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Investigation of continuous-time quantum walk via modules of Bose–Mesner and Terwilliger algebras

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Abstract

The continuous-time quantum walk on the underlying graphs of association schemes has been studied, via the algebraic combinatorics structures of association schemes, namely semi-simple modules of their Bose–Mesner and Terwilliger algebras. It is shown that the Terwilliger algebra stratifies the graph into a $(d + 1)$ disjoint union of strata which is different from the stratification based on distance, except for distance regular graphs. In underlying graphs of association schemes, the probability amplitudes and average probabilities are given in terms of dual eigenvalues of association schemes, such that the amplitudes of observing the continuous-time quantum walk on all sites belonging to a given stratum are the same, therefore there are at most $(d + 1)$ different observing probabilities. The importance of association scheme in continuous-time quantum walk is shown by some worked out examples such as arbitrary finite group association schemes followed by symmetric S_n , Dihedral D_{2m} and cyclic groups. At the end it is shown that the highest irreducible representations of Terwilliger algebras pave the way to use the spectral distributions method of Jafarizadeh and Salimi (2005 *Preprint quant-ph/0510174*) in studying quantum walk on some rather important graphs called distance regular graphs.

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1. Introduction

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

of quantum algorithms. This has led to a number of studies. Quantum walks on the line were examined by Nayak and Vishwanath [2] and on the cycle by Aharonov *et al* [3]. The latter have also considered a number of properties of quantum walks on general graphs [1]. Two distinct types of quantum walks have been identified: for the continuous-time quantum walk (CTQW) a time-independent Hamiltonian governs a continuous evolution of a single particle in a Hilbert space spanned by the vertices of a graph [1, 3–5], while the discrete-time quantum walk requires a quantum coin as an additional degree of freedom in order to allow for a discrete-time unitary evolution in the space of the nodes of a graph. The connection between both types of quantum walks is not clear up to now, but in both cases different topologies of the underlying graph have been studied (see, for example, [2, 6–10]).

Different behaviour of the quantum walk as compared to the classical random walk have been reported under various circumstances. For instance, a very promising feature of a quantum walk on a hypercube, namely an exponentially faster hitting time as compared to a classical random walk, has been presently found (numerically) by Yamasaki *et al* [11] and (analytically) by Kempe [12]. Indeed, first quantum algorithms based on quantum walks which offer an (exponential) speedup over their optimal classical counterpart have been reported in [13, 14].

On the other hand, the theory of association schemes has its origin in the design of statistical experiments. The motivation came from the investigation of special kinds of partitions of the Cartesian square of a set for the construction of partially balanced block designs. In this context association schemes were introduced by Bose and Nair. Although the concept of an association scheme was introduced by Bose and Nair, the term itself was first coined by Bose and Shimamoto in [15]. In 1973, through the work of Delsarte [16] certain association schemes were shown to play a central role in the study of error correcting codes. This connection of association schemes to algebraic codes, strongly regular graphs, distance regular graphs, design theory etc, further intensified their study. Association schemes have since then become the fundamental, perhaps the most important objects in algebraic combinatorics. To this regard association schemes have for some time been studied by various people under such names as centralizer algebras, coherent configurations, Schur rings, etc. Correspondingly, there are many different approaches to the study of association schemes.

A further step in the study of association schemes was their algebraization. This formulation was done by Bose and Mesner who introduced to each association scheme a matrix algebra generated by the adjacency matrices of the association scheme. This matrix algebra came to be known as the adjacency algebra of the association scheme or the Bose–Mesner algebra, after the names of the people who introduced them. The other formulation was done by Terwilliger, known as the Terwilliger algebra. This algebra is a finite dimensional, semi-simple and is non-commutative in general. The Terwilliger algebra has been used to study P - and Q -polynomial schemes [17], group schemes [18, 19] and Doob schemes [20].

In this paper, we study CTQW on the underlying graphs of association schemes, by using their algebraic combinatorics structures, namely semi-simple modules of their Bose–Mesner and (reference state dependent) Terwilliger algebras. By choosing the (walk) starting site as a reference state, the Terwilliger algebra connected with this choice stratifies the graph into a $(d + 1)$ disjoint union of strata (associate classes), where the amplitudes of observing the CTQW on all sites belonging to a given stratum are the same. In general, this stratification is different from the one based on distance except for distance regular graphs. Since all vertices of underlying graph of an association scheme are similar or they have a constant measure of similarity, therefore the observing probabilities can be determined by the relations or associate classes. Hence for a CTQW over a graph associated with a given scheme with diameter d , we have at most $(d + 1)$ (the number of strata) different observing probabilities.

In underlying graphs of association schemes, the probability amplitudes and average probabilities are given in terms of dual eigenvalues of association schemes. As most of association schemes arise from finite groups, hence we have studied in great details CTQW on generic group association schemes with real and complex representations, where the probability amplitudes are given in terms of characters of groups. Furthermore, as examples, we have investigated walk on graphs of association schemes of symmetric S_n , Dihedral D_{2m} and cyclic groups.

Also using the algebraic combinatorics structures of some rather important graphs called distance regular graphs (where the Hilbert space of walk consists of irreducible module of Terwilliger algebra with maximal dimension), we have established the required conditions to apply the spectral distributions method of [1], for studying CTQW on them. Actually, it is shown that these conditions are inherent in distance regular graphs, due to the existence of the scheme structure (stratification) based on distance. Then using the spectral distribution, we have evaluated the amplitudes of CTQW on distance regular graphs such as Johnson and strongly regular graphs such as Petersen graphs and normal subgroup graphs. Likewise, using the method of spectral distribution, we have evaluated the probability amplitudes of CTQW on symmetric product of trivial association schemes such as Hamming graphs, where their amplitudes are proportional to the product of amplitudes of constituent sub-graphs, and walk does not generate any entanglement between constituent sub-graphs.

The organization of this paper is as follows. In section 2, we give a brief outline of association schemes, Bose–Mesner and Terwilliger algebras and stratification. Section 3 is devoted to studying CTQW on underlying graphs of association schemes. In section 4, we work out CTQW on group association schemes. Section 5 is devoted to distance regular graphs and the required conditions (stemming from their scheme structure) to reveal their QD nature introduced in [1, 21]. In section 6, we explain how we can associate the spectral distribution μ , introduced in [1, 21], to adjacency matrix A of distance regular graphs to study CTQW, by using their algebraic combinatorics structures. In section 7, we calculate the amplitudes for CTQW on some graphs by using the prescriptions of sections 3, 4, 6. The paper is ended with a brief conclusion and three appendices, where the first appendix consists of studying the method of symmetrization of non-symmetric group schemes, the second appendix contains determination of spectral distribution by continued fractions method and the third appendix contains the list of some of the finite distance regular graphs with their corresponding spectral distributions, respectively.

2. Association scheme, Bose–Mesner algebra, Terwilliger algebra and its modules

In this section, we give a brief outline of some of the main features of association scheme, such as adjacency matrices, Bose–Mesner algebra and Terwilliger algebra. At the end by choosing the (walk) starting site as a reference state we stratify the underlying graphs of association schemes via the relevant Terwilliger algebra connected with this choice.

2.1. Association schemes

First we recall the definition of association schemes. The reader is referred to [22] for further information on association schemes.

Definition 2.1 (association schemes). *Let V be a set of vertices and let R_i ($i = 0, 1, \dots, d$) be non-empty relations on V (i.e., subset of $V \times V$). Let the following conditions (1)–(4)*

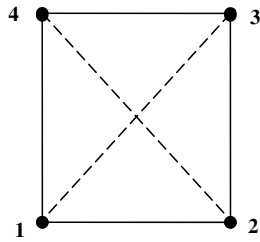


Figure 1. Hamming scheme for $n = 2$ and $d = 2$ which consist of vertices $\{1, 2, 3, 4\}$ and relations $R_0 = \{(i, i) : i = 1, 2, 3, 4\}$, $R_1 = \{(i, i + 1(\bmod 4)) : i = 1, 2, 3, 4\} \cup \{(i + 1(\bmod 4), i) : i = 1, 2, 3, 4\}$ set of solid line and $R_2 = \{(i, i + 2(\bmod 4)) : i = 1, 2, 3, 4\} \cup \{(i + 2(\bmod 4), i) : i = 1, 2, 3, 4\}$ set of dashed line, respectively. Its non-vanishing intersection numbers are $p_{11}^0 = 2, p_{22}^0 = 1, p_{01}^1 = p_{10}^1 = 1, p_{11}^2 = 2, p_{21}^1 = p_{12}^1 = 1$.

be satisfied. Then the pair $Y = (V, \{R_i\}_{0 \leq i \leq d})$ consisting of a set V and a set of relations $\{R_i\}_{0 \leq i \leq d}$ is called an association scheme:

- (1) $\{R_i\}_{0 \leq i \leq d}$ is a partition of $V \times V$,
- (2) $R_0 = \{(\alpha, \alpha) : \alpha \in V\}$,
- (3) $R_i = R_i^t$ for $0 \leq i \leq d$, where $R_i^t = \{(\beta, \alpha) : (\alpha, \beta) \in R_i\}$,
- (4) Given $(\alpha, \beta) \in R_k, p_{ij}^k = |\{\gamma \in V : (\alpha, \gamma) \in R_i \text{ and } (\gamma, \beta) \in R_j\}|$, where the constants p_{ij}^k are called the intersection numbers, depend only on i, j and k and not on the choice of $(\alpha, \beta) \in R_k$. Also condition (3) implies that $p_{ij}^k = p_{ji}^k$ for all $i, j, k \in \{0, 1, \dots, d\}$.

Then the number n of the vertices V is called the order of the association scheme and R_i is called a relation (colour) or associate class. Therefore, intersection number p_{ij}^k can be interpreted as the number of vertices which have relation i and j with vertices α and β , respectively, provided that $(\alpha, \beta) \in R_k$, and it is the same for all element of relation R_k (see figure 1). For all integers i ($0 \leq i \leq d$), set $k_i = p_{ii}^0$ and note that $k_i \neq 0$, since R_i is non-empty. We refer to k_i as the i th valency of Y . Observe that $p_{ij}^0 = \delta_{ij}k_i$ ($0 \leq i, j \leq d$).

Also for a given vertex α , we denote $R_i(\alpha) = \{\beta \in V : (\alpha, \beta) \in R_i\}$ as the set of vertices having relation R_i with it. Therefore, the set V can be written as disjoint union of $R_i(\alpha)$ for $i = 0, 1, 2, \dots, d$, i.e.,

$$V = \bigcup_{i=0}^d R_i(\alpha). \tag{2.1}$$

Finally, the underlying graph of an association scheme $\Gamma = (V, R_1)$ is an undirected connected graph, where the sets V and R_1 consist of its vertices and edges, respectively. Obviously, replacing R_1 with one of other relation such as R_i , for $i \neq 0, 1$, will also give us an underlying graph $\Gamma = (V, R_i)$ (not necessarily a connected graph) with the same set of vertices but a new set of edges R_i .

2.2. The Bose–Mesner algebra

Let C denote the field of complex numbers. By $\text{Mat}_V(C)$ we mean the C -algebra consisting of all matrices whose entries are in C and whose rows and columns are indexed by V . For each integer i ($0 \leq i \leq d$), let A_i denote the matrix in $\text{Mat}_V(C)$ with (α, β) -entry

$$(A_i)_{\alpha,\beta} = \begin{cases} 1 & \text{if } (\alpha, \beta) \in R_i, \\ 0 & \text{otherwise,} \end{cases} \quad (\alpha, \beta \in V). \tag{2.2}$$

The matrices A_i are called the adjacency matrices of the association scheme. We then have $A_0 = I$ (by (2)) and

$$A_i A_j = \sum_{k=0}^d p_{ij}^k A_k \tag{2.3}$$

(by (4)), so A_0, A_1, \dots, A_d form a basis for a commutative algebra \mathbf{A} of $\text{Mat}_V(C)$, where \mathbf{A} is known as the Bose–Mesner algebra of $Y = (V, \{R_i\}_{0 \leq i \leq d})$.

