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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 (CTQW) on graphs possessing quantum decomposition (QD graphs) have been calculated by a new method based on spectral distribution associated with their adjacency matrix. Here in this paper, it is shown that the CTQW on any arbitrary graph can be investigated by spectral analysis 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 (GQD) 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 the 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. The capability of Lanczos-based algorithm for evaluation of CTQW on 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 the limit of the large number of vertices, are in agreement with those of central limit theorem of [Phys. Rev. E **72**, 026113 (2005)]. At the end, some applications of the method such as implementation of quantum search algorithms, calculating the resistance between two nodes in regular networks and applications in solid state and condensed matter physics, have been discussed, where in all of them, the Lanczos algorithm, reduces the Hilbert space to some smaller subspaces and the problem is investigated in the subspace with maximal dimension.

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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 [4–9]. 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). Several systems have been proposed as candidates to implement quantum random walks. These proposals include atoms trapped in optical lattices [10], cavity quantum electrodynamics (CQED) [11] and nuclear magnetic resonance (NMR) in solid substrates [12,13]. In liquid-state NMR systems [14], time resolved observations of spin waves has been done [15]. It has also been pointed out that a quantum walk can be simulated using classical waves instead of matter waves [16,17].

A study of quantum walks on simple graph is well known in physics (see [18]). Recent studies of quantum walks on more general graphs were described in [4,5,7,19,20]. Some of these works studies the problem in the important context of algorithmic problems on

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graphs and suggests that quantum walks is a promising algorithmic technique for designing future quantum algorithms. One approach for investigation of CTQW 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 [21,22] for the adjacency matrix of graph. Also it is shown in [1] that by using spectral distribution one can approximate long time behavior of CTQW 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 CTQW 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 [21], 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 [1,21] are particular kinds 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 with adjacency matrix can be determined by Stieltjes/Hilbert transform. In order to see the power of Lanczos-based algorithm in the investigation of CTQW 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 introduced formalism for investigating the CTQW via Lanczos algorithm, shows the power of this algorithm in reducing the space to some smaller irreducible subspaces. Therefore, other than CTQW, in the most physical problems such as implementation of quantum search algorithms, calculating resistance between two arbitrary nodes of regular networks, investigating tight-binding Hamiltonian and special spin chain models, where the Hamiltonian is projected to the largest irreducible subspace, the introduced method (reduction together with spectral analysis method) can be applied.

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/Hilbert transform method for obtaining spectral distribution μ, and establish an isometry between orthogonal polynomials and Hilbert space of generalized stratification. Section 6 is devoted to the method for computing amplitudes of CTQW, through spectral distribution μ of the adjacency matrix A. In Section 7 we calculate the amplitudes of quantum walk on some interesting finite (infinite) graph of GQD type and finite (infinite) path graph of non-GQD type. Also, we study the asymptotic behavior of the probability amplitudes at infinite limit of number of vertices, where the obtained results are in agreement with those of central limit theorem of reference [3]. Section 8 is devoted briefly to some possible applications such as algorithmic applications mostly search algorithms, calculating resistance between two arbitrary nodes of regular networks, applications in condensed matter physics, e.g. in investigating tight-binding Hamiltonians and special spin chain models. 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 [23–26].

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

$$K_d(|\phi_0\rangle, A) = span\{|\phi_0\rangle, A|\phi_0\rangle, \ldots, A^{d-1}|\phi_0\rangle\}, \quad (2.1)$$

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 $\{|\phi_0\rangle, |\phi_1\rangle, ..., |\phi_{d-1}\rangle\}$ and satisfy the following three-term recursion relations

$$A|\phi_i\rangle = \beta_{i+1}|\phi_{i+1}\rangle + \alpha_i|\phi_i\rangle + \beta_i|\phi_{i-1}\rangle. \quad (2.2)$$

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:

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

where the scalars β_{i+1} and α_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 $\{A^i\phi_0; i = 0, ..., d-1\}$ 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 jth column of Φ and P. Then we have

$$\langle\phi_0|P_i^\dagger(A)P_j(A)|\phi_0\rangle = \langle KP_i|KP_j\rangle = \langle\phi_i|\phi_j\rangle, \qquad (2.3)$$

where $P_i = a_0 + a_1A + ... + a_iA^i$ 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 CTQW.

Lanczos algorithm

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

$$\begin{gathered} \beta_0 = 0, |\phi_0\rangle = |\phi\rangle/\||\phi\rangle\| \\ \text{for} \quad i = 0, 1, 2, ... \\ |\upsilon_i\rangle = A|\phi_i\rangle \\ \alpha_i = \langle\phi_i|\upsilon_i\rangle \\ |\upsilon_{i+1}\rangle = |\upsilon_i\rangle - \beta_i|\phi_{i-1}\rangle - \alpha_i|\phi_i\rangle \\ \beta_{i+1} = \||\upsilon_{i+1}\rangle\| \\ \text{if} \quad \beta_{i+1} \neq 0 \\ |\phi_{i+1}\rangle = |\upsilon_{i+1}\rangle/\beta_{i+1} \\ \text{else} \quad |\phi_{i+1}\rangle = 0. \end{gathered}$$

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 [21]. 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

$$A_{\alpha\beta} = \begin{cases} 1 \text{ if } \alpha \sim \beta \\ 0 \text{ otherwise.} \end{cases}$$

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 $|\ .\ |$ 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 α and β. 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 ∂.

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 [27] we define a partition (called distance partition) on $V \times V$, i.e., $V \times V = \bigcup_i \Gamma_i$ based on distance function ∂, where the subset Γ_i are defined by

$$\Gamma_i = \{(\alpha, \beta) \in V \times V | \partial(\alpha, \beta) = i\}. \qquad (3.4)$$

Using above distance partition one can define the set $\Gamma_i(\alpha)$ (ith neighborhood of vertex α) as

$$\Gamma_i(\alpha) = \{\beta \in V | (\alpha, \beta) \in \Gamma_i\}. \qquad (3.5)$$

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

$$V = \bigcup_i \Gamma_i(\alpha), \qquad (3.6)$$

(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 α, where the vertex α is referred to as a reference state (see Fig. 2).

In this stratification for any connected graph Γ, we have

$$\Gamma_1(\beta) \subseteq \Gamma_{i-1}(\alpha) \cup \Gamma_i(\alpha) \cup \Gamma_{i+1}(\alpha), \qquad (3.7)$$

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

Obviously above relations are similar to those of distance regular graphs [27], where in the later case the sets Γ_i form an association scheme and the stratification $\Gamma_i(\alpha)$ is independent of reference state α, but in an arbitrary

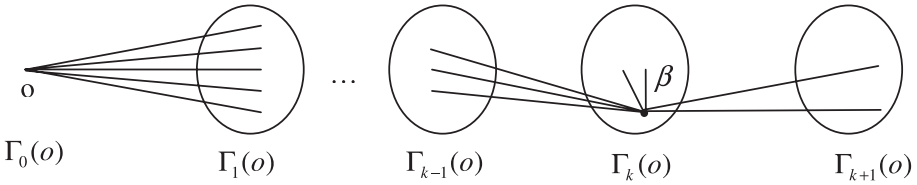


Fig. 1. The stratification with respect to distance function.

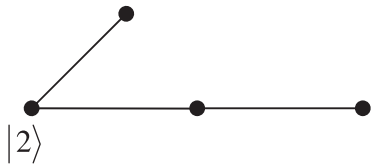


Fig. 2. The finite path graph of P_n.

graph the generalized stratification depends on the choice of reference state.

In order to study CTQW 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

For a given graph Γ, let W denotes the vector space over C consisting of column vectors whose coordinates are indexed by vertex set V of Γ, and whose entries are in C (i.e., $W = C^n$, with $n = |V|$). We observe that all $n \times n$ matrices with entries from C act on W by left multiplication. We endow W with the Hermitian inner product $\langle , \rangle$ which satisfies $\langle u, v\rangle = u^t\bar{v}$ for all $u, v \in W$, where t denotes the transpose and – denotes the complex conjugation. For all $\beta \in V$, let $|\beta\rangle$ denote the element of W with a 1 in the β coordinate and 0 in all other coordinates. We observe $\{|\beta\rangle|\beta \in V\}$ is an orthonormal basis for W, but in this basis, W is reducible and can be reduced to some irreducible subspaces. In the following we introduce an orthonormal basis for irreducible subspace of W with maximal dimension (denoted by W_0), explicitly and then explain how one can obtain basis for other irreducible subspaces via Lanczos algorithm.

