walks that motivated the study of their quantum analogs in order to explore whether they might extend the set of quantum algorithms.

Recently, the quantum analogue of classical random walks has been studied in a flurry of works [4, 5, 6, 7, 8, 9]. The works of Moore and Russell [8] and Kempe [9] showed faster bounds on instantaneous mixing and hitting times for discrete and continuous quantum walks on a hypercube (compared to the classical walk).

A study of quantum walks on simple graph is well known in physics (see [10]). Recent studies of quantum walks on more general graphs were described in [4, 5, 7, 11, 12]. Some of these works studies the problem in the important context of algorithmic problems on graphs and suggests that quantum walks is a promising algorithmic technique for designing future quantum algorithms. One approach for investigation of continuous-time quantum walk on graphs is using the spectral distribution associated with the adjacency matrix of graphs. Authors in [1, 2] have introduced a new method for calculating the probability amplitudes of quantum walk based on spectral distribution, where a canonical relation between the Hilbert space of stratification corresponding to the graph and a system of orthogonal polynomials has been established, which leads to the notion of quantum decomposition (QD) introduced in [13, 14] for the adjacency matrix of graph. Also it is shown in [1] that by using spectral distribution one can approximate long time behavior of continuous-time quantum walk on infinite graphs with finite ones and vice versa. In [1, 2], only the particular graphs of QD type have been studied .

Here in this work we try to investigate continuous-time quantum walk on arbitrary graphs.
by spectral distribution method. To this aim, first by turning the graphs into a metric space based on distance function, we have been able to generalize the stratification and quantum decomposition introduced in [13], such that the basis of Hilbert space of quantum walk consist of superposition of quantum kets of vertices belonging to the same stratum, but with different coefficients, while the coefficients are the same in QD case, therefore QD graphs introduced in [1, 13] are particular kind of graphs possessing generalized quantum decomposition (GQD).

Then we show that both in QD and GQD graphs, the unit vectors of strata are identical with the orthonormal basis produced by Lanczos algorithm. Also, in the case of GQD graphs we show that probability amplitude of observing walk at a given vertex is proportional to its coefficient in corresponding unit vector of its stratum, and it can be written in terms of the amplitude of its stratum. For more general graphs, the Lanczos algorithm transforms the adjacency matrix into a tridiagonal form (quantum decomposition) iteratively, where we use this fact for studying non-QD type graphs. Indeed, the Lanczos algorithm gives a three-term recursion structure to the graph, so the spectral distribution associated to adjacency matrix can be determined by Stieltjes transform. In order to see the power of Lanczos-based algorithm in the investigation of continuous-time quantum walk on arbitrary graphs (GQD or non-QD types), we have calculated the amplitudes of quantum walk on some interesting finite (infinite) graph of GQD type and finite (infinite) path graph of non-GQD type.

The organization of the paper is as follows. In section 2, we review the Krylov subspace methods and Lanczos algorithm. In Section 3, we give a brief outline of some of the main features of graphs and introduce generalized stratification. Section 4 is concerned with the Hilbert space of generalized stratification. In Section 5, we review the Stieltjes transform method for obtaining spectral distribution $\mu$, and establish an isometry between orthogonal polynomials and Hilbert space of generalized stratification. Section 6 is devoted to the method for computing amplitudes of continuous-time quantum walk, through spectral distribution $\mu$ of the adjacency matrix $A$. In section 7 we calculate the amplitudes of quantum walk on some
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interesting finite (infinite) graph of GQD type and finite (infinite) path graph of non-GQD type. At the end we study the asymptotic behavior the probability amplitudes at infinite limit of number of vertices, where the results thus obtained are in agreement with those of central limit theorem of Ref.[3]. Paper is ended with a brief conclusion together with two appendices.

2 Krylov subspace-Lanczos algorithm

In this section we give a brief review of some of the main features of Krylov subspace projection methods and Lanczos algorithm and more details are referred to [15, 16, 17, 18].

Krylov subspace projection methods (KSPM) are probably the most important class of projection methods for linear systems and for eigenvalue problems. In KSPM, approximations to the desired eigenpairs of an $n \times n$ matrix $A$ are extracted from a $d$-dimensional Krylov subspace

$$K_d(|\phi_0\rangle, A) = span\{|\phi_0\rangle, A|\phi_0\rangle, \cdots, A^{d-1}|\phi_0\rangle\},$$

(2-1)

where $|\phi_0\rangle$ is often a randomly chosen starting vector called reference state and $d \ll n$. In practice, the retrieval of desired spectral information is accomplished by constructing an orthonormal basis $V_d \in R^{n \times d}$ of $K_d(|\phi_0\rangle, A)$ and computing eigenvalues and eigenvectors of the $d$ by $d$ projected matrix $H_d = P_{V_d}^T A P_{V_d}$, where $P_{V_d}$ is projection operator to $d$-dimensional subspace spanned by the basis $V_d$.

The most popular algorithm for finding an orthonormal basis for the Krylov subspace, is Lanczos algorithm. The Lanczos algorithm transforms a Hermitian matrix $A$ into a tridiagonal form iteratively, i.e., the matrix $A$ will be of tridiagonal form in the $d$-dimensional projected subspace $H_d$. In fact, the Lanczos algorithm is deeply rooted in the theory of orthogonal polynomials, which builds an orthonormal sequence of vectors $\{|\phi_0\rangle, |\phi_1\rangle, \ldots, |\phi_{d-1}\rangle\}$ and satisfy the following three-term recursion relations

$$A|\phi_i\rangle = \beta_{i+1}|\phi_{i+1}\rangle + \alpha_i|\phi_i\rangle + \beta_i|\phi_{i-1}\rangle.$$  

(2-2)
The vectors \( |\phi_i\rangle, i = 0, 1, ..., d - 1 \) form an orthonormal basis for the Krylov subspace \( K_d(|\phi_0\rangle, A) \). In these basis, the matrix \( A \) is projected to the following symmetric tridiagonal matrix:

\[
L_j = \begin{pmatrix}
\alpha_0 & \beta_1 & 0 & \ldots & \ldots \\
\beta_1 & \alpha_1 & \beta_2 & 0 & \ldots \\
0 & \beta_2 & \alpha_3 & \beta_3 & \ldots \\
\ldots & \ldots & \ldots & \ldots & \ldots \\
\ldots & \ldots & 0 & \beta_{d-1} & \alpha_{d-1}
\end{pmatrix},
\]

where the scalars \( \beta_{i+1} \) and \( \alpha_i \) are computed to satisfy two requirements, namely that \( |\phi_{i+1}\rangle \) be orthogonal to \( |\phi_i\rangle \) and that \( \| |\phi_{i+1}\rangle \| = 1 \).

In fact, the Lanczos algorithm is a modified version of the classical Gram-Schmidt orthogonalization process. As it can be seen, at its heart is an efficient three-term recursion relation which arises because the matrix \( A \) is real and symmetric.