Since the matrices A_i commute, they can be diagonalized simultaneously (see [23]), that is, there exists a matrix S such that for each $A \in \mathbf{A}$, $S^{-1}AS$ is a diagonal matrix. Therefore, \mathbf{A} is semi-simple and has a second basis E_0, \dots, E_d (see [22]). These are matrices satisfying

$$E_0 = \frac{1}{n}J, \quad E_i E_j = \delta_{ij} E_i, \quad \sum_{i=0}^d E_i = I. \tag{2.4}$$

The matrix $\frac{1}{n}J$ (where J is the all-one matrix in \mathbf{A}) is a minimal idempotent (idempotent is clear, and minimal follows from the rank ($J = 1$)). E_i , for $0 \leq i, j \leq d$, are known as the primitive idempotent of Y . Let P and Q be the matrices relating our two bases for \mathbf{A} :

$$\begin{aligned} A_j &= \sum_{i=0}^d P_{ij} E_i, & 0 \leq j \leq d, \\ E_j &= \frac{1}{n} \sum_{i=0}^d Q_{ij} A_i, & 0 \leq j \leq d \end{aligned} \tag{2.5}$$

Then clearly

$$PQ = QP = nI. \tag{2.6}$$

It also follows that

$$A_j E_i = P_{ij} E_i, \tag{2.7}$$

which shows that P_{ij} (resp. Q_{ij}) is the i th eigenvalue (resp. the i th dual eigenvalue) of A_j (resp. E_j) and that the columns of E_i are the corresponding eigenvectors. Thus, $m_i = \text{rank}(E_i)$ is the multiplicity of the eigenvalue P_{ij} of A_j (provided that $P_{ij} \neq P_{kj}$ for $k \neq i$). We see that $m_0 = 1$, $\sum_i m_i = n$ and $m_i = \text{trace } E_i = n(E_i)_{jj}$ (indeed, E_i has only eigenvalues 0 and 1, so $\text{rank}(E_k)$ equals the sum of the eigenvalues). Also, by [24, 25], the eigenvalues and dual eigenvalues satisfy

$$\begin{aligned} P_{i0} = Q_{i0} = 1, & \quad P_{0i} = k_i, & \quad Q_{0i} = m_i \\ m_j P_{ji} = k_i Q_{ij}, & \quad 0 \leq i, \quad j \leq d. \end{aligned} \tag{2.8}$$

2.3. The Terwilliger algebra and its modules

We now recall the dual Bose–Mesner algebra of Y . Given a *reference vertex* $\alpha \in V$, for all integers i define $E_i^* = E_i^*(\alpha) \in \text{Mat}_V(C)$ ($0 \leq i \leq d$) to be the diagonal matrix with (β, β) -entry

$$(E_i^*)_{\beta, \beta} = \begin{cases} 1 & \text{if } (\alpha, \beta) \in R_i, \\ 0 & \text{otherwise,} \end{cases} \quad (\alpha \in V). \tag{2.9}$$

The matrix E_i^* is called the i th dual idempotent of Y with respect to α . We shall always set $E_i^* = 0$ for $i < 0$ or $i > d$. From the definition, the dual idempotents satisfy the relations

$$\sum_{i=0}^d E_i^* = I, \quad E_i^* E_j^* = \delta_{ij} E_i^*, \quad 0 \leq i, \quad j \leq d. \tag{2.10}$$

It follows that the matrices $E_0^*, E_1^*, \dots, E_d^*$ form a basis for the subalgebra $A^* = A^*(\alpha)$ of $\text{Mat}_V(R)$. A^* is known as the dual Bose–Mesner algebra of Y with respect to α . For each integer i ($0 \leq i \leq d$), let $A_i^* = A_i^*(\alpha)$ denote the diagonal matrix in $\text{Mat}_V(R)$ with (β, β) -entry:

$$(A_i^*)_{(\beta, \beta)} = n(E_i)_{\alpha, \beta} \quad (\beta \in V). \quad (2.11)$$

With reference to [24, 25] the matrices $A_0^*, A_1^*, \dots, A_d^*$ form a second basis for A^* and satisfy

$$\begin{aligned} A_0^* &= I, & A_i^{*t} &= A_i^*, & A_i^{*t} &= A_i^*, & A_0^* + A_1^* + \dots + A_d^* &= nE_0^*, \\ A_i^* A_j^* &= \sum_{h=0}^d q_{ij}^h A_h^*. \end{aligned} \quad (2.12)$$

Then by combining (2.5) with (2.9) and (2.11) we have

$$A_j^* = \sum_{i=0}^d Q_{ij} E_i^*, \quad E_j^* = \frac{1}{n} \sum_{i=0}^d P_{ij} A_i^*, \quad 0 \leq j \leq d. \quad (2.13)$$

Let $Y = (V, \{R_i\}_{0 \leq i \leq d})$ denote a scheme. Fix any $\alpha \in V$ and write $A^* = A^*(\alpha)$. Let $T = T(\alpha)$ denote the subalgebra of $\text{Mat}_V(C)$ generated by A and A^* . We call T the Terwilliger algebra of Y with respect to α .

Let $W = C^V$ denote the vector space over C consisting of column vectors whose coordinates are indexed by V and whose entries are in C . We observe $\text{Mat}_V(C)$ which acts on W by left multiplication. We endow W with the Hermitian inner product $\langle \cdot, \cdot \rangle$ which satisfies $\langle u, v \rangle = u^t \bar{v}$ for all $u, v \in W$, where t denotes the transpose and $\bar{\cdot}$ 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 that $\{|\beta\rangle \mid \beta \in V\}$ is an orthonormal basis for W . Using (2.9) we have

$$E_i^* W = \text{span}\{|\beta\rangle \mid \beta \in V, (\alpha, \beta) \in R_i\}, \quad 0 \leq i \leq d. \quad (2.14)$$

Now using relations (2.10) we can show that the operator E_i^* projects W onto $E_i^* W$, thus W can be written as direct sum of $E_i^* W$, $i = 0, 1, \dots, d$, i.e.,

$$W = E_0^* W \oplus E_1^* W \oplus \dots \oplus E_d^* W. \quad (2.15)$$

Similarly, using the idempotency relation (2.4), we can write

$$W = E_0 W \oplus E_1 W \oplus \dots \oplus E_d W. \quad (2.16)$$

We call $E_i^* W$ the i th subconstituent of $\Gamma = (V, R)$ with respect to α .

By a T -module we mean a subspace $U \subseteq W$ such that $TU \subseteq U$. Let U denote a T -module. Then U is said to be irreducible whenever U is non-zero and U contains no T -modules other than 0 and U . Let U denote an irreducible T -module. Then U is the orthogonal direct sum of the non-zero spaces among $E_0^* U, E_1^* U, \dots, E_d^* U$ ([17], lemma 3.4). By the endpoint of U we mean $\min\{i \mid 0 \leq i \leq d, E_i^* U \neq 0\}$. By the diameter of U we mean $|\{i \mid 0 \leq i \leq d, E_i^* U \neq 0\}| - 1$. We say U is thin whenever $E_i^* U$ has dimension at most 1 for $0 \leq i \leq d$. There exists a unique irreducible T -module which has endpoint 0 ([26], proposition 8.4). This module is called W_0 .

2.4. Stratification

We fix a point $o \in V$ as an origin of the underlying graph, called reference vertex. Then, relation (2.1) stratifies underlying graph into a disjoint union of associate classes $R_i(o)$.

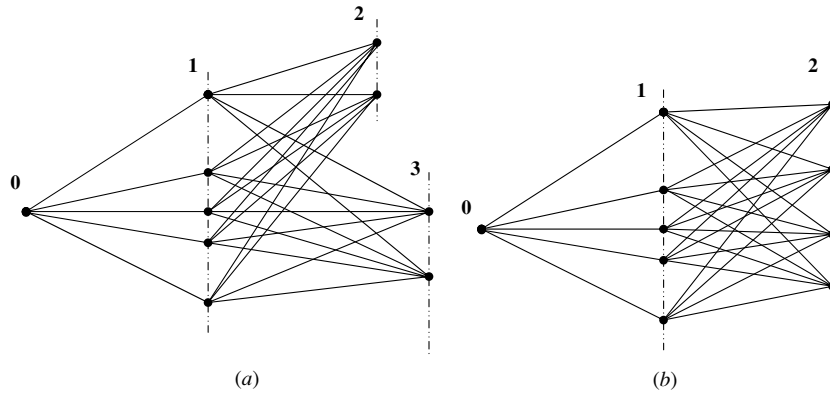


Figure 2. (a) The underlying graph of group association scheme D_{10} with diameter $d = 3$ and the stratification based on conjugacy relations, hence it has four strata, where strata 2, 3 have the same distance from the reference stratum (stratum 0). (b) The underlying graph of normal subgroup scheme D_{10} (strongly regular graph) with diameter $d = 2$ and the stratification (with three strata) based on distance function.

With each associate class $R_i(o)$ we associate a unit vector in $l^2(V)$ defined by

$$|\phi_i\rangle = \frac{1}{\sqrt{k_i}} \sum_{\alpha \in R_i(o)} |\alpha\rangle \in E_i^*W, \tag{2.17}$$

where $|\alpha\rangle$ denotes the eigenket of α th vertex at the associate class $R_i(o)$ and $k_i = |R_i(o)|$. The closed subspace of $l^2(V)$ spanned by $\{|\phi_i\rangle\}$ is denoted by $\Lambda(G)$. Since $\{|\phi_i\rangle\}$ becomes a complete orthonormal basis of $\Lambda(G)$, we often write

$$\Lambda(G) = \sum_i \oplus \mathbb{C}|\phi_i\rangle. \tag{2.18}$$

Let A_i be the adjacency matrix of a graph $\Gamma = (V, R)$ for reference state $|\phi_0\rangle$ ($|\phi_0\rangle = |o\rangle$), with $o \in V$ as reference vertex, we have

$$A_i|\phi_0\rangle = \sum_{\beta \in R_i(o)} |\beta\rangle. \tag{2.19}$$

Also, we have

$$A_i|\phi_0\rangle = E_i^*|\phi_0\rangle \in E_i^*W, \quad E_i^*A_l|\phi_0\rangle = \delta_{li}A_l|\phi_0\rangle \tag{2.20}$$

Then by using unit vectors $|\phi_i\rangle$ and equations (2.19), (2.20), we have

$$A_i|\phi_0\rangle = \sqrt{k_i}|\phi_i\rangle. \tag{2.21}$$

For $0 \leq i \leq d$, the vector $|\phi_i\rangle$ of equation (2.17) is a basis for $E_i^*W_0$ ([17], lemma 3.6).

Therefore, W_0 is thin with diameter d such that the module W_0 is orthogonal to each irreducible T -module other than W_0 ([27], lemma 3.3).

At the end one should note that sometimes we can stratify a given graph (with adjacency matrix A) in different ways, simply by considering it as the underlying graph of different association schemes. For example, as it is shown in section 7, we can associate two different association schemes for dihedral graph D_{2m} (one of them is distance regular one) with the same underlying graph (see figures 2(a) and (b)).

3. CTQW on underlying graphs of association schemes

The CTQW on graph is defined by replacing Kolmogorov's equation (master equation) of continuous-time classical random walk on a graph [28, 29]

$$\frac{dP_i(t)}{dt} = \sum_{j=1}^n H_{ij} P_j(t), \quad i = 1, 2, \dots, n \quad (3.22)$$

with Schrödinger's equation, where the matrix H is Hamiltonian of walk and $P_i(t)$ is the occupying probability of vertex i at time t . It is natural to choose the Laplacian of the graph, defined as $L = A - D$ as Hamiltonian of walk, where D is a diagonal matrix with entries $D_{jj} = \deg(\alpha_j)$. This is because we can view L as the generator matrix that describes an exponential distribution of waiting times at each vertex.

CTQW was introduced by Farhi and Gutmann [5] (see also [8, 30]). Our treatment, though, closely follow the analysis of Moore and Russell [30] which we review next. Let $l^2(V)$ denote the Hilbert space of C -valued square-summable functions on V . With each $\alpha \in V$ we associate a ket defined by $|\alpha\rangle$, then $\{|\alpha\rangle, \alpha \in V\}$ becomes a complete orthonormal basis of $l^2(V)$.

For $0 \leq i \leq d$ the vector $|\phi_i\rangle$ of equation (2.17) is a basis of $E_i^* W_0$, where W_0 is unique irreducible T -module which has endpoint 0 ([26], proposition 8.4). Therefore, Hilbert space of CTQW starting from a given site corresponds to the irreducible (with starting site of walk as a reference vertex of T -algebra) T -module W_0 with maximal dimension. Hence, other irreducible T -modules of Terwilliger algebra T are orthogonal to Hilbert space of the walk.