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 vector $|\phi_k\rangle$ in W called unit vector of kth stratum such that W_0 is spanned by $\{|\phi_k\rangle\}$. In Section 6, we will deal with CTQW, where W_0 will be referred to as walk space denoted by V_{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 W_0, one can often write

$$W_0 = \sum_k \oplus \mathbf{C}|\phi_k\rangle. \tag{4.8}$$

The unit vector associated with kth stratum $\Gamma_k(o)$ of generalized stratification, is defined by

$$|\phi_k\rangle = \frac{1}{\sqrt{\sum_\alpha g_{k,\alpha}^2}} \sum_{\alpha\in\Gamma_k(o)} g_{k,\alpha}|k,\alpha\rangle, \tag{4.9}$$

where, $|k,\alpha\rangle$ denotes the eigenket of αth 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 $\alpha \in \Gamma_k(o)$, equation (4.9) reduces to

$$|\phi_k\rangle = \frac{1}{\sqrt{|\Gamma_k(o)|}} \sum_{\alpha\in\Gamma_k(o)} |k,\alpha\rangle, \tag{4.10}$$

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

In the following we show that, for the QD type graphs the unit vectors of strata given in equation (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

$$\begin{aligned}
A|\phi_k\rangle &= \frac{1}{\sqrt{|\Gamma_k(o)|}} \sum_{\alpha\in\Gamma_k(o)} A|k,\alpha\rangle \\
&= \frac{1}{\sqrt{|\Gamma_k(o)|}} \sum_{\alpha\in\Gamma_k(o)} \sum_{\nu\in\Gamma_{k+1}(o),\nu\sim\alpha} |k+1,\nu\rangle \\
&\quad + \frac{1}{\sqrt{|\Gamma_k(o)|}} \sum_{\alpha\in\Gamma_k(o)} \sum_{\nu\in\Gamma_k(o),\nu\sim\alpha} |k,\nu\rangle \\
&\quad + \frac{1}{\sqrt{|\Gamma_k(o)|}} \sum_{\alpha\in\Gamma_k(o)} \sum_{\nu\in\Gamma_{k-1}(o),\nu\sim\alpha} |k-1,\nu\rangle \\
&= \sqrt{\frac{|\Gamma_{k+1}(o)|}{|\Gamma_k(o)|}} \frac{1}{\sqrt{|\Gamma_{k+1}(o)|}} \sum_{\nu\in\Gamma_{k+1}(o)} \lambda_{k+1}(\nu)|k+1,\nu\rangle \\
&\quad + \frac{1}{\sqrt{|\Gamma_k(o)|}} \sum_{\nu\in\Gamma_k(o)} \alpha_k(\nu)|k,\nu\rangle \\
&\quad + \sqrt{\frac{|\Gamma_{k-1}(o)|}{|\Gamma_k(o)|}} \frac{1}{\sqrt{|\Gamma_{k-1}(o)|}} \sum_{\nu\in\Gamma_{k-1}(o)} \frac{\lambda_k(\nu)|\Gamma_k(o)|}{|\Gamma_{k-1}(o)|}|k-1,\nu\rangle.
\end{aligned} \tag{4.11}$$

By defining $\beta_k = \frac{|\Gamma_k|^{1/2}}{|\Gamma_{k-1}|^{1/2}}\lambda_k(\nu)$, $\lambda_k(\nu) = |\{\alpha \in \Gamma_{k-1}(o); \alpha \sim \nu\}|$ 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.

One should notice that, by applying Krylov-subspace Lanczos algorithm to adjacency matrix A and reference state $|o\rangle$, one obtains an orthonormal basis for the irreducible subspace W_0, where in CTQW by choosing starting site of the walk as reference state, W_0 will be the same as walk space V_{walk}. Orthonormal basis for other irreducible subspaces $W_i, i \neq 0$ can be obtained by choosing new reference states orthogonal to the walk space and applying Lanczos algorithm to adjacency matrix with the new chosen reference states, respectively. Therefore W is semisimple, i.e., it can be decomposed as direct sum of irreducible subspaces as

$$W = W_0 \oplus W_1 \oplus ... \oplus W_l. \tag{4.12}$$

5 Spectral distribution of the adjacency matrix A

One of the most important applications of spectral analysis method is to analyze a set of two-state diffusion equations, which was first used by Zusman [28] to treat solvent effects on three electron transfer in the non-adiabatic limit. In [29], the spectral analysis approach developed in [30] has been employed to study the electron transfer dynamics in mixed-valence systems. The analysis allows one to characterize multiple time-scales in electron transfer processes including vibrational relaxation, electronic coherence, activated curve crossing or barrier crossing. Also, since the advent of random matrix theory (RMT), there has been considerable interest in the statistical analysis of spectra [31–34]. RMT can be viewed as a generalization of the classical probability calculus, where the concept of probability density distribution for a one-dimensional random variable is generalized onto an averaged spectral distribution of the ensemble of large, non-commuting random matrices. Such a structure exhibits several phenomena known in classical probability theory, including central limit theorems [35]. In RMT, the Poisson distribution and the Wigner-Dyson distributions have been found to be of universal relevance. The prominent features of these distributions are conveniently characterized with the help of spectral observables such as the nearest-neighbor spacing distribution and the number variance; The former stresses the correlations on a short scale, while the latter measures the stiffness of the spectrum, i.e. long-range spectral correlations.

Actually the spectral analysis of operators is an important issue in quantum mechanics, operator theory and mathematical physics [36,37]. As an example $\mu(dx) = |\psi(x)|^2 dx$ ($\mu(dp) = |\widetilde{\psi}(p)|^2 dp$) 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 [38,39].

It is well-known that, for any pair $(A, |\phi_0\rangle)$ of a matrix A and a vector $|\phi_0\rangle$, it can be assigned a measure μ as follows

$$\mu(x) = \langle\phi_0|E(x)|\phi_0\rangle, \tag{5.13}$$

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

$$A = \int xE(x)dx. \tag{5.14}$$

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

$$P(A) = \int P(x)E(x)dx, \tag{5.15}$$

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

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 (5.13) and (5.15), the expectation value of powers of adjacency matrix A over starting site $|\phi_0\rangle$ can be written as

$$\langle\phi_0|A^m|\phi_0\rangle = \int_R x^m \mu(dx), \qquad m = 0, 1, 2, ... \tag{5.16}$$

The existence of a spectral distribution satisfying (5.16) is a consequence of Hamburgers theorem, see e.g., Shohat and Tamarkin ([40], Theorem 1.2).

Obviously relation (5.16) implies an isomorphism from the Hilbert space of generalized stratification onto the closed linear span of the orthogonal polynomials with respect to the measure μ. Since, from the orthogonality of vectors $|\phi_j\rangle$ (Hilbert space of generalized stratification) produced from Lanczos algorithm process we have,

$$\begin{aligned}\delta_{ij} = \langle\phi_i|\phi_j\rangle &= \langle\phi_0|P_i^\dagger(A)P_j(A)|\phi_0\rangle \\ &= \int P_i^*(x)P_j(x)\mu(x)dx = (P_i, P_j)_\mu.\end{aligned} \tag{5.17}$$

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

$$|\phi_j\rangle = P_j(A)|\phi_0\rangle, \tag{5.18}$$

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

Now, substituting (5.18) in (2.2), we get three term recursion relations between polynomials $P_j(A)$, which leads

to the following three term recursion between polynomials $P_j(x)$

$$\beta_{k+1}P_{k+1}(x) = (x-\alpha_k)P_k(x) - \beta_k P_{k-1}(x) \quad (5.19)$$

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

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

$$\beta_1...\beta_{k+1}P_{k+1}(x) = (x-\alpha_k)\beta_1...\beta_k P_k(x) - \beta_k^2.\beta_1...\beta_{k-1}P_{k-1}(x). \quad (5.20)$$

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

$$P'_0(x) = 1, \qquad P'_1(x) = x,$$
$$xP'_k(x) = P'_{k+1}(x) + \alpha_k P'_k(x) + \beta_k^2 P'_{k-1}(x), \quad (5.21)$$

for $k \geq 1$.

If such a spectral distribution is unique, the spectral distribution μ is determined by the identity:

$$G_\mu(z) = \int_R \frac{\mu(dx)}{z-x} = \cfrac{1}{z-\alpha_0 - \cfrac{\beta_1^2}{z-\alpha_1 - \cfrac{\beta_2^2}{z-\alpha_2 - \cfrac{\beta_3^2}{z-\alpha_3-\cdots}}}} = \frac{Q^{(1)}_{n-1}(z)}{P'_n(z)} = \sum_{l=1}^{n} \frac{A_l}{z-x_l}, \quad (5.22)$$

where, x_l are the roots of polynomial $P'_n(x)$. $G_\mu(z)$ is called the Stieltjes/Hilbert transform of spectral distribution μ and polynomials $\{Q^{(1)}_k\}$ are defined recurrently as

$$Q^{(1)}_0(x) = 1, \qquad Q^{(1)}_1(x) = x - \alpha_1,$$
$$xQ^{(1)}_k(x) = Q^{(1)}_{k+1}(x) + \alpha_{k+1}Q^{(1)}_k(x) + \beta^2_{k+1}Q^{(1)}_{k-1}(x), \quad (5.23)$$

for $k \geq 1$. The coefficients A_l appearing in (5.22) are the same Guass quadrature constants which are calculated as

$$A_l = \lim_{z \longrightarrow x_l} (z-x_l)G_\mu(z). \quad (5.24)$$

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

$$\mu(y) - \mu(x) = -\frac{1}{\pi} \lim_{v \longrightarrow 0^+} \int_x^y Im\{G_\mu(u+iv)\}du. \quad (5.25)$$

Substituting the right hand side of (5.22) in (5.25), the spectral distribution can be determined in terms of $x_l, l = 1, 2, ...$ and Guass quadrature constants $A_l, l = 1, 2, ...$ as

$$\mu = \sum_l A_l \delta(x - x_l) \quad (5.26)$$

(for more details see Refs. [22,40–42]).