If we define the Krylov matrix \( K \) such that the columns of \( K \) are Krylov basis \( \{A^i|\phi_0\rangle; i = 0, ..., d - 1\} \) as:

\[
K := (|\phi_0\rangle, A|\phi_0\rangle, ..., A^{d-1}|\phi_0\rangle),
\]

the application of the orthonormalization process to the Krylov matrix is equivalent to the construction of an upper triangular matrix \( P \) such that the resulting sequence \( \Phi = KP \) satisfies \( \Phi^\dagger \Phi = 1 \). We denote by \( |\phi_j\rangle \) and \( P_j \) respectively the \( j \)-th column of \( \Phi \) and \( P \). Then we have

\[
\langle \phi_0|P_i^\dagger(A)P_j(A)|\phi_0\rangle = \langle KP_i|KP_j\rangle = \langle \phi_i|\phi_j \rangle, \tag{2-3}
\]

where \( P_i = a_0 + a_1 A + ... + a_i A^i \) is a polynomial of degree \( i \) in indeterminate \( A \).

In the remaining part of this section we give an algorithmic outline of the Lanczos algorithm, where it will be used in calculation of amplitudes of continuous-time quantum walk.

**Lanczos algorithm**

Input: Matrix \( A \in \mathbb{R}^{n \times n} \), starting vector \( |\phi_0\rangle \), \( \| |\phi_0\rangle \| = 1 \), scalar \( d \)
Output: Orthogonal basis \( \{ |\phi_0\>, ..., |\phi_{d-1}\> \} \) of Krylov subspace \( K_d(|\phi_0\>, A) \)

\[
\beta_0 = 0, |\phi_0\> = |\phi\>/\|\phi\|
\]

for \( i = 0, 1, 2, ... \)

\[
|v_i\> = A|\phi_i\>
\]

\[
\alpha_i = \langle \phi_i | v_i \rangle
\]

\[
|v_{i+1}\> = |v_i\> - \beta_i |\phi_{i-1}\> - \alpha_i |\phi_i\>
\]

\[
\beta_{i+1} = \| |v_{i+1}\> \|
\]

if

\[
\beta_{i+1} \neq 0
\]

\[
|\phi_{i+1}\> = |v_{i+1}\>/\beta_{i+1}
\]

else

\[
|\phi_{i+1}\> = 0.
\]

3 Graphs, adjacency matrix and generalized stratification

In this section we give a brief outline of some of the main features of graphs such as adjacency matrix, distance function and then by turning the graphs into a metric space based on distance function, we have been able to generalize the stratification introduced in [13]. A graph is a pair \( \Gamma = (V, E) \), where \( V \) is a non-empty set and \( E \) is a subset of \( \{ (\alpha, \beta); \alpha, \beta \in V, \alpha \neq \beta \} \). Elements of \( V \) and of \( E \) are called vertices and edges, respectively. Two vertices \( \alpha, \beta \in V \) are called adjacent if \( (\alpha, \beta) \in E \), and in that case we write \( \alpha \sim \beta \). For a graph \( \Gamma = (V, E) \) we define the adjacency matrix \( A \) by
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\[ A_{\alpha \beta} = \begin{cases} 
1 & \text{if } \alpha \sim \beta \\
0 & \text{otherwise.} 
\end{cases} \]

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 \( \alpha \in V \) is defined by

\[ \kappa(\alpha) = |\{\beta \in V; \alpha \sim \beta\}|, \]

where \( | \cdot | \) denotes the cardinality and \( \kappa(\alpha) \) is finite for all \( \alpha \in V \) (local boundedness). A finite sequence \( \alpha_0, \alpha_1, ..., \alpha_n \in V \) is called a walk of length \( n \) (or of \( n \) steps) if \( \alpha_{k-1} \sim \alpha_k \) for all \( k = 1, 2, ..., n \). For \( \alpha \neq \beta \) let \( \partial(\alpha, \beta) \) be the length of the shortest walk connecting \( \alpha \) and \( \beta \). By definition \( \partial(\alpha, \alpha) = 0 \) for all \( \alpha \in V \) and \( \partial(\alpha, \beta) = 1 \) if and only if \( \alpha \sim \beta \). Therefore, graphs become metric space with respect to above defined distance function \( \partial \).

Now, in the remaining part of this section we try to define generalized stratification based on distance function. To this aim, similar to association scheme [19] we define a partition (called distance partition) on \( V \times V \), i.e., \( V \times V = \bigcup_i \Gamma_i \) based on distance function \( \partial \), where the subset \( \Gamma_i \) are defined by

\[ \Gamma_i = \{(\alpha, \beta) \in V \times V|\partial(\alpha, \beta) = i\}. \]  

(3-4)

Using above distance partition one can define the set \( \Gamma_i(\alpha) \) (\( i \)-th neighborhood of vertex \( \alpha \)) as

\[ \Gamma_i(\alpha) = \{\beta \in V|(\alpha, \beta) \in \Gamma_i\}. \]  

(3-5)

Obviously the class of subsets \( \Gamma_i(\alpha) \) defined above partition \( V \) as

\[ V = \bigcup_i \Gamma_i(\alpha), \]  

(3-6)
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(see Fig.1). As we see the graph is stratified into a disjoint union of strata, hence we call it the generalized stratification based on distance function with respect to vertex $\alpha$, where the vertex $\alpha$ is referred to as a reference state (see Fig.2).

In this stratification for any connected graph $\Gamma$, we have

$$\Gamma_1(\beta) \subseteq \Gamma_{i-1}(\alpha) \cup \Gamma_i(\alpha) \cup \Gamma_{i+1}(\alpha),$$

for each $\beta \in \Gamma_i(\alpha)$.

Obviously above relations are similar to those of distance regular graphs [19], where in the later case the sets $\Gamma_i$ form an association scheme and the stratification $\Gamma_i(\alpha)$ is independent of reference state $\alpha$, but in an arbitrary graph the generalized stratification depends on the choice of reference state.

In order to study continuous-time quantum walk on a given graph via stratification, we define in the following section a Hilbert space which is suitable for Lanczos algorithm.

4 Hilbert space for the generalized stratification

Hereafter, we fix a point $o \in V$ as a reference state of the graph then with each stratum $\Gamma_k(o)$ we associate a unit vector $|\phi_k\rangle$ in $l^2(V)$ called unit vector of $k$-th stratum. The closed subspace of $l^2(V)$ spanned by $\{|\phi_k\rangle\}$ is denoted by $\Lambda(\Gamma)$. In section 6, we will deal with continuous-time quantum walk, where $\Lambda(\Gamma)$ will be referred as walk space denoted by $V_{\text{walk}}$, i.e., the strata $\{|\phi_k\rangle\}$ span a closed subspace, where the quantum walk remains on it forever.

Since $\{|\phi_k\rangle\}$ become a complete orthonormal basis of $\Lambda(\Gamma)$, we often write

$$\Lambda(\Gamma) = \sum_k \oplus C|\phi_k\rangle.$$  \hspace{1cm} (4-8)$$

Then for each stratum $\Gamma_k(o)$ of generalized stratification, the unit vector associated to $k$-th stratum is defined by

$$|\phi_k\rangle = \frac{1}{\sqrt{\sum_{\alpha} g_{k,\alpha}^2} \sum_{\alpha \in \Gamma_k(o)} g_{k,\alpha}} |k, \alpha\rangle,$$  \hspace{1cm} (4-9)$$
where, $|k, \alpha\rangle$ denotes the eigenket of $\alpha$-th vertex at the stratum $k$ and integers $g_{k,\alpha} \geq 1$ for each $\alpha \in \Gamma_k(o)$. We refer to a graph as GQD graph if the coefficients $g_{k,\alpha}$ satisfy conditions appearing in appendix A (the conditions (A-ii) through (A-iv)).