Let $|\phi(t)\rangle$ be a time-dependent amplitude of the quantum process on graph Γ . The wave evolution of the quantum walk is

$$i\hbar \frac{d}{dt} |\phi(t)\rangle = H |\phi(t)\rangle, \quad (3.23)$$

where we assume $\hbar = 1$ and $|\phi_0\rangle$ is the initial amplitude wavefunction of the particle. The solution 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

$$e^{-itH} = e^{-it(A - \frac{1}{d}I)} = e^{-it/d} e^{-itA}. \quad (3.24)$$

This introduces an irrelevant phase factor in the wave evolution. Hence we can consider $H = A = A_1$. Then using equation (2.5) we have

$$|\phi_0(t)\rangle = e^{-iAt} |\phi_0\rangle = e^{-i \sum_{i=0}^d P_i E_i t} |\phi_0\rangle, \quad (3.25)$$

where using the algebra of idempotents, i.e., equation (2.4), the above amplitude of wavefunction can be written as

$$|\phi_0(t)\rangle = \sum_{i=0}^d e^{-iP_i t} E_i |\phi_0\rangle. \quad (3.26)$$

Now using equations (2.5), (2.6), (2.17) and (2.21), the matrix elements of idempotent operators between eigenstates strata and eigenstates of vertices can be calculated as

$$\langle \phi_k | E_i | \phi_0 \rangle = \langle \phi_k | \frac{1}{n} \sum_{l=0}^d Q_{li} A_l | \phi_0 \rangle = \frac{1}{n} \sum_{l=0}^d Q_{li} \langle \phi_k | A_l | \phi_0 \rangle = \frac{\sqrt{k_k}}{n} Q_{ki}, \quad (3.27)$$

$$\langle \beta | E_i | \phi_0 \rangle = \frac{1}{n} Q_{ki}, \quad \text{for every } |\beta\rangle \in R_k(o), \quad (3.28)$$

respectively.

Finally multiplying (3.26) by $|\phi_k\rangle, |\beta\rangle$ and using (3.27), (3.28), we get the following expression for the amplitudes of observing the particle at vertex β and state $|\phi_k\rangle$ at time t :

$$\langle\phi_k|\phi_0(t)\rangle = \sum_{i=0}^d e^{-iP_{i1}t} \langle\phi_k|E_i|\phi_0\rangle = \frac{\sqrt{k_k}}{n} \sum_{i=0}^d e^{-iP_{i1}t} Q_{ki}. \tag{3.29}$$

$$\langle\beta|\phi_0(t)\rangle = \sum_{i=0}^d e^{-iP_{i1}t} \langle\beta|E_i|\phi_0\rangle = \frac{1}{n} \sum_{i=0}^d e^{-iP_{i1}t} Q_{ki}, \quad \text{for every } |\beta\rangle \in R_k(o), \tag{3.30}$$

respectively. Now, comparing (3.29) and (3.30), we get

$$\langle\beta|\phi_0(t)\rangle = \frac{1}{\sqrt{k_k}} \langle\phi_k|\phi_0(t)\rangle, \quad \text{for every } |\beta\rangle \in R_k(o). \tag{3.31}$$

Above relation indicates that the amplitudes of observing walk at vertices belonging to a given stratum are the same. Actually, we can straightforwardly deduce from formula (3.30) that absolute value of the matrix elements $|\langle\beta|e^{-itA}|\alpha\rangle|$ (the absolute value of probability amplitudes of observing walk at time t at vertex β provided that walk starts at vertex α) depends on the kind of relation between vertices α and β , i.e., $|\langle\beta|e^{-itA}|\alpha\rangle|$ is the same for all $(\alpha, \beta) \in R_k(o)$. This is due to the fact that in an association scheme the colouring of underlying graphs or the set of relations between vertices thoroughly determines everything. Hence for a CTQW over a graph associated with a given scheme with diameter d , we have at most $(d + 1)$ different observing probabilities (i.e., the number of strata or number of distinct eigenvalues of adjacency matrix).

At the end, by straightforward calculation, we can evaluate the average probability for finite graphs of association schemes as

$$\bar{P}(\beta) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T P_t(\beta) dt = \frac{1}{n^2} \sum_{i=0}^d Q_{ki}^2, \tag{3.32}$$

for every $|\beta\rangle \in R_k(o)$, where in obtaining above formula it is assumed that P_{i1} are all different for $i = 0, 1, \dots, d$.

Obviously, by replacing A_1 with $A_i, i \neq 0, 1$, we can study walk on underlying graph $\Gamma = (V, R_i)$. Definitely for a graph $\Gamma = (V, R_i)$, all of thus obtained results hold true (except for formula (3.32)), provided that we replace index 1 with index i everywhere, such as formulae (3.26) and (3.30).

Also we should note that the average probability of observing walk at vertex β given in (3.32) is the same for all underlying graphs with different eigenvalues.

4. CTQW on underlying graph of group schemes

In this section, we briefly discuss CTQW on group schemes with real and complex representations separately.

4.1. Group association schemes

In order to study the CTQW on group graphs, we need to study the group association schemes. One of the most important sources of association schemes is groups. Let G be a transitive group acting on a finite set V . Then G has a natural action on $V \times V$ given by $g(\alpha, \beta) = (g\alpha, g\beta)$

for $g \in G$ and $\alpha, \beta \in V$. The orbits $\{(g\alpha, g\beta) | g \in G\}$ of $V \times V$ are called orbitals. Further, we assume that the group G acting on V to be generously transitive, i.e., for every pair $(\alpha, \beta) \in V \times V$, there is a group element $g \in G$ that interchanges α and β , that is $g\alpha = \beta$ and $g\beta = \alpha$. For generously transitive G , the orbitals form the relations of the association scheme. Now, in the following, we consider the orbitals which correspond to the conjugacy classes of G . Let G be a finite group, $C_0 = \{e\}, C_1, \dots, C_d$ the conjugacy classes of G . Let $G \times G$ act on G with the action defined by $\beta(\alpha_1, \alpha_2) = \alpha_1^{-1}\beta\alpha_2$ where $\beta, \alpha_1, \alpha_2 \in G$. Then the diagonal action of $G \times G$ on $G \times G$ is given by $(\beta, \gamma)(\alpha_1, \alpha_2) = (\beta(\alpha_1, \alpha_2), \gamma(\alpha_1, \alpha_2)) = (\alpha_1^{-1}\beta\alpha_2, \alpha_1^{-1}\gamma\alpha_2)$. We can show that $(\beta_1, \beta_2), (\gamma_1, \gamma_2) \in G \times G$ belong to the same orbital of $G \times G$ if and only if $\beta_1^{-1}\beta_2, \gamma_1^{-1}\gamma_2$ belong to the same conjugacy class of G . Thus, in this case the orbitals correspond to the conjugacy classes of G . For $i = 0, 1, \dots, d$ define

$$R_i = \{(\alpha, \beta) | \alpha^{-1}\beta \in C_i\}, \quad (4.33)$$

then R_i are the orbitals of $G \times G$ and hence $X(G) = (G, \{R_i\}_{0 \leq i \leq d})$ becomes a commutative association scheme and it is called the group association scheme of the finite group G [25]. Definitely relations (4.33) imply that $R_i(e) = C_i$, where e is the unit element of group G . We define class sums \bar{C}_i for $i = 0, 1, \dots, d$ as

$$\bar{C}_i = \sum_{\gamma \in C_i} \gamma \in CG, \quad (4.34)$$

then for regular representation we have $\bar{C}_i|\alpha\rangle = \sum_{\gamma \in C_i} |\gamma\alpha\rangle$. Therefore, in regular representation the class sums \bar{C}_i ($i = 0, 1, \dots, d$) have the following matrix elements:

$$(\bar{C}_i)_{\alpha, \beta} = \begin{cases} 1 & \text{if } (\alpha, \beta) \in C_i, \\ 0 & \text{otherwise,} \end{cases} \quad (\alpha, \beta \in G). \quad (4.35)$$

Comparing the above matrix elements with those of adjacency matrices given in (2.4), we see that the class sums are the corresponding adjacency matrices of group association scheme with the relation defined through conjugation. It is well known that the class sums of finite group G form the basis of centre of its CG ring which is certainly a commutative algebra, hence they are closed under multiplication defined in CG , i.e., we have

$$\bar{C}_i \bar{C}_j = \sum_{k=0}^d p_{ij}^k \bar{C}_k$$

(see details in [31]), where p_{ij}^k ($i, j, k = 0, 1, \dots, d$) are the intersection numbers of the group association scheme $X(G)$ and have the following form:

$$p_{ij}^k = \frac{|C_i||C_j|}{|G|} \sum_{\chi} \frac{\chi(\alpha_i)\chi(\alpha_j)\overline{\chi(\alpha_k)}}{\chi(1)}, \quad (4.36)$$

where the sum is over all the irreducible characters χ of G [32]. Therefore, the idempotents $\{E_0, E_1, \dots, E_d\}$ of the group association scheme $X(G)$ are the projection operators of CG -module, i.e.,

$$E_k = \frac{\chi_k(1)}{|G|} \sum_{\alpha \in G} \chi_k(\alpha^{-1})\alpha. \quad (4.37)$$

Thus, eigenvalues of adjacency matrices of A_k and idempotents E_k , respectively, are

$$P_{ik} = \frac{d_i k_k}{m_i} \chi_i(\alpha_k), \quad Q_{ik} = d_k \overline{\chi_k(\alpha_i)}, \quad (4.38)$$

where $d_j = \chi_j(1)$. The above-defined group scheme is in general non-symmetric scheme and it can be symmetric provided that we choose a group whose whole irreducible representations of chosen group are real, such as symmetric group S_n . In appendix A, we have explained how to construct a symmetric group association scheme from a non-symmetric one.

4.1.1. *CTQW on underlying graph of group schemes with real representations.* In a finite group G with real conjugacy classes $C_0 = \{e\}, C_1, \dots, C_d$, i.e., $C(\alpha) = C(\alpha^{-1})$ for all $\alpha \in G$, all irreducible characters χ_i are real. Thus using (4.38) we can study CTQW on its underlying graph, where the amplitude of observing the particle at stratum k at time t , i.e., equation (3.30), reduces to

$$\langle \phi_k | \phi_0(t) \rangle = \frac{\sqrt{k_k}}{n} \sum_{i=0}^d d_i e^{\frac{-id_i k_1 \chi_i(\alpha_1)t}{m_i}} \overline{\chi_i(\alpha_k)}, \tag{4.39}$$

also the average probabilities over large times become

$$\bar{P}(k) = \frac{k_k}{n^2} \sum_{i=0}^d d_i^2 |\chi_i(\alpha_k)|^2, \quad k = 0, 1, \dots, d. \tag{4.40}$$

Therefore, the probability of observing the walk at starting vertex, i.e., the staying probability, is

$$\bar{P}(0) = \frac{k_0}{n^2} \sum_{i=0}^d d_i^2 |\chi_i(0)|^2 = \frac{1}{n^2} \sum_{i=0}^d d_i^4. \tag{4.41}$$

As examples we will study CTQW on $G = S_n, D_{2m}$ graphs in section 7.

4.1.2. *CTQW on underlying graph of group schemes with complex representations.* In general, all conjugacy classes of a given finite group are not real, hence some of its irreducible representations become complex and consequently we encounter with directed underlying graph or non-symmetric association scheme. But following instruction of appendix A we can generate a symmetric association scheme out of non-symmetric association scheme. Thus in this case, for CTQW on underlying graph of group schemes with complex representations, we need to use formulae (A.5) and (A.7) of appendix A, where the amplitude of observing the particle at stratum k at time t , i.e., equation (3.30), is

$$\langle \phi_k | \phi_0(t) \rangle = \begin{cases} \frac{\sqrt{k_k}}{n} \sum_{i=0}^l d_i e^{\frac{-id_i k_1 \chi_i(\alpha_1)t}{m_i}} \overline{\chi_i(\alpha_k)} & \text{for real representation,} \\ \frac{\sqrt{k_k}}{n} \sum_{i=l+1}^{\frac{d+l}{2}} d_i e^{\frac{-id_i k_1 (\chi_i(\alpha_1) + \overline{\chi_i(\alpha_1)})t}{m_i}} (\overline{\chi_i(\alpha_k)} + \chi_i(\alpha_k)) & \text{for non-real representation.} \end{cases} \tag{4.42}$$

Also, the average probabilities are

$$\bar{P}(k) = \begin{cases} \frac{k_k}{n^2} \sum_{i=0}^l d_i^2 |\chi_i(\alpha_k)|^2 & \text{for real representation,} \\ \frac{k_k}{n^2} \sum_{i=l+1}^{\frac{d+l}{2}} d_i^2 |\chi_i(\alpha_k) + \overline{\chi_i(\alpha_k)}|^2 & \text{for complex representation.} \end{cases} \tag{4.43}$$

In this case, the staying probability is

$$\bar{P}(0) = \frac{k_0}{n^2} \left(\sum_{i=0}^l d_i^2 |\chi_i(0)|^2 + 4 \sum_{i=l+1}^{\frac{d+l}{2}} d_i^2 |\chi_i(0)|^2 \right) = \frac{1}{n^2} \left(\sum_{i=0}^l d_i^4 + 4 \sum_{i=l+1}^{\frac{d+l}{2}} d_i^4 \right). \tag{4.44}$$

As an example we will study $G = C_n$ in section 7.

