ALGEBRAIC COMBINATORICS

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Volume 3, issue 3 (2020), p. 757-774.

<http://alco.centre-mersenne.org/item/ALCO_2020__3_3_757_0>

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Volume 3, issue 3 (2020), p. 757–774
https://doi.org/10.5802/alco.112

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Abstract We study the continuous-time quantum walks on graphs in the adjacency algebra of the n-cube and its related distance regular graphs.

For $k \geqslant 2$, we find graphs in the adjacency algebra of $(2^{k+2}-8)$-cube that admit instantaneous uniform mixing at time $\pi/2^k$ and graphs that have perfect state transfer at time $\pi/2^k$.

We characterize the folded n-cubes, the halved n-cubes and the folded halved n-cubes whose adjacency algebra contains a complex Hadamard matrix. We obtain the same conditions for the characterization of these graphs admitting instantaneous uniform mixing.

1. Introduction

The continuous-time quantum walk on a graph X is given by the transition operator

$$\mathrm{e}^{-\mathrm{i}\, tA} = \sum_{k\geqslant 0} \frac{(-\mathrm{i}\, t)^k}{k!} A^k,$$

where A is the adjacency matrix of X. For example, if X is the complete graph on two vertices, K_2, then

$$\begin{aligned}\mathrm{e}^{-\mathrm{i}\, tA} &= \left(1 - \frac{t^2}{2!} + \frac{t^4}{4!} - \cdots\right) I - \mathrm{i}\left(t - \frac{t^3}{3!} + \frac{t^5}{5!} - \cdots\right) A \\ &= \begin{pmatrix} \cos t & -\mathrm{i}\sin t \\ -\mathrm{i}\sin t & \cos t \end{pmatrix}.\end{aligned}$$

Being the quantum analogue of the random walks on graphs, there is a lot of research interest on quantum walks for the development of quantum algorithms. Moreover, quantum walks are proved to be universal for quantum computations [7]. In this paper, we focus on the continuous-time quantum walks introduced by Farhi and Gutmann in [10]. Please see [12] and [13] for surveys on quantum walks.

Since A is real and symmetric, the operator $\mathrm{e}^{-\mathrm{i}\, tA}$ is unitary. We say the continuous-time quantum walk on X is *instantaneous uniform mixing at time* τ if

$$|(\mathrm{e}^{-\mathrm{i}\, \tau A})_{a,b}| = \frac{1}{\sqrt{|V(X)|}}, \qquad \text{for all vertices } a \text{ and } b.$$

This condition is equivalent to $\sqrt{|V(X)|}\,\mathrm{e}^{-\mathrm{i}\, \tau A}$ being a complex Hadamard matrix. Thus if X admits instantaneous uniform mixing then its adjacency algebra contains a

Manuscript received 22nd June 2019, revised and accepted 9th February 2020.

Keywords. Association schemes, Hamming schemes, complex Hadamard matrix, continuous-time quantum walks, instantaneous uniform mixing, perfect state transfer.

complex Hadamard matrix. In K_2, the continuous-time quantum walk is instantaneous uniform mixing at time $\pi/4$.

In [14], Moore and Russell discovered that the continuous-time quantum walk on the n-cube is instantaneous uniform mixing at time $\pi/4$ which is faster than its classical analogue. Ahmadi et al. [1] showed that the complete graph K_q admits instantaneous uniform mixing if and only if $q \in \{2, 3, 4\}$. Best et al. [2] proved that instantaneous uniform mixing occurs in graphs X and Y at time τ if and only if instantaneous uniform mixing occurs in their Cartesian product at the same time. They concluded that the Hamming graph $H(n, q)$, which is the Cartesian product of n copies of K_q, has instantaneous uniform mixing if and only if $q \in \{2, 3, 4\}$. In the same paper, they also proved that a folded n-cube admits instantaneous uniform mixing if and only if n is odd.

In this paper, we give a necessary condition for the Bose–Mesner algebra of a symmetric association scheme to contain a complex Hadamard matrix. Applying this condition, we generalize the result of Best et al. to show that the adjacency algebra of $H(n, q)$ contains the adjacency matrix of a graph that admits instantaneous uniform mixing if and only if $q \in \{2, 3, 4\}$. We characterize the halved n-cubes and the folded halved n-cubes that have instantaneous uniform mixing. We obtain the same characterization for the folded n-cubes, the halved n-cubes and the folded halved n-cubes to have a complex Hadamard matrix in their adjacency algebras.

A *cubelike graph* is a Cayley graph of the elementary abelian group $\mathbb{Z}_2^d$. The graphs appear in this paper are distance regular cubelike graphs. For $k \geqslant 2$, we find graphs in the adjacency algebra of $H(2^{k+2} - 8, 2)$ that admit instantaneous uniform mixing at time $\pi/2^k$. Hence, for all $\tau > 0$, there exists graphs that admit instantaneous uniform mixing at time less than τ.

In a graph X, perfect state transfer occurs from vertex u to vertex w at time τ if

$$|(\mathrm{e}^{-\mathrm{i}\,\tau A(X)})_{u,w}| = 1.$$

In the n-cube, perfect state transfer occurs between antipodal vertices at time $\pi/4$ [8].

Given a graph X, we use $A(X)$ to denote its adjacency matrix, and X_r to denote the graph on the vertex set $V(X)$ in which two vertices are adjacent if they are at distance r in X. We use I_v and J_v to denote the $v \times v$ identity matrix and the $v \times v$ matrix of all ones, respectively. We drop the subscript if the order of the matrices is clear.

2. A Necessary Condition

The graphs we study in this paper are distance regular. The adjacency algebra of a distance regular graph is the Bose–Mesner algebra of a symmetric association scheme. In this section, we give a necessary condition for a Bose–Mesner algebra to contain a complex Hadamard matrix. This condition is also necessary for a Bose–Mesner algebra to contain the adjacency matrix of a graph that admits instantaneous uniform mixing.

A *symmetric association scheme* of order v with d classes is a set

$$\mathcal{A} = \{A_0, A_1, \dots, A_d\}$$

of $v \times v$ symmetric 01-matrices satisfying

(1) $A_0 = I$.
(2) $\sum_{j=0}^{d} A_j = J$.
(3) $A_j A_k = A_k A_j$, for $j, k = 0, \dots, d$.
(4) $A_j A_k \in \operatorname{span} \mathcal{A}$, for $j, k = 0, \dots, d$.

For example, if X is a distance regular graph with diameter d and X_j is the j-th distance graph of X, for $j = 1, \dots, d$, then the set $\{I, A(X_1), A(X_2), \dots, A(X_d)\}$ is a symmetric association scheme.

The *Bose–Mesner algebra* of an association scheme $\mathcal{A}$ is the span of $\mathcal{A}$ over $\mathbb{C}$. It is known [3] that the Bose–Mesner algebra contains another basis $\{E_0, E_1, \dots, E_d\}$ satisfying

(a) $E_j E_k = \delta_{j,k} E_j$, for $j, k = 0, \dots, d$, and
(b) $\sum_{j=0}^{d} E_j = I$.

Now there exist complex numbers $p_r(s)$'s such that

$$A_r = \sum_{s=0}^{d} p_r(s) E_s, \qquad \text{for } r = 0, \dots, d. \tag{1}$$

It follows from Condition (a) that

$$A_r E_s = p_r(s) E_s, \qquad \text{for } r, s = 0, \dots, d.$$

We call the $p_r(s)$'s *the eigenvalues of the association schemes*. Since the matrices in $\mathcal{A}$ are symmetric, the $p_r(s)$'s are real.

A $v \times v$ matrix W is *type II* if, for $a, b = 1, \dots, v$,

$$\sum_{c=1}^{v} \frac{W_{ac}}{W_{bc}} = \begin{cases} v & \text{if } a = b, \\ 0 & \text{otherwise.} \end{cases} \tag{2}$$

A *complex Hadamard matrix* is a type II matrix whose entries have absolute value one.

