New code upper bounds for the folded $n$-cube

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Abstract

Let $\Gamma$ denote a distance-regular graph. The maximum size of codewords with minimum distance at least $d$ is denoted by $A(\Gamma, d)$. Let $\square_n$ denote the folded $n$-cube $H(n, 2)$. We give an upper bound on $A(\square_n, d)$ based on block-diagonalizing the Terwilliger algebra of $\square_n$ and on semidefinite programming. The technique of this paper is an extension of the approach taken by A. Schrijver [8] on the study of $A(H(n, 2), d)$.

Key words: Code; Upper bounds; Terwilliger algebra; Semidefinite programming

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1 Introduction

Let $\Gamma$ denote a distance-regular graph with vertex set $V(\Gamma)$, path-length distance function $\partial$ and diameter $D$. We call any nonempty subset $C$ of $V(\Gamma)$ a code in $\Gamma$. For $1 < |C| < |V(\Gamma)|$, the minimum distance of $C$ is defined as $d := \min\{\partial(x, y) | x, y \in C, x \neq y\}$. The maximum size of $C$ with minimum distance at least $d$ is denoted by $A(\Gamma, d)$. In general, the problem of determining $A(\Gamma, d)$ is difficult and hence any improved upper bounds are interesting enough for the researchers in this area. In [8], A. Schrijver introduced a new method based on block-diagonalizing the Terwilliger algebra of $H(n, 2)$ and on semidefinite programming to give an upper bound on $A(H(n, 2), d)$. This method can be seen as a refinement of Delsarte’s linear programming approach [5] and the obtained new bound is stronger than the Delsarte bound. In [7] these results were extended to the $q$-Hamming scheme with $q \geq 3$. We refer the reader to [6] for more details on this method.

Motivated by above works, in this paper we will consider the folded $n$-cube $H(n, 2)$ which is denoted by $\square_n$. We first determine the Terwilliger algebra of $\square_n$ with respect to a fixed vertex. Then based on block-diagonalizing the Terwilliger algebra of $\square_n$ and on semidefinite programming, we give a new upper bound on $A(\square_n, d)$. This bound strengthens the Delsarte bound and can be calculated in time polynomial in $n$ using semidefinite programming.

We now recall the definition of $\square_n$. Let $S = \{1, 2, \ldots, n\}$ with integer $n \geq 6$. It is known that each subset of $S$ is called the support of a vertex of $H(n, 2)$ and hence we can identify all vertices of $H(n, 2)$ with their support. Then the Hamming distance of $u, v \subseteq S$ is equal to $|u \triangle v|$, where $u \triangle v = u \cup v - u \cap v$. Denote by $X$ the set of all unordered pairs $(u, u')$, where $u, u' \subseteq S$, $u \cap u' = \emptyset$, $u \cup u' = S$. $\square_n$ can be described as the graph whose vertex set is $X$, two vertices, say $z := (z_1, z_2), w := (w_1, w_2)$, are adjacent whenever $\min\{|z_i \triangle w_j| : i, j = 1, 2\} = 1$. Thus the path-length distance of $x := (x_1, x_2)$ and $y := (y_1, y_2)$ is given by

$$\partial(x, y) = \min\{|x_i \triangle y_j| : i, j = 1, 2\}.$$
Observe that $|x_1 \triangle y_1| = |x_2 \triangle y_2|$, $|x_1 \triangle y_1| = |x_2 \triangle y_1|$, and $|x_1 \triangle y_1| + |x_1 \triangle y_2| = n$. Then it follows that $\partial(x, y) = \min\{ |x_1 \triangle y_1|, |x_1 \triangle y_2| \}$ and $0 \leq \partial(x, y) \leq \left\lfloor \frac{n}{2} \right\rfloor$, where $|a|$ denotes the maximal integer less than or equal to $a$. It is well-known that $\Box_n$ is a bipartite (an almost-bipartite) distance-regular graph with diameter $\left\lfloor \frac{n}{2} \right\rfloor$ for even $n$ (odd $n$).

The paper is organized as follows. In Section 2, we recall some definitions and facts concerning the distance-regular graph and its Terwilliger algebra. In Section 3, we give a basis of the Terwilliger algebra of $\Box_n$ by considering the action of automorphism group of $\Box_n$ on $X \times X \times X$. In Section 4, we study a block-diagonalization of the Terwilliger algebra via the obtained basis. In Section 5, we estimate an upper bound on $A(\Box_n, d)$ by semidefinite programming involving the block-diagonalization of the Terwilliger algebra. Moreover, we offer several concrete upper bounds on $A(\Box_n, d)$ for $8 \leq n \leq 13$.

## 2 Preliminaries

Let $\Gamma$ denote a distance-regular graph with vertex set $V$, path-length distance function $\partial$, and diameter $D$. Let $V = \mathbb{C}^{VT}$ denote the $\mathbb{C}$-space of column vectors with coordinates indexed by $VT$, and let $\text{Mat}_{VT}(\mathbb{C})$ denote the $\mathbb{C}$-algebra of matrices with rows and columns indexed by $VT$.

For $0 \leq i \leq D$ let $A_i \in \text{Mat}_{VT}(\mathbb{C})$ denote the $i$th distance matrix of $\Gamma$: $A_i$ has $(x, y)$-entry equal to 1 if $\partial(x, y) = i$ and 0 otherwise. It is known that $A_0, A_1, \ldots, A_D$ span a commutative subalgebra of $\text{Mat}_{VT}(\mathbb{C})$, denoted by $\mathcal{M}$. It turns out that $\mathcal{M}$ can be generated by $A_1$. We call $\mathcal{M}$ the Bose-Mesner algebra of $\Gamma$. Fix a vertex $x \in VT$. For $0 \leq i \leq D$ let diagonal matrix $E_i^* = E_i^*(x)$ denote $i$th dual idempotent of $\Gamma$: $E_i^*$ has $(y, y)$-entry equal to 1 if $\partial(x, y) = i$ and 0 otherwise. It is known that $E_0^*, E_1^*, \ldots, E_D^*$ span a commutative subalgebra of $\text{Mat}_X(\mathbb{C})$, denoted by $\mathcal{M}^*$. We call $\mathcal{M}^*$ the dual Bose-Mesner algebra of $\Gamma$ with respect to $x$.

Let $T = T(x)$ denote the subalgebra of $\text{Mat}_{VT}(\mathbb{C})$ generated by $\mathcal{M}$ and $\mathcal{M}^*$, and $T$ is called the Terwilliger algebra of $\Gamma$ with respect to $x$. It is known that $T$ is semisimple and finite dimensional. In what follows, we recall some terms about $T$-modules. A subspace $W \subseteq V$ is called $T$-module if $YW \subseteq W$ for all $Y \in T$. $W$ is said to be irreducible whenever $W \neq 0$ and $W$ contains no $T$-modules besides 0 and $W$. Assume $W$ is an irreducible $T$-module. By the endpoint of $W$ (resp. diameter of $W$), we mean $\min\{ |i| : 0 \leq i \leq D, E_i^*W \neq 0 \}$ (resp. $\min\{ |i| : 0 \leq i \leq D, E_i^*W \neq 0 \} - 1 \}$. $W$ is said to be thin whenever $\text{dim}(E_i^*W) \leq 1$ for all $0 \leq i \leq D$. Note that the standard module $V$ is an orthogonal direct sum of irreducible $T$-modules. By the multiplicity with which $W$ appears in $V$, we mean the number of irreducible $T$-modules in this sum which are isomorphic to $W$. See [3, 4, 9, 10] for more information on the Terwilliger algebra.

**Lemma 2.1.** ([9 Lemma 3.9]) Let $W$ denote an irreducible $T$-module with endpoint $r$ and diameter $d^*$. Then the following (i)–(iii) hold.

(i) $A_i E_i^*W \subseteq E_{i-1}^*W + E_i^*W + E_{i+1}^*W$ ($0 \leq i \leq D$).

(ii) $E_i^*W \neq 0$ if and only if $r \leq i \leq r + d^*$.

(iii) $E_j^* A_i E_i^*W \neq 0$ if $|j - i| = 1$ ($r \leq i, j \leq d^*$).

**Lemma 2.2.** Let $W$ denote a thin irreducible $T$-module with endpoint $r$ and diameter $d^*$. Pick a nonzero vector $\xi_0 \in E_r^*W$, and let $\xi_i = E_{r+i}^* A_i E_{r+i-1}^* A_{r+i-2} \cdots E_{r+1}^* A_1 E_r^* \xi_0$ ($1 \leq i \leq d^*$). Then we have $\xi_i \in E_{r+i}^*W$ and $\xi_i$ is nonzero. Moreover, $\xi_0, \xi_1, \ldots, \xi_{d^*}$ span $W$.

**Proof.** It is easy to see that $\xi_i \in E_{r+i}^*W$. Since $W$ is thin, we have $\text{dim}(E_r^*W) = 1$ for $r \leq i \leq r + d^*$ by Lemma 2.1(ii). Then use Lemma 2.1(iii) to induct on $i$. We can have that...
each $\xi_i$ ($1 \leq i \leq d^*$) is nonzero and hence $\xi_0, \xi_1, \ldots, \xi_{d^*}$ are linearly independent. It follows from $\dim(W) = d^* + 1$ that $W = \text{span}\{\xi_0, \xi_1, \ldots, \xi_{d^*}\}$. \hfill $\square$

At end of this section, we recall some facts from number theory which are useful later.

**Lemma 2.3.** The following (i)--(iii) hold.

(i) The number of nonnegative integer solutions to the equation $x_1 + x_2 + \cdots + x_m = n$ is \(\binom{n+m-1}{m-1}\).

(ii) $\sum_{k=0}^{n} (-1)^{k-m} \binom{k}{m} \binom{n}{k} = \delta_{m,n}$.

(iii) $\sum_{k=0}^{m} (-1)^{m-k} \binom{m}{k} \binom{n-2m+k}{n-i} = \binom{n-2m}{i-m}$.

3 The Terwilliger algebra of $\square_n$

In this section, we give a basis of the Terwilliger algebra of $\square_n$ with $n \geq 6$. We treat two cases of $n$ even and odd separately.