5. Distance regular graphs

Here in this section we consider some set of important graphs called distance regular graphs, where the relations are based on distance function defined as follows: a finite sequence $\alpha_0, \alpha_1, \dots, \alpha_n \in V$ is called a walk of length n (or of n steps) if $\alpha_{k-1} \sim \alpha_k$ for all

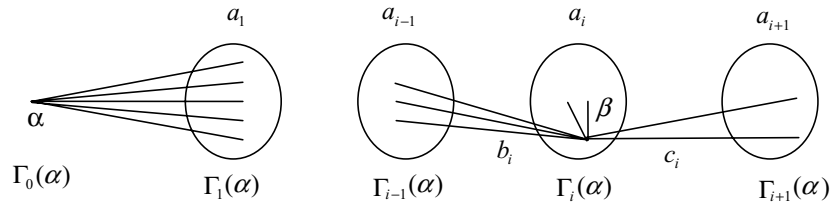


Figure 3. Edges through α and β in a distance regular graph.

$k = 1, 2, \dots, n$. For $\alpha \neq \beta$ let $\partial(\alpha, \beta)$ be the length of the shortest walk connecting α and β , therefore $\partial(\alpha, \beta)$ gives the distance between vertices α and β hence it is called the distance function and we have $\partial(\alpha, \alpha) = 0$ for all $\alpha \in V$ and $\partial(\alpha, \beta) = 1$ if and only if $\alpha \sim \beta$. Therefore, the distance regular graphs become metric spaces with the distance function ∂ .

An undirected connected graph $\Gamma = (V, R_1)$ is called distance regular graph if it is the underlying graph of an association scheme with relations defined as $(\alpha, \beta) \in R_i$ if and only if $\partial(\alpha, \beta) = i$, for $i = 0, 1, \dots, d$, where $d := \max\{\partial(\alpha, \beta) : \alpha, \beta \in V\}$ is called the diameter of graph. Usually, in distance regular graphs the relations R_i are denoted by Γ_i .

Now, in any connected graph, for every $\beta \in \Gamma_i(\alpha)$, we have

$$\Gamma_1(\beta) \subseteq \Gamma_{i-1}(\alpha) \cup \Gamma_i(\alpha) \cup \Gamma_{i+1}(\alpha). \tag{5.45}$$

Hence in a distance regular graph, $p_{j1}^i = 0$ (for $i \neq 0, j$ is not $\{i - 1, i, i + 1\}$) and the non-zero intersection numbers are denoted by

$$a_i = p_{ii}^0, \quad b_i = p_{i-1,1}^i, \quad c_i = p_{i+1,1}^i, \tag{5.46}$$

respectively (see figure 3).

Then, by using equation (5.46) and Bose–Mesner algebra (2.3), for adjacency matrices of distance regular graph Γ , we have

$$A_1 A_i = c_{i-1} A_{i-1} + (a_1 - b_i - c_i) A_i + b_{i+1} A_{i+1}, \quad \text{for } i = 1, 2, \dots, d - 1, \tag{5.47}$$

$$A_1 A_d = c_{d-1} A_{d-1} + (a_1 - b_d) A_d.$$

Using the recursion relations (5.47), we can show that A_i is a polynomial in A_1 of degree i , i.e., we have

$$A_i = P_i(A_1), \quad i = 1, 2, \dots, d, \tag{5.48}$$

and conversely A_1^i can be written as a linear combination of I, A_1, \dots, A_i .

Now, we quote a lemma which is crucial to deduce that the distance regular graphs possess natural quantum decomposition structure (introduced in [1, 21]) stemming from Terwilliger algebra representation.

Lemma 1 (Terwilliger [17]). *Let Γ denote a distance regular graph with diameter d . Fix any vertex α of Γ and write $E_i^* = E_i^*(\alpha)$ ($0 \leq i \leq d$), $A = A_1$ and $T = T(\alpha)$. Define $A^- = A^-(\alpha)$, $A^0 = A^0(\alpha)$, $A^+ = A^+(\alpha)$ as elements of Terwilliger algebra by*

$$A^- = \sum_{i=1}^d E_{i-1}^* A E_i^*, \quad A^0 = \sum_{i=1}^d E_i^* A E_i^*, \quad A^+ = \sum_{i=1}^d E_{i+1}^* A E_i^*. \tag{5.49}$$

Then,

$$A = A^+ + A^- + A^0, \tag{5.50}$$

where this is the quantum decomposition of adjacency matrix A such that

$$(A^-)^t = A^+, \quad (A^0)^t = A^0, \tag{5.51}$$

where it can be verified easily.

In the case of distance regular graphs, the strata states $|\phi_k\rangle$ are the same as defined by (2.17) of subsection 2.4, and further by using equations (5.47) and (5.50) we can show that the raising and lowering operators given by (5.49) act over them as follows:

$$A^+|\phi_k\rangle = \sqrt{\omega_{k+1}}|\phi_{k+1}\rangle, \quad k \geq 0, \tag{5.52}$$

$$A^-|\phi_0\rangle = 0, \quad A^-|\phi_k\rangle = \sqrt{\omega_k}|\phi_{k-1}\rangle, \quad k \geq 1, \tag{5.53}$$

$$A^0|\phi_k\rangle = (\alpha_{k+1})|\phi_k\rangle, \quad k \geq 0. \tag{5.54}$$

As mentioned in section 2, $|\phi_k\rangle, k = 0, 1, \dots, d$, form a basis for W_0 which is the irreducible T -module with maximal dimension, therefore all basis of the irreducible T -module W_0 can be obtained by repeated action of raising operator A^+ on reference state $|\phi_0\rangle$ and we have

$$\omega_k = c_{k-1}b_k, \quad \alpha_k = a_1 - b_{k-1} - c_{k-1} \tag{5.55}$$

similar to [1], where a_k, b_k and c_k are already defined by relations given in (5.46). The space W_0 equipped with set of operators (Γ, A^+, A^-, A^0) is an interacting Fock space associated with the Jacobi sequence $\{c_{k-1}b_k, a_1 - b_k - c_k, k = 1, 2, \dots\}$.

Summarizing all above-mentioned properties of distance regular graphs stemming from the algebraic combinatorics structures of these particular association schemes, specially existence of raising and lowering operators given by (5.49) acting on bases of irreducible T -module W_0 , and comparing these properties with those of QD graphs of [1, 21], we can deduce that distance regular graphs possess quantum decomposition and using it we can find their spectrum by spectral distribution method of [1, 21]. Of course there are some differences between distance regular graphs and those QD graphs of [1, 21]. As an example, in distance regular graphs stratification is reference state independent, namely we can choose every vertex as a reference state (therefore we can study CTQW via spectral distribution method of [1] irrespective of the starting site), while the stratification of graphs of [1] is reference dependent and we cannot stratify them for every choice of reference state.

We should know that, in general, it is hard to find the spectrum of a given Bose–Mesner algebra and the spectral distribution method works rather elegantly, only in cases of distance regular graphs (for more detail see [33]).

6. Investigation of CTQW on distance regular graphs via spectral distribution of adjacency matrix

The spectral analysis of operators is an important issue in quantum mechanics, operator theory and mathematical physics [34, 35]. As an example $\mu(dx) = |\psi(x)|^2 dx$ ($\mu(dp) = |\tilde{\psi}(p)|^2 dp$) is the spectral distribution of position (momentum) operator $\hat{X}(\hat{P})$ assigned to quantum state $|\psi\rangle$.

It is well known that for any pair $(A, |\phi_0\rangle)$ of a matrix A and a vector $|\phi_0\rangle$ a measure μ can be assigned as follows (for more details see [33]):

$$\mu(x) = \langle \phi_0 | E(x) | \phi_0 \rangle, \tag{6.56}$$

where $E(x)$ is the operator of projection onto the eigenspace of A corresponding to eigenvalue x , i.e.,

$$A = \int x E(x) dx. \tag{6.57}$$

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

$$P(A) = \int P(x)E(x) dx, \quad (6.58)$$

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

Therefore, using relations (6.56) and (6.58), the expectation value of powers of adjacency matrix $A = A_1$ over reference state $|\phi_0\rangle$ can be written as

$$\langle A^m \rangle = \int_R x^m \mu(dx), \quad m = 0, 1, 2, \dots, \quad (6.59)$$

where, according to [21], $\langle A^m \rangle$ coincides with the number of m -step walks starting and terminating at o . Then the existence of a spectral distribution satisfying (6.59) is a consequence of Hamburger's theorem, see e.g., ([36], theorem 1.2).

Now, in the case of distance regular graphs, according to (5.48), the adjacency matrices are of polynomial functions of A ; hence, using (2.21) and (6.59) the matrix elements $\langle \phi_k | A^m | \phi_0 \rangle$ can be written as

$$\begin{aligned} \langle \phi_k | A^m | \phi_0 \rangle &= \frac{1}{\sqrt{a_k}} \langle \phi_0 | A_k A^m | \phi_0 \rangle = \frac{1}{\sqrt{a_k}} \langle \phi_0 | P_k(A) A^m | \phi_0 \rangle \\ &= \frac{1}{\sqrt{a_k}} \int_R x^m P_k(x) \mu(dx), \quad m = 0, 1, 2, \dots \end{aligned} \quad (6.60)$$

One of our goals in this paper is the evaluation of amplitude for CTQW on distance regular graphs by using equation (6.60) such that we have

$$\langle \phi_k | e^{-iAt} | \phi_0 \rangle = \langle \phi_k | \phi_0(t) \rangle = \frac{1}{\sqrt{a_k}} \int_R e^{-ixt} P_k(x) \mu(dx), \quad (6.61)$$

where $\langle \phi_k | \phi_0(t) \rangle$ is the amplitude of observing the particle at level k at time t . The conservation of probability $\sum_{k=0} |\langle \phi_k | \phi_0(t) \rangle|^2 = 1$ follows immediately from equation (6.61) by using the completeness relation of orthogonal polynomials $P_n(x)$. Obviously, the evaluation of $\langle \phi_k | \phi_0(t) \rangle$ leads to the determination of the amplitudes at sites belonging to the associate scheme (stratum) $\Gamma_k(o)$. Again according to (3.30), walk has the same amplitude at all sites belonging to the same associated class or stratum (this is in agreement with the lemma proved in appendix I of [1]).

Formula (6.61) indicates a canonical isomorphism between the interacting Fock space CTQW on distance regular graphs (Hilbert space of CTQW starting from a given site, i.e., strata states or more precisely W_0 the irreducible T -module with maximal dimension) and the closed linear span of the orthogonal polynomials generated by recursion relations (5.47). This isomorphism was meant to be a reformulation of CTQW (on distance regular graphs), which describes quantum states by polynomials (describing quantum state $|\phi_k\rangle$ by $P_k(x)$), and make a correspondence between functions of operators (q -numbers) and functions of classical quantity (c -numbers), such as the correspondence between e^{-iAt} and e^{-ixt} . This isomorphism is similar to the isomorphism between Fock space of annihilation and creation operators a, a^\dagger with space of functions of coherent states parameters in quantum optics, or the isomorphism between Hilbert space of momentum and position operators, and spaces of function defined on phase space in Wigner function formalism. At the end, formula (6.61) paves the way to approximate infinite graphs with finite ones and vice versa, simply via Gauss quadrature

formula, where in cases of infinite graphs we can study asymptotic behaviour of walk at large enough times by using the method of stationary phase approximation (for more details see [1]).

Indeed, the determination of $\mu(x)$ is the main problem in the spectral theory of operators, where in the case of distance regular graphs this is quite possible by using the continued fractions method, as it is explained in appendix B.