By choosing $g_{k,\alpha} = 1$ for each $\alpha \in \Gamma_k(o)$, Eq.(4-9) reduces to

$$|\phi_k\rangle = \frac{1}{\sqrt{|\Gamma_k(o)|}} \sum_{\alpha \in \Gamma_k(o)} |k, \alpha\rangle,$$  
\hspace{1cm} (4-10)

where, $|\phi_k\rangle$, $k = 0, 1, 2, ...$ correspond to unit vectors of QD graphs of Ref.[1].

In the following we show that, for the QD type graphs the unit vectors of strata given in Eq.(4-10), are the same as the orthonormal basis produced via Lanczos algorithm (this is true for GQD graphs too, where its proof is referred to appendix A.). To do so, let us consider the action of adjacency matrix $A$ over $|\phi_k\rangle$ as

$$A|\phi_k\rangle = \frac{1}{\sqrt{|\Gamma_k(o)|}} \sum_{\alpha \in \Gamma_k(o)} A|k, \alpha\rangle$$

$$= \frac{1}{\sqrt{|\Gamma_k(o)|}} \sum_{\alpha \in \Gamma_k(o)} \sum_{\nu \in \Gamma_k(o), \nu \sim \alpha} |k+1, \nu\rangle + \frac{1}{\sqrt{|\Gamma_k(o)|}} \sum_{\alpha \in \Gamma_k(o)} \sum_{\nu \in \Gamma_k(o), \nu \sim \alpha} |k, \nu\rangle$$

$$+ \frac{1}{\sqrt{|\Gamma_k(o)|}} \sum_{\alpha \in \Gamma_k(o)} \sum_{\nu \in \Gamma_k(o), \nu \sim \alpha} |k-1, \nu\rangle = \frac{|\Gamma_{k+1}(o)|}{|\Gamma_k(o)|} \sum_{\nu \in \Gamma_{k+1}(o)} \lambda_{k+1}(\nu) |k+1, \nu\rangle$$

$$+ \frac{|\Gamma_{k-1}(o)|}{|\Gamma_k(o)|} \sum_{\nu \in \Gamma_{k-1}(o)} \lambda_k(\nu) |k, \nu\rangle + \lambda_k(\nu) |k-1, \nu\rangle.$$  
\hspace{1cm} (4-11)

By defining $\beta_k = \frac{|\Gamma_k|}{|\Gamma_{k-1}|}^{1/2} \lambda_k(\nu)$, $\lambda_k(\nu) = |\{\alpha \in \Gamma_{k-1}(o); \alpha \sim \nu\}|$ and $\alpha_k = |\{\nu \in \Gamma_k; \nu \sim \alpha\}|$ for $\alpha, \nu \in \Gamma_k(o)$, the three-term recursion relations (4-11) reduce to those given in (2-2).

Therefore, the adjacency matrix takes a tridiagonal form in the basis $|\phi_k\rangle$ (orthonormal basis associated with strata), consequently these basis are identical with the orthonormal basis produced by Lanczos algorithm.
5  Spectral distribution of the adjacency matrix $A$

It is well known that, for any pair $(A, |φ_0⟩)$ of a matrix $A$ and a vector $|φ_0⟩$, it can be assigned a measure $μ$ as follows

$$μ(x) = ⟨φ_0|E(x)|φ_0⟩, \quad (5-12)$$

where $E(x) = \sum_i |u_i⟩⟨u_i|$ is the operator of projection onto the eigenspace of $A$ corresponding to eigenvalue $x$, i.e.,

$$A = \int xE(x)dx. \quad (5-13)$$

It is easy to see that, for any polynomial $P(A)$ we have

$$P(A) = \int P(x)E(x)dx, \quad (5-14)$$

where for discrete spectrum the above integrals are replaced by summation.

Actually the spectral analysis of operators is an important issue in quantum mechanics, operator theory and mathematical physics [20, 21]. As an example $μ(dx) = |ψ(x)|^2dx$ ($μ(dp) = |ψ(p)|^2dp$) is a spectral distribution which is assigned to the position (momentum) operator $\hat{X}(\hat{P})$. Moreover, in general quasi-distributions are the assigned spectral distributions of two hermitian non-commuting operators with a prescribed ordering. For example the Wigner distribution in phase space is the assigned spectral distribution for two non-commuting operators $\hat{X}$ (shift operator) and $\hat{P}$ (momentum operator) with Wyle-ordering among them [22, 23].

Here in this paper we are concerned with spectral distribution of adjacency matrices of graphs, since the spectrum of a given graph can be determined by spectral distribution of its adjacency matrix $A$.

Therefore, using the relations (5-12) and (5-14), the expectation value of powers of adjacency matrix $A$ over starting site $|φ_0⟩$ can be written as

$$⟨φ_0|A^m|φ_0⟩ = \int_R x^mμ(dx), \quad m = 0, 1, 2, ... \quad (5-15)$$
The existence of a spectral distribution satisfying (5-15) is a consequence of Hamburgers theorem, see e.g., Shohat and Tamarkin [24, Theorem 1.2].

Obviously relation (5-15) implies an isomorphism from the Hilbert space of generalized stratification onto the closed linear span of the orthogonal polynomials with respect to the measure $\mu$. Since, from the orthogonality of vectors $|\phi_j\rangle$ (Hilbert space of generalized stratification) produced from Lanczos algorithm process we have,

$$
\delta_{ij} = \langle \phi_i | \phi_j \rangle = \langle \phi_0 | P_i^\dagger(A) P_j(A) | \phi_0 \rangle \\
= \int P_i^*(x) P_j(x) \mu(x) dx = (P_i, P_j)_\mu.
$$

(5-16)

Conversely if $P_0, ..., P_{n-1}$ is the system of orthonormal polynomials for the measure $\mu$ then the vectors

$$
|\phi_j\rangle = P_j(A) |\phi_0\rangle,
$$

(5-17)

will coincide with the sequence of orthonormal vectors produced by the Lanczos algorithm applied to $(A, |\phi_0\rangle)$.

Now, substituting (5-17) in (2-2), we get three term recursion relations between polynomials $P_j(A)$, which leads to the following three term recursion between polynomials $P_j(x)$

$$
\beta_{k+1} P_{k+1}(x) = (x - \alpha_k) P_k(x) - \beta_k P_{k-1}(x)
$$

(5-18)

for $k = 0, ..., n - 1$.

Multiplying by $\beta_1...\beta_k$ we obtain

$$
\beta_1...\beta_{k+1} P_{k+1}(x) = (x - \alpha_k) \beta_1...\beta_k P_k(x) - \beta_k^2 \beta_1...\beta_{k-1} P_{k-1}(x).
$$

(5-19)

By rescaling $P_k$ as $P'_k = \beta_1...\beta_k P_k$, the spectral distribution $\mu$ under question is characterized by the property of orthonormal polynomials $\{P'_n\}$ defined recurrently by

$$
P'_0(x) = 1, \quad P'_1(x) = x, \\
x P'_k(x) = P'_{k+1}(x) + \alpha_k P'_k(x) + \beta_k^2 P'_{k-1}(x),
$$

(5-20)
for $k \geq 1$.