### 3.1 The Terwilliger algebra of $\square_{2D}$

Recall the definition of vertex set $X$ for $n = 2D$ and we can view $X$ as the set consisting of all ordered pairs $(u, u')$ with $|u| < |u'|$ and all unordered pairs $(u, u')$ with $|u| = |u'|$. We give the following notation. To each ordered triple $(x, y, z) \in X \times X \times X$, where $x = (x_1, x_2), y = (y_1, y_2), z = (z_1, z_2)$, we associate the integers three-tuple $(i, j, t)$:

$$\partial(x, y, z) := (i, j, t), \quad \text{where } i := \partial(x, y), \quad j := \partial(x, z),$$

without loss of generality, let $|x_1 \triangle y_1| = i$ and $|x_1 \triangle z_1| = j$. Then

for $0 \leq i, j \leq D - 1$, $t := |(x_1 \triangle y_1) \cap (x_1 \triangle z_1)|$,

for $i = D, 0 \leq j \leq D - 1$, $t := \max\{|(x_1 \triangle y_1) \cap (x_1 \triangle z_1)|, |(x_1 \triangle y_2) \cap (x_1 \triangle z_1)|\}$,

for $0 \leq i \leq D - 1, j = D$, $t := \max\{|(x_1 \triangle y_1) \cap (x_1 \triangle z_1)|, |(x_1 \triangle y_1) \cap (x_1 \triangle z_2)|\}$,

for $i = j = D$, $t := \max\{|(x_1 \triangle y_1) \cap (x_1 \triangle z_1)|, |(x_1 \triangle y_1) \cap (x_1 \triangle z_2)|, |(x_1 \triangle y_2) \cap (x_1 \triangle z_1)|, |(x_1 \triangle y_2) \cap (x_1 \triangle z_2)|\}$

= $\max\{|(x_1 \triangle y_1) \cap (x_1 \triangle z_1)|, |(x_1 \triangle y_1) \cap (x_1 \triangle z_2)|\}$.

Observe that $0 \leq t \leq i, j \leq D$, $t \geq \left\lceil \frac{i+1}{2} \right\rceil$ for $i = D$, and $t \geq \left\lceil \frac{i+1}{2} \right\rceil$ for $j = D$. Note that $\partial(y, z) = \min\{|y_1 \triangle z_1|, |y_2 \triangle z_2|, |y_2 \triangle z_1|\}$. Then by simple calculation, we have that $\partial(y, z) = \min\{i + j - 2t, 2D - (i + j - 2t)\}$ for $0 \leq i, j \leq D - 1$ and $\partial(y, z) = i + j - 2t$ for $i = D$ or $j = D$. The set of three-tuples $(i, j, t)$ that occur as $\partial(x, y, z) = (i, j, t)$ for some $x, y, z \in X$ is given by

$$\mathcal{I} := \{(i, j, t) | 0 \leq t \leq i, j \leq D, i + j - t \leq 2D - 1, t \geq \left\lceil \frac{j+1}{2} \right\rceil \text{ if } i = D \text{ and } t \geq \left\lceil \frac{i+1}{2} \right\rceil \text{ if } j = D\}. \quad \text{(1)}$$

**Proposition 3.1.** We have

$$|\mathcal{I}| = \frac{(D + 1)(D^2 + 2D + 3)}{3}.$$
Proof. Let

\[ i + j - t = l \quad (0 \leq t \leq i, j \leq D, \ 0 \leq l \leq 2D - 2). \tag{2} \]

We divide the proof into three cases.

(i) the case: \(0 \leq l \leq D\). Substitute \(i' := i - t\) and \(j' := i - t\). Then the integer solutions of (2) are in bijection with the integer solutions of

\[ 0 \leq i', j', t \leq D, \ i' + j' + t = l. \tag{3} \]

By Lemma 2.3(i) the number of integer solutions of (3) is \(\binom{l + 2}{2}\) and these solutions satisfy (1).

(ii) the case: \(D + 1 \leq l \leq D + \lfloor \frac{D}{2} \rfloor\). Substitute \(i' := D - i, j' := D - j\) and \(l' := 2D - l\). Then the integer solutions of (2) are in bijection with the integer solutions of

\[ 0 \leq i', j', t \leq D, \ i' + j' + t = l'. \tag{4} \]

The number of integer solutions of (4) is \(\binom{D - l}{2} = \binom{2D - l + 2}{2}\). One easily verifies that when \(i = D\) or \(j = D\) in (2) there are total \(2(l - D)\) integer solutions satisfying (4) but not satisfying (1).

(iii) the case: \(D + \lfloor \frac{D}{2} \rfloor + 1 \leq l \leq 2D - 2\). By the argument similar to the discussion of case (ii), we have that the number of integer solutions satisfying (1) is \(\binom{2D - l + 2}{2} - 2(2D - l) - 1 = \binom{2D - 1}{2}\). Note that when \(i = D\) or \(j = D\) in (2) there are total \(2(2D - l) + 1\) integer solutions not satisfying (1).

Therefore,

\[
|I| = \sum_{l=0}^{D} \binom{l + 2}{2} + \sum_{l=D+1}^{D+\lfloor \frac{D}{2} \rfloor} \left( \binom{2D - l + 2}{2} - 2(l - D) \right) + \sum_{l=D+\lfloor \frac{D}{2} \rfloor + 1}^{2D-2} \binom{2D - l}{2} \\
= \frac{(D + 1)(D + 2)(D + 3)}{6} + \frac{D(D + 1)(D + 2)}{6} - \frac{(D - \lfloor \frac{D}{2} \rfloor)(D - \lfloor \frac{D}{2} \rfloor + 1)(D - \lfloor \frac{D}{2} \rfloor + 2)}{6} \\
- \frac{1}{2}\left(D - \lfloor \frac{D}{2} \rfloor \right)(D - \lfloor \frac{D}{2} \rfloor + 1) + \frac{(D - \lfloor \frac{D}{2} \rfloor - 2)(D - \lfloor \frac{D}{2} \rfloor - 1)(D - \lfloor \frac{D}{2} \rfloor)}{6} \\
= \frac{(D + 1)(D^2 + 2D + 3)}{3}.
\]

\[ \square \]

For each \(i, j, t \in I\), we define

\[ X_{i,j,t} := \{(x, y, z) \in \{X \times X \times X|\partial(x, y, z) = (i, j, t)\}. \tag{5} \]

Denote by \(\text{Aut}(X)\) the automorphism group of \(\square_{2D}\) and \(\text{Aut}_0(X)\) the stabilizer of vertex \(0 := (\emptyset, S)\) in \(\text{Aut}(X)\). The following proposition gives the meaning of \(X_{i,j,t}\), \((i, j, t) \in I\).

Proposition 3.2. The sets \(X_{i,j,t}\), \((i, j, t) \in I\) are the orbits of \(X \times X \times X\) under the action of \(\text{Aut}(X)\).

Proof. By \([2, p. 265]\) the \(\text{Aut}(X)\) is \(2^{2D-1}.\text{sym}(2D)\). Let \(x, y, z \in X\) and let \(\partial(x, y, z) = (i, j, t)\). By the definitions of \(i, j, t\), one easily verifies that \(i, j, t\) are unchanged under any action of \(\sigma \in \text{Aut}(X)\), that is \(\partial(\sigma x, \sigma y, \sigma z) = (i, j, t)\).

To show that \(\text{Aut}(X)\) acts transitively on \(X_{i,j,t}\) for each \((i, j, t) \in I\), it suffices to show that for fixed \(\partial(x', y', z') = (i, j, t)\) if \(\sigma \in \text{Aut}(X)\) ranges over \(\text{Aut}(X)\) then \(\partial(\sigma x', \sigma y', \sigma z')\) ranges over \(X_{i,j,t}\). By permuting on \(X\), we may assume that \(x' = 0\). Then \(\partial(0, y', z') = (i, j, t)\). Since \(\text{Aut}_0(X) = \text{sym}(2D)\), we have that if \(\psi \in \text{Aut}_0(X)\) ranges over the \(\text{Aut}_0(X)\) then \(\partial(\psi y', \psi z')\) ranges over the set \(\{(y, z) \in X \times X|\partial(0, y, z) = (i, j, t)\}\). \[\square\]
The action of Aut($X$) on $X \times X \times X$ induces an action of Aut$_0$($X$) on $\{0\} \times X \times X$. Thus we define

$$X^0_{i,j,t} := \{(x, y) \in X \times X | \partial(0, x, y) = (i, j, t)\}.$$ 

Observe that $(x, y) \in X^0_{i,j,t}$ is equivalent to $|x_1| = i, |y_1| = j$ and $t = |x_1 \cap y_1|$ when $0 \leq i, j \leq D - 1$, $t = \max\{|x_1 \cap y_1|, |x_2 \cap y_1|\}$ when $i = D, 0 \leq j \leq D - 1$, $t = \max\{|x_1 \cap y_1|, |x_1 \cap y_2|\}$ when $0 \leq i \leq D - 1, j = D$, $t = \max\{|x_1 \cap y_1|, |x_1 \cap y_2|, |x_2 \cap y_1|\}$ when $i = j = D$.

**Proposition 3.3.** The sets $X^0_{i,j,t}$, $(i, j, t) \in I$ are the orbits of $X \times X$ under the action of Aut$_0$($X$).

**Proof.** Immediate from Proposition 3.2. \qed

**Definition 3.4.** For each $(i, j, t) \in I$, define the matrix $M^t_{i,j} \in \text{Mat}_X(\mathbb{C})$ by

$$ (M^t_{i,j})_{xy} = \begin{cases} 1 & \text{if } (x, y) \in X^0_{i,j,t}, \\ 0 & \text{otherwise} \end{cases} \quad (x, y \in X).$$

Note that the transpose of $M^t_{i,j}$ is $M^t_{j,i}$. Let $\mathcal{A}$ be the linear space spanned by the matrices $M^t_{i,j}$, $(i, j, t) \in I$. It is easy to check that $\mathcal{A}$ is closed under addition, scalar, taking the adjoint and matrix multiplication which is implied by Proposition 3.3. Therefore $\mathcal{A}$ is a matrix $\mathbb{C}$-algebra with the basis $M^t_{i,j}$. Next, we show that $\mathcal{A}$ coincides with $T$, where $T := T(0)$ is the Terwilliger algebra of $\square_2 D$. To do this, we need the following propositions. Let $A_1$ and $E^*_i = E^*_i(0)$ $(0 \leq i \leq D)$ denote the adjacency matrix and the $i$th dual idempotent, respectively.

