Some 2×2 Unitary Space-Time Codes from Sphere Packing Theory with Optimal Diversity Product of Code Size 6^*

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Abstract

In this correspondence, we propose some new designs of 2×2 unitary space-time codes of sizes $6, 32, 48, 64$ with best known diversity products (or product distances) by partially using sphere packing theory. In particular, we present an optimal 2×2 unitary space-time code of size 6 in the sense that it reaches the maximal possible diversity product for 2×2 unitary space-time codes of size 6. The construction and the optimality of the code of size 6 provide the precise value of the maximal diversity product of a 2×2 unitary space-time code of size 6.

Keywords: Unitary space-time codes, differential space-time modulation, optimal diversity product, packing theory.

1 Introduction

Unitary space-time codes have been recently proposed in [6, 5] for differential space-time modulation schemes and in [1, 2, 3, 4] for possibly other space-time modulation schemes. Unitary space-time codes in differential encoding are useful not only when the channel information is not known at the receiver and non-coherent decoding is used but also when the channel information is known at the receiver and coherent decoding as a recursive trellis coding is used jointly with an error correction coding as a turbo type coding [19] where a super performance is achieved. There have been several unitary space-time code constructions in the literature: for example, group and optimal group constructions [6, 7, 5, 9]; orthogonal designs [8]; parametric codes [11]; Cayley transforms [10]; Lie groups [13, 16]; and Hamiltonian constellations or spherical codes using packing theory [9, 16]. It is known that the performance of a space-time code depends on its diversity product and having a good diversity product has become an important criterion in the design of a space-time code. In [11], some upper bounds on the diversity products of (unitary) space-time codes for a given size are presented. It is easy to reach the diversity product upper bound for 2×2 matrices of sizes below 4 and 2×2 unitary matrices of sizes 4 and 5 reaching the upper bound are also presented in [11] using the parametric forms of unitary matrices. In fact, 2×2 unitary matrices of sizes below 6 reaching the upper bound can be also constructed by

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using the Hamiltonian constellations from the packing theory, i.e., the optimal sphere packing points. However, in [11] it is shown that the upper bound is not reachable when the 2×2 unitary code size is above 5 and a tight upper bound on the diversity products remains open. The optimal or best known sphere packing points of sizes above 5 do not provide optimal 2×2 unitary space-time codes with optimal diversity products.

In this correspondence, we propose some 2×2 unitary space-time codes by partially using the optimal sphere packing points [20, 22]. We obtain a determinant relationship for difference matrices between Hamiltonian and general 2×2 unitary constellations. We present some best-known designs for size $L = 6, 32, 48, 64$, and also show that the code with size 6 reaches the optimal diversity product.

This paper is organized as follows. In Section 2, we present new best-known diversity product designs for size $L = 6, 32, 48, 64$. In Section 3, we show the optimality of the new code of size 6 presented in Section 2. Since the proof is heavily technical, we leave the most technical parts of the proof in Appendix.

2 Some 2×2 Unitary Codes with Best Known Diversity Products

In this section, we present some new 2×2 unitary codes for sizes $L = 6, 32, 48, 64$ with best known diversity products.

2.1 Diversity Product

Let $\mathcal{G} = \{V_1, V_2, \cdots, V_L\}$ be a 2×2 unitary space-time code of size L with $V_l^H V_l = I$ where ^{H} stands for the transpose and complex conjugate. Define

$$\xi(\mathcal{G}) \triangleq \min_{V_l, V_{l'} \in \mathcal{G}, l \neq l'} |\det(V_l - V_{l'})|. \tag{1}$$

and

$$d_L \triangleq \max_{\mathcal{G}} \xi(\mathcal{G}) = \max_{\mathcal{G}} \min_{V_l, V_{l'} \in \mathcal{G}, l \neq l'} |\det(V_l - V_{l'})|. \tag{2}$$

Following the convention in the literature, the diversity product for a 2×2 code $\mathcal{G}$ is defined as follows:

$$\eta(\mathcal{G}) \triangleq \frac{1}{2}\sqrt{\xi(\mathcal{G})}, \tag{3}$$

and the optimal diversity product for L-point constellation is defined as

$$\eta(L) \triangleq \max_{\mathcal{G}} \eta(\mathcal{G}) = \frac{1}{2}\sqrt{d_L}. \tag{4}$$

We are interested in designing a code $\mathcal{G}$ with large or optimal diversity product.

2.2 2×2 Unitary Matrices

The content of this subsection can be found in many literature, for example, [21, 16]. For the notational convenience for our later study, we briefly introduce some concepts on 2×2 unitary matrices below. Let $\mathbf{U}(2)$ be the set of all 2×2 unitary matrices, i.e.,

$$\mathbf{U}(2) \triangleq \{A \mid A \text{ is a } 2 \times 2 \text{ matrix with } A^H A = I\}.$$

Between $\mathbf{U}(2)$ and the unit ball $\mathbf{S}^3 \subseteq \mathbb{R}^4$, there exists a close relationship as follows.

For any 2×2 matrix A with $A^H A = I$, we have $|\det(A)| = 1$ and thus there is a unique angle $\theta \in [0, 2\pi)$ such that $\det(A) = e^{j\theta}$. For any fixed angle $\theta \in [0, 2\pi)$, let

$$\mathbf{SU}(2, \theta) \triangleq \{A \in \mathbf{U}(2) \mid \det(A) = e^{j\theta}\}. \tag{5}$$

Thus, we have

$$\mathbf{U}(2) = \bigcup_{\theta \in [0, 2\pi)} \mathbf{SU}(2, \theta).$$

We are particularly interested in the case of $\theta = 0$ and denote the set $\mathbf{SU}(2, 0)$ by $\mathbf{SU}(2)$ for short, i.e., $\mathbf{SU}(2) = \mathbf{SU}(2, 0)$. We now investigate the structure of $\mathbf{SU}(2)$. From some theory of unitary matrices (for example, see [21]), $\mathbf{SU}(2)$ can be isometrically embedded onto the 4-dimensional Euclidean real unit sphere. Let $\mathbf{S}^3$ be the unit sphere of 4-dimensional real Euclidean space $\mathbb{R}^4$, i.e.,

$$\mathbf{S}^3 = \{\mathbf{x} \in \mathbb{R}^4 \mid \|\mathbf{x}\| = 1\},$$

where $\|\cdot\|$ denotes the conventional l^2 norm. Because $\det(A) = 1$ and the unitariness for any element A in $\mathbf{SU}(2)$, it is not hard to see that there are two complex numbers, $a = a_1 + ja_2$ and $b = b_1 + jb_2$, such that

$$A = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}, \tag{6}$$

where * denotes the conjugate, and a_1, a_2, b_1, b_2 are real numbers governed by the condition $a_1^2 + a_2^2 + b_1^2 + b_2^2 = 1$, i.e., $|a|^2 + |b|^2 = 1$, [21]. From this expression, the following embedding from $\mathbf{SU}(2)$ onto $\mathbf{S}^3$ can be obtained, also see for example [16]. Let i be the mapping $i : A \mapsto i(A)$ from $\mathbf{SU}(2)$ into $\mathbf{S}^3$ defined by

$$i(A) \triangleq (a_1, a_2, b_1, b_2) = (\mathrm{Re}(a), \mathrm{Im}(a), \mathrm{Re}(b), \mathrm{Im}(b)), \tag{7}$$