If such a spectral distribution is unique, the spectral distribution $\mu$ is determined by the identity:

$$G_\mu(z) = \int_R \frac{\mu(dx)}{z-x} = \frac{1}{z-\alpha_0 - \frac{\beta_1^2}{z-\alpha_1 - \frac{\beta_2^2}{z-\alpha_2 - \frac{\beta_3^2}{z-\alpha_3 - \cdots}}} = \frac{Q^{(1)}_{n-1}(z)}{P_n'(z)} = \sum_{l=1}^{n} \frac{A_l}{z-x_l}, \quad (5-21)$$

where $G_\mu(z)$ is called the Stieltjes transform of spectral distribution $\mu$ and polynomials $\{Q_k^{(1)}\}$ are defined recurrently as

$$Q_0^{(1)}(x) = 1, \quad Q_1^{(1)}(x) = x - \alpha_1$$

and

$$xQ_k^{(1)}(x) = Q_{k+1}^{(1)}(x) + \alpha_{k+1}Q_k^{(1)}(x) + \beta_{k+1}^2Q_{k-1}^{(1)}(x), \quad (5-22)$$

for $k \geq 1$. The coefficients $A_l$ appearing in (5-21) are the same Guass quadrature constants which are calculated as

$$A_l = \lim_{z \to x_l} (z-x_l)G_\mu(z), \quad (5-23)$$

where, $x_l$ are the roots of polynomial $P_n'(x)$.

Now let $G_\mu(z)$ is known, then the spectral distribution $\mu$ can be recovered from $G_\mu(z)$ by means of the Stieltjes inversion formula as

$$\mu(y) - \mu(x) = -\frac{1}{\pi} \lim_{\nu \to 0^+} \int_x^y \text{Im}\{G_\mu(u+iv)\}du. \quad (5-24)$$

Substituting the right hand side of (5-21) in (5-24), the spectral distribution can be determined in terms of $x_l, l = 1, 2, \ldots$ and Guass quadrature constants $A_l, l = 1, 2, \ldots$ as

$$\mu = \sum_l A_l \delta(x - x_l) \quad (5-25)$$

( for more details see Ref. [14, 24, 25, 26]).

Finally, using the relation (5-17) and the recursion relations (5-20) of polynomial $P'_k(x)$, the other matrix elements $\langle \phi_k | A^m | \phi_0 \rangle$ can be calculated as

$$\langle \phi_k | A^m | \phi_0 \rangle = \frac{1}{\beta_1 \beta_2 \cdots \beta_k} \int_R x^m P'_k(x) \mu(dx), \quad m = 0, 1, 2, \ldots \quad (5-26)$$
6 Investigation of Continuous-time quantum walk on an arbitrary graph via spectral distribution of its adjacency matrix

Our main goal in this paper is the evaluation of probability amplitudes for continuous-time quantum walk by using Eq.(5-26), such that we have

\[ q_k(t) = \langle \phi_k | e^{-iAt} | \phi_0 \rangle = \frac{1}{\beta_1 \beta_2 \cdots \beta_k} \int_R e^{-ixt} P'_k(x) \mu(dx), \]  

(6-27)

where \( q_k(t) \) is the amplitude of observing the walk at stratum \( k \) at time \( t \). The conservation of probability \( \sum_{k=0} |q_k(t)|^2 = 1 \) follows immediately from Eq.(6-27), simply by using the completeness relation of orthogonal polynomials \( P'_k(x) \).

Investigation of continuous-time quantum walk via spectral distribution method, pave the way to approximate infinite graphs with finite ones and vice versa, simply via Gauss quadrature formula, where in cases of infinite graphs, one can study asymptotic behavior of walk at large enough times by using the method of stationary phase approximation (for more details see [1]).

One should note that, the spectral distribution is Fourier transform of the amplitude of observing the walk at starting site at time \( t \), i.e.,

\[ q_0(t) = \int e^{-ixt} \mu(x) dx \quad \mapsto \quad \mu(x) = \frac{1}{2\pi} \int e^{ixt} q_0(t) dt. \]  

(6-28)

Above relations imply that

\[ q_k(t) = \frac{1}{\beta_1 \beta_2 \cdots \beta_k} \int P'_k(x)e^{-ixt} \mu(x) dx = \frac{1}{2\pi \beta_1 \beta_2 \cdots \beta_k} \int P'_k(x)q_0(t')e^{-ix(t-t')} dt'dx, \]  

(6-29)

therefore, the amplitudes \( q_k(t) \) can be written in terms of the amplitude \( q_0(t) \).

Obviously for finite graphs, the formula (6-27) yields

\[ q_k(t) = \frac{1}{\beta_1 \beta_2 \cdots \beta_k} \sum_i A_i e^{-ixt} P'_k(x_i), \]  

(6-30)
where by straightforward calculation one can evaluate the average probability for the finite graphs as

\[
P(k) = \lim_{T \to \infty} \frac{1}{T} \int_{0}^{T} |q_k(t)|^2 \, dt = \frac{1}{\beta_1 \beta_2 \cdots \beta_k} \sum_{l} A_l^2 P_k^2(x_l). \tag{6-31}
\]

In appendix I of Ref.[1] it is proved that for QD graphs the amplitudes on the vertices belonging to the one stratum is the same, hence the probability of observing the walk at a site belonging to stratum \(k\) is equal to \(\frac{|q_k(t)|^2}{|\Gamma_k(0)|}\). Unfortunately for non-QD graphs the lemma appearing in appendix I of Ref.[1] is not true any more, consequently the probability amplitudes of observing walk at sites can not be obtained from those of strata in a simple way and reader can follow the details of calculation of amplitudes in appendix B.

7 Examples

7.1 Generalized QD graphs

Here in this subsection we give examples of GQD type graphs. These graphs look like kite and they are embedded in \(Z^k, k = 2, 3, \ldots\) lattices and defined as follows: Let \(K(k,n)\) be an \(k\)-dimensional lattice graph with \(n + 1\) generalized strata, which consists of vertices \((0,0,...,0), (l,0,...,0), (0,l,0,...,0), \ldots, (0,0,...0,l)\) and \((l,l,...,l)\) only for odd values of \(l\), where \(l = 0,1,...,n\). The vertex \((0,0,...,0)\) is connected to vertices \((1,0,...,0), (0,1,...,0), \ldots, (0,0,...,1)\), the vertex \((0,...,0, l,0,...,0)\) is connected to vertices \((0,...,0, l-1,0,...,0)\) and \((0,...,0, l+1,0,...,0)\) for each \(i = 1,...,k\), but for odd values of \(l\), there is an extra connection between \((0,...,0, l,0,...,0)\) and \((l,l,...,l)\) (see Fig.3 for \(k = 2, n = 6\)).