**Proposition 3.5.** With Definition 3.4, we have

(i) $M^t_{i,i} = E^*_i(0) \quad (0 \leq i \leq D)$;

(ii) $M^{-1}_{i-1,i} = E^*_{i-1} A_1 E^*_i$, $M^{-1}_{i,i-1} = E^*_i A_1 E^*_{i-1} \quad (0 \leq i \leq D)$.

**Proof.** (i) It follows from that the $(x, y)$-entry of $M^t_{i,i}$ is 1 if $x = y$, $|x_1| = i$ and 0 otherwise.

(ii) Consider the $(x, y)$-entry of both $M^{-1}_{i-1,i}$ and $E^*_{i-1} A_1 E^*_i$. For $0 \leq i \leq D - 1$, we have $(M^{-1}_{i-1,i})_{xy} = (E^*_{i-1} A_1 E^*_i)_{xy} = 1$ if $|x_1| = i - 1, |y_1| = i, |x_1 \cap y_1| = i - 1$ and 0 otherwise. For $i = D$, we have $(M^{-1}_{i-1,i})_{xy} = (E^*_{i-1} A_1 E^*_i)_{xy} = 1$ if $|x_1| = D - 1, |y_1| = |y_2| = D$, $\max\{|x_1 \cap y_1|, |x_1 \cap y_2|\} = D - 1$ and 0 otherwise. \qed

**Proposition 3.6.** With Definition 3.4, we have

(i) $M^k_{k+i,k} = \frac{1}{n} M^k_{k+i+i, k+i-1} \cdots M^k_{k+2,k+1} M^k_{k+1,k} \quad (k \neq 0, i \geq 0) \text{ or } (k = 0, 1 \leq i \leq D - 1)$;

(ii) $M^0_{D,0} = \frac{1}{2D^2} M^{D-1}_{D,D-1} \cdots M^1_{2,1} M^0_{1,0}$;

(iii) $M^k_{k+i,k} = \frac{n}{n} M^k_{k+i-i, k+i+i, k+i-1} \cdots M^k_{k+1,k} \quad (1 \leq i < k \leq D) \text{ or } (1 \leq i = k \leq D - 1)$.

**Proof.** (i) It is easy to verify $M^k_{k+i, k+i+1} M^k_{k+i+1, k+1} = 2M^k_{k+i, k+i+1}$ since the entry of this matrix in position $(x, y)$, with $|x_1| = k + 2$ and $|y_1| = k$, is equal to $|z_1| = k + 1, y_1 \subseteq z_1 \subseteq x_1|$ if $k + 2 < D$ or $|z_1| = k + 1, y_1 \subseteq z_1 \subseteq x_1$ or $y_1 \subseteq z_1 \subseteq x_2$ if $k + 2 = D$. Then by induction on $i$ ($(k \neq 0, i \geq 1)$ or $(k = 0, 1 \leq i \leq D - 1)$) we can obtain the desired result.

(ii) By use of (i), we first have $M^{D-2}_{D,D-2} \cdots M^0_{1,0} = (D - 1)! M^{D-1}_{D-1,0}$. Then we have $M^{D-1}_{D,D-1} M^0_{D,0} = 2D M^0_{D,0}$ since the entry of this matrix in position $(x, y)$, with $|x_1| = |x_2| = D$ and $|y_1| = 0$, is equal to $|z_1| = D - 1, z_1 \subseteq x_1$ or $z_1 \subseteq x_2$ $|z_1| = 2D$.

(iii) By taking transpose of both sides of (i) and replacing $k$ by $k - i$, we can obtain the desired result. \qed
Proposition 3.7. With Definition 3.4, we have

(i) for $0 \leq i, j \leq D - 1$,
$$M^t_{i,j} = \sum_{k=0}^{D-1} (-1)^{k-t} \binom{k}{t} M^k_{i,k} M^k_{k,j};$$

(ii) for $i = D, 0 \leq j \leq D - 1$ and $t \geq \left\lfloor \frac{j}{2} \right\rfloor + 1$,
$$M^t_{D,j} = \sum_{k=\left\lfloor \frac{j}{2} \right\rfloor + 1}^{D-1} (-1)^{k-t} \binom{k}{t} M^k_{D,k} M^k_{k,j};$$

(iii) for $i = D, 0 \leq j \leq D - 1$ and $t = \frac{j}{2}$ ($j$ even),
$$M^\frac{j}{2}_{D,j} = \frac{1}{2} \sum_{k=\frac{j}{2}}^{D-1} (-1)^{k-\frac{j}{2}} \binom{k}{\frac{j}{2}} M^k_{D,k} M^k_{k,j};$$

(iv) for $0 \leq i \leq D - 1, j = D$ and $t \geq \left\lfloor \frac{D}{2} \right\rfloor + 1$,
$$M^t_{i,D} = \sum_{k=\left\lfloor \frac{D}{2} \right\rfloor + 1}^{D-1} (-1)^{k-t} \binom{k}{t} M^k_{i,k} M^k_{k,D};$$

(v) for $0 \leq i \leq D - 1, j = D$ and $t = \frac{D}{2}$ ($i$ even),
$$M^\frac{D}{2}_{i,D} = \frac{1}{2} \sum_{k=\frac{D}{2}}^{D-1} (-1)^{k-\frac{D}{2}} \binom{k}{\frac{D}{2}} M^k_{i,k} M^k_{k,D};$$

(vi) for $i = j = D$ and $t \geq \left\lfloor \frac{D}{2} \right\rfloor + 1$,
$$M^t_{D,D} = \frac{1}{2} \left( \sum_{k=\left\lfloor \frac{D}{2} \right\rfloor + 1}^{D} (-1)^{k-t} \binom{k}{t} M^k_{D,k} M^k_{k,D} + (-1)^{D-t} \binom{D}{t} M^D_{D,D} \right);$$

(vii) for $i = j = D$ and $t = \frac{D}{2}$ ($D$ even),
$$M^{\frac{D}{2}}_{D,D} = \frac{1}{4} \left( \sum_{k=\frac{D}{2}}^{D} (-1)^{k-\frac{D}{2}} \binom{k}{\frac{D}{2}} M^k_{D,k} M^k_{k,D} + (-1)^{D-t} \binom{D}{\frac{D}{2}} M^D_{D,D} \right).$$

Proof. (i) For $0 \leq i, j \leq D - 1$, we have $M^k_{i,k} M^k_{k,j} = \sum_{l=0}^{D-1} \binom{l}{k} M^l_{ij}$, since the entry of this matrix in position $(x, y)$, with $|x_1| = i$ and $|y_1| = j$, is equal to $|\{z \in X||z_1| = k, z_1 \subseteq (x_1 \cap y_1)\}|$. It follows from Lemma 2.3(ii) that
$$\sum_{k=0}^{D-1} (-1)^{k-t} \binom{k}{t} M^k_{i,k} M^k_{k,j} = \sum_{k=0}^{D-1} (-1)^{k-t} \binom{k}{t} \sum_{l=0}^{D-1} \binom{l}{k} M^l_{ij},$$
$$= \sum_{l=0}^{D-1} \delta_{t,t} M^l_{ij},$$
$$= M^t_{i,j}.$$
For cases (ii)-(vii), the proofs are similar to that of (i). Note that for \(0 \leq j \leq D - 1\), \(M_{D,k}^j M_{k,D}^j = \sum_{d=0}^{D-1} \left( \binom{d}{i} + \binom{D-i}{k} \right) M_{D,j}^d (l \geq \frac{D+j}{2})\) since the entry of this matrix in position \((x,y)\), with \(|x_1| = |x_2| = D\) and \(|y_1| = j\), is equal to \(|\{ z \in X | z_1 = k, z_1 \subseteq (x_1 \cap y_1) \text{ or } z_1 \subseteq (x_2 \cap y_1) \}|\); for \(1 \leq k \leq D\), \(M_{D,k}^j M_{k,D}^j = \sum_{d=0}^{D-1} \left( \binom{d}{i} + \binom{D-i}{k} \right) M_{D,D}^d (l \geq \frac{D+j+1}{2})\) since the entry of this matrix in position \((x,y)\), with \(|x_1| = |x_2| = D\) and \(|y_1| = |y_2| = D\), is equal to \(|\{ z \in X | z_1 = k, z_1 \subseteq (x_1 \cap y_1) \text{ or } z_1 \subseteq (x_2 \cap y_1) \}|\).

**Theorem 3.8.** For \(\Box_{2D}\), the algebras \(A\) and \(T\) coincide.

**Proof.** On the one hand, we have \(T \subseteq A\) since \(A_1 = \sum_{i=1}^{D} (M_{i,i-1}^{-1} + M_{i-1,i}^{-1})\) and \(E_i^* = M_{i,i}^{-1}\) \((0 \leq i \leq D)\) by Proposition 3.9, 3.7. On the other hand, by Propositions 3.9, 3.7 we have \(A \subseteq T\) since each \(M_{ij}^* \in T\) for \((i,j,t) \in T\). So the algebras \(A\) and \(T\) coincide.

### 3.2 The Terwilliger algebra of \(\Box_{2D+1}\)

Recall the definition of \(X\) for \(n = 2D + 1\) and we view \(X\) as the set consisting of all ordered pairs \((u,u')\) with \(|u| < |u'|\). To each ordered triple \((x,y,z) \in X \times X \times X\), we define \(\partial(x,y,z) = (i,j,t)\) where \(i = \partial(x,y), j = \partial(y,z)\), without loss of generality, let \(|x_1 \cap y_1| = i\) and \(|x_1 \cap z_1| = j\). Then \(t = ||(x_1 \cap y_1) \cap (x_1 \cap z_1)|\).