Finally, using the spectral distribution $\mu(x)$ given in (B.3), formula (6.61) reduces to

$$\langle \phi_k | \phi_0(t) \rangle = \frac{1}{\sqrt{a_k}} \sum_l B_l e^{-ix_l t} P_k(x_l), \tag{6.62}$$

where by straightforward calculations we can evaluate the average probabilities of distance regular graphs as

$$\bar{P}(k) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T |\langle \phi_k | \phi_0(t) \rangle|^2 dt = \frac{1}{a_k} \sum_l B_l^2 P_k^2(x_l). \tag{6.63}$$

At the end, we should note that in the case of distance regular graphs we have exactly $(d + 1)$ different probability amplitudes.

7. Examples

7.1. Underlying graphs of group association schemes

Here in this subsection we study CTQW on underlying graphs of group association schemes by using the prescriptions of section 4.

7.1.1. Symmetric group S_n . The symmetric group S_n is ambivalent in the sense that $C(\alpha) = C(\alpha^{-1})$ for all $\alpha \in S_n$, therefore its conjugacy classes form a symmetric association scheme.

For group S_n , conjugacy classes are determined by the cycle structures of elements when they are expressed in the usual cycle notation. The useful notation for describing the cycle structure is the cycle type $[v_1, v_2, \dots, v_n]$, which is the listing of number of cycles of each length (i.e., v_1 is the number of one cycles, v_2 is that of two cycles and so on). Thus, the number of elements in a conjugacy class or stratum is given by

$$|C_{[v_1, v_2, \dots, v_n]}| = \frac{n!}{v_1! 2^{v_2} v_2! \dots n^{v_n} v_n!}. \tag{7.64}$$

On the other hand, a partition λ of n is a sequence $(\lambda_1, \dots, \lambda_n)$ where $\lambda_1 \geq \dots \geq \lambda_n$ and $\lambda_1 + \dots + \lambda_n = n$, where in terms of cycle types

$$\lambda_1 = v_1 + v_2 + \dots + v_n, \quad \lambda_2 = v_2 + v_3 + \dots + v_n, \quad \dots, \quad \lambda_n = v_n. \tag{7.65}$$

The notation $\lambda \vdash n$ indicates that λ is a partition of n . There is one conjugacy class for each partition $\lambda \vdash n$ in S_n , which consists of those permutations having cycle structure described by λ . We denote by C_λ the conjugacy class of S_n consisting of all permutations having cycle structure described by λ . Therefore, the number of conjugacy classes of S_n , namely the diameter of its scheme, is equal to the number of partitions of n , which grows approximately by $\frac{1}{4\pi\sqrt{3}} e^{\pi\sqrt{2n/3}}$. We consider the case where the generating set consists of the

set of all transposition, i.e., $C_1 = C_{[2,1,1,1,1,\dots,1]}$. For the characters at the transposition, it is known that [37]

$$\chi_\lambda(\alpha_1) = \frac{2!(n-2)!\dim(\rho_\lambda)}{n!} \sum_j \left(\binom{\lambda_j}{2} - \binom{\lambda'_j}{2} \right). \quad (7.66)$$

Here, λ' is the partition generated by transposing the Young diagram of λ , while λ'_j and λ_j are the j th components of the partitions λ' and λ , and ρ_λ is the irreducible representation corresponding to partition λ .

Then, the eigenvalues of its adjacency matrix can be written as

$$P_{\lambda 1} = \frac{d_\lambda k_1}{m_\lambda} \chi_\lambda(\alpha_1) = \sum_j \left(\binom{\lambda_j}{2} - \binom{\lambda'_j}{2} \right). \quad (7.67)$$

Therefore, by using equations (4.39) and (7.66) we can obtain the amplitudes on underlying graph of symmetric groups scheme. As an example, we obtain amplitude for associate class of conjugacy class of n -cycles as

$$\langle \phi_n | \phi_0(t) \rangle = \frac{(-2i \sin(nt/2))^{n-1}}{\sqrt{nn!}}, \quad (7.68)$$

where the results thus obtained are in agreement with those of [38].

In the above calculation, we have used the following results for the characters of the n -cycles:

$$\chi_\lambda((n)) = \begin{cases} (-1)^{n-k} & \text{for } \lambda = (k, 1, \dots, 1), k \in \{1, \dots, n\} \\ 0 & \text{otherwise} \end{cases}$$

and

$$\chi_{(k,1,\dots,1)}(\text{id}) = \dim(\rho_{(k,1,\dots,1)}) = \binom{n-1}{k-1}, \quad P_{\lambda 1} = \frac{1}{2}(2nk - n^2 - n).$$

In the remaining part of this section, we study CTQW on underlying graph of group association scheme S_4 , with diameter $d = 4$, in details. To do so, we need to have its conjugacy classes that are given by

$$\begin{aligned} C_0 &= \{1\}, & C_1 &= \{(12), (13), \dots\}, & C_2 &= \{(123), (124), \dots\}, \\ C_3 &= \{(12)(34), (13)(24), (14)(23)\}, & C_4 &= \{(1234), (1243), \dots\}. \end{aligned} \quad (7.69)$$

Now, using (4.35) we can obtain its adjacency matrices $A_i = \bar{C}_i, i = 0, 1, \dots, 4$, which satisfy the following Bose–Mesner algebra:

$$\begin{aligned} \bar{C}_1^2 &= 6\bar{C}_0 + 3\bar{C}_2 + 2\bar{C}_3, & \bar{C}_1\bar{C}_2 &= 4\bar{C}_1 + 4\bar{C}_4, & \bar{C}_1\bar{C}_3 &= \bar{C}_1 + 2\bar{C}_4, & \bar{C}_1\bar{C}_4 &= 4\bar{C}_2 + 4\bar{C}_3, \\ \bar{C}_2^2 &= 8\bar{C}_0 + 4\bar{C}_2 + 8\bar{C}_3, & \bar{C}_2\bar{C}_3 &= 3\bar{C}_2, & \bar{C}_2\bar{C}_4 &= 4\bar{C}_1 + 4\bar{C}_4, \\ \bar{C}_3^2 &= 3\bar{C}_0 + 2\bar{C}_3, & \bar{C}_3\bar{C}_4 &= 2\bar{C}_1 + \bar{C}_4, & \bar{C}_4^2 &= 6\bar{C}_0 + 3\bar{C}_2, \end{aligned} \quad (7.70)$$

above algebra indicates that group scheme S_4 is not a distance regular scheme (actually group scheme S_n is a distance regular one, only for $n = 3$).

Now, using its adjacency matrices or dual idempotents, we can stratified its underlying graph with adjacency matrix $A = \bar{C}_1$. As it is shown in figure 4, it has five strata and strata 2, 3

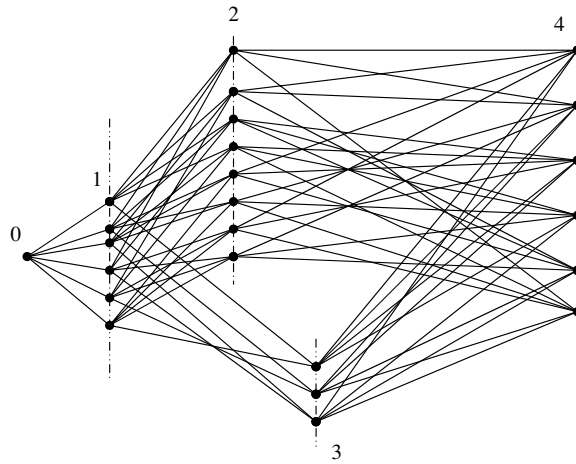


Figure 4. The graph of symmetric group S_4 , it has five strata, where strata 2, 3 have the same distance from the reference stratum (stratum number 0).

have the same distance from the reference stratum (stratum number 0). Using equations (4.39) and (7.66), we can calculate the probability amplitudes of strata as

$$\begin{aligned}
 \langle \phi_0 | \phi_0(t) \rangle &= \frac{1}{6}(1 + 2 \cos^3(2t)), \\
 \langle \phi_1 | \phi_0(t) \rangle &= \frac{-i}{\sqrt{6}}(3 \sin(2t) - 2 \sin^3(2t)), \\
 \langle \phi_2 | \phi_0(t) \rangle &= \frac{2}{3\sqrt{8}}(-1 + 4 \cos^3(2t) - 3 \cos(2t)), \\
 \langle \phi_3 | \phi_0(t) \rangle &= \frac{1}{4\sqrt{3}}(1 + 4 \cos^3(2t) - 6 \cos(2t)), \\
 \langle \phi_4 | \phi_0(t) \rangle &= \frac{2i}{\sqrt{6}} \sin^3(2t).
 \end{aligned}
 \tag{7.71}$$

We should note that even though strata 2 and 3 have the same distance from the reference stratum, but have different amplitudes, therefore the probability amplitudes of CTQW on underlying graph of association scheme S_4 do not depend on their distance from walk starting site (we expect that this holds true for all non-distance regular schemes). Also the number of different amplitudes is the same as the number of strata.

7.1.2. Dihedral group D_{2m} . The dihedral group $G = D_{2m}$ is the semi-direct product of cyclic groups Z_m and Z_2 with corresponding generators a and b . Hence, it is generated by generators a and b with following relations:

$$D_{2m} = \langle a, b : a^m = b^2 = 1, b^{-1}ab = a^{-1} \rangle.
 \tag{7.72}$$

In finding its conjugacy classes, it is convenient to consider whether m is odd or even. Hence, we will study CTQW on underlying graph of dihedral group D_{2m} scheme for odd and even m separately.

1. $m = \text{odd}$. The dihedral group D_{2m} has precisely $\frac{1}{2}(m + 3)$ conjugacy classes (see figure 2(a)):

$$\begin{aligned} C_0 &= \{1\}, & C_1 &= \{b, ab, a^2b, \dots, a^{m-1}b\}, \\ C_2 &= \{a, a^{-1}\}, \dots, & C_{\frac{m+1}{2}} &= \{a^{(m-1)/2}, a^{-(m-1)/2}\} \end{aligned} \quad (7.73)$$

(for more details see [31]).

By using equations (4.38) and (3.30) we obtain the following amplitudes:

$$\langle \phi_k | \phi_0(t) \rangle = \begin{cases} \frac{1}{m}((m-1) + \cos(mt)) & \text{for } k = 0 \\ \frac{1}{\sqrt{m}}(-i \sin(mt)) & \text{for } k = 1 \\ \frac{\sqrt{2}}{m}(\cos(mt) - 1) & \text{for } k = 2, 3, \dots, (m+1)/2. \end{cases} \quad (7.74)$$

Using equation (3.32) we obtain the following average probabilities for strata k at time t :

$$\bar{P}(k) = \begin{cases} \frac{1}{m^2}((m-1)^2 + \frac{1}{2}) & \text{for } k = 0 \\ \frac{1}{2m} & \text{for } k = 1 \\ \frac{3}{m^2} & \text{for } k = 2, 3, \dots, (m+1)/2. \end{cases} \quad (7.75)$$

2. $m = \text{even}$. The dihedral group D_{2m} ($m = 2l$) has precisely $l + 3$ conjugacy classes:

$$\begin{aligned} C_0 &= \{1\}, & C_1 &= \{a^l\}, & C_2 &= \{a, a^{-1}\}, \dots, & C_l &= \{a^{l-1}, a^{-l+1}\} \\ C_{l+1} &= \{a^{2j}b : 0 \leq j \leq l-1\}, & C_{l+2} &= \{a^{2j+1}b : 0 \leq j \leq l-1\} \end{aligned} \quad (7.76)$$

(for more details see [31]).

Now, in order to get an association scheme with connected underlying graph, we have to define a new scheme based on the following conjugacy classes:

$$\tilde{C}_0 = C_0, \quad \tilde{C}_1 = C_{l+1} \cup C_{l+2}, \quad \tilde{C}_2 = C_1, \quad \tilde{C}_3 = C_2, \quad \tilde{C}_4 = C_3, \dots, \tilde{C}_{l+1} = C_l. \quad (7.77)$$

In this case, the calculation of amplitudes and average probabilities of CTQW on connected underlying graph with adjacency matrix $A = \sum_{\gamma \in \tilde{C}_1} \gamma$ is similar to that of dihedral groups with odd m .

Formula (7.74) indicates that we have only three different probability amplitudes, even through the association schemes (7.73) associated with dihedral group D_{2m} (for odd m) have diameter $d = \lfloor \frac{n}{2} \rfloor + 1$, namely the number of different amplitudes is less than $(d + 1)$. This is true for even values of m too.