Now, we define unit vectors of generalized strata in such a way that, they coincide with the orthonormal basis produced by lanczos algorithm (see appendix A)

\[
|\phi_0\rangle = |0,0,...,0\rangle
\]
continuous-time Quantum walk

\[ |\phi_1\rangle = \frac{1}{\sqrt{k}} \sum_{\text{perm.}} |1, 0, ..., 0\rangle \]

\[ |\phi_2\rangle = \frac{1}{\sqrt{k(k+1)}} \left( \sum_{\text{perm.}} |2, 0, ..., 0\rangle + k|1, 1, ..., 1\rangle \right) \]

\[ \vdots \]

\[ |\phi_{2l-1}\rangle = \frac{1}{\sqrt{k}} \sum_{\text{perm.}} |2l-1, 0, ..., 0\rangle \]

\[ |\phi_{2l}\rangle = \frac{1}{\sqrt{k(k+1)}} \left( \sum_{\text{perm.}} |2l, 0, ..., 0\rangle + k|2l-1, 2l-1, ..., 2l-1\rangle \right), \tag{7-32} \]

where, the summations are taken over all possible permutations. Using the relations (A-ii)-(A-iv), one can show that the coefficients \( \beta_i \) and \( \alpha_i \) are

\[ \beta_1^2 = k, \quad \beta_2^2 = \beta_3^2 = \ldots = k + 1 \quad \text{and} \quad \alpha_i = 0, \quad i = 1, 2, \ldots \tag{7-33} \]

Now, one can study quantum continuous time walk on these graphs for finite values of \( n \) simply by following the general prescriptions, but here we restrict ourselves to infinite \( n \). Substituting coefficients \( \beta_i \) and \( \alpha_i \) in (5-21), the Stieltjes transform \( G_\mu(z) \) of spectral distribution \( \mu \) takes the following form

\[ G_\mu(z) = \frac{1}{z - \frac{k}{z - \frac{k+1}{z - \frac{k+1}{z - \ldots}}}}. \tag{7-34} \]

In order to evaluate above infinite continued fraction, we need first to evaluate the following infinite continued fraction defined as

\[ \tilde{G}(z) = \frac{1}{z - \frac{k+1}{z - \frac{k+1}{z - \ldots}}} = \frac{1}{z - (k+1)\tilde{G}(z)}, \tag{7-35} \]

where by solving above equation, we get

\[ \tilde{G}(z) = \frac{z - \sqrt{z^2 - 4(k+1)}}{2(k+1)}. \tag{7-36} \]

Inserting (7-36) in (7-35), we get

\[ G_\mu(z) = \frac{1}{z - k\tilde{G}_\mu(z)}, \tag{7-37} \]
then substituting (7-36) in (7-37), we obtain the following expression for Stieltjes transform of $\mu$

$$G_{\mu}(z) = \frac{(k + 2)z - k\sqrt{z^2 - 4(k + 1)}}{2(k^2 + z^2)}, \quad (7-38)$$

finally by applying Stieltjes inversion formula, we get the absolutely continuous part of spectral distribution $\mu$ as follows

$$\mu(x) = \frac{k}{2\pi} \frac{\sqrt{4(k + 1) - x^2}}{k^2 + x^2}, \quad |x| \leq 2\sqrt{k + 1}. \quad (7-39)$$

Now, we study the probability amplitudes of walk at time $t$ in the limit of large $k$, i.e.,

$$q_l(t) = \lim_{k \to \infty} \langle \phi_l | e^{\frac{-iAt}{k}} | \phi_0 \rangle = \lim_{k \to \infty} \frac{1}{\sqrt{k(k + 1)^{l-1}}} \int_{-2\sqrt{k+1}}^{2\sqrt{k+1}} e^{-ixt} P'_l(x) \frac{k}{2\pi} \sqrt{4(k + 1) - x^2} dx$$

$$= \lim_{k \to \infty} \frac{1}{2\pi \sqrt{k(k + 1)^{l-1}}} \int_{-2\sqrt{k+1}}^{2\sqrt{k+1}} e^{-ixt} P'_l(\sqrt{kx}) \frac{\sqrt{4(k + 1)/k - x^2}}{1 + x^2/k} dx \quad (7-40)$$

$$= \frac{1}{2\pi} \int_{-2}^{2} e^{-ixt} P'_{l,\infty}(x) \sqrt{4 - x^2} dx = \frac{2}{\pi} \int_{-1}^{1} e^{-2ixt} P'_{l,\infty}(2x) \sqrt{1 - x^2} dx,$$

where the polynomial $P'_{l,\infty}(x)$ is defined by

$$P'_{l,\infty}(x) = \lim_{k \to \infty} \frac{1}{\sqrt{k(k + 1)^{l-1}}} P'_l(\sqrt{kx}). \quad (7-41)$$

Now, substituting $\beta_i$ and $\alpha_i$ from (7-33) in three-term recursion relations (5-20), we obtain the following relations for polynomials $P'_l(x)$

$$P'_0(\sqrt{kx}) = 1,$$

$$P'_1(\sqrt{kx}) = \sqrt{kx},$$

$$P'_2(\sqrt{kx}) = kx^2 - k,$$

$$\sqrt{kx} P'_1(\sqrt{kx}) = P'_{l+1}(\sqrt{kx}) + (k + 1)P'_{l-1}(\sqrt{kx}), \quad l = 3, 4, \ldots . \quad (7-42)$$

Then dividing left and right hand sides of the recursion relations in (7-42) by $\sqrt{k(k + 1)^{l-1}}$ and taking the limit at $k \to \infty$, one can obtain the following recursion relations for $P'_{l,\infty}(x)$

$$P'_{0,\infty}(x) = 1,$$
continuous-time Quantum walk

\[
P'_{1,\infty}(x) = \lim_{k \to \infty} \frac{\sqrt{kx}}{\sqrt{k}} = x,
\]

\[
P'_{2,\infty}(x) = \lim_{k \to \infty} \frac{kx^2 - k}{\sqrt{k(k+1)}} = x^2 - 1,
\]

\[xP'_{l,\infty}(x) = P'_{l+1,\infty}(x) + P'_{l-1,\infty}(x), \quad l = 3, 4, \ldots . \tag{7-43}\]

By comparing the recursion relations (7-43) of \(P'_{l,\infty}(x)\) with those of Tchebichef polynomials of second kind, we conclude that

\[P'_{l,\infty}(x) = U_l(x/2), \tag{7-44}\]

where, \(U_l(x)\)’s are Tchebichef polynomials of second kind. Therefore the probability amplitudes in Eq.(7-40) can be rewritten as

\[q_l(t) = \frac{2}{\pi} \int_{-1}^{1} e^{-2ixt} U_l(x) \sqrt{1 - x^2} dx = \frac{2}{\pi} \int_{-1}^{1} e^{-2ixt} \sin((l + 1) \cos^{-1} x) dx. \tag{7-45}\]

Now, by doing the change the variable \(x = \cos \theta\), the integral(7-45) can be written as

\[q_l(t) = \frac{2}{\pi} \int_{0}^{\pi} e^{-2it\cos \theta} \sin((l + 1) \theta) \sin \theta d\theta. \tag{7-46}\]