Observe that \(0 \leq t \leq i,j \leq D\) and \(\partial(y,z) = \min\{i + j - 2t, 2D + 1 - (i + j - 2t)\}\). The set of such tuples \((i,j,t)\), that occur as \(\partial(x,y,z) = (i,j,t)\) for some \(x,y,z \in X\), is given by \(T' := \{(i,j,t)|0 \leq t \leq i,j \leq D, i + j - t \leq 2D\}\).

**Proposition 3.9.** We have \(|T'| = \frac{(D+1)(D+2)(2D+3)}{6}\).

**Proof.** Similar to the proof of Proposition 3.1(i), (ii): \(|T'| = \sum_{i=0}^{D} \binom{i+2}{2} + \sum_{i=D+1}^{2D} \binom{2D-i+2}{2}\).

For each \((i,j,t) \in T'\), define the sets \(X_{i,j,t}\) and \(X_{i,j,t}^0\) as in Subsection 3.1. Note that \(X_{i,j,t}^0 = \{(x,y) \in X \times X | x_1 = i, |y_1| = j, |x_1 \cap y_1| = t\}\). Similar to the proof of Proposition 3.2 we have the following proposition.

**Proposition 3.10.** The sets \(X_{i,j,t}\) \((i,j,t) \in T'\) are the orbits of \(X \times X \times X\) under the action of \(\text{Aut}(X)\), where \(\text{Aut}(X)\) is the automorphism group of \(\Box_{2D+1}\). The sets \(X_{i,j,t}^0\) \((i,j,t) \in T'\) are the orbits of \(X \times X\) under the action of \(\text{Aut}_0(X)\), where \(\text{Aut}_0(X)\) is the stabilizer of vertex 0 in \(\text{Aut}(X)\).

**Definition 3.11.** For each \((i,j,t) \in T'\), define the matrix \(M_{i,j}^t \in \text{Mat}_X(C)\) by

\[
(M_{i,j}^t)_{xy} = \begin{cases} 
1 & \text{ if } (x,y) \in X_{i,j,t}^0, \\
0 & \text{ otherwise, } (x,y) \in X.
\end{cases}
\]

Let \(A'\) be the linear space spanned by the matrices \(M_{i,j}^t\) \((i,j,t) \in T'\). It is easy to check that \(A'\) is a matrix \(C^*\)-algebra with the basis \(M_{i,j}^t\), \((i,j,t) \in T'\). We next show \(A'\) coincides with \(T\), where \(T := T(0)\) is the Terwilliger algebra of \(\Box_{2D+1}\). Let \(A_1\) and \(E_i^* = E_i^*(0)\) be the adjacency matrix and the ith dual idempotent of \(\Box_{2D+1}\), respectively.

**Proposition 3.12.** With Definition 3.11 we have

(i) \(M_{i,i}^t = E_i^*\) \((0 \leq i \leq D)\);

(ii) \(M_{i-1,i}^{-1} = E_{i-1}^* A_i E_i^*\), \(M_{i,i-1}^{-1} = E_i^* A_i E_{i-1}^*\) \((0 \leq i \leq D)\);

(iii) \(M_{k+i,k}^k = \frac{1}{D} M_{k+i,k+i-1} M_{k+i-1,k+i-2} \cdots M_{k+1,k} (1 \leq i \leq D - k)\).
(iv) $M_{k-i,k}^i = \frac{1}{n} M_{k,i+1,k-1}^{i+1} M_{k-1,k-1,k-2}^{i+1} \cdots M_{k-1,k-1}^1 (1 \leq i \leq k)$;

(v) $M_{i,j}^k = \sum_{k=0}^{D} (-1)^{k-t} \binom{k}{t} M_{i,k} M_{k,j}^D$.

Proof. Similar to the proofs of Propositions 3.5, 3.6 and 3.7(i).

Theorem 3.13. For $\Box_{2D+1}$, the algebras $\mathcal{A}$ and $T$ coincide.

Proof. Similar to the proof of Theorem 3.8. Note that $A_1 = \sum_{i=1}^{D} (M_{i,i-1}^{-1} + M_{i-1,i}^{-1}) + M_{D,D}^0$.

4 Block diagonalization of $T$ of $\Box_n$

In this section, we study a block-diagonalization of $T$ of $\Box_n$ by using the theory of irreducible $T$-modules together with the obtained basis in Section 3. We treat two cases of $n$ even and odd separately.

4.1 Block diagonalization of $T$ of $\Box_{2D}$

Proposition 4.1. For $\Box_{2D}$, let $W$ denote an irreducible $T$-module with endpoint $r$ and diameter $d^*$ ($0 \leq r, d^* \leq D$). Then $W$ is thin, $r + d^* = D$ (even) or $r + d^* = D - 1$ (odd), and the isomorphism class of $W$ is determined only by $r$.

Proof. See [3] Lemma 9.2, Theorem 13.1 and [10] pp. 204–205]. Note that the endpoint here is denoted by dual endpoint in $\Box_n$.

Based on Definition 3.3 and Proposition 4.1 for $r = 0, 1, \ldots, D$ define the linear vector space $L_r$ as follows.

$$L_r := \{ \xi \in V := \mathbb{C}^X | M_{r-r}^{-1} \xi = 0, \xi(x_1,x_2) = 0 \text{ if } |x_1| \neq r \}.$$ 

The space $L_r$ is in fact connected to the irreducible $T$-modules. For discusional convenience, denote by $W_r$ ($0 \leq r \leq D$) the $T$-module spanned by all the irreducible $T$-modules with endpoint $r$, and define $W_r := 0$ if there does not exist such irreducible $T$-module.

Proposition 4.2. For $\Box_{2D}$, let $W$ denote an irreducible $T$-module with endpoint $r$, diameter $d^*$ ($0 \leq r, d^* \leq D$) and let $W_r$ be defined as above. Then the following (i)–(iv) hold.

(i) $L_r = E_r^r W_r$.

(ii) Up to isomorphism, $W_r$ is $(\frac{2D}{r}) - (\frac{2D}{r-1})$ copies of $W$ for $0 \leq r \leq D - 1$; $W_D$ is $\frac{1}{2} (\frac{2D}{D}) - \frac{D-1}{2D} (\frac{2D}{D-1})$ copies of $W$ for $r = D$ (D even); $W_D = 0$ for $r = D$ (D odd).

(iii) Pick any $0 \neq \xi \in L_r$, then $0 \neq M_{r+i,r}^i \xi \in E_{r+i}^r W_r$ for $0 \leq i \leq d^*$.

(iv) Pick any $0 \neq \xi \in L_r$, then $M_{r-i,r}^{-i} \xi = 0$ for $1 \leq i \leq r$.

Proof. (i) We suppose $L_r \neq 0$ and $W_r \neq 0$. It is easy to see that $0 \neq \xi \in L_r$ if and only if $E_r^r \xi \neq 0, E_r^r \xi = 0 (i \neq r)$ and $E_{r-1}^r A_1 E_r^r \xi = 0$. Pick any $0 \neq \xi' \in E_r^r W_r$. We have $\xi' \in L_r$ since $E_r^r \xi' \neq 0, E_r^r \xi' = 0 (i \neq r)$ and $E_{r-1}^r A_1 E_r^r \xi' \in E_{r-1}^r (E_{r-1}^r W_r + E_r^r W_r + E_{r+1}^r W_r) = 0$, which is from Lemma 2.1(i),(ii). Thus $E_r^r W_r \subseteq L_r$. Conversely, pick any $0 \neq \xi \in L_r$. By $E_r^r \xi' \neq 0$ and $E_r^r \xi' = 0 (i \neq r)$, we have $\xi' \in E_r^r V$. Then by $E_{r-1}^r A_1 E_r^r \xi' = 0$ and Lemma 2.1(i),(iii), we have $\xi' \in E_r^r W_r$ since $V$ is the orthogonal direct sum of $W_0 + W_1 + \cdots + W_D$. Thus $L_r \subseteq E_r^r W_r$.

(ii) To prove this claim, it suffices to give the multiplicity of $W$ since the isomorphism class
Applying $E^*_r$ $(0 \leq r \leq D)$ to the both sides of (6), we obtain $\dim(E^*_r V) = \sum_{h=0}^n \dim(E^*_h W_h)$.

(ii) For $0 \leq r \leq D-1$, by Proposition 4.1 we know that for each $h$ $(0 \leq h \leq n)$, $\dim(E^*_h W_h) = 1$ if the endpoint of $W_h$ is at most $r$, and $\dim(E^*_h W_h) = 0$ if the endpoint of $W_h$ is greater than $r$. Moreover, for every $\rho$ $(0 \leq \rho \leq D)$, there exist exactly $m(\rho, d_\rho)$ modules in (6) with endpoint $\rho$ and diameter $d_\rho$, where $m(\rho, d_\rho)$ denotes the multiplicity of the module with endpoint $\rho$ and diameter $d_\rho$. Thus we have

$$\dim(E^*_r V) = \sum_{\rho \leq r} m(\rho, d_\rho),$$

which implies

$$m(r, d^*) = \dim(E^*_r V) - \dim(E^*_{r-1} V) = \binom{2D}{r} - \binom{2D}{r-1}. \quad \text{(by [2, p. 264] and [1, p. 195])}$$

(iib) For $r = D$, it is easy to see $m(D, 0) = 0$ if $D$ is odd. Now, we suppose that $D$ is even. Similar to obtaining (7), we have $\dim(E^*_D V) = \sum_{\rho \in \text{even}} m(\rho, D-\rho)$. So

$$m(D, 0) = \dim(E^*_D V) - (m(0, D) + m(2, D-2) + \cdots + m(D-2, 2)) = \frac{1}{2} \binom{2D}{D} - \frac{D-1}{2D} \binom{2D}{D-1}.$$

(iii) Immediate from above (i), Proposition 3.6(ii) and Lemma 2.1(ii).

(iv) Immediate from above (i), Proposition 4.1(ii) and Lemma 2.2(ii).

**Corollary 4.3.** For $\square_{2D}$, the following (i), (ii) hold.

(i) For $0 \leq r \leq D-1$, $\dim(L_r) = \binom{2D}{r} - \binom{2D}{r-1}$.