7.1.3. Cycle graph C_n . A cycle graph or cycle is a graph that consists of some number of vertices connected in a closed chain. The cycle graph with n vertices is denoted by C_n , where its graphical representation cyclic group $Z_n = \langle \alpha \rangle$, with $\alpha^n = 1$. In this case, we consider the orbitals to correspond to the conjugacy classes of cyclic group. Also, we give $\tilde{C} = C(\alpha) \cup C(\alpha^{-1})$ for all $\alpha \in Z_n$, therefore the relations R_i form a symmetric association scheme with d classes on C_n (called the conjugacy scheme of C_n). Let $\omega_j = e^{2\pi ij/n}$ for $j = 0, 1, \dots, n-1$. Using the properties of characters of cyclic group, and equations (A.4) and (A.5), we obtain

$$\begin{aligned} \tilde{P}_{j1} &= \chi_j(1) + \chi_j(n-1) = \omega_j + \omega_j^{n-1} = 2 \cos(2\pi j/n), \\ \tilde{Q}_{kj} &= \overline{\chi_k(j)} + \overline{\chi_k(n-j)} = 2 \cos(2\pi jk/n). \end{aligned} \quad (7.78)$$

Therefore by using equation (3.30), for strata k , we have

$$\langle \phi_k | \phi_0(t) \rangle = \begin{cases} \frac{1}{n} (e^{-it} + 2 \sum_{j=0}^d e^{-it \cos(2\pi j/n)}) & \text{for } k = 0 \\ \frac{\sqrt{2}}{n} (e^{-it} + 2 \sum_{j=0}^d e^{-it \cos(2\pi j/n)} \cos(2\pi jk/n)) & \text{for } k = 1, 2, \dots, d, \end{cases} \quad (7.79)$$

where the results thus obtained are in agreement with those of [1, 39]. Thus, we can evaluate the average probability of staying at origin for large time as follows (equation (4.44)):

$$\bar{P}(0) = \frac{1}{n^2} \left(1 + 4 \sum_{j=1}^d \cos^2(0) \right) = \frac{1}{n^2} (1 + 4d), \quad (7.80)$$

and using equation (3.32) we get the following average probabilities to stratum k :

$$\bar{P}(k) = \frac{2}{n^2} (1 + 4 \sum_{j=1}^d \cos^2(2\pi jk/n)). \quad (7.81)$$

Here we have considered odd n , and the calculation for even n is similar to that of cycle graph with the odd one.

7.2. Examples of distance regular graphs

In this subsection, we study CTQW on some important distance regular graphs via spectral distributions of their corresponding adjacency matrices.

7.2.1. Strongly regular graphs. Here, we study CTQW on some important distance regular graphs of diameter 2, called strongly regular graphs.

A graph (simple, undirected and loopless) of order n is strongly regular with parameters n, κ, λ, η whenever it is not complete or edgeless and

- (i) each vertex is adjacent to κ vertices,
- (ii) for each pair of adjacent vertices there are λ vertices adjacent to both,
- (iii) for each pair of non-adjacent vertices there are η vertices adjacent to both.

For strongly regular graph, the intersection numbers are given by

$$a_1 = \kappa; \quad b_1 = 1, \quad b_2 = \eta; \quad c_0 = \kappa, \quad c_1 = \kappa - \lambda - 1. \quad (7.82)$$

By using formula (B.4) we can straightforwardly get the following spectral distribution:

$$\mu = B_1 \delta(x - x_1) + B_2 \delta(x - x_2) + B_3 \delta(x - x_3), \quad (7.83)$$

where we obtain x_i and B_i for $i = 1, 2, 3$, respectively, as

$$\begin{aligned} x_1 &= \kappa, \\ x_2 &= \frac{1}{2} (\lambda - \eta + \sqrt{(\lambda - \eta)^2 - 4(\eta - \kappa)}), \\ x_3 &= \frac{1}{2} (\lambda - \eta - \sqrt{(\lambda - \eta)^2 - 4(\eta - \kappa)}), \end{aligned} \quad (7.84)$$

$$\begin{aligned} B_1 &= \frac{\eta}{\kappa^2 - \kappa(\lambda - \eta) + (\eta - \kappa)}, \\ B_2 &= \frac{-\kappa \sqrt{(\lambda - \eta)^2 - 4(\eta - \kappa)} + \kappa(\lambda - \eta) + 2\kappa}{(\lambda - \eta - 2\kappa) \sqrt{(\lambda - \eta)^2 - 4(\eta - \kappa)} + (\lambda - \eta)^2 - 4(\eta - \kappa)}, \\ B_3 &= \frac{\kappa \sqrt{(\lambda - \eta)^2 - 4(\eta - \kappa)} + \kappa(\lambda - \eta) + 2\kappa}{(-\lambda + \eta + 2\kappa) \sqrt{(\lambda - \eta)^2 - 4(\eta - \kappa)} + (\lambda - \eta)^2 - 4(\eta - \kappa)}. \end{aligned} \quad (7.85)$$

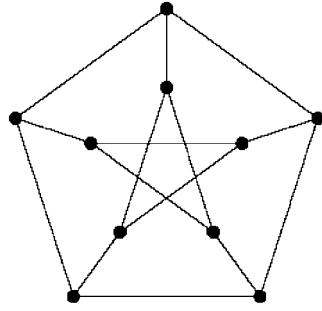


Figure 5. The Petersen graph.

Again using equation (6.61) we can obtain the amplitudes for quantum walk at strata k and time t .

In the remaining part of subsection (7.2.1), we study CTQW on the following two well-known strongly regular graphs.

(A) *Petersen graph*

Petersen graph [22] is strongly regular graph with parameters $(n, \kappa, \lambda, \eta) = (10, 3, 0, 1)$ (see figure 5).

The intersection numbers and spectral distribution are

$$\begin{aligned} a_1 = 3, \quad a_2 = 6; \quad b_1 = b_2 = 1; \quad c_0 = 3, \quad c_1 = 2. \\ \mu = \frac{1}{10}\delta(x-3) + \frac{1}{2}\delta(x-1) + \frac{2}{5}\delta(x+2). \end{aligned} \quad (7.86)$$

Therefore, the amplitudes for walk at time t are

$$\begin{aligned} \langle \phi_0 | \phi_0(t) \rangle &= \int_R e^{-ixt} \mu(dx) = \frac{1}{2} e^{-it} + \frac{2}{5} e^{2it} + \frac{1}{10} e^{-i3t} \\ \langle \phi_1 | \phi_0(t) \rangle &= \frac{1}{\sqrt{3}} \int_R x e^{-ixt} \mu(dx) = \frac{1}{\sqrt{3}} \left(\frac{1}{2} e^{-it} - \frac{4}{5} e^{2it} + \frac{3}{10} e^{-i3t} \right) \\ \langle \phi_2 | \phi_0(t) \rangle &= \frac{1}{\sqrt{6}} \int_R (x^2 - 3) e^{-ixt} \mu(dx) = \frac{1}{\sqrt{6}} \left(-e^{-it} + \frac{2}{5} e^{2it} + \frac{2}{5} e^{-i3t} \right). \end{aligned} \quad (7.87)$$

(B) *Normal subgroup scheme*

A partition of finite group G into sets $P = \{P_0, P_1, \dots, P_d\}$ is a blueprint [22] if

- (i) $P_0 = \{e\}$,
 - (ii) for $i = 1, 2, \dots, d$ if $g \in P_i$ then $g^{-1} \in P_i$,
 - (iii) the set of relations $R_i = \{(\alpha, \beta) \in G \otimes G | \alpha^{-1}\beta \in P_i\}$ on G form an association scheme.
- The set of real conjugacy classes given in appendix A is an example of blueprint on G . Also similar to group symmetric scheme, we can show that in regular representation the class sums \bar{P}_i for $i = 0, 1, \dots, d$ defined as

$$\bar{P}_i = \sum_{\gamma \in P_i} \gamma \in CG, \quad i = 0, 1, \dots, d \quad (7.88)$$

are the adjacency matrices of blueprint scheme.

Now, we define a blueprint scheme for group G which is a strongly regular graph. If H is a normal subgroup of G , we define the blueprint classes by

$$P_0 = \{e\}, \quad P_1 = G - \{H\}, \quad P_2 = H - \{e\}. \tag{7.89}$$

This blueprint scheme is a strongly regular graph with the following Bose–Mesner algebra:

$$\begin{aligned} \bar{P}_1^2 &= (|G| - |H|)\bar{P}_0 + (|G| - 2|H|)\bar{P}_1 + (|G| - |H|)\bar{P}_2, & \bar{P}_1\bar{P}_2 &= (|H| - 1)\bar{P}_2, \\ \bar{P}_2^2 &= (|H| - 1)\bar{P}_0 + (|H| - 2)\bar{P}_2. \end{aligned} \tag{7.90}$$

Hence, it has the following intersection numbers and parameters:

$$a_1 = |G| - |H|; \quad b_1 = 1, \quad b_2 = |G| - |H|; \quad c_0 = |G| - |H|, \quad c_1 = |H| - 1; \tag{7.91}$$

and parameters $(n, \kappa, \lambda, \eta) = (|G|, |G| - |H|, |G| - 2|H|, |G| - |H|)$, respectively.

It is interesting to note that in the normal subgroup scheme the intersections numbers and other parameters depend only on the cardinalities of group and its normal subgroup.

As an example, we consider $G = D_{2m}$, where its normal subgroup is $H = Z_m$. Therefore, the blueprint classes are given by

$$P_0 = \{e\}, \quad P_1 = \{b, ab, a^2b, \dots, a^{m-1}b\}, \quad P_2 = \{a, a^2, \dots, a^{m-1}\}, \tag{7.92}$$

which form a strongly regular graph (see figure 2(b)) with the following intersection numbers and parameters:

$$a_1 = m, \quad a_2 = m - 1; \quad b_1 = 1, \quad b_2 = m; \quad c_0 = m, \quad c_1 = m - 1; \tag{7.93}$$

and parameters $(2m, m, 0, m)$, respectively. Using equations (7.83)–(7.85), we get the following expressions for the spectral distribution:

$$\mu = \frac{1}{2m}\delta(x - m) + \frac{m - 1}{m}\delta(x) + \frac{1}{2m}\delta(x + m). \tag{7.94}$$

Therefore, the amplitudes for walk at time t are

$$\begin{aligned} \langle \phi_0 | \phi_0(t) \rangle &= \frac{1}{m}((m - 1) + \cos(mt)), & \langle \phi_1 | \phi_0(t) \rangle &= \frac{1}{\sqrt{m}}(-i \sin(mt)) \\ \langle \phi_2 | \phi_0(t) \rangle &= \frac{\sqrt{m - 1}}{m}(\cos(mt) - 1). \end{aligned} \tag{7.95}$$

Also using equation (6.63) we evaluate the average probabilities as

$$\bar{P}(k) = \begin{cases} \frac{1}{m^2}((m - 1)^2 + \frac{1}{2}) & \text{for } k = e \\ \frac{1}{2m} & \text{for } k = 1 \\ \frac{3(m-1)}{2m^2} & \text{for } k = 2. \end{cases} \tag{7.96}$$

Formula (7.95) indicates that these amplitudes are the same as those given in (7.73), since the dihedral scheme D_{2m} of subsection 7.1.2 and normal subgroup scheme D_{2m} have the same underlying graph (see figures 2(a) and (b)). Also we have three different probability amplitudes, which are the same as the number of its strata, namely the number of different amplitudes is exactly equal to $(d + 1)$ in this case (because it is a distance regular graph).

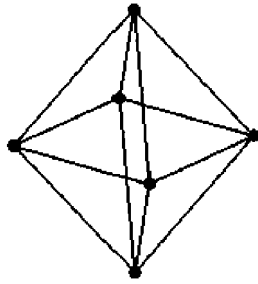


Figure 6. The Johnson graph $J(4, 2)$.