Proposition 2.1. *Let $\mathcal{A} = \{A_0, A_1, \dots, A_d\}$ be a symmetric association scheme. Let $t_0, \dots, t_d \in \mathbb{C}\backslash\{0\}$. The matrix $W = \sum_{j=0}^{d} t_j A_j$ is type II if and only if*

$$\left[\sum_{h=0}^{d} p_h(s) t_h\right] \left[\sum_{j=0}^{d} p_j(s) \frac{1}{t_j}\right] = v, \qquad \textit{for } s = 0, 1, \dots, d.$$

Proof. The matrix W is type II if and only if

$$\left[\sum_{h=0}^{d} t_h A_h\right] \left[\sum_{j=0}^{d} \frac{1}{t_j} A_j\right] = vI.$$

It follows from Equation (1) and Condition (b) that

$$\left[\sum_{h=0}^{d} \sum_{l=0}^{d} t_h p_h(l) E_l\right] \left[\sum_{j=0}^{d} \sum_{k=0}^{d} \frac{1}{t_j} p_j(k) E_k\right] = v \sum_{r=0}^{d} E_r.$$

By Condition (a), the left-hand side becomes

$$\sum_{r=0}^{d} \left[\sum_{h=0}^{d} t_h p_h(r)\right] \left[\sum_{j=0}^{d} \frac{1}{t_j} p_j(r)\right] E_r,$$

multiplying E_s to both sides yields the equations of this proposition. □

Finding type II matrices in the Bose–Mesner algebra of a symmetric association scheme amounts to solving the system of equations in Proposition 2.1, which is not easy as d gets large. When we limit the scope of the search to complex Hadamard matrices, we get the following necessary condition which can be checked efficiently.

Proposition 2.2. *If the Bose–Mesner algebra of $\mathcal{A}$ contains a complex Hadamard matrix, then*

$$v \leqslant \left[\sum_{r=0}^{d} |p_r(s)|\right]^2, \qquad \textit{for } s = 0, 1, \ldots, d.$$

Proof. Suppose $W = \sum_{j=0}^{d} t_j A_j$ is a complex Hadamard matrix. By Proposition 2.1, for $s = 0, \ldots, d$,

$$v = \sum_{r=0}^{d} p_r(s)^2 + \sum_{0 \leqslant h < j \leqslant d} \left(\frac{t_h}{t_j} + \frac{t_j}{t_h}\right) p_h(s) p_j(s).$$

Since $|\frac{t_h}{t_j}| = 1$, we have $|\frac{t_h}{t_j} + \frac{t_j}{t_h}| \leqslant 2$ and

$$v \leqslant \sum_{r=0}^{d} |p_r(s)|^2 + \sum_{0 \leqslant h < j \leqslant d} 2|p_h(s) p_j(s)| = \left[\sum_{r=0}^{d} |p_r(s)|\right]^2. \qquad \square$$

Suppose $A(X)$ belongs to the Bose–Mesner algebra of $\mathcal{A}$. If instantaneous uniform mixing occurs in X at time τ then $\sqrt{v}\, \mathrm{e}^{-\mathrm{i}\,\tau A(X)}$ is a complex Hadamard matrix and the eigenvalues of $\mathcal{A}$ satisfy the inequalities in Proposition 2.2. For example, the association scheme $\{I_q, J_q - I_q\}$ has eigenvalues $p_0(1) = 1$ and $p_1(1) = -1$. By Proposition 2.2, if the adjacency algebra of K_q contains a complex Hadamard matrix then $q \leqslant 4$. Hence instantaneous uniform mixing does not occur in K_q, for $q \geqslant 5$.

Proposition 2.3. *Let X be a graph whose adjacency matrix belongs to the Bose–Mesner algebra of $\mathcal{A}$. Let $\theta_0, \ldots, \theta_d$ be the eigenvalues of $A(X)$ satisfying*

$$A(X) = \sum_{s=0}^{d} \theta_s E_s.$$

The continuous-time quantum walk of X is instantaneous uniform mixing at time τ if and only if there exist scalars $t_0, \ldots, t_d$ such that

$$|t_0| = \ldots = |t_d| = 1$$

and

$$\sqrt{v}\, \mathrm{e}^{-\mathrm{i}\,\tau\theta_s} = \sum_{j=0}^{d} p_j(s) t_j, \qquad \textit{for } s = 0, \ldots, d.$$

Proof. It follows from Condition (a) that $A(X)^k = \sum_{s=0}^{d} \theta_s^k E_s$, for $k \geqslant 0$. Therefore,

$$\sqrt{v}\, \mathrm{e}^{-\mathrm{i}\,\tau A(X)} = \sqrt{v} \sum_{s=0}^{d} \mathrm{e}^{-\mathrm{i}\,\tau\theta_s} E_s \tag{3}$$

belongs to $\operatorname{span} \mathcal{A}$, and there exists $t_0, \ldots, t_d$ such that

$$\sqrt{v}\, \mathrm{e}^{-\mathrm{i}\,\tau A(X)} = \sum_{j=0}^{d} t_j A_j.$$

By Equation (1), we get

$$\sqrt{v}\, \mathrm{e}^{-\mathrm{i}\,\tau\theta_s} = \sum_{j=0}^{d} p_j(s) t_j, \qquad \text{for } s = 0, \ldots, d.$$

Lastly, $\sqrt{v}\, \mathrm{e}^{-\mathrm{i}\,\tau A(X)}$ is a complex Hadamard matrix exactly when

$$|t_0| = \cdots = |t_d| = 1. \qquad \square$$

For $n, q \geqslant 2$, the *Hamming graph* $H(n,q)$ is the Cartesian product of n copies of K_q. Equivalently, the vertex set V of the Hamming graph $H(n,q)$ is the set of words of length n over an alphabet of size q, and two words are adjacent if they differ in exactly one coordinate. The Hamming graph is a distance regular graph on q^n vertices with diameter n. For $j = 1, \dots, n$, X_j is the graph with vertex set V where two vertices are adjacent when they differ in exactly j coordinates. Let $A_0 = I$ and $A_j = A(X_j)$, for $j = 1, \dots, n$. Then $\mathcal{H}(n,q) = \{A_0, A_1, \dots, A_n\}$ is a symmetric association scheme, called the *Hamming scheme*. For more information on Hamming scheme, please see [3] and [11].

It follows from Equation (4.1) of [11] that

$$\sum_{j=0}^{n} x^j A_j = [I_q + x(J_q - I_q)]^{\otimes n},$$

and the eigenvalues of $\mathcal{H}(n,q)$ satisfy

$$\sum_{j=0}^{n} p_j(s) x^j = (1 + (q-1)x)^{n-s} (1-x)^s, \quad \text{for } s = 0, \dots, n. \tag{4}$$

Using $[x^k]g(x)$ to denote the coefficient of x^k in a polynomial $g(x)$, we have for $r, s = 0, \dots, n$,

$$\begin{aligned} p_r(s) &= [x^r]\,(1 + (q-1)x)^{n-s}\,(1-x)^s \\ &= [x^r]\,(1 + (q-1)x)^{n-s}\,((1 + (q-1)x) - qx)^s \\ &= [x^r] \sum_h \binom{s}{h} (1 + (q-1)x)^{n-h}\,(-qx)^h \\ &= \sum_h (-q)^h (q-1)^{r-h} \binom{n-h}{r-h} \binom{s}{h}. \qquad (5) \end{aligned}$$

We now quote the following characterization from [14] and [2].

Theorem 2.4. *The Hamming graph $H(n,q)$ admits instantaneous uniform mixing if and only if $q \in \{2,3,4\}$.*

We see from Proposition 2.3 that whether a graph X admits instantaneous uniform mixing depends on only the spectrum of X and the eigenvalues of the Bose–Mesner algebra containing $A(X)$. A *Doob graph* $D(m_1, m_2)$ is a Cartesian product of m_1 copies of the Shrikhande graph and m_2 copies of K_4. It is a distance regular graph with the same parameters as the Hamming graph $H(2m_1 + m_2, 4)$, see Section 9.2B of [3]. Since instantaneous uniform mixing occurs in $H(n,4)$ for all $n \geqslant 1$, we see that the Doob graph $D(m_1, m_2)$ admits instantaneous uniform mixing for all $m_1, m_2 \geqslant 1$.

Corollary 2.5. *The Bose–Mesner algebra of $\mathcal{H}(n,q)$ contains a complex Hadamard matrix if and only if $q \in \{2,3,4\}$.*

Proof. It follows from Equation (4) that

$$p_r(n) = (-1)^r \binom{n}{r}.$$

By Proposition 2.2, if the Bose–Mesner algebra of $\mathcal{H}(n,q)$ contains a complex Hadamard matrix, then

$$q^n \leqslant \left[\sum_{r=0}^{n} |p_r(n)|\right]^2 = 4^n.$$

Hence $q \in \{2,3,4\}$.

The converse follows directly from Theorem 2.4. □

We conclude that if $A(X)$ belongs to the Bose–Mesner algebra of $\mathcal{H}(n,q)$, for $q \geqslant 5$, then instantaneous uniform mixing does not occur in X.