(ii) For $r = D$, $\dim(L_D) = \left\{ \begin{array}{ll} \frac{1}{2} \binom{2D}{D} - \frac{D-1}{2D} \binom{2D}{D-1} & \text{if } D \text{ is even} \\ 0 & \text{if } D \text{ is odd} \end{array} \right.$

**Proof.** Immediate from Proposition 4.2(ii), (i). □

Propositions 4.1, 4.2 and Corollary 4.3 imply the block sizes and block multiplicity of $T$. To describe this block diagonalization, we need consider the action of matrices $M^t_{i,j}$, $(i, j, t) \in I$ on $M^r_{j, r, \xi}$, where $0 \neq \xi \in \mathcal{L}_r$ $(0 \leq r \leq D)$.

**Proposition 4.4.** For all $(i, j, t) \in I$, $r \in \{0, 1, \ldots, D\}$ and for $\xi \in \mathcal{L}_r$, we have

(i) for $0 \leq i, j \leq D-1$,

$$\binom{2D-2r}{i-r} M^t_{i,j} M^r_{j, r, \xi} = \beta^r_{i,j,t} M^r_{i, r, \xi},$$

where $\beta^r_{i,j,t} = \binom{2D-2r}{i-r} \sum_{l=0}^{D-1} (-1)^{r-l} \binom{r-l}{i-l} (2D-2r+l)$;
(ii) For \( i = D, 0 \leq j \leq D - 1 \),

\[
2 \left( \frac{2D - 2r}{D - r} \right) M_{D,j}^r \xi = \beta_{D,i}^r M_{D,j}^r \xi,
\]

where \( \beta_{D,i}^r = 2 \left( \frac{2D - 2r}{D - r} \right) \left( \sum_{l=0}^{D-1} (-1)^{r-l} \binom{l}{i} \left( \binom{D-r}{i} \right) \left( \binom{D-r+i}{j} \right) + \left( \binom{D-r}{i} \right) \left( \binom{D-r+i}{j} \right) \right) \).

(iii) For \( 0 \leq i \leq D - 1, j = D \),

\[
2 \left( \frac{2D - 2r}{D - r} \right) M_{i,D}^r \xi = \beta_{i,D}^r M_{i,D}^r \xi,
\]

where \( \beta_{i,D}^r = 2 \left( \frac{2D - 2r}{D - r} \right) \left( \sum_{i=0}^{D-1} (-1)^{r-l} \binom{l}{i} \left( \binom{2D-r-i+l}{D} \right) \right) \) + 2(-1)^r \delta \binom{D-r+i}{j} \).

(iv) For \( i = j = D \) and \( 0 \leq r \leq D - 1, \)

\[
2 \left( \frac{2D - 2r}{D - r} \right) M_{D,D}^r \xi = \beta_{D,D}^r M_{D,D}^r \xi,
\]

where \( \beta_{D,D}^r = 2 \left( \frac{2D - 2r}{D - r} \right) \left( \sum_{i=0}^{D-1} (-1)^{r-l} \binom{l}{i} \left( \binom{D-r-i+l}{D} \right) \right) \) + 2(-1)^r \delta \binom{D-r+i}{j} \).

(v) For \( i = j = D \) and \( r = D \) (\( D \) is even),

\[
M_{D,D}^r \xi = \beta_{D,D}^r \xi,
\]

where \( \beta_{D,D}^r = (-1)^{r-l} \binom{D}{i} \) if \( t \geq \frac{D}{2} + 1 \) and \( \beta_{D,D}^r = \frac{1}{2}(-1)^{l} \binom{D}{l} \) if \( t = \frac{D}{2} \).

**Proof.** (i) For \( 0 \leq i, j \leq D - 1 \), we first have \( M_{i,j}^r \xi = \sum_{l=0}^{D-1} (-1)^{r-l} \binom{l}{i} \binom{2D-r-i+l}{j} M_{i,D}^r \xi \). Then by Propositions 3.7(i) and 4.2(iv), we have \( M_{i,r}^r \xi = (-1)^{r-l} \binom{l}{i} M_{i,r}^r \xi \). So

\[
M_{i,j}^r \xi = \sum_{l=0}^{D-1} (-1)^{r-l} \binom{l}{i} \binom{2D-r-i+l}{j} M_{i,D}^r \xi.
\]

For cases (ii)–(iv), by the argument similar to proof of case (i) we can obtain the desired results. (v) is immediate from Proposition 3.7(vi), (vii). Note that \( M_{D,D}^D \xi = \xi \). □

In the following, we describe a block-diagonalization of \( T \) of \( \square_{2D} \). We first consider the case \( D \) even.

### 4.1.1 Block diagonalization of \( T \) of \( \square_{2D} \) with even \( D \)

In this subsection, we suppose \( D > 3 \) is even. Based on Propositions 4.1, 4.2 and Corollary 4.3 for each \( r = 0, 1, \ldots, D \) denote by \( B_r \) the set of an orthonormal basis of \( \mathcal{L}_r \) and let

\[
\mathcal{B}_1 \{ (r, \xi, i) | r = 0, 1, \ldots, D, \xi \in B_r, i = r, r + 1, \ldots, D \text{ for even } r \}
\]

\[
i = r, r + 1, \ldots, D - 1 \text{ for odd } r \}.
\]

It is not difficult to calculate

\[
|\mathcal{B}_1| = \sum_{r=0}^{D-2} (D - r + 1) \left( \binom{2D}{r} - \binom{2D}{r-1} \right) + \frac{1}{2} \binom{2D}{D} - \frac{D-1}{2D} \binom{2D}{D-1}
\]

\[
+ \sum_{r=1}^{D-1} (D-r) \left( \binom{2D}{r} - \binom{2D}{r-1} \right) = 2^{2D-1}.
\]

(8)
For each \((r, \xi, i) \in B_1\), define the vector \(u_{r,\xi,i} \in V\) by

\[
\begin{align*}
\forall & \leq i \leq D - 1, \\
\end{align*}
\]

\[
\begin{align*}
u_{r,\xi,i} := \left(2D - 2r\right)^{-\frac{1}{2}} M_{r,i}^r \xi \quad (r \leq i \leq D - 1),
\end{align*}
\]

\[
\begin{align*}
u_{r,\xi,D} := \sqrt{2} \left(2D - 2r\right)^{-\frac{1}{2}} M_{r,D}^r \xi \quad (i = D \text{ and } 0 \leq r < D \text{ even}),
\end{align*}
\]

\[
\begin{align*}
u_{D,\xi,D} := \xi \quad (i = r = D).
\end{align*}
\]

**Proposition 4.5.** The vectors \(u_{r,\xi,i}, (r, \xi, i) \in B_1\) form an orthonormal basis of the standard module \(V\).

**Proof.** For \(r \leq i \leq D - 1\),

\[
\begin{align*}
\xi^T M_{r,i}^r M_{r,i}^r \xi &= \sum_{l=0}^{r} \left(2D - 2r + l\right)^{\frac{1}{2}} \left(i - 2r + l\right)^{-\frac{1}{2}} \xi^T M_{r,i}^r \xi \\
&= \sum_{l=0}^{r} \left(2D - 2r + l\right)(-1)^{r-l} \left(i\right)^{\frac{1}{2}} \xi^T \xi \quad \text{(by Propositions 3.7(i) and 4.2(iv))} \\
&= \left(2D - 2r\right)^{-\frac{1}{2}} \xi^T \xi; \quad \text{(by Lemma 2.3(iii))}
\end{align*}
\]

For \(i = D\),

\[
\begin{align*}
\xi^T M_{r,D}^r M_{r,D}^r \xi &= \sum_{l=0}^{r} \left(2D - 2r + l\right)^{\frac{1}{2}} \left(D - 2r + l\right)^{-\frac{1}{2}} \xi^T M_{r,D}^r \xi + \left(2D - 2r\right)^{\frac{1}{2}} \xi^T M_{r,D}^r \xi \\
&= 2 \left(2D - 2r\right)^{-\frac{1}{2}} \xi^T \xi. \quad \text{(by Propositions 3.7(i), 4.2(iv), Lemma 2.3(iii))}
\end{align*}
\]

It follows that \(u_{r,\xi,i}, (r, \xi, i) \in B_1\) are normal. Next, we show that \(u_{r,\xi,i}\) is pairwise orthogonal. By Proposition 4.2(i), (iii), the vectors \(u_{r,\xi,i}\) and \(u_{r',\xi,j'}\) are orthogonal if \(r \neq r'\) or \(i \neq i'\). One can easily verify that \(u_{r,\xi,i}\) and \(u_{r',\xi,j'}\) are also orthogonal if \(r = r', i = i', \xi \neq \xi'\) by the argument similar to the proof of normality since \(\xi^T \xi' = 0\).

Let \(U_1\) be the \(X \times B_1\) matrix with \(u_{r,\xi,i}\) as the \((r, \xi, i)\)-th column. For each triple \((i, j, t) \in I\), define the matrix \(M_{i,j} := U_1^T M_{i,j} U_1\). The following proposition shows that \(M_{i,j}\) is in block diagonal form.

**Proposition 4.6.** For \((i, j, t) \in I\) and \((r, \xi, i')\), \((r', \xi', j') \in B_1\), the following (i)–(iv) hold.