where a_1, a_2, b_1, b_2 are the real numbers defined in (6) and Re and Im stand for the real and imaginary parts of a complex number, respectively. Clearly, the mapping i is one-to-one and onto. Furthermore, the following relationship holds:

$$\det(A - B) = \|i(A) - i(B)\|^2. \tag{8}$$

This equation also implies that all determinants of difference matrices of two distinct 2×2 unitary matrices in $\mathbf{SU}(2)$ are positive. From (8), one can see that the problem to find an optimal 2×2 space-time code in $\mathbf{SU}(2)$, i.e., it is restricted to have determinant 1, becomes to find optimal packing points on the sphere $\mathbf{S}^3$, which is called *Hamiltonian constellations* in [9]. Thus, as indicated in [9], if we denote D_L as the maximal minimum-distance of L-point packing on $\mathbf{S}^3$, then

$$d_L \geq D_L^2,$$

i.e., the square of the maximal minimum-distance of L-point packing on $\mathbf{S}^3$ is a lower bound for d_L. However, as we shall see later, the above Hamiltonian constellation may not be enough to have good codes and we need to consider the entire 2×2 unitary matrix space $\mathbf{U}(2)$. To do so, we need a determinant formula.

2.3 A Useful Determinant Formula

Let us consider a relationship between $\mathbf{SU}(2)$ and $\mathbf{U}(2)$ or equivalently between $\mathbf{SU}(2)$ and $\mathbf{SU}(2,\theta)$ for any $\theta \in [0, 2\pi)$.

For a fixed θ, we define a mapping J_θ from $\mathbf{SU}(2,\theta)$ to $\mathbf{SU}(2)$ as follows:

$$J_\theta(A) \stackrel{\Delta}{=} e^{-j\theta/2}A, \quad \text{for } A \in \mathbf{SU}(2,\theta). \tag{9}$$

Since $\det(J_\theta(A)) = e^{-j\theta}\det(A) = e^{-j\theta}e^{j\theta} = 1$, this mapping is well-defined. Furthermore, it is not hard to see that it is one-to-one and onto. With this notation, one can see that any 2×2 unitary matrix A can be represented by

$$A = e^{j\theta/2}J_\theta(A), \quad \text{for some} \quad \theta \in [0, 2\pi).$$

An important property from this mapping is that it also provides a determinant formula for a difference matrix of two matrices selected from different sets $\mathbf{SU}(2,\theta_1)$ and $\mathbf{SU}(2,\theta_2)$, which is stated in the following proposition.

Proposition 1 *For any $A_0 \in \mathbf{SU}(2)$ and $A \in \mathbf{SU}(2,\theta)$, we have*

$$|\det(A - A_0)| = |\det(A_0 - J_\theta(A)) - 4\sin^2(\theta/4)|.$$

Proof: Assume

$$A_0 = \begin{pmatrix} a_0 & b_0 \\ -b_0^* & a_0^* \end{pmatrix}, \quad \text{and} \quad J_\theta(A) = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix},$$

where $|a_0|^2 + |b_0|^2 = 1$ and $|a|^2 + |b|^2 = 1$. Then

$$\begin{aligned} \det(A_0 - J_\theta(A)) &= \det(\begin{pmatrix} a_0 & b_0 \\ -b_0^* & a_0^* \end{pmatrix} - \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}) \\ &= 2 - (a_0a^* + b_0b^* + a_0^*a + b_0^*b), \end{aligned}$$

By the definition of J_θ in (5), we have $A = e^{j\theta/2}J_\theta(A)$. Therefore,

$$\begin{aligned}
|\det(A_0 - A)| &= \left|\det\left(\left(\begin{array}{cc} a_0 & b_0 \\ -b_0^* & a_0^* \end{array}\right) - \left(\begin{array}{cc} e^{j\theta/2}a & e^{j\theta/2}b \\ -e^{j\theta/2}b^* & e^{j\theta/2}a^* \end{array}\right)\right)\right| \\
&= |1 + e^{j\theta} - e^{j\theta/2}(a_0a^* + b_0b^* + a_0^*a + b_0^*b)| \\
&= |1 + e^{j\theta} - e^{j\theta/2}(2 - \det(A_0 - J_\theta(A)))| \\
&= |e^{-j\theta/2} + e^{j\theta/2} - (2 - \det(A_0 - J_\theta(A)))|,
\end{aligned}$$

which is the same as the one in the proposition. **q.e.d.**

From this proposition, we immediately have the following corollary

Corollary 1 *For any $A_1 \in \mathbf{SU}(2, \theta_1)$ and $A_2 \in \mathbf{SU}(2, \theta_2)$, we have*

$$|\det(A_1 - A_2)| = |\det(J_{\theta_1}(A_1) - J_{\theta_2}(A_2)) - 4\sin^2((\theta_1 - \theta_2)/4)|.$$

From the above proposition and corollary, one can see that the determinant absolute value of the difference matrix of two 2×2 unitary matrices depends on the distance between their embeddings and their angle difference. This motivates us to design a 2×2 unitary space-time code using two steps: *one is to select good packing points on the sphere $\mathbf{S}^3$ and the other is to select good angles θ.*

2.4 Some New Codes with Best-Known Diversity Products

With the help of the above determinant formulas, we can construct some 2×2 unitary codes with best-known diversity products.

2.4.1 Size $L = 6$

Let $d = -5/2 + \sqrt{22}$. Select a 4-point packing on $\mathbf{S}^3$ as follows:

$$\mathbf{a}_1 = (-a, -b, b, -b),\ \mathbf{a}_2 = (-a, b, b, b),\ \mathbf{a}_3 = (-a, -b, -b, b),\ \mathbf{a}_4 = (-a, b, -b, -b),$$

where $a = \sqrt{1 - 3d/8}$ and $b = \sqrt{(1 - a^2)/3}$. By mapping these points back to $\mathbf{SU}(2)$, we have the following four unitary matrices:

$$A_1 = \left(\begin{array}{cc} -a - bj & b - bj \\ -b - bj & -a + bj \end{array}\right),\quad A_2 = \left(\begin{array}{cc} -a + bj & b + bj \\ -b + bj & -a - bj \end{array}\right),$$
$$A_3 = \left(\begin{array}{cc} -a - bj & -b + bj \\ b + bj & -a + bj \end{array}\right),\quad A_4 = \left(\begin{array}{cc} -a + bj & -b - bj \\ b - bj & -a - bj \end{array}\right).$$

For other two unitary matrices, we use angle θ. Let

$$\theta_1 = 2\arccos(d/2 - a),\ \text{ and }\ \theta_2 = 2\pi - \theta_1,$$

and

$$A_5 = e^{j\theta_1/2}I \in \mathbf{SU}(2, \theta_1),\ A_6 = -e^{j\theta_2/2}I \in \mathbf{SU}(2, \theta_2).$$

It is easy to check that the diversity product of the code $\{A_1, A_2, \cdots, A_6\}$ is $\frac{1}{2}\sqrt{-5/2+\sqrt{22}} \approx 0.7400$. In next section, we shall prove that $\eta(6) = \frac{1}{2}\sqrt{-5/2+\sqrt{22}}$, i.e., this code reaches the optimal diversity product of any 2×2 unitary space-time codes of size $L = 6$.

2.4.2 Sizes $L = 32, 48, 64$

To construct 32, 48 or 64 unitary matrices with large diversity products, at first, we first construct four diamonds in $\mathbf{S}^3$ as follows.