Then, using the following integral representation of Bessel polynomials

\[J_l(x) = \frac{i^{-l}}{\pi} \int_{0}^{\pi} e^{-ix \cos \theta} \cos \theta d\theta, \tag{7-47}\]

the integral in (7-46) can be written as

\[q_l(t) = i^l (J_l(2t) + J_{l+2}(2t)). \tag{7-48}\]

Now, from the recursion relations for Bessel polynomials, i.e.,

\[J_{l+1}(x) = \frac{2l}{x} J_l(x) - J_{l-1}(x), \tag{7-49}\]

we obtain the following expression for the probability amplitudes of walk in the limit of large \(k\)

\[q_l(t) = (l + 1) i^l \frac{J_{l+1}(2t)}{t}, \tag{7-50}\]

where the results are in agreement with the corresponding quantum central limit theorem of Ref.[3].
7.2 Non-GQD type graphs

In this subsection we study an example of non-GQD type graphs, those graphs that do not possess three term recursion property. In order to obtain spectral distribution of adjacency matrix of a given non-GQD graph, we need to find the basis in which the adjacency matrix has tridiagonal form. To this aim we have to choose starting site of walk as a reference state and then apply Lanczos algorithm to its adjacency matrix. Then by using spectral distribution, we will be able to calculate the amplitudes of walk as will be explained in the following example.

7.2.1 Walk on finite path graph with second vertex as the starting site of the walk

Finite path graph $\mathbb{P}_n = \{1, 2, \ldots\}$ is a $n$-vertex graph with $n - 1$ edges all on a single open path [1]. For this graph, the stratification depends on the choice of starting site of walk. If we choose the second vertex as starting site of the walk, as it is shown in Fig.2, the graph does not satisfy a three term recursion relations, i.e., the adjacency matrix has not tridiagonal form.

Therefore, in order to find the basis in which the adjacency matrix has tridiagonal form, we have to apply Lanczos algorithm to the adjacency matrix $A$ of the graph $\mathbb{P}_n$, where starting site $|\phi_0\rangle = |1\rangle$ is chosen as a reference state. Also, the Lanczos algorithm provides the coefficients $\alpha$ and $\beta$ from which the Stieltjes transform $G_\mu(z)$ of $\mu$, Eq.(5-21) can be calculated.

Hence, following the prescription of Lanczos algorithm given in section 2, we get the following results for $\mathbb{P}_n$, which are different for even and odd values of $n$.

A. $n = 2k$

$\alpha_i = 0, \quad i = 0, 1, \ldots, 2k - 1,$

$\beta_{2i} = \sqrt{\frac{i}{i+1}},$

$\beta_{2i-1} = \sqrt{\frac{i+1}{i}}, \quad i = 1, \ldots, k - 1,$

$\beta_{2k-1} = \frac{1}{\sqrt{k}}.$

B. $n = 2k + 1$
\[ \alpha_i = 0, \quad i = 0, 1, \ldots, 2k - 1, \]
\[ \beta_{2i} = \sqrt{\frac{i}{i+1}}, \quad i = 1, \ldots, k - 1 \]
\[ \beta_{2i-1} = \sqrt{\frac{i+1}{i}}, \quad i = 1, \ldots, k, \] respectively.

Substituting the coefficients \( \alpha_i \) and \( \beta_i \) in (5-20) and (5-22), and using (5-21), we get the following closed form of the Stieltjes transform of \( \mu \)

\[ G_\mu(z) = \frac{z U_{n-2}(z/2)}{U_n(z/2)} \] (7-51)

where, \( U_n \)'s are Tchebichef polynomials of second kind. Therefore, the roots \( x_i \) appearing in (5-21) are roots of Tchebichef polynomials of second kind, i.e., \( x_i = 2 \cos\left(\frac{ln}{n+1}\right) \). Also, using (5-23) we get the following expression for the coefficients \( A_l \)

\[ A_l = \frac{2}{n+1} \sin^2\left(\frac{2l\pi}{n+1}\right). \] (7-52)

Thus, spectral distribution is given by

\[ \mu = \frac{2}{n+1} \sum_{l=1}^{n} \sin^2\left(\frac{2l\pi}{n+1}\right) \delta(x - 2 \cos\left(\frac{ln}{n+1}\right)). \] (7-53)

Then the probability amplitude of the walk at starting site at time \( t \) is

\[ q_0(t) = \frac{1}{n+1} \sum_{l=1}^{n} \sin^2\left(\frac{2l\pi}{n+1}\right) e^{-2i t \cos\left(\frac{ln}{n+1}\right)}, \] (7-54)

again one can calculate the other amplitudes by using Eq.(6-30).

It should be noticed that, for odd \( n \) the Lanczos algorithm produces \( n - 1 \) orthonormal basis, therefore for calculating the amplitudes on vertices we need to construct an extra vector orthogonal to the walk space \( V_{walk} \).

Finally, in the limit of large \( n \), the continuous part of spectral distribution \( \mu(x) \) is obtained as follows

\[ \mu(x) = \frac{2}{\pi} \int_{0}^{\pi} dy \sin^2(2y) \delta(x - 2 \cos(y)) \]
\[ = \frac{2}{\pi} \int_{0}^{\pi} dy \frac{\sin^2(2y) \delta(y - \arccos(x/2))}{2 \sin(y)} \]
continuous-time Quantum walk

\[
\begin{align*}
\theta(x) &= \frac{4}{\pi} \int_0^\pi dy \sin(y) \cos^2(y) \delta(y - \arccos(x/2)) \\
&= \frac{1}{2\pi} x^2 \sqrt{4 - x^2}, \quad -2 \leq x \leq 2, 
\end{align*}
\]

therefore, the probability amplitude of the walk at starting site at time \( t \) is

\[
q_0(t) = \frac{1}{2\pi} \int_{-2}^{2} e^{-ixt} x^2 \sqrt{4 - x^2} dx = \frac{4J_1(2t)}{t} - \frac{6J_2(2t)}{t^2},
\]

where above result is obtained by making the change of variable \( x = \cos \theta \), and using the integral representation of Bessel polynomials given in (7-47). Similarly, other amplitudes of walk can be calculated by using Eq.(6-27).

8 Conclusion

By turning the graphs into a metric space based on distance function, we have been able to generalize the stratification and quantum decomposition introduced in [13]. Then the continuous-time quantum walk on arbitrary graphs are investigated by spectral distribution method based on Krylov subspace-Lanczos algorithm. We have showed that both in QD and GQD graphs, the unit vectors of strata are identical with the orthonormal basis produced by Lanczos algorithm. For more general graphs, we have used the Lanczos algorithm to get a basis in which the adjacency matrix has tridiagonal form, where it is necessary for determination of spectral distribution of adjacency matrix by using inverse Stieltjes transform. We believe that the introduced algorithm is a powerful and general tool to investigate the continuous-time quantum walk on any arbitrary graph.