Finally, using the relation (5.18) and the recursion relations (5.21) of polynomial $P'_k(x)$, the other matrix elements $\langle \phi_k | A^m \mid \phi_0 \rangle$ can be calculated as

$$\langle \phi_k | A^m \mid \phi_0 \rangle = \frac{1}{\beta_1\beta_2\cdots\beta_k} \int_R x^m P'_k(x)\mu(dx), \qquad m = 0, 1, 2, ... \quad (5.27)$$

6 Investigation of CTQW on an arbitrary graph via spectral distribution of its adjacency matrix

For a given undirected graph Γ with n vertices and adjacency matrix A, one can define the Laplacian $L = A - D$, where D is the diagonal matrix with $D_{jj} = \deg(j)$, the degree of vertex j. Classically, the continuous time random walk (CTRW) on Γ is a Markov process with a fixed probability per unit time γ of hopping from a given vertex to one of its neighbors. In other words, the probability of hopping to any connected vertex in a time ϵ is $\gamma\epsilon$ (in the limit $\epsilon \to 0$). This walk is governed by the master equation (Kolmogorov's equation) [43]

$$\frac{dq_j(t)}{dt} = \gamma \sum_k L_{jk} q_k(t), \quad (6.28)$$

where, $q_j(t)$ is the probability of being at vertex j at time t. Since the columns of L sum to zero, probability is conserved. Equation (6.28), is spatially discrete, but it also admits extensions to continuous spaces, e.g., leading to the disordered Lorentz gas model, which describes the dynamics of an electron through a disordered substrate [44]. The derivation of master equation for random walks on unweighted, undirected graphs, has been studied in [45,46].

We now turn to one quantum mechanical extension of the problem, the so-called CTQW. The CTQW on the graph Γ is defined by replacing master equation of continuous-time classical random walk (Eq. (6.28)) with Schrödinger's equation [43,47] where, γ is set to 1 for convenience and L (the Laplacian of the graph) is chosen as the Hamiltonian of the walk. This is because we can view L as the generator matrix that describes an exponential distribution of waiting times at each vertex.

Although, CTQW was introduced by Farhi and Gutmann [4] (see also [5,8]), our treatment, follow closely the analysis of Moore and Russell [8]. As illustrated in Section 4, for $0 \leq i \leq d$, the unit vectors $|\phi_i\rangle$ of equation (4.10) form a basis for Hilbert space of CTQW starting from a given site [2]. Let $|\phi(t)\rangle$ be a time-dependent amplitude of the quantum process on graph Γ. The wave evolution of the quantum walk is governed by

$$i\hbar \frac{d}{dt}|\phi(t)\rangle = H|\phi(t)\rangle, \quad (6.29)$$

where we assume $\hbar = 1$. Let, $|\phi_0\rangle$ be the initial amplitude wave function of the particle. Then, the solution to (6.29), is given by $|\phi_0(t)\rangle = e^{-iHt}|\phi_0\rangle$. On d-regular graphs, $D = \frac{1}{d}I$, and since A and D commute, we get

$$e^{-itH} = e^{-it(A-\frac{1}{d}I)} = e^{-it/d}e^{-itA}. \quad (6.30)$$

This introduces an irrelevant phase factor in the wave evolution. Hence we can consider $H = A = A_1$. Thus, we have

$$|\phi_0(t)\rangle = e^{-iAt}|\phi_0\rangle. \quad (6.31)$$

One of our main goals in this paper is the evaluation of probability amplitudes for CTQW by using equation (5.27), such that we have

$$q_{k0}(t) \equiv q_k(t) = \langle \phi_k | e^{-iAt} \mid \phi_0 \rangle = \frac{1}{\beta_1\beta_2\cdots\beta_k} \int_R e^{-ixt} P'_k(x)\mu(dx), \quad (6.32)$$

where $q_k(t)$ is the amplitude of observing the walk at stratum k at time t. The conservation of probability $\sum_{k=0} \mid q_k(t) \mid^2 = 1$ follows immediately from equation (6.32), simply by using the completeness relation of orthogonal polynomials $P'_k(x)$.

Investigation of CTQW 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.,

$$q_0(t) = \int e^{-ixt}\mu(x)dx \longmapsto \mu(x) = \frac{1}{2\pi}\int e^{ixt} q_0(t)dt. \quad (6.33)$$

Above relations imply that

$$q_k(t) = \frac{1}{\beta_1\beta_2\cdots\beta_k}\int P'_k(x)e^{-ixt}\mu(x)dx = \frac{1}{2\pi\beta_1\beta_2\cdots\beta_k}\int P'_k(x)q_0(t')e^{-ix(t-t')}dt'dx, \quad (6.34)$$

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

Obviously for finite graphs, the formula (6.32) yields

$$q_k(t) = \frac{1}{\beta_1\beta_2\cdots\beta_k}\sum_l A_l e^{-ix_l t} P'_k(x_l), \quad (6.35)$$

where by straightforward calculation one can evaluate the average probability for the finite graphs as

$$P(k) = \lim_{T\to\infty}\frac{1}{T}\int_0^T \mid q_k(t) \mid^2 dt = \frac{1}{\beta_1\beta_2\cdots\beta_k}\sum_l A_l^2 P'^2_k(x_l). \quad (6.36)$$

In Appendix I of reference [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 $\frac{|q_k(t)|^2}{|\Gamma_k(o)|}$. Unfortunately for non-QD graphs the lemma appearing in Appendix I of reference [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.

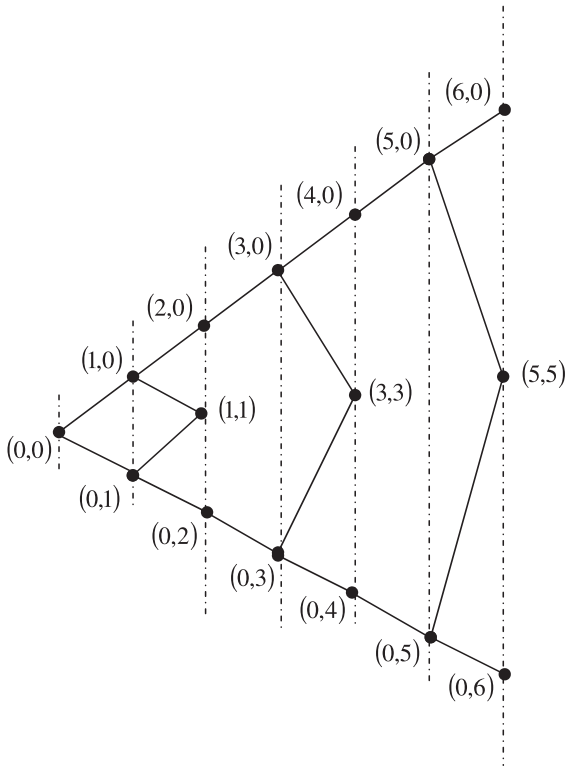


Fig. 3. Generalized QD graph.