Let t is a parameter, and

$$a = \sqrt{1 - \frac{3}{8}t^2}, \quad r = \sqrt{1-a^2}, \quad b = -\frac{\sqrt{6}}{12}t, \quad r_1 = \frac{\sqrt{3}}{3}t, \quad \beta = \frac{2\pi}{3}.$$

The four point coordinates of the first diamond are

$$\begin{array}{ll} \mathbf{a}_1 = (a, r, 0, 0), & \mathbf{a}_2 = (a, b, r_1, 0), \\ \mathbf{a}_3 = (a, b, r_1\cos(\beta), r_1\sin(\beta)), & \mathbf{a}_4 = (a, b, r_1\cos(2\beta), r_1\sin(2\beta)). \end{array}$$

The ones of the second diamond are

$$\begin{array}{ll} \mathbf{a}_5 = (a, -r, 0, 0), & \mathbf{a}_6 = (a, -b, -r_1, 0), \\ \mathbf{a}_7 = (a, -b, -r_1\cos(\beta), -r_1\sin(\beta)), & \mathbf{a}_8 = (a, -b, -r_1\cos(2\beta), -r_1\sin(2\beta)). \end{array}$$

The ones of the third diamond are

$$\begin{array}{ll} \mathbf{a}_9 = (-a, r, 0, 0), & \mathbf{a}_{10} = (-a, b, r_1, 0), \\ \mathbf{a}_{11} = (-a, b, r_1\cos(\beta), r_1\sin(\beta)), & \mathbf{a}_{12} = (-a, b, r_1\cos(2\beta), r_1\sin(2\beta)). \end{array}$$

The ones of the forth diamond are

$$\begin{array}{ll} \mathbf{a}_{13} = (-a, -r, 0, 0), & \mathbf{a}_{14} = (-a, -b, -r_1, 0), \\ \mathbf{a}_{15} = (-a, -b, -r_1\cos(\beta), -r_1\sin(\beta)), & \mathbf{a}_{16} = (-a, -b, -r_1\cos(2\beta), -r_1\sin(2\beta)). \end{array}$$

Mapping these points back to $\mathbf{SU}(2)$ using the map i^{-1} given in (7), we obtain 16 matrices, denoted by Q_j, i.e., $Q_j \stackrel{\Delta}{=} i^{-1}(\mathbf{a}_j)$ for $j = 1, 2, \cdots, 16$. These matrices can be used to generate best-known diversity product unitary codes with $L = 32$, 48 and 64 as follows.

For $L = 32$, let $t = \sqrt{2}$, $\gamma = \arccos(3/4)$ and define

$$\begin{array}{ll} U_i = Q_i, \;\; i = 1,2,3,4; & U_i = Q_{8+i}, \;\; i = 5,6,7,8 \\ U_i = e^{\mathbf{j}(\pi/4+\gamma/2)}Q_{i-8}, \;\; i = 9,10,11,12; & U_i = e^{\mathbf{j}(\pi/4+\gamma/2)}Q_i, \;\; i = 13,14,15,16; \\ U_i = e^{\mathbf{j}(\pi/2)}Q_{i-12}, \;\; i = 17,18,19,20; & U_i = e^{\mathbf{j}(\pi/2)}Q_{i-12}, \;\; i = 21,22,23,24; \\ U_i = e^{\mathbf{j}(3\pi/4+\gamma/2)}Q_{i-20}, \;\; i = 25,26,27,28; & U_i = e^{\mathbf{j}(3\pi/4+\gamma/2)}Q_{i-20}, \;\; i = 29,30,31,32. \end{array}$$

and put $\mathcal{G}_{32} = \{U_1, \cdots, U_{32}\}$, then the minimum determinant $\xi(\mathcal{G}_{32}) = \frac{\sqrt{7}-1}{2}$, and the diversity product $\eta(\mathcal{G}_{32})$ is $\frac{1}{2}\sqrt{\frac{\sqrt{7}-1}{2}} \cong 0.4536$, which is best-known for size $L = 32$.

For $L = 48$, let $t = \sqrt{2}$ and

$$\begin{array}{ll} V_i = Q_i, \;\; i = 1,2,3,4; & V_i = Q_{8+i}, \;\; i = 5,6,7,8 \\ V_i = e^{\mathbf{j}(\pi/6)}Q_{i-4}, \;\; i = 9,10,11,12; & V_i = e^{\mathbf{j}(\pi/6)}Q_{i-4}, \;\; i = 13,14,15,16; \\ V_i = e^{\mathbf{j}(\pi/3)}Q_{i-16}, \;\; i = 17,18,19,20; & V_i = e^{\mathbf{j}(\pi/6)}Q_{i-8}, \;\; i = 21,22,23,24; \\ V_i = e^{\mathbf{j}(\pi/2)}Q_{i-20}, \;\; i = 25,26,27,28; & V_i = e^{\mathbf{j}(\pi/2)}Q_{i-20}, \;\; i = 29,30,31,32; \\ V_i = e^{\mathbf{j}(2\pi/3)}Q_{i-32}, \;\; i = 33,34,35,36; & V_i = e^{\mathbf{j}(2\pi/3)}Q_{i-24}, \;\; i = 37,38,39,40; \\ V_i = e^{\mathbf{j}(5\pi/6)}Q_{i-36}, \;\; i = 41,42,43,44; & V_i = e^{\mathbf{j}(5\pi/6)}Q_{i-36}, \;\; i = 45,46,47,48. \end{array}$$

and define $\mathcal{G}_{48} = \{V_1, \cdots, V_{48}\}$, then the minimum determinant $\xi(\mathcal{G}_{48}) = \sqrt{3} - 1$, and the diversity product $\eta(\mathcal{G}_{48})$ is $\frac{1}{2}\sqrt{\sqrt{3}-1} \cong 0.4278$, which is best-known for size $L = 48$.

For $L = 64$, let $t = \sqrt{1.3880}$, and define

$$\begin{array}{ll}
W_i = Q_i, \;\; i = 1,2,3,4; & W_i = Q_{8+i}, \;\; i = 5,6,7,8 \\
W_i = e^{\mathbf{j}(\pi/8)} Q_{i-4}, \;\; i = 9,10,11,12; & W_i = e^{\mathbf{j}(\pi/8)} Q_{i-4}, \;\; i = 13,14,15,16; \\
W_i = e^{\mathbf{j}(\pi/4)} Q_{i-16}, \;\; i = 17,18,19,20; & W_i = e^{\mathbf{j}(\pi/4)} Q_{i-8}, \;\; i = 21,22,23,24; \\
W_i = e^{\mathbf{j}(3\pi/8)} Q_{i-20}, \;\; i = 25,26,27,28; & W_i = e^{\mathbf{j}(3\pi/8)} Q_{i-20}, \;\; i = 29,30,31,32; \\
W_i = e^{\mathbf{j}(\pi/2)} Q_{i-32}, \;\; i = 33,34,35,36; & W_i = e^{\mathbf{j}(\pi/2)} Q_{i-24}, \;\; i = 37,38,39,40; \\
W_i = e^{\mathbf{j}(5\pi/8)} Q_{i-36}, \;\; i = 41,42,43,44; & W_i = e^{\mathbf{j}(5\pi/8)} Q_{i-36}, \;\; i = 45,46,47,48; \\
W_i = e^{\mathbf{j}(3\pi/4)} Q_{i-48}, \;\; i = 49,50,51,52; & W_i = e^{\mathbf{j}(3\pi/4)} Q_{i-40}, \;\; i = 53,54,55,56; \\
W_i = e^{\mathbf{j}(7\pi/8)} Q_{i-52}, \;\; i = 57,58,59,60; & W_i = e^{\mathbf{j}(7\pi/8)} Q_{i-52}, \;\; i = 61,62,63,64.
\end{array}$$

and define $\mathcal{G}_{64} = \{W_1, \cdots, W_{64}\}$, then the minimum determinant $\xi(\mathcal{G}_{64}) = 0.5406$, and the diversity product $\eta(\mathcal{G}_{64})$ is $\frac{1}{2}\sqrt{0.5406} \cong 0.3676$, which is best-known for size $L = 64$.