(i) For \(0 \leq i, j \leq D - 1\),

\[
\begin{align*}
\left(M_{i,j}_{r,\xi,i''),(r',\xi',j'')\right) &= \left\{
\begin{align*}
\left(2D - 2r\right)^{-\frac{1}{2}} \left(2D - 2r\right)^{-\frac{1}{2}} \beta_{i,j,t}' & \text{if } r = r', \xi = \xi', i = i', j = j', \\
0 & \text{otherwise}.
\end{align*}
\right.
\end{align*}
\]

(ii) For \(i = D, 0 \leq j \leq D - 1\),

\[
\begin{align*}
\left(M_{D,j}_{r,\xi,i''),(r',\xi',j'')\right) &= \left\{
\begin{align*}
\sqrt{2} \left(2D - 2r\right)^{-\frac{1}{2}} \left(2D - 2r\right)^{-\frac{1}{2}} \beta_{D,j,t}' & \text{if } r = r', \xi = \xi', i = D, j = j', \\
0 & \text{otherwise}.
\end{align*}
\right.
\end{align*}
\]

(iii) For \(0 \leq i \leq D - 1, j = D\),

\[
\begin{align*}
\left(M_{i,D}_{r,\xi,i''),(r',\xi',j'')\right) &= \left\{
\begin{align*}
\sqrt{2} \left(2D - 2r\right)^{-\frac{1}{2}} \left(2D - 2r\right)^{-\frac{1}{2}} \beta_{i,D,t}' & \text{if } r = r', \xi = \xi', i = i', j' = D, \\
0 & \text{otherwise}.
\end{align*}
\right.
\end{align*}
\]

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(iv) For \( i = j = D \) and \( 0 \leq r \leq D - 1 \),
\[
(\widetilde{M}_{D,D}^t)_{(r,\xi,j),(r',\xi',j')} = \begin{cases} \frac{1}{2}(2D-2r)^{-1} \beta_{D,D,t} \beta_{D,D,t}^{-1} & \text{if } r = r', \xi = \xi', i' = j' = D, \\ 0 & \text{otherwise.} \end{cases}
\]

(v) For \( i = j = D \) and \( r = D \),
\[
(\widetilde{M}_{D,D}^t)_{(r,\xi,j),(r',\xi',j')} = \begin{cases} \beta_{D,D,t} & \text{if } r = r' = D, \xi = \xi', i' = j' = D, \\ 0 & \text{otherwise.} \end{cases}
\]

Note that the numbers \( \beta_{i,j,t} \) are from Proposition 4.4 and \( r \) is even in (ii)–(v).

Proof. (i) For \( 0 \leq i, j \leq D - 1 \), it is clear that \( (\widetilde{M}_{i,j}^t)_{(r,\xi,j),(r',\xi',j')} = u_{r,j,i}^\top M_{i,j}^t u_{r',\xi,j'} \). By (ii), we have
\[
M_{i,j}^t u_{r',\xi,j'} = \left( 2D - 2r' \right)^{-\frac{1}{2}} M_{i,j}^t M_{r',r}^t
\]
\[
= \delta_{j,j'}\left( 2D - 2r' \right)^{-\frac{1}{2}} \left( 2D - 2r' \right)^{-1} \beta_{i,j,t} \beta_{i,j,t}^{-1} \quad \text{(by Proposition 4.3(1))}
\]
\[
= \delta_{j,j'}\left( 2D - 2r' \right)^{-\frac{1}{2}} \left( 2D - 2r' \right)^{-\frac{1}{2}} \beta_{i,j,t} u_{r',\xi,j'}
\]
from which (i) follows.

The proofs of (ii)–(v) are similar to that of (i).

Proposition 4.6 implies that each matrix \( \widetilde{M}_{i,j}^t \), \( (i,j,t) \in I \) has a block diagonal form: for each even \( 0 \leq r \leq D - 1 \) there are \( (2D) - (\frac{2D}{r-1}) \) copies of a \( (D + 1 - r) \times (D + 1 - r) \) block on the diagonal; for each odd \( 0 \leq r \leq D - 1 \) there are \( (\frac{2D}{r}) - (\frac{2D}{r-1}) \) copies of a \( (D - r) \times (D - r) \) block on the diagonal; for \( r = D \) there are \( \frac{2D}{2(r-1)} \) copies of a \( 1 \times 1 \) block on the diagonal. For each \( r \) the copies are indexed by the elements of \( B_r \), and in each copy the rows and columns are indexed by the integers \( i \in \{ r, r + 1, \ldots, D \} \) (even) or \( i \in \{ r, r + 1, \ldots, D - 1 \} \) (odd). Thus by deleting copies of blocks and using the identity
\[
\sum_{r=0}^{D-1} (D - r + 1)^2 + \sum_{r=1}^{D-1} (D - r)^2 = \frac{(D+1)(D^2+2D+3)}{3}
\]
we have the following theorem.

**Theorem 4.7.** For \( \square_{2D} \) with even \( D > 3 \), the above matrix \( U_1 \) gives a block-diagonalization of \( T \) and \( T \) is isomorphic to \( \mathbb{C}^{D+1 \times N_r} \) where \( N_r := \{ r, r + 1, \ldots, D \} \) (even) or \( N_r := \{ r, r + 1, \ldots, D - 1 \} \) (odd).

### 4.1.2 Block diagonalization of \( T \) of \( \square_{2D} \) with odd \( D \)

In this subsection, we suppose \( D \geq 3 \) is odd. Based on Propositions 4.1 and 4.2 and Corollary 4.3, for each \( r = 0, 1, \ldots, D - 1 \), denote by \( B_r \) the set of an orthonormal basis of \( L_r \) and let
\[
B_2 = \{ (r, \xi, i) | r = 0, 1, \ldots, D - 1, \xi \in B_r, i = r, r + 1, \ldots, D \} \text{ for even } r
\]
\[
i = r, r + 1, \ldots, D - 1 \text{ for odd } r \}
\]
It is not difficult to calculate
\[
|B_2| = \sum_{\substack{r=0 \text{ even} \atop r=1 \text{ odd}}}^{D-1} (D - r + 1) \left( \frac{2D}{r} \right) - \left( \frac{2D}{r-1} \right) + \sum_{r=1}^{D-2} (D - r) \left( \frac{2D}{r} \right) - \left( \frac{2D}{r-1} \right)
\]
\[
= 2^{2D-1}.
\]
For each \((r, \xi, i) \in \mathcal{B}_2\), define the vector \(u_{r, \xi, i} \in V\) by the forms of (9) and (10). One can easily verify that the vectors \(u_{r, \xi, i}\), \((r, \xi, i) \in \mathcal{B}\) form an orthonormal basis of the standard module \(V\). Let \(U_2\) be the \(X \times \mathcal{B}_2\) matrix with \(u_{r, \xi, i}\) as the \((r, \xi, i)\)-th column. It follows from Proposition 4.14(i)–(iv) that for each triple \((i, j, t) \in \mathcal{I}\) the matrix \(M_{i,j}^t := U_2^T M_{i,j}^t U_2\) is in block diagonal form: for each even \(0 \leq r \leq D - 1\) there are \((2^D) - (2^D)\) copies of a \((D + 1 - r) \times (D + 1 - r)\) block on the diagonal; for each odd \(0 \leq r \leq D - 1\) there are \((2^D) - (2^D)\) copies of a \((D - r) \times (D - r)\) block on the diagonal. By deleting copies of blocks and using the identity 
\[
\sum_{r=0}^{D-1} (D - r + 1)^2 + \sum_{r=0}^{D-1} (D - r)^2 = \frac{(D+1)(D^2+2D+3)}{3},
\]
we have the following theorem.

**Theorem 4.8.** For \(\square_{2D}\) with odd \(D \geq 3\), the above matrix \(U_2\) gives a block diagonalization of \(T\) and \(T\) is isomorphic to \(\bigoplus_{r=0}^{D-1} \mathbb{C}^{N_r} \times N_r\), where \(N_r := \{r, r + 1, \ldots, D\}\) (\(r\) even) or \(N_r := \{r, r + 1, \ldots, D - 1\}\) (\(r\) odd).

### 4.2 Block diagonalization of \(T\) of \(\square_{2D+1}\)

**Proposition 4.9.** For \(\square_{2D+1}\) with \(D \geq 2\), let \(W\) denote an irreducible \(T\)-module with endpoint \(r\) and diameter \(d^*\) \((0 \leq r, d^* \leq D)\). Then \(W\) is thin, \(r + d^* = D\) and the isomorphism class of \(W\) is determined only by \(r\).

**Proof.** From [4] we know that \(W\) is thin, \(r + d^* = D\) and the isomorphism class of \(W\) is determined by its dual endpoint and \(d^*\). By [11] pp. 305-306 and [10] p. 196 we have that \(\square_{2D+1}\) is isomorphic to \(\frac{4}{4} H(2D + 1, 2)^{n^*}\). Then it follows from [9] p. 204 that both \(W\)'s dual endpoint and \(d^*\) can be determined by \(r\). \(\Box\)

Based on Definition 3.11 and Proposition 4.9, for \(r = 0, 1, \ldots, D\), define the linear vector space \(\mathcal{L}'_r\) as follows.

\[
\mathcal{L}'_r := \{\xi \in V | M^{-1}_{r+1,i}\xi = 0, \xi(x_1, x_2) = 0 \text{ if } |x_1| \neq r\}.
\]

**Proposition 4.10.** For \(\square_{2D+1}\) with \(D \geq 2\), let \(W\) denote an irreducible \(T\)-module with endpoint \(r\), diameter \(d^*\) \((0 \leq r, d^* \leq D)\) and let \(W_r\) be defined as in Subsection 4.1. Then the following (i)–(iv) hold.

(i) \(\mathcal{L}'_r = E^*_r W_r\).

(ii) Up to isomorphism, \(W_r\) is \((2^D) - (2^D)\) copies of \(W\) for \(0 \leq r \leq D\).

(iii) Pick any \(0 \neq \xi \in \mathcal{L}'_r\), then \(0 \neq M_{r+i,r}\xi \in E^*_r W_r\) for \(0 \leq i \leq d^*\).

(iv) Pick any \(0 \neq \xi \in \mathcal{L}'_r\), then \(M_{r-i,r}\xi = 0\) for \(1 \leq i \leq r\).

**Proof.** Similar to the proof of Proposition 1.2 \(\Box\)

**Corollary 4.11.** We have \(\dim(\mathcal{L}'_r) = \binom{2D+1}{r} - \binom{2D+1}{r-1}\) for \(0 \leq r \leq D\).

**Proposition 4.12.** For all \((i, j, t) \in \mathcal{I}'\), \(r \in \{0, 1, \ldots, D\}\) and for \(\xi \in \mathcal{L}'_r\), we have

\[
\binom{2D + 1 - 2r}{i-r} M_{i,j}^t \xi = \beta^r_{i,j,t} M_{i,r}^t \xi,
\]

where \(\beta^r_{i,j,t} = \binom{2D+1-2r}{i-r} \sum_{l=0}^{D} (-1)^{r-l} \binom{r}{l} \binom{2D+1+1-r}{l} \binom{2D+1+1-r+l}{D}\).