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 $Z^k, k = 2, 3, ...$ lattices and defined as follows: let $K(k, n)$ be an k-dimensional lattice graph with $n + 1$ generalized strata, which consists of vertices $\underbrace{(0, 0, ..., 0)}_{k}, (l, 0, ..., 0), (0, l, 0, ..., 0), ..., (0, 0, ...0, l)$ and $\underbrace{(l, l, ..., l)}_{k}$ only for odd values of l, where $l = 0, 1, ..., n$. The vertex $(0, 0, ..., 0)$ is connected to vertices $(1, 0, ..., 0), (0, 1, ..., 0), ..., (0, 0, ..., 1)$, the vertex $(0, ..., 0, \underbrace{l}_{i}, 0, ..., 0)$ is connected to vertices $(0, ..., 0, \underbrace{l-1}_{i}, 0, ..., 0)$ and $(0, ..., 0, \underbrace{l+1}_{i}, 0, ..., 0)$ for each $i = 1, ..., k$, but for odd values of l, there is an extra connection between $(0, ..., 0, \underbrace{l}_{i}, 0, ..., 0)$ 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)

$$
\begin{aligned}
|\phi_0\rangle &= |\underbrace{0,0,...,0}_{k}\rangle \\
|\phi_1\rangle &= \frac{1}{\sqrt{k}}\sum_{perm.}|1,0,...,0\rangle \\
|\phi_2\rangle &= \frac{1}{\sqrt{k(k+1)}}(\sum_{perm.}|2,0,...,0\rangle + k|1,1,...,1\rangle) \\
&\vdots \\
|\phi_{2l-1}\rangle &= \frac{1}{\sqrt{k}}\sum_{perm.}|2l-1,0,...,0\rangle \\
|\phi_{2l}\rangle &= \frac{1}{\sqrt{k(k+1)}}(\sum_{perm.}|2l,0,...,0\rangle \\
&\quad + k|2l-1,2l-1,...,2l-1\rangle),
\end{aligned}
\tag{7.37}
$$

where, the summations are taken over all possible permutations. Using the relations (A.ii)–(A.iv), one can show that the coefficients β_i and α_i are

$$
\beta_1^2 = k,\ \ \beta_2^2 = \beta_3^2 = ... = k+1 \ \text{ and } \ \alpha_i = 0,\ i = 1,2,... \tag{7.38}
$$

Now, one can study CTQW on these graphs for finite values of n simply by following the general prescriptions, but here we restrict ourselves to infinite n. Substituting coefficients β_i and α_i in (5.22), the Stieltjes/Hilbert transform $G_\mu(z)$ of spectral distribution μ takes the following form

$$
G_\mu(z) = \frac{1}{z - \frac{k}{z - \frac{k+1}{z - \frac{k+1}{z-\cdots}}}}. \tag{7.39}
$$

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

$$
\tilde{G}(z) = \frac{1}{z - \frac{k+1}{z - \frac{k+1}{z - \frac{k+1}{z-\cdots}}}} = \frac{1}{z-(k+1)\tilde{G}(z)}, \tag{7.40}
$$

where by solving above equation, we get

$$
\tilde{G}(z) = \frac{z - \sqrt{z^2 - 4(k+1)}}{2(k+1)}. \tag{7.41}
$$

Inserting (7.41) in (7.40), we get

$$
G_\mu(z) = \frac{1}{z - kG'_\mu(z)}, \tag{7.42}
$$

then substituting (7.41) in (7.42), we obtain the following expression for Stieltjes/Hilbert transform of μ

$$
G_\mu(z) = \frac{(k+2)z - k\sqrt{z^2-4(k+1)}}{2(k^2+z^2)}, \tag{7.43}
$$

finally by applying Stieltjes/Hilbert inversion formula, we get the absolutely continuous part of spectral distribution μ as follows

$$
\mu(x) = \frac{k}{2\pi}\frac{\sqrt{4(k+1)-x^2}}{k^2+x^2}, \quad |x| \le 2\sqrt{k+1}. \tag{7.44}
$$

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

$$
\begin{aligned}
q_l(t) &= \lim_{k\to\infty}\langle\phi_l|e^{\frac{-iAt}{\sqrt{k}}}\mid\phi_0\rangle \\
&= \lim_{k\to\infty}\frac{1}{\sqrt{k(k+1)^l}}\int_{-2\sqrt{k+1}}^{2\sqrt{k+1}} e^{\frac{-ixt}{\sqrt{k}}} \\
&\quad \times P'_l(x)\frac{k}{2\pi}\frac{\sqrt{4(k+1)-x^2}}{k^2+x^2}dx \\
&= \lim_{k\to\infty}\frac{1}{2\pi\sqrt{k(k+1)^l}}\int_{-2\sqrt{(k+1)/k}}^{2\sqrt{(k+1)/k}} e^{-ixt} \\
&\quad \times P'_l(\sqrt{k}x)\frac{\sqrt{4(k+1)/k-x^2}}{1+x^2/k}dx \\
&= \frac{1}{2\pi}\int_{-2}^{2} e^{-ixt}P'_{l,\infty}(x)\sqrt{4-x^2}dx \\
&= \frac{2}{\pi}\int_{-1}^{1} e^{-i2xt}P'_{l,\infty}(2x)\sqrt{1-x^2}dx,
\end{aligned}
\tag{7.45}
$$

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

$$
P'_{l,\infty}(x) = \lim_{k\to\infty}\frac{1}{\sqrt{k(k+1)^{l-1}}}P'_l(\sqrt{k}x). \tag{7.46}
$$

Now, substituting β_i and α_i from (7.38) in three-term recursion relations (5.21), we obtain the following relations for polynomials $P'_l(x)$

$$
\begin{aligned}
P'_0(\sqrt{k}x) &= 1, \\
P'_1(\sqrt{k}x) &= \sqrt{k}x, \\
P'_2(\sqrt{k}x) &= kx^2 - k, \\
\sqrt{k}xP'_l(\sqrt{k}x) &= P'_{l+1}(\sqrt{k}x) + (k+1)P'_{l-1}(\sqrt{k}x), \\
&\qquad\qquad l = 3,4,...
\end{aligned}
\tag{7.47}
$$

Then dividing left and right hand sides of the recursion relations in (7.47) by $\sqrt{k(k+1)^{l-1}}$ and taking the limit at $k\to\infty$, one can obtain the following recursion relations for $P'_{l,\infty}(x)$

$$
\begin{aligned}
P'_{0,\infty}(x) &= 1, \\
P'_{1,\infty}(x) &= \lim_{k\to\infty}\frac{\sqrt{k}x}{\sqrt{k}} = x, \\
P'_{2,\infty}(x) &= \lim_{k\to\infty}\frac{kx^2-k}{\sqrt{k(k+1)}} = x^2 - 1, \\
xP'_{l,\infty}(x) &= P'_{l+1,\infty}(x) + P'_{l-1,\infty}(x), \ \ l = 3,4,...
\end{aligned}
\tag{7.48}
$$

By comparing the recursion relations (7.48) of $P'_{l,\infty}(x)$ with those of Tchebichef polynomials of second kind, we conclude that

$$
P'_{l,\infty}(x) = U_l(x/2), \tag{7.49}
$$

where, $U_l(x)$'s are Tchebichef polynomials of second kind. Therefore the probability amplitudes in equation (7.45)

can be rewritten as

$$q_l(t) = \frac{2}{\pi}\int_{-1}^{1} e^{-2ixt}U_l(x)\sqrt{1-x^2}dx$$
$$= \frac{2}{\pi}\int_{-1}^{1} e^{-2ixt}\sin((l+1)\cos^{-1}x)dx. \quad (7.50)$$

Now, by doing the change the variable $x = \cos\theta$, the integral (7.50) can be written as

$$q_l(t) = \frac{2}{\pi}\int_0^{\pi} e^{-2it\cos\theta}\sin((l+1)\theta)\sin\theta d\theta. \quad (7.51)$$

Then, using the following integral representation of Bessel polynomials

$$J_l(x) = \frac{i^{-l}}{\pi}\int_0^{\pi} e^{-ix\cos\theta}\cos\theta d\theta, \quad (7.52)$$

the integral in (7.51) can be written as

$$q_l(t) = i^l(J_l(2t) + J_{l+2}(2t)). \quad (7.53)$$

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

$$J_{l+1}(x) = \frac{2l}{x}J_l(x) - J_{l-1}(x), \quad (7.54)$$

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

$$q_l(t) = (l+1)i^l\frac{J_{l+1}(2t)}{t}, \quad (7.55)$$

where the results are in agreement with the corresponding quantum central limit theorem of reference [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 give 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 $\mathsf{P}_n = \{1, 2, ...\}$ 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 Figure 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 P_n, where starting site $|\phi_0\rangle = |1\rangle$ is chosen as a reference state. Also, the Lanczos algorithm provides the coefficients α and β from which the Stieltjes/Hilbert transform $G_\mu(z)$ of μ, equation (5.22) can be calculated.

Hence, following the prescription of Lanczos algorithm given in Section 2, we get the following results for P_n, which are different for even and odd values of n.

A. $n = 2k$

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

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

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

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

B. $n = 2k+1$

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

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

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

Substituting the coefficients α_i and β_i in (5.21) and (5.23), and using (5.22), we get the following closed form of the Stieltjes/Hilbert transform of μ

$$G_\mu(z) = \frac{zU_{n-2}(z/2)}{U_n(z/2)} \quad (7.56)$$

where, U_n's are Tchebichef polynomials of second kind. Therefore, the roots x_l appearing in (5.22) are roots of Tchebichef polynomials of second kind, i.e., $x_l = 2\cos(\frac{l\pi}{n+1})$. Also, using (5.24) we get the following expression for the coefficients A_l

$$A_l = \frac{2}{n+1}\sin^2\left(\frac{2l\pi}{n+1}\right). \quad (7.57)$$

Thus, spectral distribution is given by

$$\mu = \frac{2}{n+1}\sum_{l=1}^{n}\sin^2\left(\frac{2l\pi}{n+1}\right)\delta\left(x - 2\cos\left(\frac{l\pi}{n+1}\right)\right). \quad (7.58)$$

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

$$q_0(t) = \frac{1}{n+1}\sum_{l=1}^{n}\sin^2\left(\frac{2l\pi}{n+1}\right)e^{-2it\cos l\pi/(n+1)}, \quad (7.59)$$

again one can calculate the other amplitudes by using equation (6.35).