7.2.2. *Johnson graph.* The Johnson graph $J(v, d)$ has all d -subsets of a fixed v -subset as its vertices, with two d -subsets adjacent if and only if they intersect in exactly $d - 1$ elements. Two d -subsets are then at distance i if and only if they have exactly $d - i$ elements in common (see figure 6). Its intersection numbers are given by

$$\begin{aligned}
 a_i &= \frac{d!(v-d)!}{(i!)^2(d-i-1)!(v-d-i-1)!}, & 1 \leq i \leq d, \\
 b_i &= i^2, & 1 \leq i \leq d, \\
 c_i &= (v-d-i)(d-i), & 0 \leq i \leq d-1,
 \end{aligned}
 \tag{7.97}$$

By symmetry we may assume that $2d \leq v$. Consider the growing family of Johnson graphs $J(v, d)$, where $d \rightarrow \infty$ and $\frac{2d}{v} \rightarrow p \in (0, 1]$. Then, the associated orthogonal polynomials are as follows (for more details see [40]):

(A) For $p = 1$, we have Laguerre polynomials $L_n(x)$ with the following recurrence formula:

$$\begin{aligned}
 L_0(x) &= 1, \\
 L_1(x) &= x - 1, \\
 xL_n(x) &= L_{n+1}(x) + (2n + 1)L_n(x) + n^2L_{n-1}(x), & n \geq 1.
 \end{aligned}
 \tag{7.98}$$

By using the fact that the Laguerre polynomials are orthogonal polynomials with respect to the spectral distribution $e^{-x} dx$ and following paper [1] we obtain the following amplitudes:

$$\langle \phi_k | \phi_0(t) \rangle = \frac{(it)^k}{(1 + it)^{k+1}}.
 \tag{7.99}$$

(B) For $0 \leq p \leq 1$, by modifying the Meixner polynomials $M_n(x)$ we have the recurrence formula

$$\begin{aligned}
 M_0(x) &= 1, & M_1(x) &= x, \\
 xM_n(x) &= M_{n+1}(x) + \frac{2n}{\sqrt{p(2-p)}}M_n(x) + n^2M_{n-1}(x), & n \geq 1.
 \end{aligned}
 \tag{7.100}$$

Hence by using the fact that the Meixner polynomials are orthogonal polynomials with respect to the spectral distribution $\sum_{k=0}^{\infty} \frac{2(1-p)}{2-p} \left(\frac{p}{2-p}\right)^k \delta\left(x - \frac{-p+2(1-p)k}{\sqrt{p(2-p)}}\right)$ and equation (6.61) we can obtain the amplitudes. As an example, we obtain the amplitude at the origin at time t as

$$\langle \phi_0 | \phi_0(t) \rangle = \sum_{k=0}^{\infty} \frac{2(1-p)}{2-p} \left(\frac{p}{2-p}\right)^k e^{-i\frac{-p+2(1-p)k}{\sqrt{p(2-p)}}t}.
 \tag{7.101}$$

7.2.3. *Product of association schemes.* In this section, we recall some basic facts about the symmetric product of trivial schemes (see [41] for more details). This product is important not only as a means of constructing new association schemes from the old ones, but also for describing the structure of certain schemes in term of particular sub-schemes or schemes whose structure may already be known. Then using equation (3.30) and (6.61) we can evaluate amplitudes of CTQW on new association schemes. The symmetric product of d -tuples of trivial scheme K_n with adjacency matrices of $I_n, J_n - I_n$ is association scheme with the following adjacency matrices (generators of its Bose–Mesner algebra):

$$\begin{aligned}
 A_0 &= I_n \otimes I_n \otimes \cdots \otimes I_n, \\
 A_1 &= \sum_{\text{permutation}} (J_n - I_n) \otimes I_n \otimes \cdots \otimes I_n, \\
 &\vdots \\
 A_i &= \sum_{\text{permutation}} \underbrace{(J_n - I_n) \otimes (J_n - I_n) \cdots \otimes (J_n - I_n)}_i \otimes I_n \otimes \cdots \otimes I_n,
 \end{aligned}
 \tag{7.102}$$

where J_n is $n \times n$ matrix with all matrix elements equal to 1. This scheme is the well-known Hamming scheme (see figure 1) with intersection number

$$\begin{aligned}
 a_i &= \frac{(n-1)^i d(d-1) \cdots (d-i+1)}{i!}, & 1 \leq i \leq d, \\
 b_i &= i, & 1 \leq i \leq d, \\
 c_i &= (n-1)(d-i), & 0 \leq i \leq d-1,
 \end{aligned}
 \tag{7.103}$$

where its underlying graph is the Cartesian product of d -tuples of cyclic group Z_n . Following [1], the amplitudes of walk and the spectral distribution in the symmetric product of graphs can be obtained in terms of sub-graphs. Finally, we obtain the following expression for the amplitude at origin and spectral distribution:

$$\begin{aligned}
 \mu &= \sum_{l=0}^d \frac{(n-1)^{d-l} d!}{n^d l! (d-l)!} \delta(x - nl + d), \\
 \langle \phi_0 | \phi_0(t) \rangle &= \sum_{l=0}^d \frac{(n-1)^{d-l} d!}{n^d l! (d-l)!} e^{-it(nl-d)},
 \end{aligned}
 \tag{7.104}$$

respectively.

Also we can show that its idempotents $\{E_0, E_1, \dots, E_d\}$ are symmetric product of d -tuples of corresponding idempotents of trivial schemes K_n . That is, we have

$$\begin{aligned}
 E_0 &= \frac{J_n}{n} \otimes \frac{J_n}{n} \otimes \cdots \otimes \frac{J_n}{n}, \\
 E_1 &= \sum_{\text{permutation}} \left(I_n - \frac{J_n}{n} \right) \otimes \frac{J_n}{n} \otimes \cdots \otimes \frac{J_n}{n}, \\
 &\vdots \\
 E_i &= \sum_{\text{permutation}} \underbrace{\left(I_n - \frac{J_n}{n} \right) \otimes \left(I_n - \frac{J_n}{n} \right) \cdots \otimes \left(I_n - \frac{J_n}{n} \right)}_i \otimes \frac{J_n}{n} \otimes \cdots \otimes \frac{J_n}{n}.
 \end{aligned}
 \tag{7.105}$$

Therefore, for the eigenvalues P_{ij} and dual ones Q_{ij} we get

$$\begin{aligned} P_{ij} &= C_i^d (C_j^d)^{-1} (n-1)^{i-j} K_j(i), \\ Q_{ij} &= \frac{m_j}{k_i} C_j^d (C_i^d)^{-1} (n-1)^{j-i} K_i(j), \end{aligned} \quad (7.106)$$

where $K_k(x)$ is the Krawtchouk polynomials defined as

$$K_k(x) = \sum_{i=1}^k C_i^x C_{k-i}^{n-x} (-1)^i (d-1)^{k-i}, \quad (7.107)$$

and $C_k^l = \frac{l!}{k!(l-k)!}$. Then by using equation (2.7) we obtain the amplitude as

$$\langle \phi_k | \phi_0(t) \rangle = \frac{\sqrt{a_k}}{n^d} \sum_{j=0}^k e^{-it \frac{j(d-1)!(n-1)^{j-1}}{j!(d-j)!}} Q_{kj}. \quad (7.108)$$

8. Conclusion

CTQW on underlying graphs of the association schemes has been studied by using the irreducible modules of Bose–Mesner and Terwilliger algebras connected with them, where the irreducible modules of Terwilliger algebra and dual eigenvalues of association schemes play an important role. It is shown that the Terwilliger algebra stratifies the graph into a $(d+1)$ disjoint union of strata (associate classes), which is different from stratification based on distance, except for distance regular graphs. Also similar to QD graphs of [1], the amplitudes of observing the CTQW are the same for the vertices belonging to a given stratum. Hence, for a CTQW on underlying graph of a give association scheme with diameter d we have at most $(d+1)$ different probability amplitudes. Some worked out examples connected with group association schemes show the importance of the algebraic combinatorics structures of association schemes in CTQW. Using the algebraic combinatorics structures of some rather important graphs called distance regular graphs, particularly the irreducible representation of Terwilliger algebras, we have established the required conditions to apply the spectral distributions method of [1], for studying CTQW on them. We expect that, using algebraic combinatorics structures of association schemes, we can study CTQW on some underlying graphs of non-distance regular association schemes by spectral distribution method. At the end, even though it is possible to study CTQW on some graphs which lack association scheme structure by spectral distribution method (for details see [33]), but the formalism is not as elegant as the cases of underlying graphs association schemes.

Appendix A.

In this appendix, we study the method of symmetrization of group schemes of non-symmetric one. If we have $\alpha \in C_i$ but α^{-1} is not in C_i , then the association scheme is non-symmetric. In order to construct a symmetric group scheme from a give non-symmetric one, we need to define the following class sums:

$$\tilde{C}_i = \begin{cases} \bar{C}_i & \text{for } i = 0, 1, \dots, l, \\ \bar{C}_i + \bar{C}_i^{-1} & \text{for } i = l+1, \dots, \frac{d+1+l}{2}, \end{cases} \quad (A.1)$$

where \tilde{C}_i and \bar{C}_i for $i = 0, 1, \dots, l$ are real and for $i = l+1, \dots, \frac{d+1+l}{2}$ are complex.

We can show that the above-defined class sums yield the following relations among themselves:

$$\begin{aligned} \tilde{C}_i \tilde{C}_j = \frac{|\tilde{C}_i| |\tilde{C}_j|}{|G|} & \left(\sum_{v,k=0}^l \frac{\chi_v(\alpha_i) \chi_v(\alpha_j) \overline{\chi_v(\alpha_k)}}{\chi_v(1)} \tilde{C}_k \right. \\ & \left. + \frac{1}{2} \sum_{v,r=l+1}^{\frac{d+1+l}{2}} \frac{\chi_v(\alpha_i) \chi_v(\alpha_j) (\overline{\chi_v(\alpha_r)} + \chi_v(\alpha_r))}{\chi_v(1)} \tilde{C}_r \right) \end{aligned}$$

for $i, j = 0, 1, \dots, l$, and

$$\begin{aligned} \tilde{C}_i \tilde{C}_j = \frac{|\tilde{C}_i| |\tilde{C}_j|}{2|G|} & \left(\sum_{v,k=0}^l \frac{\chi_v(\alpha_i) (\chi_v(\alpha_j) + \overline{\chi_v(\alpha_j)}) \overline{\chi_v(\alpha_k)}}{\chi_v(1)} \tilde{C}_k \right. \\ & \left. + \sum_{v,r=l+1}^{\frac{d+1+l}{2}} \frac{\chi_v(\alpha_i) (\chi_v(\alpha_j) + \overline{\chi_v(\alpha_j)}) (\overline{\chi_v(\alpha_r)} + \chi_v(\alpha_r))}{\chi_v(1)} \tilde{C}_r \right) \end{aligned}$$

for $i = 0, 1, \dots, l$ and $j = l + 1, \dots, \frac{d+1+l}{2}$,

$$\begin{aligned} \tilde{C}_i \tilde{C}_j = \frac{|\tilde{C}_i| |\tilde{C}_j|}{2|G|} & \left(\sum_{v,k=0}^l \frac{(\chi_v(\alpha_i) + \overline{\chi_v(\alpha_i)}) (\chi_v(\alpha_j) + \overline{\chi_v(\alpha_j)}) \overline{\chi_v(\alpha_k)}}{\chi_v(1)} \tilde{C}_k \right. \\ & \left. + \sum_{v,r=l+1}^{\frac{d+1+l}{2}} \frac{(\chi_v(\alpha_i) + \overline{\chi_v(\alpha_i)}) (\chi_v(\alpha_j) + \overline{\chi_v(\alpha_j)}) (\overline{\chi_v(\alpha_r)} + \chi_v(\alpha_r))}{\chi_v(1)} \tilde{C}_r \right) \end{aligned} \tag{A.2}$$

for $i, j = l + 1, \dots, \frac{d+1+l}{2}$. Therefore, the corresponding idempotents $\{\tilde{E}_0, \tilde{E}_1, \dots, \tilde{E}_{\frac{d+1+l}{2}}\}$ of group association scheme are its irreducible CG -modules projection operators, i.e.,

$$\tilde{E}_k = \begin{cases} \frac{\chi_k(1)}{|G|} \sum_{j=0}^l \overline{\chi_k(\alpha_j)} \tilde{C}_j \\ \frac{\chi_k(1)}{|G|} \sum_{j=l+1}^{\frac{d+1+l}{2}} (\overline{\chi_k(\alpha_j)} + \chi_k(\alpha_j)) \tilde{C}_j \end{cases} \tag{A.3}$$

for $k = 0, 1, \dots, l$ and

$$\tilde{E}_k = \begin{cases} \frac{\chi_k(1)}{|G|} \sum_{j=0}^l 2 \overline{\chi_k(\alpha_j)} \tilde{C}_j \\ \frac{\chi_k(1)}{|G|} \sum_{j=l+1}^{\frac{d+1+l}{2}} (\overline{\chi_k(\alpha_j)} + \chi_k(\alpha_j)) \tilde{C}_j \end{cases} \tag{A.4}$$

for $k = l + 1, \dots, \frac{d+1+l}{2}$.