3. The Cubes

The Hamming graph $H(n,2)$ is also called the *n-cube*. It is a distance regular graph on 2^n vertices with intersection numbers

$$a_j = 0, \quad b_j = (n-j) \quad \text{and} \quad c_j = j, \qquad \text{for } j = 0, \dots, n.$$

It is both bipartite and antipodal, see Section 9.2 of [3] for details.

It follows from Equation (4) that the eigenvalues of $\mathcal{H}(n,2)$ satisfy

$$p_r(n-s) = (-1)^r p_r(s) \qquad \text{and} \qquad p_{n-r}(s) = (-1)^s p_r(s), \tag{6}$$

for $r, s = 0, \dots, n$.

The proof of Lemma 3.3 uses the following equations, which are Propositions 2.1(3) and 2.3 of [6].

Proposition 3.1. *The eigenvalues of $\mathcal{H}(n,2)$ satisfy*

(a) $p_r(s+1) - p_r(s) = -p_{r-1}(s+1) - p_{r-1}(s)$, *for* $s = 0, \dots, n-1$, $r = 1, \dots, n$ *and*

(b) $p_{r-1}(s) - p_{r-1}(s+2) = 4\sum_h (-2)^h \binom{n-2-h}{r-2-h}\binom{s}{h}$, *for* $s = 0, \dots, n-2$ *and* $r = 1, \dots, n$.

Note that the Kronecker product of two complex Hadamard matrices is a complex Hadamard matrix. Hence for $\epsilon \in \{-1, 1\}$,

$$[I_2 + \epsilon\,\mathrm{i}(J_2 - I_2)]^{\otimes n} = \sum_{j=0}^{n} (\epsilon\,\mathrm{i})^j A_j$$

is a complex Hadamard matrix in the Bose–Mesner algebra of $\mathcal{H}(n,2)$.

Suppose $A(X)$ belongs to the Bose–Mesner algebra of $\mathcal{H}(n,2)$ and

$$A(X)E_s = \theta_s E_s, \quad \text{for } s = 0, \dots, n.$$

It follows from Equations (3) and (4) that

$$\sqrt{2^n}\,\mathrm{e}^{-\mathrm{i}\,\tau A(X)} = \mathrm{e}^{\mathrm{i}\,\beta}\,[I_2 + \epsilon\,\mathrm{i}(J_2 - I_2)]^{\otimes n}$$

if and only if

$$\begin{aligned} \sqrt{2^n}\,\mathrm{e}^{-\mathrm{i}\,\tau\theta_s} &= \mathrm{e}^{\mathrm{i}\,\beta}(1+\epsilon\,\mathrm{i})^{n-s}(1-\epsilon\,\mathrm{i})^s \\ &= \sqrt{2^n}\,\mathrm{e}^{\mathrm{i}\,\beta}\,\mathrm{e}^{\epsilon\,\mathrm{i}\,\pi(n-2s)/4}, \qquad \text{for } s = 0, \dots, n. \end{aligned}$$

This system of equations holds exactly when

$$\mathrm{e}^{\mathrm{i}\,\beta} = \mathrm{e}^{-\mathrm{i}\,\tau\theta_0 - \epsilon\,\mathrm{i}\,\pi n/4}$$

and

$$\mathrm{e}^{-\mathrm{i}\,\tau(\theta_s - \theta_0)} = \mathrm{e}^{-\epsilon\,\mathrm{i}\,\pi s/2}, \qquad \text{for } s = 0, \dots, n.$$

Lemma 3.2. *Suppose $A(X)$ belongs to the Bose–Mesner algebra of $\mathcal{H}(n,2)$ and $A(X)E_s = \theta_s E_s$, for $s = 0, \dots, n$. If there exist k and $\epsilon \in \{-1, 1\}$ satisfying*

$$\theta_s - \theta_0 \equiv \epsilon s 2^{k-1} \pmod{2^{k+1}}, \qquad \text{for } s = 0, \dots, n,$$

then there exists $\beta \in \mathbb{R}$ such that

$$\sqrt{2^n}\,\mathrm{e}^{-\mathrm{i}\,\frac{\pi}{2^k} A(X)} = \mathrm{e}^{\mathrm{i}\,\beta}[I_2 + \epsilon\,\mathrm{i}(J_2 - I_2)]^{\otimes n}.$$

That is, X admits instantaneous uniform mixing at time $\pi/2^k$.

Lemma 3.3. *Let $r \geqslant 1$. Let α be the largest integer such that $\binom{n-1}{r-1}$ is divisible by 2^α. Suppose*

$$\binom{n-2-h}{r-2-h} \equiv 0 \pmod{2^{\alpha+1-h}}, \quad \text{for } h = 0, \dots, \alpha.$$

Then there exists $\beta \in \mathbb{R}$ such that

$$\sqrt{2^n}\, \mathrm{e}^{-\mathrm{i}\, \frac{\pi}{2^{\alpha+2}} A_r} = \mathrm{e}^{\mathrm{i}\,\beta}[I_2 + \epsilon\, \mathrm{i}(J_2 - I_2)]^{\otimes n},$$

where $\epsilon \in \{-1, 1\}$ satisfies

$$\binom{n-1}{r-1} \equiv -\epsilon 2^\alpha \pmod{2^{\alpha+2}}.$$

In particular, X_r admits instantaneous uniform mixing at time $\pi/2^{\alpha+2}$.

Further, if n is even and r is odd, then there exists $\beta' \in \mathbb{R}$ such that

$$\sqrt{2^n}\, \mathrm{e}^{-\mathrm{i}\, \frac{\pi}{2^{\alpha+2}} A_{n-r}} = \mathrm{e}^{\mathrm{i}\,\beta'}[I_2 + (-1)^{\frac{n+2}{2}} \epsilon\, \mathrm{i}(J_2 - I_2)]^{\otimes n}.$$

In particular, X_{n-r} admits instantaneous uniform mixing at time $\pi/2^{\alpha+2}$.

Proof. Since $2^{\alpha+3}$ divides the right-hand side of Proposition 3.1 (b), we have

$$p_{r-1}(s+2) \equiv p_{r-1}(s) \pmod{2^{\alpha+3}}, \qquad \text{for } s = 0, \dots, n-2.$$

Applying this congruence repeatedly gives, for $s = 0, \dots, n-1$,

$$-p_{r-1}(s+1) - p_{r-1}(s) \equiv -p_{r-1}(1) - p_{r-1}(0) \pmod{2^{\alpha+3}}.$$

It follows from Equation (5) that $-p_{r-1}(1) - p_{r-1}(0) = -2\binom{n-1}{r-1}$, which is divisible by $2^{\alpha+1}$ but not by $2^{\alpha+2}$. Let $\epsilon \in \{-1, 1\}$ satisfy

$$\binom{n-1}{r-1} \equiv -\epsilon 2^\alpha \pmod{2^{\alpha+2}}.$$

Then

$$-p_{r-1}(1) - p_{r-1}(0) \equiv \epsilon 2^{\alpha+1} \pmod{2^{\alpha+3}}$$

and

$$-p_{r-1}(s+1) - p_{r-1}(s) \equiv \epsilon 2^{\alpha+1} \pmod{2^{\alpha+3}}, \quad \text{for } s = 0, \dots, n-1.$$

By Proposition 3.1 (a), we have

$$p_r(s+1) - p_r(s) \equiv \epsilon 2^{\alpha+1} \pmod{2^{\alpha+3}}$$

and therefore

$$p_r(s) - p_r(0) \equiv \epsilon s 2^{\alpha+1} \pmod{2^{\alpha+3}}, \quad \text{for } s = 0, \dots, n. \tag{7}$$

By Lemma 3.2,

$$\sqrt{2^n}\, \mathrm{e}^{-\mathrm{i}\, \frac{\pi}{2^{\alpha+2}} A_r} = \mathrm{e}^{\mathrm{i}\,\beta}[I_2 + \epsilon\, \mathrm{i}(J_2 - I_2)]^{\otimes n},$$

for some $\beta \in \mathbb{R}$, and X_r admits instantaneous uniform mixing at time $\pi/2^{\alpha+2}$.