**Proof.** Similar to the proof of Proposition 4.1(i). \(\Box\)
Based on Propositions 4.9, 4.10 and Corollary 4.11 for each \( r = 0, 1, \ldots, D \), denote by \( B'_r \) the set of an orthonormal basis of \( L'_r \) and let \( B' = \{(r, \xi, i)| r = 0, 1, \ldots, D, \xi \in B'_r, i = r, r + 1, \ldots, D\} \). Then it is not difficult to calculate

\[
|B'| = \sum_{r=0}^{D} (D - r + 1) \left( \begin{pmatrix} 2D + 1 \\ r \end{pmatrix} - \begin{pmatrix} 2D + 1 \\ r - 1 \end{pmatrix} \right)
= 2^{2D}. \tag{13}
\]

For each \((r, \xi, i) \in B'\), define the vector \( u_{r, \xi, i} \in \mathbb{C}^X \) by

\[
u_{r, \xi, i} := \left( \begin{pmatrix} 2D + 1 - 2r \\ i - r \end{pmatrix} \right)^{-\frac{1}{2}} M'_{r, i, \xi} \tag{14}\]

The form of \( u_{r, \xi, i} \) is from \( \xi^T M'_{r, i, \xi} = \begin{pmatrix} 2D + 1 - 2r \end{pmatrix}^{\frac{1}{2}} \xi^T \).

By the argument similar to proof of Proposition 4.6, we can easily prove that the vectors \( u_{r, \xi, i}, (r, \xi, i) \in B' \) form an orthonormal basis of the standmodule \( V \). Let \( U' \) be the \( X \times B' \) matrix with \( u_{r, \xi, i} \) as the \((r, \xi, i)\)-th column. For each triple \((i, j, \xi, i') \in I'\) define the martices \( M'_{i, j} := U'^T M'_{i, j} U' \).

**Proposition 4.13.** For \((i, j, \xi, i') \in I'\), \((r, \xi, i) \in B'\),

\[
(M'_{i, j})^{\xi, i'} = \begin{cases} \left( \begin{pmatrix} 2D + 1 - 2r \\ i - r \end{pmatrix} \right)^{-\frac{1}{2}} \left( \begin{pmatrix} 2D + 1 - 2r \\ j - r \end{pmatrix} \right)^{-\frac{1}{2}} \beta_{i, j}^{r, \xi, i'} & \text{if } r = r', \xi = \xi', i = i', j = j', \\ 0 & \text{otherwise}, \end{cases}
\]

where the numbers \( \beta_{i, j}^{r, \xi, i'} \) are from Proposition 4.12.

**Proof.** Similar to the proof of Proposition 4.11. \( \square \)

**Theorem 4.14.** For \( \square_{2D+1} \) with \( D \geq 3 \), the above matrix \( U' \) gives a block-diagonalization of \( T \) and \( T \) is isomorphic to \( \bigoplus_{r=0}^{D} \mathbb{C}^{N_r \times N_r} \), where \( N_r = \{r, r + 1, \ldots, D\} \).

5 Semidefinite programming bound on \( A(\square_n, d) \)

In this section, we give an upper bound on \( A(\square_n, d) \) by semidefinite programming involving the block-diagonalization of \( T \). We treat two cases of \( n \) even and odd separately.

5.1 Semidefinite programming bound on \( A(\square_{2D}, d) \)

Given code \( C \), for each \((i, j, t) \in I\) define the numbers \( \gamma_{i, j}^t := |(C \times C \times C) \cap X_{i, j, t}| \) and numbers \( x_{i, j}^t := |(C \gamma_{i, j}^t)|^{-1} \gamma_{i, j}^t \), where \( \gamma_{i, j}^t \) denotes the number of nonzero entries of \( M'_{i, j} \). Observe that

\[
|C| = \sum_{i=0}^{D} \sum_{j=0}^{D} x_{i, 0} x_{0, j}^t. \tag{15}\]
Define the matrix \( M_C \in \text{Mat}_X(\mathbb{C}) \) by
\[
(M_C)_{xy} = \begin{cases} 
1 & \text{if } x, y \in C, \\
0 & \text{otherwise}.
\end{cases}
\]
Observe that \( M_C = \chi_c\chi_c^T \) is positive semidefinite, where \( \chi_c \) is the characteristic column vector of \( C \). In the following, we define two important matrices by

\[
M' := \frac{1}{|C| |\text{Aut}_0(X)|} \sum_{\sigma \in \text{Aut}(X)} M_{\sigma C}, \quad M'' := \frac{1}{(|X| - |C|) |\text{Aut}_0(X)|} \sum_{\sigma \in \text{Aut}(X)} M_{\sigma C}.
\]

Observe that the matrices \( M' \) and \( M'' \) are positive semidefinite and invariant under any permutation of \( \text{Aut}_0(X) \) of rows and columns, and hence they are in \( T \) by Proposition 3.3.

**Proposition 5.1.** With above notation, we have

(i) \( M' = \sum_{(i,j,t) \in I} x_{i,j} M_{i,j}^t \).

(ii) \( M'' = \sum_{(i,j,t) \in I} (x_{i,j}^0 - x_{i,j}^t) M_{i,j}^t \), where \( \zeta = \min\{i + j - 2t, 2D - (i + j - 2t)\} \).

**Proof.** (i) Let \( \Phi = \{\sigma \in \text{Aut}(X) | \mathbf{0} \in \sigma C\} \). Let \( x, y, z \in C \) and let \((x, y, z) \in X_{i,j,t} \). Then there exists \( \sigma' \in \Phi \) that map \( x \) to \( \mathbf{0} \) and hence \((\sigma' y, \sigma' z) \in X_{i,j,t}^0 \). If \( \psi \in \text{Aut}_0(X) \) ranges over the \( \text{Aut}_0(X) \), then \((\psi \sigma' y, \psi \sigma' z) \) ranges over \( X_{i,j,t}^0 \). Note that the set \( \{\psi \sigma' | \psi \in \text{Aut}_0(X)\} \) consists of all automorphisms in \( \Phi \) that map \( x \) to \( \mathbf{0} \). Hence by \( M' \in T \) we have

\[
M' = \frac{1}{|C| |\text{Aut}_0(X)|} \sum_{(i,j,t) \in I} M_{\sigma C}^t,
\]

\[
= \sum_{(i,j,t) \in I} x_{i,j} M_{i,j}^t.
\]

(ii) Let \( M = |C| M' + (|X| - |C|) M'' \), that is \( M = \frac{1}{|\text{Aut}_0|} \sum_{\sigma \in \text{Aut}(X)} M_{\sigma C} \). Note that the matrix \( M \) is \( \text{Aut}(X) \)-invariant and hence an element of the Bose-Mesner algebra of \( \Box_{2D} \), and we write \( M = \sum_{k=0}^D \alpha_k A_k \). Then for any \( x \in X \) with \( \partial(x, \mathbf{0}) = k \), we have \( \alpha_k = (M)_{x,0} = (|C|M')_{x,0} = |C|x_{x,0}^0 \). So

\[
M'' = \frac{1}{|X| - |C|} (M - |C|M')
\]

\[
= \frac{1}{|X| - |C|} \left( \sum_{k=0}^D |C|x_{x,0}^0 A_k - |C| \sum_{(i,j,t) \in I} x_{i,j} M_{i,j}^t \right)
\]

\[
= \frac{|C|}{|X| - |C|} \sum_{(i,j,t) \in I} (x_{x,0}^0 - x_{i,j}^t) M_{i,j}^t,
\]

where \( \zeta = \min\{i + j - 2t, 2D - (i + j - 2t)\} \). \( \square \)

**Proposition 5.2.** \( x_{i,j}^t, (i,j,t) \in I \) satisfy the following linear constraints, where (v) holds
if $C$ has minimum distance at least $d$:

(i) $x_{0,0}^0 = 1$.

(ii) $0 \leq x_{i,j}^t \leq x_{i,j}^0$.

(iii) For $0 \leq i, j \leq D$, $0 \leq i + j - 2t \leq D$, $x_{i,j}^t = x_{i',j'}^t$, if $(i', j', i + j - 2t')$ is a permutation of $(i, j, i + j - 2t)$.

(iv) For $0 \leq i, j \leq D$, $D + 1 \leq i + j - 2t \leq 2D - 2$, $x_{i,j}^t = x_{i',j'}^t$, if $(i', j', 2D - (i' + j' - 2t'))$ is a permutation of $(i, j, 2D - (i + j - 2t))$.

(v) $x_{i,j}^t = 0$ if $\{i, j, i + j + 2t, 2D - (i + j + 2t)\} \cap \{1, 2, \ldots, d - 1\} \neq \emptyset$.

Proof. It is easy to see that the above constraints (i), (iii)–(v) follow directly from the definition of $x_{i,j}^t$. We now consider constraint (ii). Let $\Phi = \{\sigma \in \text{Aut}(X) | 0 \in \sigma C\}$. For any fixed $(i, j, t) \in T$, let $y, z \in X$ and let $(0, y, z) \in X_0^{i,j,t}$. Then by the definition of the matrix $M'$ and Proposition 5.1, we have that $x_{i,j}^t = \frac{1}{|C||\text{Aut}(X)|} \left| \{\sigma \in \Phi | y, z \in \sigma C\} \right| \leq x_{i,j}^0 = \frac{1}{|C||\text{Aut}(X)|} \left| \{\sigma \in \Phi | y \in \sigma C, 0 \in \sigma C\} \right|$. □

5.1.1 Semidefinite programming bound on $A(\square_{2D}, d)$ with even $D \geq 2$

Based on Proposition 4.6, Theorem 4.7 and Proposition 5.1, the positive semidefiniteness of $M'$ is equivalent to

for each even $r = 0, 2, \ldots, D$, the matrices

$$\left( \sum_t \beta_{i,j,t}^r x_{i,j}^t \right)_i^D$$

and for each odd $r = 1, 3, \ldots, D - 1$, the matrices

$$\left( \sum_t \beta_{i,j,t}^r x_{i,j}^t \right)_{i,j=0}^{D-1}$$

are positive semidefinite, and $M''$ is equivalent to

for each even $r = 0, 2, \ldots, D$, the matrices

$$\left( \sum_t \beta_{i,j,t}^r (x_{i,j}^0 - x_{i,j}^t) \right)_i^D$$

and for each odd $r = 1, 3, \ldots, D - 1$, the matrices

$$\left( \sum_t \beta_{i,j,t}^r (x_{i,j}^0 - x_{i,j}^t) \right)_{i,j=0}^{D-1}$$

are positive semidefinite, where $\zeta = \min \{i + j - 2t, 2D - (i + j - 2t)\}$.