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

$$\begin{aligned}\mu(x) &= \frac{2}{\pi}\int_0^\pi dy \sin^2(2y)\delta(x-2\cos(y)) \\ &= \frac{2}{\pi}\int_0^\pi dy \frac{\sin^2(2y)\delta(y-\arccos(x/2))}{2\sin(y)} \\ &= \frac{4}{\pi}\int_0^\pi dy \sin(y)\cos^2(y)\delta(y-\arccos(x/2)) \\ &= \frac{1}{2\pi}x^2\sqrt{4-x^2}, \qquad -2\le x\le 2. \end{aligned} \tag{7.60}$$

Therefore, the probability amplitude of the walk at starting site at time t is

$$\begin{aligned} q_0(t) &= \frac{1}{2\pi}\int_{-2}^{2} e^{-ixt}x^2\sqrt{4-x^2}dx \\ &= \frac{4J_1(2t)}{t} - \frac{6J_2(2t)}{t^2}, \end{aligned} \tag{7.61}$$

where, the 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 equation (6.32).

8 Some applications

In this section, some applications of CTQW and the introduced spectral analysis approach based on Krylov subspace-Lanczos algorithm are discussed briefly. The applications include algorithmic applications, computation of the resistance between two nodes in a resistor network and applications in solid state and condensed matter physics which are discussed in the following.

8.1 Algorithmic applications

Random walks provide a nice description of how classical particles diffuse toward some kind of equilibrium. Because quantum particles can become delocalized (i.e. can go many directions simultaneously), one might expect algorithms based on a quantum version of a random walk to outperform those based on classical random walks. Indeed, polynomial speed-ups are standard and some exponential improvements have also been found. As illustrated in Section 6, a CTQW on a graph is indistinguishable from ordinary Schrödinger time-evolution under the influence of some Hamiltonian/adjacency matrix. This implies that any efficient algorithm to simulate a Hamiltonian can be effected by a quantum walk over some graph, and vice versa.

To illustrate the power of quantum walks, we describe a way to implement Grover's algorithm [48] using CTQW, designed to find with high probability a marked element of some unsorted database. Consider the complete graph with n vertices. One of the eigenstates of the associated Hamiltonian $H = A$ is the uniform superposition

$$|\psi\rangle = \frac{1}{\sqrt{n}}\sum_j |j\rangle. \tag{8.62}$$

This is because other than a factor of I, the Hamiltonian itself is $H = n|\psi\rangle\langle\psi|$. Now suppose that the vertex q is marked, and we would like to evolve the initial state $|\psi\rangle$ under the influence of some Hamiltonian, so that $|\psi\rangle \to |q\rangle$ after some time t. To approach the Grover problem with a CTQW, we need to modify the Hamiltonian so that the vertex q is special. It turns out that for the complete graph, one simply needs to use the following Hamiltonian

$$H = -\frac{1}{n}A - |q\rangle\langle q| = -|\psi\rangle\langle\psi| - |q\rangle\langle q| + \frac{1}{n}I. \tag{8.63}$$

The extra factor of $\frac{1}{n}I$ just gives a constant shift to the energy and has no effect on the time dynamics except to shift the wavefunction's phase. The solution requires inverting the Schrödinger equation (6.29), so that $q_j(t) = \exp(-iHt)q_j(0)$. But to obtain an analytical solution for $U(t) = \exp(-iHt)$, we need to expand in an orthogonal basis, and the vectors $|\psi\rangle$ and $|q\rangle$ are not orthogonal; rather, $\langle q|\psi\rangle \equiv x = \frac{1}{\sqrt{n}}$ for any q. To make further progress, we first need to use an orthogonal basis; let's define a vector $|p\rangle$ that is explicitly orthogonal to $|q\rangle$:

$$|p\rangle = \frac{1}{\sqrt{1-x^2}}(|\psi\rangle - x|q\rangle). \tag{8.64}$$

It should be noticed that, the new orthonormal basis $\{|q\rangle, |p\rangle\}$ is the same as the stratification basis produced by Krylov-subspace Lanczos algorithm applied to to the pair $(A, |q\rangle)$. Now the restriction of the Hamiltonian and initial state $|\psi\rangle$ to the subspace W_0 with the basis $\{|q\rangle, |p\rangle\}$ (irreducible subspace of adjacency matrix with maximal dimension, see Sect. 4 for more details) reads as

$$-H = \begin{pmatrix} 1+x^2 & x\sqrt{1-x^2} \\ x\sqrt{1-x^2} & 1-x^2 \end{pmatrix} \quad \text{and} \quad |\psi\rangle = x|q\rangle + \sqrt{1-x^2}|p\rangle, \tag{8.65}$$

respectively. The eigenvalues of H are given by $1\pm x$. Then, one can easily obtain

$$|\psi(t)\rangle = (x\cos(xt) - i\sin(xt))|q\rangle + \sqrt{1-x^2}\cos(xt)|p\rangle. \tag{8.66}$$

So, the probability of being in the marked state $|q\rangle$, i.e., $x^2\cos^2(xt) + \sin^2(xt)$ is exactly one when $t = \pi/2x = \pi\sqrt{n}/2$, so that the search time scales like $\sqrt{n}$ as hoped. While similar algorithms have been devised for other kinds of graphs, the efficiency with which the marked state can be found varies considerably. For the case of the complete graph, the resulting algorithm is simply the continuous time search algorithm of Farhi and Gutmann [49]. It has be shown that, unless special tricks are used, a regular lattice needs to have dimension greater than 3 for a quantum algorithm to give any advantage over brute-force searching [50].

8.2 The resistance between two arbitrary nodes of a finite regular lattice

A classic problem in electric circuit theory studied by numerous authors over many years, is the computation of the resistance between two nodes in a resistor network (see, e.g., [51]). The two-point resistance has a probabilistic interpretation based on classical random walker walking on the network. Indeed, the connection between random walks and electric networks has been recognized for some time (see e.g. [52–54]), where one can establish a connection between the electrical concepts of current and voltage and corresponding descriptive quantities of random walks regarded as finite state Markov chains (for more details see [55]). Also, by adapting the random-walk dynamics and mean-field theory it has been studied that [56], how the growth of a conducting network, such as electrical or electronic circuits, interferes with the current flow through the underlying evolving graphs. Our results in this subsection show that, there is also connection between the introduced mathematical techniques for investigating CTQW on graphs, such as Hilbert space of the walk based on stratification and spectral analysis through Lanczos algorithm and electrical concept of resistance between two arbitrary nodes of regular networks and the same techniques can be employed for calculating the resistance. In reference [57], this problem is investigated in terms of the eigenvalues and eigenfunctions of the Laplacian matrix associated with the network. Here, we obtain the same results based on stratification and spectral techniques used through the paper for investigation of CTQW.

For a given regular graph Γ with n vertices and adjacency matrix A, let $r_{ij} = r_{ji}$ be the resistance of the resistor connecting vertices i and j. Hence, the conductance is $c_{ij} = r_{ij}^{-1} = c_{ji}$ so that $c_{ij} = 0$ if there is no resistor connecting i and j. Denote the electric potential at the ith vertex by V_i and the net current flowing into the network at the ith vertex by I_i (which is zero if the ith vertex is not connected to the external world). Since there exist no sinks or sources of current including the external world, we have the constraint $\sum_{i=1}^{n} I_i = 0$. The Kirchhoff law states

$$\sum_{j=1,j\neq i}^{n} c_{ij}(V_i - V_j) = I_i, \quad i = 1, 2, ..., n. \tag{8.67}$$

Explicitly, equation (8.67) reads

$$L\vec{V} = \vec{I}, \tag{8.68}$$

where, $\vec{V}$ and $\vec{I}$ are n-vectors whose components are V_i and I_i, respectively and

$$L = \upsilon I - \sum_{i,j} c_{ij}|i\rangle\langle j| \tag{8.69}$$

is the Laplacian of the graph Γ with $\upsilon = \deg(\alpha)$, for each vertex α. Hereafter, we will assume that all nonzero resistances are equal to 1, then the off-diagonal elements of $-L$ are precisely those of the adjacency matrix A of the graph, i.e.,

$$L = \upsilon I - A. \tag{8.70}$$

It should be noticed that, L has eigenvector $(1, 1, ..., 1)^t$ with eigenvalue 0. Therefore, L is not invertible and so we define the psudo-inverse of L as

$$L^{-1} = \sum_{i,\lambda_i\neq 0} \lambda_i^{-1} E_i, \tag{8.71}$$

where, E_i is the operator of projection onto the eigenspace of L^{-1} corresponding to eigenvalue λ_i. Following the result of [57] and that L^{-1} is a real matrix, the resistance between vertices α and β is given by

$$R_{\alpha\beta} = \langle\alpha|L^{-1}|\alpha\rangle - 2\langle\alpha|L^{-1}|\beta\rangle + \langle\beta|L^{-1}|\beta\rangle. \tag{8.72}$$