Suppose n is even and r is odd. By Lemma 3.2, it suffices to show

$$p_{n-r}(s) - p_{n-r}(0) \equiv (-1)^{\frac{n+2}{2}} \epsilon s 2^{\alpha+1} \pmod{2^{\alpha+3}}, \qquad \text{for } s = 0, \dots, n.$$

When s is even, $2^{\alpha+2}$ divides $s2^{\alpha+1}$ and $(-1)^{(n+2)/2}\epsilon s 2^{\alpha+1} \equiv \epsilon s 2^{\alpha+1} \pmod{2^{\alpha+3}}$. Applying Equations (6) and (7), we have

$$\begin{aligned} p_{n-r}(s) - p_{n-r}(0) &= p_r(s) - p_r(0) \\ &\equiv (-1)^{\frac{n+2}{2}} \epsilon s 2^{\alpha+1} \pmod{2^{\alpha+3}}. \end{aligned}$$

When s is odd, Equation (6) gives $p_{n-r}(s)-p_{n-r}(0)=-p_r(s)-p_r(0)$. Applying Equations (5) and (7), we get

$$p_r(1)-p_r(0)=\frac{-2r}{n}\binom{n}{r}\equiv \epsilon 2^{\alpha+1} \pmod{2^{\alpha+3}}, \tag{8}$$

so $2^{\alpha+1}$ is the largest power of 2 that divides $\frac{2r}{n}\binom{n}{r}$.

If $n\equiv 0 \pmod 4$, then $2^{\alpha+3}$ divides $2\binom{n}{r}=2p_r(0)$ and

$$\begin{aligned} p_{n-r}(s)-p_{n-r}(0) &= -[p_r(s)-p_r(0)]-2p_r(0) \\ &\equiv -[p_r(s)-p_r(0)] \pmod{2^{\alpha+3}} \\ &\equiv (-1)^{\frac{n+2}{2}}\epsilon s 2^{\alpha+1} \pmod{2^{\alpha+3}}. \end{aligned}$$

Suppose $n\equiv 2 \pmod 4$. By Equation (5),

$$2p_r(s)=\sum_j (-1)^j 2^{j+1}\binom{n-j}{r-j}\binom{s}{j}.$$

The hypothesis of this lemma ensures that $2^{\alpha+3}$ divides $2^{j+1}\binom{n-j}{r-j}\binom{s}{j}$ for $j\geqslant 2$. Thus

$$2p_r(s)\equiv 2\binom{n}{r}-2^2\binom{n-1}{r-1}s \pmod{2^{\alpha+3}}.$$

We see from Equation (8) that $2^{\alpha+1}$ is the highest power of 2 that divides $\frac{2r}{n}\binom{n}{r}$. Since r is odd and $n\equiv 2 \pmod 4$, $2^{\alpha+1}$ is the largest power of 2 that divides $\binom{n}{r}$. Using our assumption on $\binom{n-1}{r-1}$,

$$2p_r(s)\equiv 2^{\alpha+2}(\gamma_1-\gamma_2) \pmod{2^{\alpha+3}},$$

for some odd integers γ_1 and γ_2. Therefore, $2p_r(s)$ is divisible by $2^{\alpha+3}$ and

$$\begin{aligned} p_{n-r}(s)-p_{n-r}(0) &= [p_r(s)-p_r(0)]-2p_r(s) \\ &\equiv (-1)^{\frac{n+2}{2}}\epsilon s 2^{\alpha+1} \pmod{2^{\alpha+3}}. \end{aligned}$$

By Lemma 3.2, there exists $\beta'\in\mathbb{R}$ such that

$$\sqrt{2^n}\,\mathrm{e}^{-\mathrm{i}\frac{\pi}{2^{\alpha+2}}A_{n-r}}=\mathrm{e}^{\mathrm{i}\beta'}[I_2+(-1)^{\frac{n+2}{2}}\epsilon\,\mathrm{i}(J_2-I_2)]^{\otimes n},$$

and instantaneous uniform mixing occurs in X_{n-r} at time $2^{\alpha+2}$. □

To find the n's and r's that satisfy the condition in Lemma 3.3, we need the following results from number theory, due to Lucas and Kummer, respectively (see Chapter IX of [9]).

Theorem 3.4. *Let p be a prime. Suppose the representation of N and M in base p are $n_k\dots n_1n_0$ and $m_k\dots m_1m_0$, respectively.*

Then

$$\binom{N}{M}\equiv\binom{n_k}{m_k}\cdots\binom{n_0}{m_0} \pmod p.$$

Theorem 3.5. *Let p be a prime. The largest integer k such that p^k divides $\binom{N}{M}$ is the number of carries in the addition of $N-M$ and M in base p representation.*

Let 2^α be the highest power of 2 that divides $\binom{n-1}{r-1}$. That is, there are exactly α carries in the addition of $n-r$ and $r-1$ in base 2 representation. If both n and r are even, then no carry takes place in the right-most digit. Therefore, there are exactly α carries in the addition of $n-r$ and $r-2$ in base 2 representation. Similarly, when n is odd and r is even, there are exactly $\alpha-1$ carries in the addition of $n-r$ and $r-2$ in base 2 representation. In both cases, $2^{\alpha+1}$ does not divide $\binom{n-2}{r-2}$, so the hypothesis of Lemma 3.3 does not hold when r is even.

Corollary 3.6. *Suppose n is even. If r is an odd positive integer with $1 \leqslant r \leqslant n$, and*
$$\binom{n-1}{r-1} \equiv 1 \pmod 2,$$
then there exist $\beta, \beta' \in \mathbb{R}$ such that
$$\sqrt{2^n}\, \mathrm{e}^{-\mathrm{i}\, \frac{\pi}{4} A_r} = \mathrm{e}^{\mathrm{i}\, \beta} [I_2 + \epsilon\, \mathrm{i}(J_2 - I_2)]^{\otimes n}$$
and
$$\sqrt{2^n}\, \mathrm{e}^{-\mathrm{i}\, \frac{\pi}{4} A_{n-r}} = \mathrm{e}^{\mathrm{i}\, \beta'} [I_2 + (-1)^{\frac{n+2}{2}} \epsilon\, \mathrm{i}(J_2 - I_2)]^{\otimes n},$$
where $\epsilon \in \{-1, 1\}$ satisfies $\binom{n-1}{r-1} \equiv -\epsilon \pmod 4$.

In particular, X_r and X_{n-r} admit instantaneous uniform mixing at time $\pi/4$.

Proof. When $r = 1$, we have $\binom{n-2}{r-2} = 0$. For $r \geqslant 3$, both $n-r$ and $r-2$ are odd, there is at least one carry (in the rightmost digit) in the addition of $n-r$ and $r-2$ in base 2 representation. By Theorem 3.5, 2 divides $\binom{n-2}{r-2}$. The result follows from applying Lemma 3.3 with $\alpha = 0$. ☐

Corollary 3.7. *Let $n = 2^m(2l+1)$, for integers $l \geqslant 0$ and $m \geqslant 1$. For each odd r satisfying $1 \leqslant r < 2^m$, there exist $\beta, \beta' \in \mathbb{R}$ such that*
$$\sqrt{2^n}\, \mathrm{e}^{-\mathrm{i}\, \frac{\pi}{4} A_r} = \mathrm{e}^{\mathrm{i}\, \beta} [I_2 + \epsilon\, \mathrm{i}(J_2 - I_2)]^{\otimes n}$$
and
$$\sqrt{2^n}\, \mathrm{e}^{-\mathrm{i}\, \frac{\pi}{4} A_{n-r}} = \mathrm{e}^{\mathrm{i}\, \beta'} [I_2 + (-1)^{\frac{n+2}{2}} \epsilon\, \mathrm{i}(J_2 - I_2)]^{\otimes n},$$
where $\epsilon \in \{-1, 1\}$ satisfies $\binom{n-1}{r-1} \equiv -\epsilon \pmod 4$.

In particular, X_r and X_{n-r} admit instantaneous uniform mixing at time $\pi/4$.

Proof. Let r be an odd integer between 1 and 2^m. In base 2 representation, let $(n-1)$ and $(r-1)$ be $v_k \dots v_0$ and $u_k \dots u_0$, respectively. Then $v_j = 1$ for $j \leqslant m-1$ and $u_h = 0$ for $h \geqslant m$, so $\binom{v_j}{u_j} = 1$ for all j. By Lucas' Theorem, we have
$$\binom{n-1}{r-1} \equiv 1 \pmod 2.$$
The result follows from Corollary 3.6. ☐

We are now ready to show the existence of graphs that admit instantaneous uniform mixing earlier than time $\pi/4$.

Theorem 3.8. *Let $n = 2^{k+2} - 8$, for some $k \geqslant 2$. For $j = 1, 3, 5, 7$, there exists $\beta_j \in \mathbb{R}$ such that*
$$\sqrt{2^n}\, \mathrm{e}^{-\mathrm{i}\, \frac{\pi}{2^k} A_{(2^{k+1}-j)}} = \mathrm{e}^{\mathrm{i}\, \beta_j} [I_2 + \epsilon_j\, \mathrm{i}(J_2 - I_2)]^{\otimes n}, \tag{9}$$
where $\epsilon_j \in \{-1, 1\}$ satisfies
$$\binom{n-1}{(2^{k+1}-j)-1} \equiv -\epsilon_j 2^{k-2} \pmod{2^k}.$$
That is, $X_{2^{k+1}-1}$, $X_{2^{k+1}-3}$, $X_{2^{k+1}-5}$ and $X_{2^{k+1}-7}$ in $\mathcal{H}(2^{k+2}-8, 2)$ admit instantaneous uniform mixing at time $\pi/2^k$.