The following table summarizes the above results and compares with some existing codes, where diversity sum means the minimum Euclidean distance between codeword matrices [11]. From Table 1, one can see that the optimal diversity sum, 0.7746, of the 2 by 2 unitary code of size 6 presented in [11] is slightly better than the one, 0.7400, of the 2 by 2 unitary code of size 6 with optimal diversity product presented in this paper. Fig. 1 shows the symbol error rates (SER) of these two codes of size 6 over a quasi static fading channel and one can see that the one with the optimal diversity product performs slightly better than the one with the optimal diversity sum at high SNR, which also confirms the argument between diversity product and diversity sum in [11].

Table 1: Diversity product and sum comparisons

	Hamiltonian Codes [9]		Parametric Codes [11]		New Codes	
Size	Diversity product	Diversity sum	Diversity product	Diversity sum	Diversity product	Diversity sum
6	0.7071	0.7071	0.7071	0.7746 (opt.)	0.7400 (opt.)	0.7400
32	0.4496	0.4496	0.4461	0.5621	0.4536	0.5217
48	0.3938	0.3938	0.3875		0.4278	0.5000
64	0.3609	0.3609	0.3535	0.4852	0.3676	0.3827

3 Optimality of 2×2 Unitary Space-time Codes of Size $L = 6$.

The main goal of this section is to prove the optimality of the code of size 6 presented in Section 2.4.1.

Theorem 1 *The maximal diversity product of a* 2×2 *unitary space-time code of size* 6 *is* $\frac{1}{2}\sqrt{-5/2+\sqrt{22}}$, *i.e.,*

$$\eta(6) = \frac{1}{2}\sqrt{-5/2+\sqrt{22}}.$$

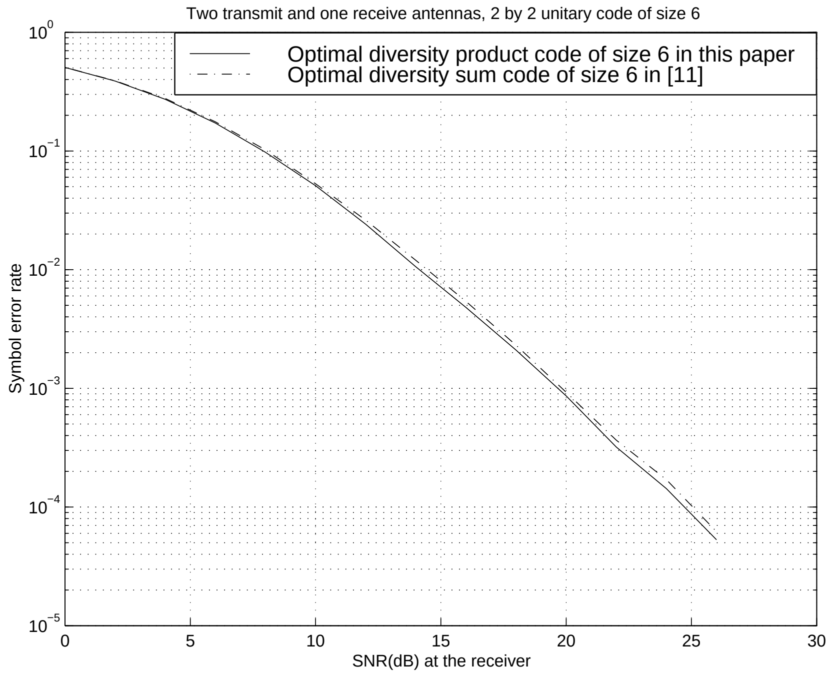

Figure 1: Symbol error rate comparison.

This theorem implies that the code presented in Section 2.4.1 has already reached the maximal diversity product.

To prove this theorem, we need some preparations.

First, we introduce the concept of *dual*. For any unitary matrix $A = e^{j\theta/2}J_\theta(A)$, its dual is defined as $e^{j(2\pi-\theta)/2}(-J_\theta(A))$ and denoted by $\tilde{A}$. If $\theta = 0$, then $\tilde{A} = e^{j2\pi/2}(-J_\theta(A)) = A$, i.e., the dual of $A \in \mathbf{SU}(2)$ is itself. With the definition of a dual matrix we have the following corollary.

Lemma 1 *For any unitary matrices A_1 and A_2 with their duals $\tilde{A}_1$ and $\tilde{A}_2$, respectively, we have*

$$\begin{array}{ll} (i) & |\det(A_1 - B)| = |\det(\tilde{A}_1 - B)|, \quad \text{for any unitary matrix } B \in \mathbf{SU}(2), \\ (ii) & |\det(A_1 - A_2)| = |\det(\tilde{A}_1 - \tilde{A}_2)|. \end{array}$$

This lemma is a direct result of Proposition 1, we omit its proof. In what follows, for the notational convenience, we use $\hat{A}$ to denote $J_\theta(A)$ for a matrix $A \in \mathbf{SU}(2,\theta)$ by dropping the subscript θ without causing any confusion. Since there exists an embedding i from $\mathbf{SU}(2)$ onto $\mathbf{S}^3$, we do not distinguish a matrix in $\mathbf{SU}(2)$ and a vector on $\mathbf{S}^3$ and use the same notation A to express a matrix in $\mathbf{SU}(2)$ and a point on $\mathbf{S}^3$. If A is treated as a point on $\mathbf{S}^3$, it means its embedding, i.e., $i(A)$ in (7).

Lemma 2 *Let $A_i \in \mathbf{SU}(2,\theta_i)$, $i = 1, 2, \cdots, L$, and $\{A_1, A_2, \cdots, A_L\}$ be an optimal unitary space-time code of size L with the maximal diversity product $d_L \geq 2$. Then,*

$$|\det(A_i - A_j)| = \det(\hat{A}_i - \hat{A}_j) - 4\sin^2((\theta_i - \theta_j)/4) \geq d_L, \quad \text{if} \quad |\theta_i - \theta_j| \leq \pi,$$
$$|\det(A_i - A_j)| = 4\sin^2((\theta_i - \theta_j)/4) - \det(\hat{A}_i - \hat{A}_j) \geq d_L, \quad \text{if} \quad |\theta_i - \theta_j| \geq \pi,$$

where $\hat{A}_l = J_\theta(A_l)$ *is the projection of* A_l *from* $\mathbf{SU}(2,\theta_l)$ *to* $\mathbf{SU}(2)$ *as defined in Section 2.2.*

Its proof is in Appendix. Lemma 2 basically provides an expression of the absolute value of a difference matrix determinant from the one of their projections to $\mathbf{SU}(2)$ and their angles for an optimal constellation.