Now, for calculating the matrix elements of L^{-1} in (8.72), we employ the spectral techniques based on Lanczos algorithm. For diagonal elements, one can use the Stieltjes/Hilbert transform

$$\langle\gamma|L^{-1}|\gamma\rangle = \int \frac{\mu_\gamma(\lambda)}{\upsilon - \lambda} d\lambda, \tag{8.73}$$

where, λ's are eigenvalues of adjacency matrix A and vertex depending spectral measure $\mu_\gamma(\lambda)$, is defined by (5.26). Therefore, for calculating the elements $L^{-1}_{\alpha\alpha}$ and $L^{-1}_{\beta\beta}$ in (8.72), we must stratify the graph with respect to the vertices α and β (each time, one of α and β is chosen as reference state in Lanczos algorithm). For calculating $L^{-1}_{\beta\alpha}$, we choose one of the vertices, say α, as reference state. From the fact that, the vertices belonging to the same stratum with respect to α, have equal circumstances, it follows that for $\beta \in \Gamma_k(\alpha)$, the matrix elements $\langle\beta|L^{-1}|\alpha\rangle$ and $\langle\phi_k|L^{-1}|\alpha\rangle$ are equal up to constant $\frac{1}{\sqrt{|\Gamma_k(\alpha)|}}$ (see Appendix B), where the vector $|\phi_k\rangle$ is defined in (4.10). In other words, the resistances between α and β is the same for all $\beta \in \Gamma_k(\alpha)$. Therefore, it is sufficient to calculate the matrix elements $\langle\phi_k|L^{-1}|\alpha\rangle$. By using equation (5.18), we calculate these elements via spectral method as follows

$$\begin{aligned} L^{-1}_{\beta\alpha} &= \frac{1}{\sqrt{|\Gamma_k(\alpha)|}}\langle\phi_k|L^{-1}|\alpha\rangle \\ &= \frac{1}{\sqrt{|\Gamma_k(\alpha)|}}\int \frac{\mu_\alpha(\lambda)}{\upsilon - \lambda} P_k(\lambda) d\lambda, \quad \lambda \neq \upsilon \end{aligned} \tag{8.74}$$

where, the polynomial P_k associated with unit vector $|\phi_k\rangle$, is defined by (5.18). One can notice that, the only difference with CTQW is that e^{-iAt} is replaced by $(\upsilon I - A)^{-1}$. Also, it should be noticed that, all computations are done in the irreducible subspace W_0. For the sake of clarity, we give three examples of complete graph, Peterson graph and cyclic one.

8.2.1 Example 1: Complete graph

For, a complete graph with n vertices shown in Figure 5a, we have $\upsilon = n - 1$. The adjacency matrix is $A = J - I$,

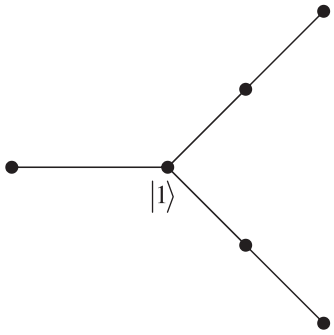


Fig. 4. The tree graph.

where J is a matrix with all entries equal to 1. Then, by using continued fraction (5.22) and the relations (5.24) and (5.26), one can obtain vertex independent spectral measure as

$$\mu(\lambda) = \frac{1}{n}((n-1)\delta(\lambda+1) + \delta(\lambda-n+1)). \tag{8.75}$$

Therefore, by using Stieltjes/Hilbert transform (8.73), we obtain $L^{-1}_{\alpha\alpha} = \frac{n-1}{n^2}$, for all α. From (8.74) and (8.75), we obtain for $L^{-1}_{\beta\alpha}$ (with α as reference state, i.e., $|\phi_0\rangle = |\alpha\rangle$)

$$L^{-1}_{\beta\alpha} = \frac{1}{n-1}\int \frac{\mu(\lambda)}{n-1-\lambda}\lambda d\lambda = -\frac{1}{n^2}, \tag{8.76}$$

where, we have used the fact that $\beta \in \Gamma_1(\alpha)$ and $|\phi_1\rangle = \frac{1}{\sqrt{n-1}}A|\alpha\rangle$, i.e., $P_1(\lambda) = \frac{1}{\sqrt{n-1}}\lambda$. Therefore, by using (8.72), we obtain

$$R_{\alpha\beta} = \frac{2}{n^2} + \frac{2(n-1)}{n^2} = \frac{2}{n}. \tag{8.77}$$

This result is in agreement with those of reference [57].

8.2.2 Example 2: Peterson graph

As another example, we consider the Peterson graph and calculate the resistance between the vertices 1 and 2 in Figure 5b. For Peterson graph, we have $\upsilon = 3$. By using continued fraction (5.22) and the relations (5.24) and (5.26), one can obtain

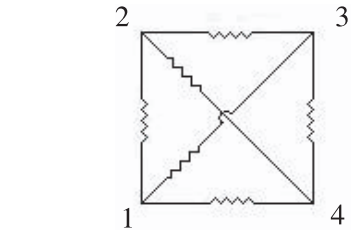
$$\begin{aligned}\mu(\lambda) \equiv \mu_1(\lambda) &= \mu_2(\lambda) \\ &= \frac{1}{10}\delta(\lambda-3) + \frac{1}{2}\delta(\lambda-1) + \frac{2}{5}\delta(\lambda+2).\end{aligned} \tag{8.78}$$

Now, by using Stieltjes/Hilbert transform (8.73), we calculate

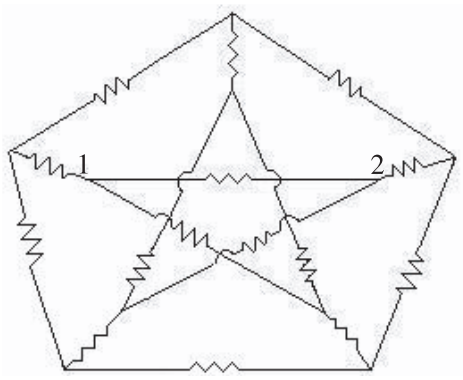
$$L^{-1}_{11} = L^{-1}_{22} = \int \frac{\mu(\lambda)}{3-\lambda}d\lambda = \frac{33}{100}. \tag{8.79}$$

By using $P_1(\lambda) = \frac{\lambda}{\sqrt{3}}$ and (8.74), we obtain

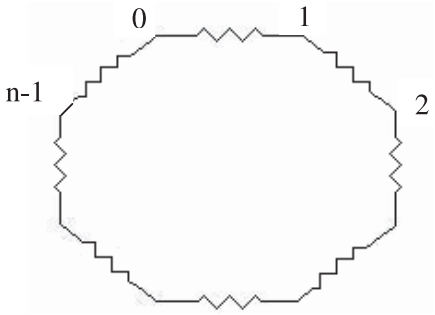
$$L^{-1}_{21} = L^{-1}_{12} = \frac{1}{3}\int \frac{\lambda\mu(\lambda)}{3-\lambda}d\lambda = \frac{3}{100}. \tag{8.80}$$



(a)



(b)



(c)

Fig. 5. (a) The complete network. (b) The Peterson network. (c) The cyclic network.