Appendix A

In this appendix we show that in the case of GQD graphs the unit vectors of strata (i.e., Eq.(4-9)), are the same as the orthonormal basis produced via Lanczos algorithm. To do so,
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Let us consider the action of adjacency matrix $A$ over $|\phi_k\rangle$ as

$$A|\phi_k\rangle = \frac{1}{\sqrt{\sum_{\alpha} g_{k,\alpha}^2}} \sum_{\alpha \in \Gamma_k(o)} g_{k,\alpha} A|k,\alpha\rangle = \frac{1}{\sqrt{\sum_{\alpha} g_{k,\alpha}^2}} \sum_{\nu \in \Gamma_{k+1}(o), \alpha \sim \nu} g_{k,\alpha} \sum_{\nu \in \Gamma_k(o)} |k+1,\nu\rangle$$

$$+ \frac{1}{\sqrt{\sum_{\alpha} g_{k,\alpha}^2}} \sum_{\alpha \in \Gamma_k(o)} g_{k,\alpha} \sum_{\nu \in \Gamma_k(o), \alpha \sim \nu} |k,\nu\rangle + \frac{1}{\sqrt{\sum_{\alpha} g_{k,\alpha}^2}} \sum_{\alpha \in \Gamma_k(o)} g_{k,\alpha} \sum_{\nu \in \Gamma_{k-1}(o), \alpha \sim \nu} |k-1,\nu\rangle,$$  \hspace{1cm} (A-i)

Now in order to have a GQD graph the coefficients $g_{k,\alpha}$ should satisfy the following conditions

$$\sum_{\alpha \in \Gamma_k(o)} g_{k,\alpha} = \gamma_{k+1} g_{k+1,\nu},$$  \hspace{1cm} (A-ii)

for all $\nu \in \Gamma_{k+1}(o)$ and $\alpha \sim \nu$,

$$\sum_{\alpha \in \Gamma_k(o)} g_{k,\alpha} = \eta_k g_{k,\nu},$$  \hspace{1cm} (A-iii)

for all $\nu \in \Gamma_k(o)$ and $\alpha \sim \nu$,

$$\sum_{\alpha \in \Gamma_k(o)} g_{k,\alpha} = \gamma_k \left( \sum_{\xi \in \Gamma_{k-1}(o)} g_{k-1,\xi}^2 \right) g_{k-1,\nu},$$  \hspace{1cm} (A-iv)

for all $\nu \in \Gamma_{k-1}(o)$ and $\alpha \sim \nu$. One should note that the constants $\gamma_k$ and $\eta_k$ depend only on strata number.

Then by defining $\beta_k = \gamma_k \sqrt{\sum_{\alpha \in \Gamma_k(o)} g_{k,\alpha}^2}$ and $\alpha_k = \eta_k$ for all $\alpha \in \Gamma_k(o), \xi \in \Gamma_{k-1}(o)$ and $\xi \sim \alpha$, the three-term recursion relations (A-i) reduce to those given in (2-2).

Therefore similar to the QD case, the adjacency matrix takes a tridiagonal form in the basis $|\phi_k\rangle$ (orthonormal basis associated with strata of GQD graphs), consequently these basis are identical with the orthonormal basis produced by Lanczos algorithm.

### Appendix B

Here in this appendix we first prove that in GQD graphs, the ratio of amplitude of a vertex in a given stratum to its coefficient appearing in (4-9) is constant, i.e., $\frac{\phi_k}{g_{k,\alpha}}$ is independent of $\alpha \in \Gamma_k(o)$. To do so, let us consider the eigenket $|\phi_k\rangle$ given in (4-9), it is straightforward to see that, the eigenket $|\phi_k\rangle$ together with the following set of states

$$|\phi_{k,l}^\perp\rangle = \frac{1}{\sqrt{\sum_{\nu \in \Gamma_k(o)} |\nu,\alpha\rangle}} \sum_{\alpha \in \Gamma_k(o)} g_{k,\alpha} \omega_{l\alpha}^k |k,\alpha\rangle, \quad l = 1, 2, ..., |\Gamma_k(o)| - 1,$$  \hspace{1cm} (B-i)
form a set of orthonormal basis for a complex space formed by linear span of eigenkets belonging to stratum $k$ where $\omega = e^{-\frac{2\pi i}{|\Gamma_k(o)|}}$.

The above given states are actually orthogonal to all states of walk space ($V_w$), since the eigenket of other stratum do not contain any of $|k,\alpha\rangle, \alpha \in \Gamma_k(o)$. Therefore, $e^{-iAt}|\phi_o\rangle$ is orthogonal to set of orthogonal vectors $|\phi_k^l\rangle$, for all $l = 1, 2, ..., |\Gamma_k(o)| - 1; k = 0, 1, ..., d$ since it is a state which remains in $V_w$ for all $t$. Now, substituting (4-9) in (6-27) and $\langle\phi_k^l|e^{-iAt}|\phi_0\rangle = 0, l = 1, 2, ..., |\Gamma_k(o)| - 1$, we get the following set of equations for amplitudes of vertices belonging to stratum $k$,

$$q_k(t) = \frac{1}{\sqrt{\sum_{\nu \in \Gamma_k(o)} g_{k,\nu}^2}} \sum_{\alpha \in \Gamma_k(o)} g_{k,\alpha} q_{k,\alpha}(t), \quad \text{(B-ii)}$$

$$0 = \frac{1}{\sqrt{\sum_{\nu \in \Gamma_k(o)} \frac{1}{g_{k,\nu}^2}}} \sum_{\alpha \in \Gamma_k(o)} \frac{\omega^{-\alpha}}{g_{k,\alpha}} q_{k,\alpha}(t), \quad l = 1, 2, ..., |\Gamma_k(o)| - 1, \quad \text{(B-iii)}$$

where $q_{k,\alpha}(t)$ denotes the amplitude of vertex $\alpha \in \Gamma_k(o)$. To solve equations (B-ii) and (B-iii), first we multiply equations (B-iii) by $\omega^{l\alpha}$ and sum over $l = 1, 2, ..., |\Gamma_k(o)| - 1$, where by using the identity $\sum_{l=0}^{|\Gamma_k(o)|-1} \omega^{l(\nu-\alpha)} = |\Gamma_k(o)| \delta_{\alpha \nu}$, we get for $\nu \neq \alpha$

$$\frac{q_{k,\alpha}(t)}{g_{k,\alpha}} = \frac{1}{|\Gamma_k(o)|} \sum_{\nu \neq \alpha} \frac{q_{k,\nu}(t)}{g_{k,\nu}}, \quad \text{for all} \quad \alpha \in \Gamma_k(o). \quad \text{(B-iv)}$$

Above equations imply that $\frac{q_{k,\alpha}(t)}{g_{k,\alpha}} = \frac{q_{k,\xi}(t)}{g_{k,\xi}} = B_k$ for all $\alpha, \xi \in \Gamma_k(o)$ where, $B_k$ is some constant independent of vertices of stratum $k$, and it can be determined by substituting $q_{k,\alpha}(t) = B_k g_{k,\alpha}$ in (B-ii) as

$$B_k = \frac{1}{\sqrt{\sum_{\nu \in \Gamma_k(o)} g_{k,\nu}^2}} q_k(t). \quad \text{(B-v)}$$

Therefore, probability amplitude of observing walk at given vertex is proportional to its coefficient $g_{k,\alpha}$ and it can be written in terms of amplitude of the $k$-th stratum $q_k(t)$ as

$$q_{k,\alpha}(t) = \frac{g_{k,\alpha}}{\sqrt{\sum_{\nu \in \Gamma_k(o)} g_{k,\nu}^2}} q_k(t). \quad \text{(B-vi)}$$
In QD graphs we have $g_{k,\alpha} = 1$, for all $\alpha \in \Gamma_k(o)$, hence vertices belonging to the same stratum, have the same amplitude which is in agreement with the result of appendix I of Ref.[1].