Lemma 3 *Let* $\{A_1, \cdots, A_L\}$ *be an unitary space-time code with the optimal diversity product* $d_L > 2$ *and* $A_j \in \mathbf{SU}(2,\theta_j)$, $j = 1,2,\cdots,L \geq 6$. *If* $0 = \theta_1 \leq \cdots \leq \theta_L < 2\pi$, *then* $\theta_{i+1} - \theta_i < \pi$ *for* $i = 1,2,\cdots,L-1$, *i.e., the difference of two adjacent angles is less than* π.

Its proof is in Appendix.

Lemma 4 *Let* $\{\mathbf{P}_1, \cdots, \mathbf{P}_L\}$ *be* L *points on the sphere* $\mathbf{S}^3$. *Assume that* $\|\mathbf{P}_i - \mathbf{P}_j\|^2 \geq d$ *for a constant* $d \geq 2$ *and* $1 \leq i < j \leq L$. *Let* $\mathbf{P}_0$ *be any a point on this sphere. Then,*

- *if* $L = 4$, *there exist* s *and* t, $1 \leq s,t \leq L$, *such that*

$$\|\mathbf{P}_0 - \mathbf{P}_s\|^2 \geq 2 - 2\sqrt{1-3d/8} \quad \textit{and} \quad \|\mathbf{P}_0 - \mathbf{P}_t\|^2 \leq 2 + 2\sqrt{1-3d/8},$$

- *if* $L = 3$, *there exist* s *and* t, $1 \leq s,t \leq L$, *such that*

$$\|\mathbf{P}_0 - \mathbf{P}_s\|^2 \geq 2 - 2\sqrt{1-d/3} \quad \textit{and} \quad \|\mathbf{P}_0 - \mathbf{P}_t\|^2 \leq 2 + 2\sqrt{1-d/3},$$

- *if* $L = 2$, *there exist* s *and* t, $1 \leq s,t \leq L$, *such that*

$$\|\mathbf{P}_0 - \mathbf{P}_s\|^2 \geq 2 - 2\sqrt{1-d/4}, \quad \textit{and} \quad \|\mathbf{P}_0 - \mathbf{P}_t\|^2 \leq 2 + 2\sqrt{1-d/4}.$$

Its proof is in Appendix.

Lemma 5 *For any* L *points* $\{\mathbf{P}_1, \cdots, \mathbf{P}_L\}$ *on the unit sphere* $\mathbf{S}^n$ *in the* $n+1$*-dimensional real Euclidean space* $\mathbb{R}^{n+1}$, *we have*

$$\sum_{1 \leq i < j \leq L} \|\mathbf{P}_i - \mathbf{P}_j\|^2 \leq L^2.$$

Its proof can be found in, for example, [11].

Lemma 6 *Let* $A_i = e^{j\theta_i/2}\hat{A}_i \in \mathbf{SU}(2,\theta_i)$, $i = 1,2,3$, *be three unitary matrices. Assume* $\theta_1 \leq \theta_2 \leq \theta_3$. *If* $\theta_3 - \theta_1 \leq \pi$, *and for* $i \neq j$, $|\det(A_i - A_j)| \geq d_6 \geq \sqrt{22} - 5/2$, *then,*

$$\theta_3 - \theta_1 \leq 5\pi/6.$$

Its proof is in Appendix.

Lemma 7 *Let $2 < d \leq 2.5$ and $-1 < a, b \leq 1 - d/2$. If $\arccos(d/2 + a) + \arccos(d/2 + b) \geq \pi/2$, then,*

$$2\sin(\arccos(a + d/2)/2) - \frac{b - \cos(\arccos(d/2 + b) + \arccos(d/2 + a)) - d/2}{\cos(\arccos(-a)/2)} \geq d, \tag{10}$$

where $0 \leq \arccos(x) \leq \pi$.

Its proof is in Appendix.

Proposition 2 *Let $\{A_1, A_2, \cdots, A_6\}$ be an optimal constellation with $A_j = e^{j\theta_j/2}\hat{A}_j$ of the maximal diversity product d_6. Assume that $0 = \theta_1 \leq \cdots \leq \theta_5 \leq \pi \leq \theta_6$ and $\theta_6 - \theta_5 \leq \pi$, $\theta_6 - \theta_4 \geq \pi$. Then, $d_6 \leq -5/2 + \sqrt{22}$.*

Its proof is in Appendix.

Proposition 3 *Let $\{A_1, A_2, \cdots, A_6\}$ be an optimal constellation with $A_j = e^{j\theta_j/2}\hat{A}_j$. Assume that $0 = \theta_1 \leq \cdots \leq \theta_5 \leq \pi \leq \theta_6$ and $\theta_6 - \theta_4 \leq \pi$, $\theta_6 - \theta_3 \geq \pi$. Then, $d_6 < -5/2 + \sqrt{22}$.*

Its proof is in Appendix.

Proposition 4 *Let $\{A_1, A_2, \cdots, A_6\}$ be an optimal constellation with $A_j = e^{j\theta_j/2}\hat{A}_j$. Assume that $0 = \theta_1 \leq \cdots \leq \theta_4 \leq \pi \leq \theta_5 \leq \theta_6$ and $\theta_6 - \theta_4 \leq \pi$, $\theta_6 - \theta_3 \geq \pi$. Then, $d_6 < -5/2 + \sqrt{22}$.*

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Proposition 5 *Let $\{A_1, A_2, \cdots, A_6\}$ be an optimal constellation with $A_j = e^{j\theta_j/2}\hat{A}_j$. Assume that $0 = \theta_1 \leq \cdots \leq \theta_4 \leq \pi \leq \theta_5 \leq \theta_6$ and $\theta_6 - \theta_3 \leq \pi$, $\theta_6 - \theta_2 \geq \pi$. Then, $d_6 < -5/2 + \sqrt{22}$.*

Its proof is in Appendix.

Now we begin to prove Theorem 1.

Proof of Theorem 1: Assume signal constellation $\mathcal{G} = \{A_1, A_2, \cdots, A_6\}$ is an optimal constellation with the maximal diversity product d_6 and $A_i \in \mathbf{SU}(2, \theta_i)$, $i = 1, 2, \cdots, 6$. By the construction in Section 2.4 (1), we have $d_6 \geq -5/2 + \sqrt{22}$. We next need to show that $d_6 \leq -5/2 + \sqrt{22}$. To do so, let us consider the different cases of the number of the zero angles of A_i: $p \triangleq \sharp\{i \mid \theta_i = 0\}$. Without loss of generality, we can assume that $1 \leq p \leq 6$. In this proof and the proofs in Appendix, we always use $0 \leq \arccos(x) \leq \pi$.

(i) $p = 6$.

$p = 6$ means that all $A_i \in \mathbf{SU}(2)$, i.e., all six matrices A_i are on the sphere $\mathbf{S}^3$. In other words, there exist 6-point packing such that the minimal distance is greater than $\sqrt{2}$, which contradicts with the packing result on $\mathbf{S}^3$ (according to the result [20], the packing angle on $\mathbf{S}^3$ is $\pi/2$, that is, the maximal minimum distance is $\sqrt{2}$).

(ii) $p = 5$.