Proof. Let $n = 2^{k+2} - 8$ and $r = \frac{n}{2} - 1$. Then
$$n - r = 2^{k+1} - 3 = 2^k + 2^{k-1} + \dots + 1 \cdot 2^3 + 1 \cdot 2^2 + 0 \cdot 2^1 + 1 \cdot 2^0$$
and
$$r - 1 = 2^{k+1} - 6 = 2^k + 2^{k-1} + \dots + 1 \cdot 2^3 + 0 \cdot 2^2 + 1 \cdot 2^1 + 0 \cdot 2^0.$$
There are $(k-2)$ carries in the addition of $n-r$ and $r-1$ in base 2 representation. By Kummer's Theorem, the highest power of 2 that divides $\binom{n-1}{r-1}$ is 2^{k-2}.

We want to show that 2^{k-1-h} divides $\binom{n-2-h}{r-2-h}$, for $0 \leqslant h \leqslant k-2$. When $h=0$,

$$r-2 = 2^{k+1}-7 = 2^k + 2^{k-1} + \cdots + 1\cdot 2^3 + 0\cdot 2^2 + 0\cdot 2^1 + 1\cdot 2^0,$$

so there are $(k-1)$ carries in the addition of $n-r$ and $r-2$ in base 2 representation. By Kummer's Theorem, 2^{k-1} divides $\binom{n-2}{r-2}$.

Similarly, there are $(k-2)$ carries in the addition of $n-r$ and $r-3$ in base 2 representation, so 2^{k-2} divides $\binom{n-3}{r-3}$.

As h increments by 1, the number of 1's in the leftmost $(k-2)$ digits in the base 2 representation of $r-2-h$ decreases by at most one. Hence there are at least $k-1-h$ carries in the addition of $n-r$ and $r-2-h$ in base 2 representation, and 2^{k-1-h} divides $\binom{n-2-h}{r-2-h}$, for $h=0,\dots,k-2$.

Applying Lemma 3.3 with $r = 2^{k+1}-5$ and $\alpha = k-2$, Equation (9) holds for $j=5$ and $j=3$, and $X_{2^{k+1}-5}$ and $X_{2^{k+1}-3}$ admit instantaneous uniform mixing at time $\pi/2^k$.

A similar analysis shows that Equation (9) holds for $j=1$ and $j=7$, and instantaneous uniform mixing occurs in $X_{2^{k+1}-1}$ and $X_{2^{k+1}-7}$ at the same time. $\square$

4. Perfect State Transfer

Let u and w be distinct vertices in X. We say that *perfect state transfer* occurs from u to w in the continuous-time quantum walk on X at time τ if

$$|(\mathrm{e}^{-\mathrm{i}\,\tau A(X)})_{u,w}| = 1.$$

We say that X is *periodic* at u with period τ if

$$|(\mathrm{e}^{-\mathrm{i}\,\tau A(X)})_{u,u}| = 1.$$

If $A(X)$ belongs to the Bose–Mesner algebra of an association scheme $\mathcal{A}$ and X is periodic at some vertex u, then X is periodic at every vertex because $I \in \mathcal{A}$. In this case, we simply say that X is *periodic*.

Consider X_r in the Hamming scheme $\mathcal{H}(2^m,2)$ when r is odd. We see from the proof of Corollary 3.7 that $\binom{2^m-1}{r-1}$ is odd. It follows from Theorem 2.3 of [5] that perfect state transfer occurs in X_r at time $\pi/2$. Moreover, let $1 \leqslant r' \leqslant 2^m$ be an odd integer distinct from r, then the graph $X_r \cup X_{r'}$ is periodic with period $\pi/2$.

Let X be one of the graphs considered in Corollary 3.7 or Theorem 3.8. At the time τ of instantaneous uniform mixing in X, we have

$$\mathrm{e}^{-\mathrm{i}\,\tau A(X)} = \frac{\mathrm{e}^{\mathrm{i}\,\beta}}{\sqrt{2^n}} \begin{pmatrix} 1 & \epsilon\,\mathrm{i} \\ \epsilon\,\mathrm{i} & 1 \end{pmatrix}^{\otimes n}, \qquad \text{for some } \beta \in \mathbb{R} \text{ and } \epsilon \in \{-1,1\}.$$

Observe that, for $\epsilon, \epsilon' \in \{-1,1\}$,

$$\begin{pmatrix} 1 & \epsilon\,\mathrm{i} \\ \epsilon\,\mathrm{i} & 1 \end{pmatrix}\begin{pmatrix} 1 & \epsilon' i \\ \epsilon'\,\mathrm{i} & 1 \end{pmatrix} = \begin{cases} 2\begin{pmatrix} 0 & \epsilon\,\mathrm{i} \\ \epsilon\,\mathrm{i} & 0 \end{pmatrix} & \text{if } \epsilon = \epsilon', \\ 2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \text{if } \epsilon \neq \epsilon'. \end{cases} \tag{10}$$

We see that

$$\mathrm{e}^{-\mathrm{i}\,2\tau A(X)} = \mathrm{e}^{2\beta\,\mathrm{i}} \begin{pmatrix} 0 & \epsilon\,\mathrm{i} \\ \epsilon\,\mathrm{i} & 0 \end{pmatrix}^{\otimes n},$$

and X has perfect state transfer at time 2τ.

We generalize the above observation by applying Equation (10) to the union of two graphs in $\mathcal{H}(n,2)$.

Lemma 4.1. *Let X and X' be graphs in $\mathcal{H}(n,2)$ such that $E(X)\cap E(X')=\varnothing$, and there exist $\beta,\beta'\in\mathbb{R}$ and $\epsilon,\epsilon'\in\{-1,1\}$ such that*

$$\mathrm{e}^{-\mathrm{i}\,\tau A(X)}=\frac{\mathrm{e}^{\mathrm{i}\,\beta}}{\sqrt{2^n}}\begin{pmatrix}1 & \epsilon\,\mathrm{i}\\ \epsilon\,\mathrm{i} & 1\end{pmatrix}^{\otimes n}\quad \text{and}\quad \mathrm{e}^{-\mathrm{i}\,\tau A(X')}=\frac{\mathrm{e}^{\mathrm{i}\,\beta'}}{\sqrt{2^n}}\begin{pmatrix}1 & \epsilon'\,\mathrm{i}\\ \epsilon'\,\mathrm{i} & 1\end{pmatrix}^{\otimes n}.$$

If $\epsilon=\epsilon'$ then $X\cup X'$ has perfect state transfer at time τ. Otherwise, $X\cup X'$ is periodic at time τ.

Proof. As $A(X)$ and $A(X')$ commute, it follows from Equation (10) that

$$\mathrm{e}^{-\mathrm{i}\,\tau A(X\cup X')}=\mathrm{e}^{-\mathrm{i}\,\tau A(X)}\,\mathrm{e}^{-\mathrm{i}\,\tau A(X')}=\begin{cases}\mathrm{e}^{(\beta+\beta')\,\mathrm{i}}\begin{pmatrix}0 & \epsilon\,\mathrm{i}\\ \epsilon\,\mathrm{i} & 0\end{pmatrix}^{\otimes n} & \text{if } \epsilon=\epsilon',\\ \mathrm{e}^{(\beta+\beta')\,\mathrm{i}}\,I_{2^n} & \text{otherwise.}\end{cases}$$

□

With the help of the following result in number theory, Theorem 1 of [4], we find graphs in $\mathcal{H}(2^m,2)$ and $\mathcal{H}(2^{k+2}-8,2)$ that have perfect state transfer earlier than $\pi/2$.

Theorem 4.2. *Let p be prime, n and k be positive integers. If p^k divides n then*

$$\binom{n-1}{s}\equiv(-1)^{s-\lfloor s/p\rfloor}\binom{n/p-1}{\lfloor s/p\rfloor}\pmod{p^k},$$

for $s=0,\dots,n-1$.

Proposition 4.3. *For $m\geqslant 3$, and for odd integers r and r' satisfying*

$$1\leqslant r<r'<2^{m-1}\qquad \text{or}\qquad 2^{m-1}<r<r'<2^m, \tag{11}$$

perfect state transfer occurs in the graph $X_r\cup X_{r'}$ of $\mathcal{H}(2^m,2)$ at time $\pi/4$.