Now, by using (8.72), one obtains

$$R_{12} = 2\frac{33}{100} - 2\frac{3}{100} = \frac{3}{5}. \tag{8.81}$$

8.2.3 Example 3: Cyclic graph

Now, we consider cyclic graph with n vertices shown in Figure 5c. Clearly $\upsilon = 2$ and the adjacency matrix reads $A = S + S^{-1}$, where

$$S = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & 1 & 0 \\ 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & \dots & 0 & 0 \end{pmatrix}, \tag{8.82}$$

is circulant matrix with period n, i.e., $S^n = I$. The spectral measure is reference independent and is given by

$$\mu(\lambda) = \frac{1}{n}\sum_{l=0}^{n-1}\delta\bigg(\lambda - 2\cos\frac{2\pi l}{n}\bigg). \tag{8.83}$$

For two arbitrary vertices α and β, with α as reference vertex for stratification, we obtain

$$L^{-1}_{\alpha\alpha} = L^{-1}_{\beta\beta} = \int \frac{\mu(\lambda)}{2-\lambda}d\lambda = \frac{1}{2n}\sum_{l=1}^{n-1}\frac{1}{1-\cos\frac{2\pi l}{n}}. \tag{8.84}$$

By using Lanczos algorithm applied to $|\alpha\rangle$, one can easily obtain the polynomials $P_k(x)$ as follows

$$P_0(x) = 1, \quad P_k(x) = \sqrt{2}T_k\bigg(\frac{x}{2}\bigg), \tag{8.85}$$

where, T_k are Tchebichef polynomials of the first kind defined by

$$T_k(x) = \cos(k\cos^{-1}x). \tag{8.86}$$

If β belongs to the kth stratum $\Gamma_k(\alpha)$, in this case we have $\beta - \alpha = k$, then we will have

$$\begin{aligned} L^{-1}_{\beta\alpha} &= \frac{1}{\sqrt{2}}\int\frac{\mu(\lambda)}{2-\lambda}P_k(\lambda)d\lambda \\ &= \frac{1}{\sqrt{2}n}\sum_{l=1}^{n-1}\frac{P_k(2\cos\frac{2\pi l}{n})}{2(1-\cos\frac{2\pi l}{n})} \\ &= \frac{1}{2n}\sum_{l=1}^{n-1}\frac{\cos\frac{2\pi kl}{n}}{1-\cos\frac{2\pi l}{n}}, \end{aligned} \tag{8.87}$$

where, we have used $P_k(2\cos\frac{2\pi l}{n}) = \sqrt{2}\cos(\frac{2\pi kl}{n})$. Now, by using (8.84), (8.87) and (8.72) we obtain

$$R_{\beta\alpha} = \frac{1}{n}\sum_{l=1}^{n-1}\frac{1-\cos\frac{2\pi kl}{n}}{1-\cos\frac{2\pi l}{n}}, \tag{8.88}$$

where, the result is in agreement with those of reference [57].

8.3 Tight-binding on a generic structure

The tight-binding approximation [58] is widely used when dealing with quantum particles on discrete structures, such as solids, molecules, atomic clusters. The Hamiltonian of such a system has the form

$$H = \sum_{i,j} h_{ij}a_i^\dagger a_j, \tag{8.89}$$

where, $a_i^\dagger$ and a_i are the creation and annihilation operator at site i with $[a_i, a_j^\dagger] = \delta_{ij}$. The Hamiltonian matrix h_{ij} is defined as [59]

$$h_{ij} = tA_{ij} + az_i\delta_{ij}, \tag{8.90}$$

where, the off-diagonal term, called hopping term, contains the adjacency matrix describing the topological arrangement of the structure and the so-called hopping parameter t and the diagonal term, called local term, contains the local parameter a and the coordination number $z_i = \sum_j A_{ij}$, namely the number of nearest neighbours of the ith site. On a periodic lattice (with homogeneous elementary cell) this term is site-independent and it can be dropped without loss of generality, since it simply results in a rigid shift of the spectrum.

A route to the spectrum of the Hamiltonian (8.90) (on a periodic lattice) alternative to direct diagonalization, passes through the so-called Local Density of States (LDOS), which is related to Green's functions by the formula [60]

$$\rho_i(\omega) = -\frac{1}{\pi}\lim_{\epsilon\to 0}\mathrm{Im}(G_{ii}(\omega + i\epsilon)). \tag{8.91}$$

The Green's function is defined by

$$G(\omega) = \frac{1}{\omega - tA}. \tag{8.92}$$

Denoting $|i\rangle$ the eigenfunction of the position operator at site i and ϕ_k the eigenfunction of the Hamiltonian operator relevant to the eigenvalue ω_k, $H|\phi_k\rangle = \omega_k|\phi_k\rangle$, one gets

$$G(\omega) = \sum_k \frac{|\phi_k\rangle\langle\phi_k|}{\omega - \omega_k}, \tag{8.93}$$

thus one can write $G_{ij}(\omega) = \langle i|G(\omega)|j\rangle = \sum_k\langle i|\phi_k\rangle\langle\phi_k|j\rangle(\omega - \omega_k)^{-1}$. Plugging this result into equation (8.91) and recalling that $\lim_{\epsilon\to 0} Im(\omega \pm i\epsilon)^{-1} = \mp\pi\delta(\omega)$, one gets

$$\rho_i(\omega) = \sum_k \delta(\omega - \omega_k)|\langle i|\phi_k\rangle|^2. \tag{8.94}$$

Equation (8.94) sheds light on the significance of the LDOS at site i. The density of states (DOS), is recovered by summing the LDOS over all sites:

$$\begin{aligned} \sum_i \rho_i(\omega) &= \sum_k \delta(\omega - \omega_k)\sum_i |\langle i|\phi_k\rangle|^2 \\ &= \sum_k \delta(\omega - \omega_k) = \rho(\omega). \end{aligned} \tag{8.95}$$

One could notice that, $G_{ii}(\omega)$ is the same Stieltjes/Hilbert transform defined in (5.22) and from (5.26), it is seen that $\rho_i(\omega)$ is the inverse Stieltjes/Hilbert transform of $G_{ii}(\omega)$. Therefore, inverse Fourier transform of $\rho_i(\omega)$ gives the probability amplitude of observing the CTQW at starting site i at time t. Depending on starting site of the walk as reference vertex, the graph may be of QD, GQD or non-GQD type, e.g., the finite path graph with first vertex as reference vertex is a graph of QD type, while with second one as reference vertex is of non-GQD type, as we considered in Section 7.2.1. Therefore, calculating the DOS $\rho(\omega)$ from (8.95) is not an easy work.

8.3.1 Infinite line as a hopping model

Consider a periodic potential in one dimension, where $V(x+a) = V(x)$. Realistically, we may consider the motion of an electron in a chain of regularly spaced positive ions. Clearly, the Hamiltonian H is invariant under the translation $T(a)$, where $T(a)$ has the property $T(a)|x\rangle = |x+a\rangle$. Now, let us assume that the particle is localized at the nth site and denote the corresponding ket by $|n\rangle$. This is an energy eigenket with energy eigenvalue E_0, namely, $H|n\rangle = E_0|n\rangle$. In the case that the barrier between two adjacent sites is not infinitely high, we expect that there is some leakage possible into neighboring sites due to quantum tunneling. The diagonal elements of H in the $\{|n\rangle\}$ basis, are all equal because of translation invariance, i.e., $\langle n|H|n\rangle = E_0$, for all n. However, we suspect that H is not diagonal in this basis due to leakage. One can assume that

$$\langle n'|H|n\rangle \neq 0, \quad \text{only if} \quad n' = n, n \pm 1. \tag{8.96}$$

In solid state physics this assumption is known as the tight-binding approximation. By defining $\langle n \pm 1|H|n\rangle = -\Delta$, one obtains

$$H|n\rangle = E_0|n\rangle - \Delta|n+1\rangle - \Delta|n-1\rangle. \tag{8.97}$$

In fact, H is symmetric tridiagonal in the $\{|n\rangle\}$ basis. One could notice that, this Hamiltonian can be viewed as adjacency matrix of infinite path graph which is projected to the subspace W_0 with basis produced by lanczos algorithm applied to adjacency matrix and starting site of the walk as reference state. The problem of finding probability amplitude of observing the electron at kth ion at time t if electron be localized at ith ion initially, can be solved by CTQW on infinite path, where we investigated it in Section 7.2.1 via spectral methods.

In references [20,61], CTQW on some ideally perfect quantum graphs called G_n first studied in [5], has been investigated where the exponential speed-up of quantum walks on these graphs relative to classical particles diffusing on the same graphs, has been discussed as a striking observation. Also, by using well-established ideas from the theory of Anderson localization applied to these quantum walks, the authors of reference [61] showed that when the graphs have imperfections, as they surely will in any real physical implementation, the propagation of quantum information is suppressed exponentially in the amount of imperfection. The techniques such as generalized stratification and Krylov-subspace Lanczos algorithm employed in this paper, enable us to investigate the same problems on more general graphs due to the fact that these techniques cause us to give a tridiagonal form to the Hamiltonians (adjacency matrices of the graphs) in the subspaces spanned by the stratification basis (called also column subspace), i.e., any given graph can be projected to a weighted line graph in which each vertex $|i\rangle$ is adjacent with vertices $|i-1\rangle$ and $|i+1\rangle$.

8.4 A spin chain model

In [62], a spin chain model was introduced to describe a system of n qubits containing imperfections which generate a residual inter-qubit coupling and fluctuations in the energy spacings between the two states of one qubit. The Hamiltonian of this model reads as

$$H = \sum_{i<j} J_{ij}\sigma_i^x\sigma_j^x + \sum_i \Gamma_i\sigma_i^z, \tag{8.98}$$

where, the σ_i are the Pauli matrices for the qubit i. Γ_i represent the energy spacing between the two states of a qubit and the couplings J_{ij} represent the residual static interaction between qubits (this model is called standard generic quantum computer model, for more details see [62, 63]). For special case where, the energy spacing Γ_i and coupling parameters J_{ij} are the same for all qubits, the Hamiltonian (8.98) reads as

$$H = \sum_{i<j} \sigma_i^x\sigma_j^x + \sum_i \sigma_i^z. \tag{8.99}$$

Now, one could notice that, in the special Hamiltonian (8.99), the first term can be viewed as adjacency matrix of underlying graph of Hamming association scheme $H(2,n)$ [27] and can be block-diagonalized via Krylov subspace-Lanczos algorithm as illustrated in Section 4. On the other hand, the Hamiltonian (8.99) belongs to a semisimple algebra known as Terwilliger algebra [64] associated with Hamming scheme $H(2,n)$. The basis for irreducible subspaces of this algebra are equal with those of adjacency matrix and therefore, the corresponding Hamiltonian can be block-diagonalized via Lanczos algorithm process, in order to evaluating corresponding spectrum.