Assume $\theta_1 = \cdots = \theta_5 = 0$ and $\theta_6 > 0$. Thus, $A_i = \hat{A}_i, i = 1, 2, \cdots, 5$. By Lemma 3, we have $\theta_6 - \theta_5 \leq \pi$, i.e., $\theta_6 \leq \pi$. By Lemma 2,

$$\det(\hat{A}_i - \hat{A}_6) \geq d_6 + 4\sin^2(\theta_6/4) > 2, \ i = 1, 2, \cdots, 5.$$

For $1 \leq i \neq j \leq 5$, from the condition, $\det(\hat{A}_i - \hat{A}_j) > 2$. Therefore, there exists six points $\{\hat{A}_1, \cdots, \hat{A}_6\}$ on the sphere $\mathbf{S}^3$ such that the minimum distance is greater than $\sqrt{2}$, which contradicts with the packing result as in (i).

(iii) $p = 4$.

Assume $\theta_1 = \cdots = \theta_4 = 0$ and $0 < \theta_5 \leq \theta_6 < 2\pi$. By Lemma 3, we have $\theta_5 \leq \pi$ and $\theta_6 - \theta_5 \leq \pi$. If $\theta_6 \leq \pi$, then, as shown as (ii), $\{\hat{A}_1, \cdots, \hat{A}_4, \hat{A}_5, \hat{A}_6\}$ consists of a 6-point packing on $\mathbf{S}^3$ with minimum distance greater than $\sqrt{2}$, which results in a contradiction. Therefore, we can assume that $\theta_5 \leq \pi \leq \theta_6$ and $\theta_6 - \theta_5 \leq \pi$.

We next investigate the packing position of $\{\hat{A}_1, \cdots, \hat{A}_4, \hat{A}_5, -\hat{A}_6\}$ on $\mathbf{S}^3$. Denote $\hat{A}_i = (a_i, b_i, c_i, e_i)$, $i = 1, \cdots, 6$. By a unitary transformation, we can assume $\hat{A}_5 = I$, i.e., $a_5 = 1, b_5 = c_5 = e_5 = 0$. We then convert this problem to a packing problem on the 3-dimensional unit sphere $\mathbf{S}^2$ as follows. If $a_i \neq 1, -1$, define

$$\mathbf{b}_i = \frac{1}{r_i}(b_i, c_i, e_i), \quad i = 1, 2, 3, 4, 6, \tag{11}$$

where $r_i = \sqrt{1 - a_i^2}$. Then $\mathbf{b}_i \in \mathbf{S}^2$ and clearly,

$$\det(\hat{A}_i - \hat{A}_j) = 2(1 - a_i a_j) + r_i r_j (\|\mathbf{b}_i - \mathbf{b}_j\|^2 - 2), \tag{12}$$

$$\|\mathbf{b}_i - \mathbf{b}_j\|^2 = 2 - \frac{2(1 - a_i a_j) - \det(\hat{A}_i - \hat{A}_j)}{r_i r_j}. \tag{13}$$

Two remarks about this conversion are as follows. The mapping $\mathbf{S}^3 \ni (a, b, c, e) \to \mathbf{b} = (b/r, c/r, e/r) \in \mathbf{S}^2$ is *not* one-to-one. It is because, for different two points (a, b, c, e) and $(-a, b, c, e)$, the images are the same. However, when we restrict $a \geq 0$ or $a \leq 0$, the mapping becomes one-to-one and onto. Another remark is that an image point $\mathbf{b}$ does *not* depend on a, when we restrict a to $a \leq 0$ or $a \geq 0$. To explain this, we use the polar coordination. For any point $(a, b, c, e) \in \mathbf{S}^3$, there exist three angles ϕ_1, ϕ_2, ϕ_3, such that $a = \sin(\phi_1)$ and $b = \cos(\phi_1)\sin(\phi_2), c = \cos(\phi_1)\cos(\phi_2)\sin(\phi_3), e = \cos(\phi_1)\cos(\phi_2)\cos(\phi_3)$. Hence $\mathbf{b} = (b/r, c/r, e/r) = (\sin(\phi_2), \cos(\phi_2)\sin(\phi_3), \cos(\phi_2)\cos(\phi_3))$, which is independent of ϕ_1, i.e., a. Therefore, when we restrict a to $a \leq 0$ or $a \geq 0$, the distance $\|\mathbf{b}_i - \mathbf{b}_j\|$ is independent of a_i and a_j.

For $1 \leq i \leq 4$ and $i = 6$, because $\theta_5 \leq \pi$ and $\theta_6 - \theta_5 \leq \pi$, by Lemma 2, we have

$$2 < d_6 \leq |\det(A_5 - A_i)| = \det(\hat{A}_5 - \hat{A}_i) - 4\sin^2(\theta_5/4) = 2 - 2a_i - 4\sin^2(\theta_5/4).$$

Therefore, $a_i < 0$ for $i = 1, 2, 3, 4, 6$.

Since $\theta_1 = \theta_2 = \theta_3 = \theta_4 = 0$, without loss of generality, we may assume that $-1 \leq a_1 \leq a_2 \leq a_3 \leq a_4 < 0$. If $a_1 = -1$, then $b_1 = c_1 = e_1 = 0$ and it is not hard to see that $\det(\hat{A}_4 - \hat{A}_1) = 2 + 2a_4$. It implies $d_6 \le 2+2a_4$, i.e., $a_4 > 0$, which contradicts with the result $a_4 < 0$ we derived before. Therefore, $a_1 > -1$.

For $1 \le i \ne j \le 4$, from (12) and the fact that $\theta_i = \theta_j = 0$, we have

$$\begin{aligned} d_6 &\le |\det(A_i - A_j)| = \det(\hat{A}_i - \hat{A}_j) - 4\sin^2((\theta_i - \theta_j)/4) \\ &= 2 - 2a_i a_j + r_i r_j (\|\mathbf{b}_i - \mathbf{b}_j\|^2 - 2). \end{aligned}$$

Because $a_i a_j > 0$ and $r_i r_j > 0$, we have $\|\mathbf{b}_i - \mathbf{b}_j\|^2 - 2 > 0$. Furthermore, it is easy to see that for a fixed a_i, the right hand side of the above inequality is increasing for a_j. Therefore,

$$d_6 \le 2 - 2a_i a_j + r_i r_j (\|\mathbf{b}_i - \mathbf{b}_j\|^2 - 2) \le 2 - 2a_4^2 + r_4^2 (\|\mathbf{b}_i - \mathbf{b}_j\|^2 - 2),$$

which implies that $a_4 \ge -\sqrt{1 - d_6/\|\mathbf{b}_i - \mathbf{b}_j\|^2}$. Because $\{\mathbf{b}_1, \cdots, \mathbf{b}_4\}$ are on $\mathbf{S}^2$, by the packing theory on $\mathbf{S}^2$, there is at least one pair $\{\mathbf{b}_i, \mathbf{b}_j\}$ such that $\|\mathbf{b}_i - \mathbf{b}_j\|^2 \le 8/3$. Hence,

$$a_4 \ge -\sqrt{1 - 3d_6/8}. \tag{14}$$

Since $a_5 = 1, -1 \le a_6 < 0$, and $0 \le \theta_6 - \theta_5 \le \pi$, from Lemma 2 we have

$$\begin{aligned} d_6 &\le |\det(A_6 - A_5)| = \det(\hat{A}_6 - \hat{A}_5) - 4\sin^2((\theta_6 - \theta_5)/4) \\ &= 2 - 2a_6 - 4\sin^2((\theta_6 - \theta_5)/4) \le 2 - 2(-1) - 4\sin^2((\theta_6 - \theta_5)/4). \end{aligned}$$