In non-GQD type graphs, the coefficients of unit vectors $|\phi_k\rangle$ do not satisfy the conditions (A-ii)-(A-iv) , and we can not obtain vectors orthogonal to $V_{walk}$ by the above explained prescription of GQD graphs. Therefore, one should use Lanczos algorithm for obtaining $n$ independent linear equations, where the amplitudes of vertices of the graph can be determined by solving them. Let the Krylov subspace generated by the adjacency matrix $A$ and starting site $|\phi_0\rangle$ has dimension $d$, then we will have $d$ unit vectors of strata produced from Lanczos algorithm applied to the pair $(A,|\phi_0\rangle)$ (one should note that the walk space $V_{walk}$ is generated by applying the Lanczos algorithm to adjacency matrix and starting site of the walk ). In the most cases, the dimension of $V_{walk}$ is less than the number of vertices ($d < n$), i.e., the Lanczos algorithm applied to the pair $(A,|\phi_0\rangle)$, does not produce the enough basis, therefore for obtaining remaining equations we choose new reference states orthogonal to walk space $V_{walk}$ and then we apply the Lanczos algorithm to the adjacency matrix with new reference states, respectively. In the following, we explain the procedure in details for the following example.

Example

We consider tree graph of Fig.4, with six vertices and complete orthonormal basis

$$\{|1\rangle, |2\rangle, |3\rangle, |4\rangle, |5\rangle, |6\rangle\},$$

where vertex $|1\rangle$ is considered as starting site of the walk. We apply the Lanczos algorithm to adjacency matrix $A$ and starting site $|\phi_0\rangle = |1\rangle$, where orthonormal basis and coefficients $\alpha_k, \beta_k$ produced from Lanczos algorithm are

$$|\phi_0\rangle = |1\rangle, \quad |\phi_1\rangle = \frac{1}{\sqrt{3}}(|2\rangle + |3\rangle + |4\rangle)$$

$$|\phi_2\rangle = \frac{1}{\sqrt{2}}(|5\rangle + |6\rangle), \quad |\phi_3\rangle = \frac{1}{\sqrt{6}}(-2|2\rangle + |3\rangle + |4\rangle),$$
\[ \beta_1 = \sqrt{3}, \quad \beta_2 = \sqrt{2/3}, \quad \beta_3 = \sqrt{1/3}; \quad \alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 0, \]  
respectively. One can straightforwardly show that the corresponding Stieltjes transform of \( \mu \) and spectral distribution are

\[
G_{\mu}(z) = \frac{z^3 - (1 + \sqrt{2})z/\sqrt{3}}{z^4 - (4 + \sqrt{2})z^2/\sqrt{3} + 1},
\]

\[ \mu = 0.2851952676(\delta(x - 1.662563892) + \delta(x + 1.662563892)) + 0.2148047323(\delta(x - 0.6014806445) + \delta(x + 0.6014806445)), \]  
respectively, which yield the following probability amplitudes of walk at \( k \)-th stratum at time \( t \), for \( k = 0, 1, 2, 3 \)

\[
q_0(t) = \int_{\mathbb{R}} e^{-ixt} \mu(dx) = 0.2851952676 \cos(1.662563892t) + 0.2148047323 \cos(0.6014806445t).
\]

\[
q_1(t) = \frac{1}{\sqrt{3}} \int_{\mathbb{R}} e^{-ixt} P_1'(x) \mu(dx) = \frac{1}{\sqrt{3}} \int_{\mathbb{R}} xe^{-ixt} \mu(dx)
\]

\[ = \frac{2}{i\sqrt{3}}[0.2851952676 \sin(1.662563892t) + 0.2148047323 \sin(0.6014806445t)], \]

\[
q_2(t) = \frac{1}{\sqrt{2}} \int_{\mathbb{R}} e^{-ixt} P_2'(x) \mu(dx) = \frac{1}{\sqrt{2}} \int_{\mathbb{R}} (x^2 - \sqrt{3})e^{-ixt} \mu(dx)
\]

\[ = \frac{1}{\sqrt{2}}[0.2943408772 \cos(1.662563892t) - 0.2943408762 \cos(0.6014806445t)], \]

\[
q_3(t) = \frac{3}{\sqrt{2}} \int_{\mathbb{R}} e^{-ixt} P_3'(x) \mu(dx) = \frac{3}{\sqrt{2}} \int_{\mathbb{R}} (x^3 - 3 + \sqrt{2})x e^{-ixt} \mu(dx)
\]

\[ = \frac{6}{i\sqrt{6}}[0.102214289 \sin(1.662563892t) - 0.282324240 \sin(0.6014806445t)]. \]  

Obviously, we need two extra equations for obtaining amplitudes on sites of the graph. According to the above explained prescription we can consider

\[ |\psi_0\rangle = \frac{1}{\sqrt{2}}(|5\rangle - |6\rangle), \]

as new reference state \( (|\psi_0\rangle \in V_{\text{walk}}^\perp) \) and then by applying Lanczos algorithm to the pair \((A, |\psi_0\rangle)\) we obtain

\[ |\psi_1\rangle = \frac{1}{\sqrt{2}}(|3\rangle - |4\rangle), \]
which leads to two following extra equations

\[ \langle \psi_0 | e^{-itA} | \phi_0 \rangle = 0, \]
\[ \langle \psi_1 | e^{-itA} | \phi_0 \rangle = 0. \]  

(B-xii)

Now, by solving the above six equations, one can obtain amplitudes of continuous-time quantum walk on vertices of the graph as

\[ \langle 1 | e^{-iAt} | \phi_0 \rangle = q_0(t), \]
\[ \langle 2 | e^{-iAt} | \phi_0 \rangle = \frac{1}{\sqrt{3}} (q_1(t) - \sqrt{2} q_3(t)), \]
\[ \langle 3 | e^{-iAt} | \phi_0 \rangle = \langle 4 | e^{-iAt} | \phi_0 \rangle = \frac{1}{\sqrt{3}} (q_1(t) + \frac{1}{\sqrt{2}} q_3(t)), \]
\[ \langle 5 | e^{-iAt} | \phi_0 \rangle = \langle 6 | e^{-iAt} | \phi_0 \rangle = \frac{1}{\sqrt{2}} q_2(t), \]  

(B-xiii)

where \( q_0(t), q_1(t), q_2(t) \) and \( q_3(t) \) have been given in Eq.(B-ix).

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**Figure Captions**

**Figure.1**: Shows the stratification with respect to distance function.

**Figure.2**: Shows the finite path graph of $P_n$, where walk starts at vertex 2.

**Figure.3**: Kite graph with $k = 2$ and $n = 6$, where walk starts at vertex $(0,0)$. All vertices lying on a given vertical dashed line belong to the same statum.

**Figure.4**: Shows the tree graph, where walk starts at vertex 1.
\begin{figure}
\centering
\includegraphics{fig1}
\caption{Fig. 1}
\end{figure}
Fig. 2
Fig. 3