Proof. Let r be an odd integer between 2^b and 2^{b+1} for some $b\leqslant m-1$. Let $s_0=r-1$ and $s_i=\lfloor s_{i-1}/2\rfloor$, for $i=1,\dots,b$. Let $n=2^m$. Applying Theorem 4.2 repeatedly gives

$$\binom{n-1}{r-1}\equiv(-1)^{s_0-s_i}\binom{2^{m-i}-1}{s_i}\pmod{2^{m-i+1}},\qquad \text{for } 1\leqslant i\leqslant b.$$

Since $s_b=1$ and $m-b+1\geqslant 2$, applying the above equation with $i=b$ yields

$$\binom{n-1}{r-1}\equiv(-1)^{r-2}(2^{m-b}-1)\pmod 4.$$

If $r<2^{m-1}$, we have $b\leqslant m-2$ and

$$\binom{n-1}{r-1}\equiv 1\pmod 4.$$

If $2^{m-1}<r$, we have $b=m-1$ and

$$\binom{n-1}{r-1}\equiv -1\pmod 4.$$

It follows from Corollary 3.7 that there exist $\beta,\beta'\in\mathbb{R}$ such that

$$\mathrm{e}^{-\mathrm{i}\,\frac{\pi}{4}A_r}=\frac{\mathrm{e}^{\mathrm{i}\,\beta}}{\sqrt{2^n}}\begin{pmatrix}1 & \epsilon\,\mathrm{i}\\ \epsilon\,\mathrm{i} & 1\end{pmatrix}^{\otimes n}\quad \text{and}\quad \mathrm{e}^{-\mathrm{i}\,\frac{\pi}{4}A_{r'}}=\frac{\mathrm{e}^{\mathrm{i}\,\beta'}}{\sqrt{2^n}}\begin{pmatrix}1 & \epsilon\,\mathrm{i}\\ \epsilon\,\mathrm{i} & 1\end{pmatrix}^{\otimes n},$$

where

$$\epsilon=\begin{cases}-1 & \text{if } r \text{ and } r' \text{ are odd integers between } 1 \text{ and } 2^{m-1},\\ 1 & \text{if } r \text{ and } r' \text{ are odd integers between } 2^{m-1} \text{ and } 2^m.\end{cases}$$

By Lemma 4.1, perfect state transfer occurs in $X_r\cup X_{r'}$ at time $\frac{\pi}{4}$. □

Proposition 4.4. *For integer $k \geqslant 2$, perfect state transfer occurs in graphs*

$$X_{2^{k+1}-5} \cup X_{2^{k+1}-7} \quad \textit{and} \quad X_{2^{k+1}-1} \cup X_{2^{k+1}-3}$$

of $\mathcal{H}(2^{k+2}-8, 2)$ at time $\pi/2^k$.

Proof. Let $n = 2^{k+2} - 8$ and $m = \frac{n}{8}$. Let $\epsilon_1, \epsilon_3, \epsilon_5, \epsilon_7$ be the integers defined in Theorem 3.8.

Consider $4m-1 = 2^{k+1}-5$ and $4m-3 = 2^{k+1}-7$. From

$$\binom{8m-1}{4m-4} = \left[1 - 4\frac{5m}{(4m+3)(2m+1)}\right]\binom{8m-1}{4m-2},$$

we get

$$\begin{aligned}\binom{n-1}{(2^{k+1}-7)-1} &= \left[1 - 4\frac{5m}{(4m+3)(2m+1)}\right]\binom{n-1}{(2^{k+1}-5)-1} \\ &\equiv \left[1 - 4\frac{5m}{(4m+3)(2m+1)}\right](-\epsilon_5 2^{k-2}) \pmod{2^k}.\end{aligned}$$

Since $4m+3$ and $2m+1$ are coprime with 2^k, we have

$$\binom{n-1}{(2^{k+1}-7)-1} \equiv -\epsilon_5 2^{k-2} \pmod{2^k},$$

and $\epsilon_7 = \epsilon_5$. It follows from Theorem 3.8 and Lemma 4.1 that perfect state transfer occurs in $X_{2^{k+1}-5} \cup X_{2^{k+1}-7}$ at time $\pi/2^k$.

For $X_{2^{k+1}-3}$ and $X_{2^{k+1}-1}$, we have $4m+1 = 2^{k+1}-3$ and $4m+3 = 2^{k+1}-1$. From

$$\binom{8m-1}{4m+2} = \left[1 - 4\frac{3m}{(4m+1)(2m+1)}\right]\binom{8m-1}{4m},$$

we have

$$\begin{aligned}\binom{n-1}{(2^{k+1}-1)-1} &= \left[1 - 4\frac{3m}{(4m+1)(2m+1)}\right]\binom{n-1}{(2^{k+1}-3)-1} \\ &\equiv \left[1 - 4\frac{3m}{(4m+1)(2m+1)}\right](-\epsilon_3 2^{k-2}) \pmod{2^k}.\end{aligned}$$

Since $4m+1$ and $2m+1$ are coprime with 2^k, we have

$$\binom{n-1}{(2^{k+1}-1)-1} \equiv -\epsilon_3 2^{k-2} \pmod{2^k},$$

and $\epsilon_1 = \epsilon_3$. It follows from Theorem 3.8 and Lemma 4.1 that perfect state transfer occurs in $X_{2^{k+1}-1} \cup X_{2^{k+1}-3}$ at time $\pi/2^k$. □

5. Halved n-Cube

The n-cube X is a connected bipartite graph of diameter n. When $n \geqslant 2$, X_2 has two components, one of which has the set $\mathcal{E}$ of binary words of even weights as its vertex set. The *halved n-cube*, denoted by $\widehat{X}$, is the subgraph of X_2 induced by $\mathcal{E}$. It is a distance regular graph on 2^{n-1} vertices with diameter $\lfloor \frac{n}{2} \rfloor$. The intersection numbers of $\widehat{X}$ are

$$\widehat{a}_j = 2j(n-2j), \quad \widehat{b}_j = \frac{(n-2j)(n-2j-1)}{2} \quad \text{and} \quad \widehat{c}_j = j(2j-1),$$

for $j = 0, \ldots, \lfloor \frac{n}{2} \rfloor$, and the eigenvalues of $\widehat{X}$ are $p_2(0), p_2(1), \ldots, p_2(\lfloor n/2 \rfloor)$.

Let $\widehat{\mathcal{A}} = \{I, \widehat{A}_1, \dots, \widehat{A}_{\lfloor n/2 \rfloor}\}$ where $\widehat{A}_r = A(\widehat{X}_r)$. We use $\widehat{p}_r(s)$ to denote the eigenvalues of $\widehat{\mathcal{A}}$ and let $\widehat{p}_{-1}(s) = 0$. Equation (11) on page 128 of [3] states that, for $r, s = 0, \dots, \lfloor n/2 \rfloor$,

$$\widehat{p}_1(s)\widehat{p}_r(s) = \widehat{c}_{r+1}\widehat{p}_{r+1}(s) + \widehat{a}_r\widehat{p}_r(s) + \widehat{b}_{r-1}\widehat{p}_{r-1}(s).$$

It is straightforward to verify that $\widehat{p}_r(s) = p_{2r}(s)$ satisfies these recursions, so the eigenvalues of $\widehat{\mathcal{A}}$ are

$$\widehat{p}_r(s) = p_{2r}(s), \qquad \text{for } r, s = 0, \dots, \lfloor \frac{n}{2} \rfloor. \tag{12}$$

For more information on the halved n-cube, please see Sections 4.2 and 9.2D of [3].

When $n = 2m+1$, Equation (4) yields

$$\sum_{h=0}^{n} p_h(s) i^h = (1+i)^{2m+1-s}(1-i)^s = 2^m i^{m-s}(1+i), \qquad \text{for } s = 0, \dots, n.$$

The real part of this sum is

$$\begin{aligned} \sum_{r=0}^{m} p_{2r}(s)(-1)^r &= \sum_{r=0}^{m} \widehat{p}_r(s)(-1)^r \\ &= \begin{cases} 2^m & \text{if } m-s \equiv 0 \pmod 4 \text{ or } m-s \equiv 3 \pmod 4, \\ -2^m & \text{otherwise.} \end{cases} \end{aligned} \tag{13}$$

By Proposition 2.1, $\sum_{r=0}^{m}(-1)^r \widehat{A}_r$ is a (complex) Hadamard matrix.