Therefore,

$$\cos((\theta_6 - \theta_5)/2) \ge d_6/2 - 1. \tag{15}$$

Using the fact that $d_6 \le |\det(A_5 - A_4)| = \det(\hat{A}_5 - \hat{A}_4) - 4\sin^2(\theta_5/4)$, and noting that $\det(\hat{A}_5 - \hat{A}_4) = 2 - 2a_4$, we have

$$\begin{aligned} d_6 &\le 2 - 2a_4 - 4\sin^2(\theta_5/4) \le 2 + 2\sqrt{1 - 3d_6/8} - 4\sin^2(\theta_5/4) \\ &= 2\cos(\theta_5/2) + 2\sqrt{1 - 3d_6/8}, \end{aligned} \tag{16}$$

where the second inequality is from (14). Inequality (16) implies

$$\cos(\theta_5/2) \ge d_6/2 - \sqrt{1 - 3d_6/8}. \tag{17}$$

We now replace A_5, A_6 by their duals $\tilde{A}_5, \tilde{A}_6$. From the definition, we have

$$\tilde{A}_6 = e^{j(2\pi - \theta_6)/2}(-\hat{A}_6), \quad \tilde{A}_5 = e^{j(2\pi - \theta_5)/2}(-\hat{A}_5).$$

Furthermore, $\{A_1, \cdots, A_4, \tilde{A}_6, \tilde{A}_5\}$ is also an optimal signal constellation by Lemma 1. We make a normalization by multiplying $-\hat{A}_6^H$ from left to the constellation to get a new constellation:

$$\begin{aligned} \mathcal{G}_1 &\triangleq \{-\hat{A}_6^H A_1, -\hat{A}_6^H A_2, -\hat{A}_6^H A_3, -\hat{A}_6^H A_4, -\hat{A}_6^H \tilde{A}_6, -\hat{A}_6^H \tilde{A}_5\} \\ &= \{-\hat{A}_6^H A_1, -\hat{A}_6^H A_2, -\hat{A}_6^H A_3, -\hat{A}_6^H A_4, e^{j(2\pi - \theta_6)/2} I, -\hat{A}_6^H \tilde{A}_5\}. \end{aligned}$$

Since $-\hat{A}_6^H$ is a unitary matrix, $\mathcal{G}_1$ is also an optimal constellation. Furthermore, $\mathcal{G}_1$ and $\{A_1, \cdots, A_6\}$ have the same angle relationships. Therefore, inequality (17) corresponding to this new constellation $\mathcal{G}_1$ also holds:

$$\cos((2\pi - \theta_6)/2) \geq d_6/2 - \sqrt{1 - 3d_6/8}. \tag{18}$$

From (17) and (18), we have

$$\theta_5 \leq 2\arccos(d_6/2 - \sqrt{1 - 3d_6/8}), \quad \theta_6 \geq 2\pi - 2\arccos(d_6/2 - \sqrt{1 - 3d_6/8}).$$

Hence,

$$\theta_6 - \theta_5 \geq 2\pi - 4\arccos(d_6/2 - \sqrt{1 - 3d_6/8}).$$

From (15), we know that $\theta_6 - \theta_5 \leq 2\arccos(d_6/2 - 1)$. Therefore,

$$2\pi - 4\arccos(d_6/2 - \sqrt{1 - 3d_6/8}) \leq 2\arccos(d_6/2 - 1).$$

Hence,

$$d_6 \leq -4(d_6/2 - \sqrt{1 - 3d_6/8})^2 + 4,$$

which implies the desired result $d_6 \leq -5/2 + \sqrt{22}$.

(iv) $p \leq 3$.

Assume $0 = \theta_1 \leq \theta_2 \leq \theta_3 \leq \cdots \leq \theta_6$. Using the same argument as in the beginning of Case (iii) when $p = 4$ and Lemma 3, we can also assume that $\pi \leq \theta_6$ and $\theta_2 \leq \pi$, $\theta_6 - \theta_5 \leq \pi$. We divide the proof into several cases according to the relationships among the angles θ_j.

Case I $\theta_6 \geq \pi$ **and** $\theta_5 \leq \pi$**.**

We divide this case into 4 subcases.

Case I.1 $\theta_6 \geq \pi$**,** $\theta_5 \leq \pi$ **and** $\theta_6 - \theta_4 \geq \pi$**.**

This subcase is Proposition 2.

Case I.2 $\theta_6 \geq \pi$**,** $\theta_5 \leq \pi$ **and** $\theta_6 - \theta_4 \leq \pi$**,** $\theta_6 - \theta_3 \geq \pi$**.**

This subcase is Proposition 3.

Case I.3 $\theta_6 \geq \pi$**,** $\theta_5 \leq \pi$ **and** $\theta_6 - \theta_3 \leq \pi$**,** $\theta_6 - \theta_2 \geq \pi$**.**

By taking the rotation of angle $-\theta_5$ to $\mathcal{G}$, we obtain a new constellation

$$\mathcal{G}' = \{A'_1, A'_2, \cdots, A'_6\},$$

where $A'_j = e^{-j\theta_5/2}A_j$. For $j = 1, 2, 3, 4$,

$$A'_j = e^{-j\theta_5/2}e^{j\theta_j/2}\hat{A}_j = e^{(2\pi - (\theta_5 - \theta_j))/2}(-\hat{A}_5).$$

For $j = 5$, we have $A'_5 = e^{-j\theta_5/2}A_5 = \hat{A}_5$. For $j = 6$, we have

$$A'_6 = e^{-j\theta_5/2}e^{j\theta_6/2}\hat{A}_6 = e^{(\theta_6 - \theta_5)/2}\hat{A}_6.$$

Therefore, the relationship between $\mathcal{G}'$ and $\mathcal{G}$ is

$$\{\hat{A}'_1, \hat{A}'_2, \hat{A}'_3, \hat{A}'_4, \hat{A}'_5, \hat{A}'_6\} = \{-\hat{A}_1, -\hat{A}_2, -\hat{A}_3, -\hat{A}_4, \hat{A}_5, \hat{A}_6\},$$

and

$$\{\theta'_1, \theta'_2, \theta'_3, \theta'_4, \theta'_5, \theta'_6\} = \{2\pi - \theta_5, 2\pi - (\theta_5 - \theta_2), 2\pi - (\theta_5 - \theta_3), 2\pi - (\theta_5 - \theta_4), 0, \theta_6 - \theta_5\}.$$

Clearly, the diversity product of $\mathcal{G}'$ is still d_6.

We now consider the dual of $\mathcal{G}'$, denoted by $\tilde{\mathcal{G}}'$, which has the same diversity product as $\mathcal{G}'$ by Corollary 1: $\tilde{\mathcal{G}}' = \{\tilde{A}'_1, \tilde{A}'_2, \cdots, \tilde{A}'_6\}$, where $\tilde{A}'_j = e^{\theta''_j/2}\hat{\hat{A}}'_j$, $1 \le j \le 6$. By the definition of a dual, the relationship between $\tilde{\mathcal{G}}'$ and $\mathcal{G}'$ or $\mathcal{G}$ is

$$\begin{aligned}\{\hat{\hat{A}}'_1, \hat{\hat{A}}'_2, \hat{\hat{A}}'_3, \hat{\hat{A}}'_4, \hat{\hat{A}}'_5, \hat{\hat{A}}'_6\} &= \{-\hat{A}'_1, -\hat{A}'_2, -\hat{A}'_3, -\hat{A}'_4, \hat{A}'_5, -\hat{A}'_6\} \\ &= \{\hat{A}_1, \hat{A}_2, \hat{A}_3, \hat{A}_4, \hat{A}_5, -\hat{A}_6\},\end{aligned}$$

and the corresponding angles are

$$\begin{aligned}\{\theta''_1, \theta''_2, \theta''_3, \theta''_4, \theta''_5, \theta''_6\} &= \{2\pi - \theta'_1, 2\pi - \theta'_2, 2\pi - \theta'_3, 2\pi - \theta'_4, 0, 2\pi - \theta'_6\} \\ &= \{\theta_5, \theta_5 - \theta_2, \theta_5 - \theta_3, \theta_5 - \theta_4, 0, 2\pi - (\theta_6 - \theta_5)\}.\end{aligned}$$