Note that (i) we have deleted the factors $(\frac{2D-2r}{1})^{-\frac{r}{4}}(\frac{2D-2r}{j-r})^{-\frac{r}{4}}$, $(\frac{2D-2r}{D-r})^{-\frac{r}{2}}(\frac{2D-2r}{j-r})^{-\frac{r}{2}}$ as they make the coefficients integer, while the positive semidefiniteness is maintained; (ii) in (17) and (19), $t \geq \left[ \frac{j+1}{2} \right]$ for $i = D$ and $t \geq \left[ \frac{i+1}{2} \right]$ for $j = D$.

Theorem 5.3. For $\square_{2D}$ with even $D \geq 2$, the semidefinite programming problem: maximize $\sum_{i=0}^{D-1} \left( \frac{2D}{i} \right) x_{i,0}^t + \frac{1}{2} \left( \frac{2D}{D} \right) x_{D,0}^t$ subject to conditions (16)–(20) is an upper bound on $A(\square_{2D}, d)$.

Proof. Let $C$ be a code with minimum distance $d$ and we view $x_{i,j}^t$ as variables. Then $x_{i,j}^t$ subject to conditions (16)–(20) yields a feasible solutions with objective value $|C|$.
5.1.2 Semidefinite programming bound on $A(\Box_{2D}, d)$ with odd $D \geq 3$

Based on Proposition 4.6, Theorem 4.8 and Proposition 5.1, the positive semidefiniteness of $M'$ is equivalent to

for each even $r = 0, 2, \ldots, D - 1$, the matrices

$$
\left( \sum_t \beta^r_{i,j,t} x^t_{i,j} \right)^D_{i,j=r}
$$

and for each odd $r = 1, 3, \ldots, D - 2$, the matrices

$$
\left( \sum_t \beta^r_{i,j,t} x^t_{i,j} \right)^{D-1}_{i,j=r}
$$

are positive semidefinite, and $M''$ is equivalent to

for each even $r = 0, 2, \ldots, D - 1$, the matrices

$$
\left( \sum_t \beta^r_{i,j,t} (x^0_{\zeta,0} - x^t_{i,j}) \right)^D_{i,j=r}
$$

and for each odd $r = 1, 3, \ldots, D - 2$, the matrices

$$
\left( \sum_t \beta^r_{i,j,t} (x^0_{\zeta,0} - x^t_{i,j}) \right)^{D-1}_{i,j=r}
$$

are positive semidefinite, where $\zeta = \min\{i + j - 2t, 2D - 1 , (i + j - 2t)\}$.

**Theorem 5.4.** For $\Box_{2D}$ with odd $D \geq 3$, the semidefinite programming problem: maximize $\sum_{i=0}^{D-1} (2D)x^0_{i,0} + \frac{1}{2}(2D)x^0_{D,0}$ subject to conditions (16) and (21)–(24) is an upper bound on $A(\Box_{2D}, d)$.

**Proof.** Similar to the proof of Theorem 5.3. \(\square\)

5.2 Semidefinite programming bound on $A(\Box_{2D+1}, d)$

In this subsection, we give an upper bound on $A(\Box_{2D+1}, d)$. Given a code $C$ of $\Box_{2D+1}$, for each $(i,j,t) \in \mathcal{I}'$ define the numbers $\lambda^t_{i,j} := \left|(C \times C \times C) \cap X_{i,j,t}\right|$ and numbers $x^t_{i,j} := \left|(C \times \gamma^t_{i,j})^{-1} \lambda^t_{i,j}\right|$, where $\gamma^t_{i,j}$ denotes the number of nonzero entries of $M^t_{i,j}$.

Recall the matrices $M'$ and $M''$ defined as in Subsection 5.1. By the argument similar to proofs of Propositions 5.4 and 5.5 we can obtain the following propositions.

**Proposition 5.5.** We have

$$
M' = \sum_{(i,j,t) \in \mathcal{I}'} x^t_{i,j} M^t_{i,j}, \quad M'' = \frac{|C|}{|X| - |C|} \sum_{(i,j,t) \in \mathcal{I}'} (x^0_{v,0} - x^t_{i,j}) M^t_{i,j},
$$

where $\nu = \min\{i + j - 2t, 2D + 1 - (i + j - 2t)\}$.

**Proposition 5.6.** $x^t_{i,j}, (i,j,t) \in \mathcal{I}'$ satisfy the following linear constraints, where (v) holds
if $C$ has minimum distance at least $d$:

(i) $x_{0,0}^t = 1$.
(ii) $0 \leq x_{i,j}^t \leq x_{i,0}^0$.
(iii) For $0 \leq i, j \leq D$, $0 \leq i + j - 2t \leq D$, $x_{i,j}^t = x_{i',j'}^t$ if $(i', j', i' + j' - 2t')$ is a permutation of $(i, j, i + j - 2t)$.
(iv) For $0 \leq i, j \leq D$, $D + 1 \leq i + j - 2t \leq 2D$, $x_{i,j}^t = x_{i',j'}^t$ if $(i', j', 2D + 1 - (i' + j' - 2t'))$ is a permutation of $(i, j, 2D + 1 - (i + j - 2t))$.
(v) $x_{i,j}^t = 0$ if $\{i, j, i + j - 2t, 2D + 1 - (i + j - 2t)\} \cap \{1, 2, \ldots, d - 1\} = \emptyset$.

Based on Proposition 4.13, Theorem 4.14 and Proposition 5.5, the positive semidefiniteness of $M'$ and $M''$ is equivalent to

$$\sum_{i,j,t} \beta_{i,j,t}^r x_{i,j}^t$$

subject to conditions (25) is an upper bound on $A(\Box_{2D+1}, d)$.

Theorem 5.7. For $\Box_{2D+1}$, the semidefinite programming problem: maximize $\sum_{i=0}^D (2D+1)_i x_{i,0}^0$ subject to conditions (25) is an upper bound on $A(\Box_{2D+1}, d)$.

Proof. Similar to the proof of Theorem 5.3.

We remark that the above semidefinite programming problems in Theorems 5.3, 5.4 and 5.7 with $O(n^3)$ variables can be solved in time polynomial in $n$. The obtained new bound is at least as strong as the Delsarte’s linear programming bound [3]. Indeed, diagonalizing the Bose-Mesner algebra of $\Box_n$ yields the Delsarte bound, which is equal to the maximum of $\sum_{i=0}^D \sum_{x_{i,0}^0} x_{i,0}^0$ subject to the conditions $x_{0,0}^0 = 1$, $x_{1,0}^0 = \cdots = x_{d-1,0}^0$, $x_{d,0}^0 = x_{d+1,0}^0 = \cdots = x_{d+\frac{d}{2},0}^0 \geq 0$ and

$$\sum_{i=0}^D x_{i,0}^0 A_i$$

is positive semidefinite, (28)

where $A_i$ is the $i$th distance matrix of $\Box_n$. Note that condition (28) can be implied by the condition that $M'$ and $M''$ is positive semidefinite.

5.3 Computational results

In this subsection we give, in the range $8 \leq n \leq 13$, several concrete semidefinite programming bounds and Delsarte’s linear programming bounds on $A(\Box_n, d)$, respectively. The latter involves the second eigenmatrix of $\Box_n$.

Lemma 5.8. Let $\bar{q}_j(i)$ ($0 \leq i, j \leq \lfloor \frac{n}{2} \rfloor$) be the $(i, j)$-entry of this eigenmatrix. Then we have

$$\bar{q}_j(i) = \sum_{k=0}^j (-1)^k \binom{j}{k} \binom{n-1-j}{\frac{n-j}{2}}$$.
Proof. We first recall the following fact. Let $\Gamma$ denote a distance-regular graph with diameter $D$ and intersection numbers $c_i, a_i, b_i$ ($0 \leq i \leq D$). Without loss of generality, we assume its eigenvalues $\theta_0 > \theta_1 > \cdots > \theta_D$. Let $q_j(i)$ ($0 \leq i, j \leq D$) be the $(i,j)$-entry of the second eigenmatrix of $\Gamma$. Then we have $c_i q_j(i - 1) + a_i q_j(i) + b_i q_j(i + 1) = \theta_j q_j(i)$ ($0 \leq j \leq D$) by [2, p. 128].

When $\Gamma$ is $H(n, 2)$, it is known that $q_j(i) = \sum_{k=0}^i (-1)^k \binom{i}{k} \binom{n-i}{j-k} (0 \leq i, j \leq n)$ is the $(i, j)$-entry of the second eigenmatrix of $H(n, 2)$. Then by comparing the above identity for $H(n, 2)$ with that for $\square_n$, one can easily finds that $\bar{q}_j(i) = q_{2j}(i)$ ($0 \leq i, j \leq \lfloor \frac{n}{2} \rfloor$).

The followings are our computational resuls.

| New upper bounds on $A(\square_{2D}, d)$ | New upper bounds on $A(\square_{2D+1}, d)$ |
|----------------------------------------|----------------------------------------|
| $D$ $d$ | New bound | Delsarte bound | $D$ $d$ | New bound | Delsarte bound |
| 4 2 28 | 64 | 4 2 93 | 112 |
| 5 2 256 | 256 | 6 2 1348 | 1877 |
| 5 3 24 | 32 | 5 3 85 | 85 |
| 6 3 87 | 128 | 6 3 213 | 213 |
| 5 4 16 | 16 | 5 4 20 | 27 |
| 6 4 54 | 85 | 6 4 111 | 120 |

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