Theorem 5.1. *For $n \geqslant 3$, the adjacency algebra of the halved n-cube contains a complex Hadamard matrix if and only if n is odd.*

Proof. Suppose $n = 2m$. Using Proposition 2.2, it is sufficient to show that

$$\left[\sum_{r=0}^{m} |\widehat{p}_r(m-1)|\right]^2 < 2^{2m-1}, \qquad \text{for } m \geqslant 2.$$

It follows from Equations (4) and (12) that for $r \geqslant 0$,

$$\begin{aligned} \widehat{p}_r(m-1) &= [x^{2r}](1+x)^{m+1}(1-x)^{m-1} \\ &= [x^{2r}](1+2x+x^2)(1-x^2)^{m-1} \\ &= (-1)^r \left[\binom{m-1}{r} - \binom{m-1}{r-1}\right]. \end{aligned}$$

Hence

$$|\widehat{p}_r(m-1)| = \begin{cases} \binom{m-1}{r} - \binom{m-1}{r-1} & \text{if } 0 \leqslant r \leqslant \frac{m}{2} \\ \binom{m-1}{r-1} - \binom{m-1}{r} & \text{if } \frac{m}{2} < r \leqslant m \end{cases}$$

and

$$\begin{aligned} \sum_{r=0}^{m} |\widehat{p}_r(m-1)| &= \sum_{r=0}^{\lfloor \frac{m}{2} \rfloor} \left[\binom{m-1}{r} - \binom{m-1}{r-1}\right] + \sum_{r=\lfloor \frac{m}{2} \rfloor + 1}^{m} \left[\binom{m-1}{r-1} - \binom{m-1}{r}\right] \\ &= 2\binom{m-1}{\lfloor \frac{m}{2} \rfloor}. \end{aligned}$$

A simple mathematical induction on m shows that $4\binom{m-1}{\lfloor \frac{m}{2} \rfloor}^2 < 2^{2m-1}$, for $m \geqslant 2$.

When n is odd, $\sum_{r=0}^{m}(-1)^r \widehat{A}_r$ is a complex Hadamard matrix. $\square$

Theorem 5.2. *For $n \geqslant 3$, the halved n-cube admits instantaneous uniform mixing if and only if n is odd.*

Proof. From the above theorem, the halved n-cube does not admit instantaneous uniform mixing when $n \geqslant 4$ is even.

Suppose $n = 2m+1$ and $\mathrm{e}^{-2\,\mathrm{i}\,\tau} \in \{-i, i\}$. For $s = 0, \ldots, m$, we have

$$\widehat{p}_1(s) = 2(m-s)(m-s+1) - m$$

and

$$\begin{aligned}
\mathrm{e}^{-\,\mathrm{i}\,\tau \widehat{p}_1(s)} &= (\mathrm{e}^{-2\,\mathrm{i}\,\tau})^{(m-s)(m-s+1)}\,\mathrm{e}^{\mathrm{i}\,\tau m} \\
&= \begin{cases} \mathrm{e}^{\mathrm{i}\,\tau m} & \text{if } m-s \equiv 0 \pmod 4 \text{ or } m-s \equiv 3 \pmod 4, \\ -\,\mathrm{e}^{\mathrm{i}\,\tau m} & \text{otherwise.} \end{cases}
\end{aligned}$$

We see from Equation (13) that

$$2^m\,\mathrm{e}^{-\,\mathrm{i}\,\tau \widehat{p}_1(s)} = \mathrm{e}^{\mathrm{i}\,\tau m} \sum_{r=0}^{m} (-1)^r \widehat{p}_r(s), \qquad \text{for } s = 0, \ldots, m.$$

Since $|\,\mathrm{e}^{\mathrm{i}\,\tau m}(-1)^r| = 1$, it follows from Proposition 2.3 that $\widehat{X}_1$ admits instantaneous uniform mixing at time $\frac{\pi}{4}$. □

The halved 2-cube is the complete graph on two vertices and it admits instantaneous uniform mixing (see [1]).

When $n \geqslant 3$, the halved n-cube is isomorphic to the cubelike graph of $\mathbb{Z}_2^{n-1}$ with connection set

$$C = \{\mathbf{a} : \text{weight of } \mathbf{a} \text{ is 1 or 2}\}.$$

Applying Theorem 2.3 of [5] to the halved n-cube with even n, we see that perfect state transfer occurs from $\mathbf{a}$ to $\mathbf{a} \oplus \mathbf{1}$ at time $\pi/2$. But this graph does not have instantaneous uniform mixing.

6. Folded n-Cube

Let Γ be a distance regular graph on v vertices with diameter d and intersection array $\{b_0, b_1, \ldots, b_{d-1}; c_1, \ldots, c_d\}$. We say Γ is *antipodal* if Γ_d is a union of complete graph K_R's, for some fixed R. The vertex sets of the K_R's in Γ_d form an equitable partition $\mathcal{P}$ of Γ and the quotient graph of Γ with respect to $\mathcal{P}$ is called the *folded graph* $\widetilde{\Gamma}$ of Γ. When $d > 2$, $\widetilde{\Gamma}$ is a distance regular graph on $\frac{v}{R}$ vertices with diameter $\lfloor \frac{d}{2} \rfloor$, see Proposition 4.2.2 (ii) of [3]. Moreover $\widetilde{\Gamma}$ has intersection numbers $\widetilde{a}_j = a_j$, $\widetilde{b}_j = b_j$ and $\widetilde{c}_j = c_j$ for $j = 0, \ldots \lfloor \frac{d}{2} \rfloor - 1$ and

$$\widetilde{c}_{\lfloor \frac{d}{2} \rfloor} = \begin{cases} c_{\lfloor \frac{d}{2} \rfloor} & \text{if } d \text{ is odd,} \\ Rc_{\frac{d}{2}} & \text{if } d \text{ is even.} \end{cases}$$

From Proposition 4.2.3 (ii) of [3], we see that if the eigenvalues of Γ are $p_1(0) \geqslant p_1(1) \geqslant \ldots \geqslant p_1(d)$, then $\widetilde{\Gamma}$ has eigenvalues $\widetilde{p}_1(j) = p_1(2j)$ for $j = 0, \ldots, \lfloor \frac{d}{2} \rfloor$. The eigenvalues for $\widetilde{A}_j$'s and A_j's satisfy the same recursive relation (Equation (11) on Page 128 of [3]) for $j = 0, \ldots, \lfloor \frac{d}{2} \rfloor$ when d is odd and for $j = 0, \ldots, \frac{d}{2} - 1$ when d is even. When d is even, $\widetilde{p}_{\frac{d}{2}}(s) = \frac{1}{R} p_{\frac{d}{2}}(2s)$. Therefore

$$\widetilde{p}_r(s) = \begin{cases} p_r(2s) & \text{if } 0 \leqslant r < \lfloor \frac{d}{2} \rfloor, \\ p_{\lfloor \frac{d}{2} \rfloor}(2s) & \text{if } d \text{ is odd and } r = \lfloor \frac{d}{2} \rfloor, \\ \frac{1}{R} p_{\frac{d}{2}}(2s) & \text{if } d \text{ is even and } r = \frac{d}{2}. \end{cases} \tag{14}$$

For each vertex $\mathbf{a}$ in the n-cube X, $\mathbf{1} \oplus \mathbf{a}$ is the unique vertex at distance n from $\mathbf{a}$. Therefore X_n is a union of K_2's. The *folded n-cube* $\widetilde{X}$ has 2^{n-1} vertices, diameter $\lfloor \frac{n}{2} \rfloor$, and eigenvalues

$$\widetilde{p}_r(s) = \begin{cases} [x^r](1+x)^{n-2s}(1-x)^{2s} & \text{if } 0 \leqslant r < \lfloor \frac{n}{2} \rfloor, \\ [x^{\lfloor \frac{n}{2} \rfloor}](1+x)^{n-2s}(1-x)^{2s} & \text{if } n \text{ is odd and } r = \lfloor \frac{n}{2} \rfloor, \\ [x^{\frac{n}{2}}]\frac{1}{2}(1+x)^{n-2s}(1-x)^{2s} & \text{if } n \text{ is even and } r = \frac{n}{2}. \end{cases} \tag{15}$$

The folded n-cube is isomorphic to the graph obtained from an $(n-1)$-cube by adding the perfect matching in which a vertex $\mathbf{a}$ is adjacent to $\mathbf{1} \oplus \mathbf{a}$. Best et al. proved the following result, see Theorem 1 of [2].

Theorem 6.1. *For $n \geqslant 3$, the folded n-cube admits instantaneous uniform mixing if and only if n is odd.*

In particular, the adjacency algebra of the folded n-cube contains a complex Hadamard matrix when n is odd.