9 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 [21]. Then the CTQW 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/Hilbert transform. We believe that, the introduced formalism (reduction to subspace W_0 together with spectral analysis method) is a powerful and general tool which can be applied not only for investigating the CTQW on any arbitrary graph, but also for studying the most physical problems such as implementation of quantum search algorithms, resistor circuit theory,

tight-binding Hamiltonian and particular spin chain models where, the Hamiltonian is projected to the largest irreducible subspace. We have discussed that, the CTQW on complete graph implements Grover's algorithm. It is naturally expected that CTQW on more general graphs such as finite path graph, Hamming graph, etc. can implement other spatial search problems, where this problem is under investigation. Also, our method was applied to calculating the resistance between two arbitrary vertices of regular graphs. Although in the present paper we gave three examples of complete graph, Peterson and cyclic ones, the method can be applied for any finite or infinite regular graph similarly.

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, let us consider the action of adjacency matrix A over $|\phi_k\rangle$ as

$$\begin{aligned} A|\phi_k\rangle &= \frac{1}{\sqrt{\sum_\alpha g_{k,\alpha}^2}} \sum_{\alpha\in\Gamma_k(o)} g_{k,\alpha} A|k,\alpha\rangle \\ &= \frac{1}{\sqrt{\sum_\alpha g_{k,\alpha}^2}} \sum_{\alpha\in\Gamma_k(o)} g_{k,\alpha} \sum_{\nu\in\Gamma_{k+1}(o),\alpha\sim\nu} |k+1,\nu\rangle \\ &+ \frac{1}{\sqrt{\sum_\alpha g_{k,\alpha}^2}} \sum_{\alpha\in\Gamma_k(o)} g_{k,\alpha} \sum_{\nu\in\Gamma_k(o),\alpha\sim\nu} |k,\nu\rangle \\ &+ \frac{1}{\sqrt{\sum_\alpha g_{k,\alpha}^2}} \sum_{\alpha\in\Gamma_k(o)} g_{k,\alpha} \sum_{\nu\in\Gamma_{k-1}(o),\alpha\sim\nu} |k-1,\nu\rangle, \end{aligned} \tag{A.i}$$

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

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

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

$$\sum_{\alpha\in\Gamma_k(o)} g_{k,\alpha} = \eta_k g_{k,\nu}, \tag{A.iii}$$

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

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

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

Then by defining $\beta_k = \gamma_k\sqrt{\frac{\sum_{\alpha\in\Gamma_k(o)} g_{k,\alpha}^2}{\sum_{\xi\in\Gamma_{k-1}(o)} g_{k-1,\xi}^2}}$ 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., $\frac{\phi_{k,\alpha}}{g_{k,\alpha}}$ 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

$$|\phi_{k,l}^{\perp}\rangle = \frac{1}{\sqrt{\sum_{\nu\in\Gamma_k(o)}\frac{1}{|g_{k,\nu}|^2}}} \sum_{\alpha\in\Gamma_k(o)} \frac{\omega^{l\alpha}}{g_{k,\alpha}}|k,\alpha\rangle, \quad l=1,2,...,|\Gamma_k(o)|-1, \tag{B.i}$$

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 $|\phi_{k,l}^{\perp}\rangle$, 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 (6.32) and $\langle\phi_{k,l}^{\perp}|e^{-iAt}|\phi_0\rangle = 0, l=1,2,...,|\Gamma_k(o)|-1$, we get the following set of equations for amplitudes of vertices belonging to stratum k,

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

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

$$l=1,2,...,|\Gamma_k(o)|-1, \tag{B.iv}$$

where $q_{k,\alpha}(t)$ denotes the amplitude of vertex $\alpha\in\Gamma_k(o)$. To solve equations (B.ii) and (B.iv), first we multiply equations (B.iv) by $\omega^{l\nu}$ 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 $\nu\neq\alpha$

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

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

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

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 kth stratum $q_k(t)$ as

$$q_{k,\alpha}(t) = \frac{g_{k,\alpha}}{\sqrt{\sum_{\nu\in\Gamma_k(o)} g_{k,\nu}^2}} q_k(t). \qquad \text{(B.vii)}$$

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 reference [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 deteremined 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 $(A, |\phi_0\rangle)$, dose 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 Figure 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 α_k, β_k produced from Lanczos algorithm are

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

$$|\phi_2\rangle = \frac{1}{\sqrt{2}}(|5\rangle + |6\rangle), \qquad |\phi_3\rangle = \frac{1}{\sqrt{6}}(-2|2\rangle + |3\rangle + |4\rangle),$$

$$\beta_1 = \sqrt{3}, \quad \beta_2 = \sqrt{2/3}, \quad \beta_3 = \sqrt{1/3}; \quad \alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 0, \qquad \text{(B.viii)}$$

respectively. One can straightforwardly show that the corresponding Stieltjes/Hilbert transform of μ and spectral distribution are

$$G_\mu(z) = \frac{z^3 - (1+\sqrt{2})z/\sqrt{3}}{z^4 - (4+\sqrt{2})z^2/\sqrt{3} + 1},$$
$$\mu = 0.2851952676(\delta(x - 1.662563892) + \delta(x + 1.662563892)) + 0.2148047323(\delta(x - 0.6014806445) + \delta(x + 0.6014806445)), \qquad \text{(B.ix)}$$

respectively, which yield the following probability amplitudes of walk at kth stratum at time t, for $k = 0, 1, 2, 3$

$$q_0(t) = \int_R e^{-ixt}\mu(dx) = 0.2851952676\cos(1.662563892t) + 0.2148047323\cos(0.6014806445t).$$

$$q_1(t) = \frac{1}{\sqrt{3}}\int_R e^{-ixt}P_1'(x)\mu(dx) = \frac{1}{\sqrt{3}}\int_R xe^{-ixt}\mu(dx) = \frac{2}{i\sqrt{3}}[0.2851952676\sin(1.662563892t) + 0.2148047323\sin(0.6014806445t)],$$

$$q_2(t) = \frac{1}{\sqrt{2}}\int_R e^{-ixt}P_2'(x)\mu(dx) = \frac{1}{\sqrt{2}}\int_R (x^2 - \sqrt{3})e^{-ixt}\mu(dx) = \frac{1}{\sqrt{2}}[0.2943408772\cos(1.662563892t) - 0.2943408762\cos(0.6014806445t)],$$

$$q_3(t) = \frac{\sqrt{3}}{\sqrt{2}}\int_R e^{-ixt}P_3'(x)\mu(dx) = \frac{\sqrt{3}}{\sqrt{2}}\int_R (x^3 - \frac{3+\sqrt{2}}{\sqrt{3}}x)e^{-ixt}\mu(dx) = \frac{6}{i\sqrt{6}}[0.102214289\sin(1.662563892t) - 0.2825324240\sin(0.6014806445t)]. \qquad \text{(B.x)}$$

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

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}(|5\rangle - |6\rangle), \qquad \text{(B.xi)}$$

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

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|3\rangle - |4\rangle), \qquad \text{(B.xii)}$$

which leads to two following extra equations

$$\langle\psi_0|e^{-itA}|\phi_0\rangle = 0,$$

$$\langle\psi_1|e^{-itA}|\phi_0\rangle = 0. \qquad \text{(B.xiii)}$$

Now, by solving the above six equations, one can obtain amplitudes of CTQW on vertices of the graph as

$$\langle 1|e^{-iAt} \mid \phi_0\rangle = q_0(t),$$
$$\langle 2|e^{-iAt} \mid \phi_0\rangle = \frac{1}{\sqrt{3}}(q_1(t) - \sqrt{2}q_3(t)),$$
$$\langle 3|e^{-iAt} \mid \phi_0\rangle = \langle 4|e^{-iAt} \mid \phi_0\rangle = \frac{1}{\sqrt{3}}(q_1(t) + \frac{1}{\sqrt{2}}q_3(t)),$$
$$\langle 5|e^{-iAt} \mid \phi_0\rangle = \langle 6|e^{-iAt} \mid \phi_0\rangle = \frac{1}{\sqrt{2}}q_2(t), \qquad \text{(B.xiv)}$$

where $q_0(t), q_1(t), q_2(t)$ and $q_3(t)$ have been given in equation (B.x).

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