Obviously, the above-defined association scheme is symmetric. It is rather straightforward to see that its eigenvalues \tilde{P}_{ik} and dual ones \tilde{Q}_{ik} are

$$\tilde{P}_{ik} \longrightarrow \begin{cases} \frac{d_i \kappa_k}{m_i} \chi_i(\alpha_k) & \text{for } i = 0, 1, \dots, l, \\ \frac{d_i \kappa_k}{m_i} (\chi_i(\alpha_k) + \overline{\chi_i(\alpha_k)}) & \text{for } i = l + 1, \dots, \frac{d+1+l}{2}, \end{cases} \tag{A.5}$$

for $k = 0, 1, \dots, l$,

$$\tilde{P}_{ik} \longrightarrow \begin{cases} \frac{d_i \kappa_k}{m_i} (\chi_i(\alpha_k) + \overline{\chi_i(\alpha_k)}) & \text{for } i = 0, 1, \dots, l, \\ 2 \frac{d_i \kappa_k}{m_i} (\chi_i(\alpha_k) + \overline{\chi_i(\alpha_k)}) & \text{for } i = l + 1, \dots, \frac{d+1+l}{2}, \end{cases} \tag{A.6}$$

for $k = 0, 1, \dots, \frac{d+1+l}{2}$,

$$\tilde{Q}_{ik} \rightarrow \begin{cases} d_k \overline{\chi_k(\alpha_i)} & \text{for } i = 0, 1, \dots, l, \\ d_k (\overline{\chi_k(\alpha_i)} + \chi_k(\alpha_i)) & \text{for } i = l+1, \dots, \frac{d+1+l}{2}, \end{cases} \quad (\text{A.7})$$

for $k = 0, 1, \dots, l$ and

$$\tilde{Q}_{ik} \rightarrow \begin{cases} 2d_k \overline{\chi_k(\alpha_i)} & \text{for } i = 0, 1, \dots, l, \\ d_k (\overline{\chi_k(\alpha_i)} + \chi_k(\alpha_i)) & \text{for } i = l+1, \dots, \frac{d+1+l}{2}, \end{cases} \quad (\text{A.8})$$

for $k = 0, 1, \dots, \frac{d+1+l}{2}$.

In fact, eigenvalues (dual eigenvalues) are sum of real and non-real contributions.

In section 7, using the above prescription we have studied the CTQW on cyclic groups.

Appendix B. Determination of spectral distribution by continued fractions method

Here in this appendix we explain how we can determine spectral distribution $\mu(x)$ of distance regular graphs by using the Szegő–Jacobi sequences $(\{\omega_k\}, \{\alpha_k\})$; the parameters ω_k and α_k are defined in (5.55).

To this aim let us consider the orthogonal polynomials $\{Q_n\}$ defined recursively by

$$\begin{aligned} Q_0(x) &= 1, & Q_1(x) &= x - \alpha_1, \\ x Q_n(x) &= Q_{n+1}(x) + \alpha_{n+1} Q_n(x) + \omega_n Q_{n-1}(x), \end{aligned} \quad (\text{B.1})$$

for $n \geq 1$. As it is shown in [42], the spectral distribution μ can be determined by the following identity:

$$G_\mu(x) = \int_R \frac{\mu(dy)}{x-y} = \frac{1}{x - \alpha_1 - \frac{\omega_1}{x - \alpha_2 - \frac{\omega_2}{x - \alpha_3 - \frac{\omega_3}{x - \alpha_4 - \dots}}}} = \frac{Q_{n-1}^{(1)}(x)}{Q_n(x)} = \sum_{l=1}^n \frac{B_l}{x - x_l}, \quad (\text{B.2})$$

where $G_\mu(x)$ is called the Stieltjes transform of μ and B_l is the coefficient in the Gauss quadrature formula corresponding to the roots x_l of the polynomial $Q_n(x)$ where the polynomials $\{Q_n^{(1)}\}$ are defined recursively as

$$\begin{aligned} Q_0^{(1)}(x) &= 1, \\ Q_1^{(1)}(x) &= x - \alpha_2, \\ x Q_n^{(1)}(x) &= Q_{n+1}^{(1)}(x) + \alpha_{n+2} Q_n^{(1)}(x) + \omega_{n+1} Q_{n-1}^{(1)}(x), \end{aligned}$$

for $n \geq 1$.

Now if $G_\mu(x)$ is known, then the spectral distribution μ can be recovered from $G_\mu(x)$ by means of the Stieltjes inversion formula:

$$\mu(y) - \mu(x) = -\frac{1}{\pi} \lim_{v \rightarrow 0^+} \int_x^y \text{Im}\{G_\mu(u + iv)\} du. \quad (\text{B.3})$$

Substituting the right-hand side of (B.2) into (B.3), the spectral distribution can be determined in terms of x_l , $l = 1, 2, \dots$, the roots of the polynomial $Q_n(x)$ and Gauss quadrature constant B_l , $l = 1, 2, \dots$, as

$$\mu = \sum_l B_l \delta(x - x_l) \quad (\text{B.4})$$

(for more details see [36, 40, 42, 43]).

Appendix C. List of some important distance regular graphs [44–46]

1. *Collinearity graph gen. octagon* $GO(s, t)$

$$\begin{aligned} \mu = & \frac{1}{(s+1)(st+1)(s^2t^2+1)}\delta(x-s(t+1)) + \frac{st(t+1)}{4(st+1-\sqrt{2st})(s+t+\sqrt{2st})} \\ & \times \delta(x-s+1-\sqrt{2st}) + \frac{st(t+1)}{2(st+1)(s+t)}\delta(x-s+1) \\ & + \frac{st(t+1)}{4(st+1-\sqrt{2st})(s+t+\sqrt{2st})}\delta(x-s+1+\sqrt{2st}) \\ & + \frac{s^4}{(s+1)(s+t)(s^2+t^2)}\delta(x+t+1). \end{aligned}$$

Intersection numbers:

$$\begin{aligned} c_0 = s(t+1), & & c_1 = st, & & c_2 = st, & & c_3 = st, \\ b_1 = 1, & & b_2 = 1, & & b_3 = 1, & & b_4 = t+1. \end{aligned}$$

2. *Collinearity graph gen. dodecagon* $GD(s, 1)$

$$\begin{aligned} \mu = & \frac{1}{((s+1)^2-3s)((s+1)^2-s)(s+1)^2}\delta(x-2s) + \frac{s-1+\sqrt{3s}}{12((s+1)^2-3s)}\delta(x-s+1-\sqrt{3s}) \\ & + \frac{s-1-\sqrt{3s}}{12((s+1)^2-3s)}\delta(x-s+1+\sqrt{3s}) + \frac{s-1+\sqrt{s}}{4((s+1)^2-s)}\delta(x-s+1+\sqrt{s}) \\ & + \frac{s-1-\sqrt{s}}{4((s+1)^2-s)}\delta(x-s+1-\sqrt{s}) + \frac{s^5}{((s+1)^2-3s)((s+1)^2-s)(s+1)^2}\delta(x+2). \end{aligned}$$

Intersection numbers:

$$\begin{aligned} c_0 = 2s, & & c_1 = s, & & c_2 = s, & & c_3 = s, & & c_4 = s, & & c_5 = s, \\ b_1 = 1, & & b_2 = 1, & & b_3 = 1, & & b_4 = 1, & & b_5 = 1, & & b_6 = 2. \end{aligned}$$

3. M_{22} graph

$$\mu = \frac{7}{110}\delta(x+4) + \frac{3}{10}\delta(x+3) + \frac{7}{15}\delta(x-1) + \frac{1}{6}\delta(x-4) + \frac{1}{330}\delta(x-7).$$

Intersection numbers:

$$\begin{aligned} c_0 = 7, & & c_1 = 6, & & c_2 = 4, & & c_3 = 4, \\ b_1 = 1, & & b_2 = 1, & & b_3 = 1, & & b_4 = 6. \end{aligned}$$

4. *Incidence graph* $pg(k-1, k-1, k-1)$, $k = 4, 5, 7, 8$

$$\mu = \frac{1}{2k^2}(\delta(x-k) + \delta(x+k)) + \frac{k-1}{k^2}\delta(x) + \frac{k-1}{2k}(\delta(x-\sqrt{k}) + \delta(x+\sqrt{k})).$$

Intersection numbers:

$$\begin{aligned} c_0 = k, & & c_1 = k-1, & & c_2 = k-1, & & c_3 = 1, \\ b_1 = 1, & & b_2 = 1, & & b_3 = k-1, & & b_4 = k. \end{aligned}$$

5. *Coset graph doubly truncated binary Golay*

$$\mu = \frac{21}{512}\delta(x+11) + \frac{35}{64}\delta(x+3) + \frac{105}{256}\delta(x-5) + \frac{1}{512}\delta(x-21).$$

Intersection numbers:

$$\begin{aligned} c_0 &= 21, & c_1 &= 20, & c_2 &= 16, \\ b_1 &= 1, & b_2 &= 2, & b_3 &= 12. \end{aligned}$$

6. *Coset graph extended ternary Golay code*

$$\mu = \frac{8}{243}\delta(x+12) + \frac{440}{729}\delta(x+3) + \frac{88}{243}\delta(x-6) + \frac{1}{729}\delta(x-24).$$

Intersection numbers:

$$\begin{aligned} c_0 &= 24, & c_1 &= 22, & c_2 &= 20, \\ b_1 &= 1, & b_2 &= 2, & b_3 &= 12. \end{aligned}$$

7. *Wells graph*

$$\mu = \frac{1}{16}\delta(x+3) + \frac{1}{4}(\delta(x+\sqrt{5}) + \delta(x-\sqrt{5}) + \delta(x-1)) + \frac{3}{16}\delta(x-5).$$

Intersection numbers:

$$\begin{aligned} c_0 &= 5, & c_1 &= 4, & c_2 &= 1, & c_3 &= 1, \\ b_1 &= 1, & b_2 &= 1, & b_3 &= 4, & b_4 &= 5. \end{aligned}$$

8. *3-Cover GQ(2, 2)*

$$\mu = \frac{1}{9}\delta(x+3) + \frac{2}{5}\delta(x+2) + \frac{4}{15}\delta(x-3) + \frac{1}{5}\delta(x-1) + \frac{1}{45}\delta(x-6).$$

Intersection numbers:

$$\begin{aligned} c_0 &= 6, & c_1 &= 4, & c_2 &= 2, & c_3 &= 1, \\ b_1 &= 1, & b_2 &= 1, & b_3 &= 4, & b_4 &= 6. \end{aligned}$$

9. *Double Hoffman–Singleton*

$$\mu = \frac{7}{25}(\delta(x+2) + \delta(x-2)) + \frac{21}{100}(\delta(x+3) + \delta(x-3)) + \frac{1}{100}(\delta(x+7) + \delta(x-7)).$$

Intersection numbers:

$$\begin{aligned} c_0 &= 7, & c_1 &= 6, & c_2 &= 6, & c_3 &= 1, & c_4 &= 1, \\ b_1 &= 1, & b_2 &= 1, & b_3 &= 6, & b_4 &= 6, & b_5 &= 7. \end{aligned}$$

10. *Foster graph*

$$\begin{aligned} \mu &= \frac{1}{9}\delta(x) + \frac{1}{5}(\delta(x+1) + \delta(x-1)) + \frac{1}{10}(\delta(x+2) + \delta(x-2)) + \frac{1}{90}(\delta(x+3) + \delta(x-3)) \\ &\quad + \frac{2}{15}(\delta(x+\sqrt{6}) + \delta(x-\sqrt{6})). \end{aligned}$$

Intersection numbers:

$$\begin{aligned} c_0 &= 3, & c_1 &= 2, & c_2 &= 2, & c_3 &= 2, & c_4 &= 2, & c_5 &= 1, & c_6 &= 1, & c_7 &= 1, \\ b_1 &= 1, & b_2 &= 1, & b_3 &= 1, & b_4 &= 1, & b_5 &= 2, & b_6 &= 2, & b_7 &= 2, & b_8 &= 3. \end{aligned}$$

In all of the above examples, a_k is defined in terms of b_k and c_k as

$$a_k = \frac{c_0 c_1 \cdots c_{k-1}}{b_1 b_2 \cdots b_k}. \quad (\text{C.1})$$

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