Theorem 6.2. *For $n \geqslant 3$, the adjacency algebra of the folded n-cube contains a complex Hadamard matrix if and only if n is odd.*

Proof. Suppose $n = 4m$, for some $m \geqslant 1$. We have, for $r = 0, \dots, 2m-1$,

$$\begin{aligned} \widetilde{p}_r(m) &= [x^r](1+x)^{2m}(1-x)^{2m} \\ &= \begin{cases} (-1)^{\frac{r}{2}} \binom{2m}{\frac{r}{2}} & \text{if } r \text{ is even,} \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

and

$$\widetilde{p}_{2m}(m) = (-1)^m \frac{1}{2} \binom{2m}{m}.$$

Now

$$\begin{aligned} \sum_{r=0}^{2m} |\widetilde{p}_r(m)| &= \sum_{r=0}^{m-1} \binom{2m}{r} + \frac{1}{2}\binom{2m}{m} \\ &= \frac{1}{2}\left[\sum_{r=0}^{2m} \binom{2m}{r}\right] \\ &= 2^{2m-1}. \end{aligned}$$

We have $\left[\sum_{s=0}^{2m} |\widetilde{p}_s(m)|\right]^2 < 2^{4m-1}$. By Proposition 2.2, the adjacency algebra of the folded $4m$-cube does not contain a complex Hadamard matrix.

Suppose $n = 4m+2$. By Equation (15),

$$\widetilde{p}_r(m) = \begin{cases} 1 & \text{if } r = 0, \\ (-1)^{\lfloor \frac{r}{2} \rfloor} 2\binom{2m}{\lfloor \frac{r}{2} \rfloor} & \text{if } 1 \leqslant r < 2m \text{ is odd,} \\ (-1)^{\frac{r}{2}} \left[\binom{2m}{\frac{r}{2}} - \binom{2m}{\frac{r}{2}-1}\right] & \text{if } 2 \leqslant r \leqslant 2m \text{ is even,} \\ (-1)^m \binom{2m}{m} & \text{if } r = 2m+1. \end{cases}$$

Now

$$\begin{aligned} \sum_{s=0}^{2m+1} |\widetilde{p}_s(m)| &= 1 + \sum_{r=0}^{m-1} 2\binom{2m}{r} + \sum_{r=1}^{m} \left[\binom{2m}{r} - \binom{2m}{r-1}\right] + \binom{2m}{m} \\ &= 2^{2m} + \binom{2m}{m}. \end{aligned}$$

A simple mathematical induction on m shows that $\left[2^{2m}+\binom{2m}{m}\right]^2 < 2^{4m+1}$, for all integer $m \geqslant 2$. We conclude that the adjacency algebra of the folded $(4m+2)$-cube does not contain a complex Hadamard matrix, for $m \geqslant 2$.

The folded 6-cube has eigenvalues

$$p_0(1) = p_0(2) = 1, \qquad p_1(1) = -p_1(2) = 2,$$
$$p_2(1) = p_2(2) = -1 \qquad \text{and} \qquad p_3(1) = -p_3(2) = -2.$$

Let $W = \sum_{j=0}^{3} t_j \widetilde{A}_j$ be a type II matrix. Adding the equations in Proposition 2.1 for $s = 1$ and $s = 2$ gives

$$-\left(\frac{t_0}{t_2}+\frac{t_2}{t_0}\right) - 4\left(\frac{t_1}{t_3}+\frac{t_3}{t_1}\right) = 22.$$

The left-hand side is at most ten if $|t_0| = |t_1| = |t_2| = |t_3| = 1$. Therefore, the adjacency algebra of the folded 6-cube does not contain a complex Hadamard matrix. □

The folded 2-cube is the complete graph on two vertices and it admits instantaneous uniform mixing (see [1]).

7. Folded Halved $2m$-Cube

According to Page 141 of [3], the halved $2m$-cube $\widehat{X}$ is antipodal with antipodal classes of size two and the folded $2m$-cube $\widetilde{X}$ is bipartite for $m \geqslant 2$. In addition, the folded graph of $\widehat{X}$ is isomorphic to the halved graph of $\widetilde{X}$. We use $\mathcal{X}$ to denoted the folded graph of $\widehat{X}$ which is a distance regular graph on 2^{2m-2} vertices with diameter $\lfloor \frac{m}{2} \rfloor$. Let $\mathcal{A}_r = A(\mathcal{X}_r)$, for $r = 0, \ldots, \lfloor \frac{m}{2} \rfloor$.

By Equations (12) and (14), the eigenvalues of the folded halved $2m$-cube are

$$\mathcal{P}_r(s) = \begin{cases} p_{2r}(2s) & \text{if } 0 \leqslant r < \lfloor \frac{m}{2} \rfloor, \\ p_{2\lfloor \frac{m}{2} \rfloor}(2s) & \text{if } m \text{ is odd and } r = \lfloor \frac{m}{2} \rfloor, \\ \frac{1}{2} p_m(2s) & \text{if } m \text{ is even and } r = \frac{m}{2}. \end{cases} \tag{16}$$

Theorem 7.1. *The adjacency algebra of the folded halved $2m$-cube contains a complex Hadamard matrix if and only if m is even.*

Proof. Suppose $m = 2u+1$. Then

$$\begin{aligned} \mathcal{P}_r(u) &= [x^{2r}](1+2x+x^2)(1-x^2)^{2u} \\ &= \begin{cases} 1 & \text{if } r = 0 \\ (-1)^r \binom{2u}{r} + (-1)^{r-1}\binom{2u}{r-1} & \text{if } 1 \leqslant r \leqslant u. \end{cases} \end{aligned}$$

Then

$$\sum_{r=0}^{u} |\mathcal{P}_r(u)| = 1 + \sum_{r=1}^{u} \left[\binom{2u}{r} - \binom{2u}{r-1}\right] = \binom{2u}{u}.$$

Hence

$$\left[\sum_{r=0}^{u} |\mathcal{P}_r(u)|\right]^2 < \left[\sum_{r=0}^{2u} \binom{2u}{r}\right]^2 = 2^{4u}.$$

By Proposition 2.2, the adjacency algebra of the folded halved $(4u+2)$-cube does not contain a complex Hadamard matrix.

Suppose $m = 2u$. By Equations (16) and (6),

$$\begin{aligned}\sum_{r=0}^{u}(-1)^r\mathcal{P}_r(s) &= \sum_{r=0}^{u-1}(-1)^r p_{2r}(2s) + \frac{1}{2}(-1)^u p_{2u}(2s)\\ &= \frac{1}{2}\sum_{r=0}^{u-1}(-1)^r p_{2r}(2s) + \frac{1}{2}(-1)^u p_{2u}(2s) + \frac{1}{2}\sum_{r=0}^{u-1}(-1)^r(-1)^{2s}p_{4u-2r}(2s)\\ &= \frac{1}{2}\sum_{r=0}^{2u}(-1)^r p_{2r}(2s),\end{aligned}$$

which is equal to the real part of $\frac{1}{2}\sum_{j=0}^{4u} i^j p_j(2s)$. By Equation (4),

$$\frac{1}{2}\sum_{j=0}^{4u} i^j p_j(2s) = \frac{1}{2}(1+i)^{4u-2s}(1-i)^{2s} = (-1)^{u-s}2^{2u-1}. \tag{17}$$

By Proposition 2.1, $\sum_{s=0}^{u}(-1)^s\mathcal{A}_s$ is a complex Hadamard matrix. □

Theorem 7.2. *The folded halved $2m$-cube admits instantaneous uniform mixing if and only if m is even.*

Proof. Suppose $m = 2u$ and $\mathrm{e}^{-8\,\mathrm{i}\,\tau} = -1$. For $s = 0, \dots, u$,

$$\mathcal{P}_1(s) = 8(u-s)^2 - 2u$$

and

$$2^{2u-1}\,\mathrm{e}^{-\mathrm{i}\,\tau\mathcal{P}_1(s)} = 2^{2u-1}(-1)^{(u-s)^2}\,\mathrm{e}^{2\,\mathrm{i}\,u\tau},$$

which is equal to $\mathrm{e}^{2\,\mathrm{i}\,u\tau}\sum_{r=0}^{u}(-1)^r\mathcal{P}_r(s)$ from Equation (17). By Proposition 2.3, the folded halved $4u$-cube admits instantaneous uniform mixing at time $\pi/8$. □

Acknowledgements. The author would like to thank Chris Godsil, Natalie Mullin and Aidan Roy for many interesting discussions. The author is grateful for Akihiro Munemasa's advice on the exposition.

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