It is easy to see that $\theta''_6 \ge \pi$ and $\theta''_j \le \pi$ for $j = 1, 2, 3, 4, 5$. Furthermore,

$$\theta''_6 - \theta''_1 \le \pi, \quad \theta''_6 - \theta''_2 \le \pi, \theta''_6 - \theta''_j \ge \pi, \quad j = 3, 4, 5.$$

Thus, if we rearrange $\tilde{\mathcal{G}}'$ into

$$\mathcal{G}'' = \{\tilde{A}'_5, \tilde{A}'_4, \tilde{A}'_3, \tilde{A}'_2, \tilde{A}'_1, \tilde{A}'_6\},$$

then the conditions on $\mathcal{G}''$ are exactly the same as the ones in Case I.2. By Proposition 3, we have proved this theorem in this subcase.

Case I.4 $\quad \theta_6 \ge \pi$**,** $\theta_5 \le \pi$ **and** $\theta_6 - \theta_2 \le \pi$

Make a rotation angle $-\theta_2$ to the constellation $\mathcal{G}$ as done in Case I.3 and we find that the new constellation has the same conditions as in Case I.1. Therefore, by Proposition 2, we have proved this theorem in this subcase.

Case II $\quad \theta_6, \theta_5 \ge \pi$ **and** $\theta_4 \le \pi$**.**

We divide this proof into 4 subcases.

Case II.1 $\quad \theta_6, \theta_5 \ge \pi$**,** $\theta_4 \le \pi$ **and** $\theta_6 - \theta_4 \ge \pi$**.**

In this case, we make a rotation to the constellation as follows. Let $A'_j = e^{-j\theta_6/2}A_j$ for $j = 1, 2, \cdots, 6$. Then $\{A'_1, A'_2, \cdots, A'_6\}$ is also an optimal constellation. Since, for $j = 1, 2, 3, 4, 5$, $A'_j = e^{-j\theta_6/2}A_j = e^{j(2\pi - (\theta_6 - \theta_j))/2} \cdot (-\hat{A}_j)$, we obtain $\hat{A}'_j = -\hat{A}_j$ and the angle θ'_j of A'_j is $2\pi - (\theta_6 - \theta_j)$. For $j = 6$, $\theta'_6 = 0$, i.e., A'_6 belongs to $\mathbf{SU}(2)$ and $A'_6 = \hat{A}_6$. Furthermore, we have that $\theta'_6, \theta'_1, \theta'_2, \theta'_3, \theta'_4$ are all less than or equal to π, and θ_5' is greater than or equal to π. Therefore, $\{A_1', A_2', \cdots, A_6'\}$ satisfies the conditions in Case I. Thus we have proved this theorem in this subcase.

Case II.2 $\theta_6, \theta_5 \geq \pi$, $\theta_4 \leq \pi$ **and** $\theta_6 - \theta_4 \leq \pi$, $\theta_6 - \theta_3 \geq \pi$.

It is proved in Proposition 4.

Case II.3 $\theta_6, \theta_5 \geq \pi$, $\theta_4 \leq \pi$ **and** $\theta_6 - \theta_3 \leq \pi$, $\theta_6 - \theta_2 \geq \pi$.

It is proved in Proposition 5.

Case II.4 $\theta_6, \theta_5 \geq \pi$, $\theta_4 \leq \pi$ **and** $\theta_6 - \theta_2 \leq \pi$.

Let $A_{j-1}' = e^{-j\theta_2/2} A_j$ for $j = 2, 3, 4, 5, 6$, and $A_6' = e^{(2\pi - j\theta_2)/2} A_1$. Note that $\hat{A}_1 = A_1$ since $\theta_1 = 0$. Then, $\{A_1', A_2', A_3', A_4', A_5', A_6'\}$ satisfies the conditions of Case I.

Case III $\theta_6, \theta_5, \theta_4 \geq \pi$ **and** $\theta_3 \leq \pi$.

Under this assumption, we consider the dual constellation: $\theta_1 = 0$ is fixed, and θ_2, θ_3 are changed to $2\pi - \theta_2, 2\pi - \theta_3$, which belong to $[\pi, 2\pi]$, and $\theta_4, \theta_5.\theta_6$ are transferred to $2\pi - \theta_4, 2\pi - \theta_5, 2\pi - \theta_6$, which belong to $[0, \pi]$. Therefore, through this duality, we change this subcase into Case II.

Case IV $\theta_6, \theta_5, \theta_4, \theta_3 \geq \pi$ **and** $\theta_2 \leq \pi$.

Also we consider its dual constellation and find that this case can be converted to Case I.

By summarizing all the above cases, this theorem is proved. **q.e.d.**

4 Conclusion

In this correspondence, we have partially used sphere packing theory to construct 2×2 unitary space-time codes. Although the optimal ones of sizes L below 6 can be constructed from the sphere packings on $\mathbf{S}^3$, i.e., Hamiltonian constellations [9, 16] that reach the upper bound $\frac{1}{2}\sqrt{2L/(L-1)}$ of the maximal diversity products derived in [11]. This upper bound can not be reached when the sizes are above 5 as shown in [11]. The critical boundary on the sizes is size $L = 6$. In this correspondence, we have constructed 2×2 unitary space-time code of size 6 that has been shown in this correspondence to have the optimal diversity product. The optimal diversity product $d_6 = \frac{1}{2}\sqrt{-5/2 + \sqrt{22}} \approx 0.74 < 0.7746 \approx \frac{1}{2}\sqrt{2L/(L-1)}$ when $L = 6$. Some constructions of 2×2 unitary space-time codes of sizes $32, 48, 64$ of non-Hamiltonian constellations with best known diversity products have been also presented by partially using sphere packing theory. To obtain these results, we have presented a determinant identity between the difference matrices of two matrices in a Hamiltonian constellation and two matrices in non-Hamiltonian constellations.

Appendix

In this Appendix, we always assume that $0 \leq \arccos(x) \leq \pi$.

Proof of Lemma 2

Condition $d_L \geq 2$ implies that for any i, j, $|\det(A_i - A_j)| \geq 2$. Therefore, from Corrollary 1, we have

$$|\det(\hat{A}_i - \hat{A}_j) - 4\sin^2((\theta_i - \theta_j)/4)| \geq 2.$$

If $|\theta_i - \theta_j| \leq \pi$, then

$$0 \leq 4\sin^2((\theta_i - \theta_j)/4) \leq 2.$$

Therefore, by noting that $\det(\hat{A}_i - \hat{A}_j) \geq 0$ from (4) and Corollary 1, we obtain

$$|\det(A_i - A_j)| = \det(\hat{A}_i - \hat{A}_j) - 4\sin^2((\theta_i - \theta_j)/4).$$

The second inequality can be similarly proved. **q.e.d.**

Proof of Lemma 3

Assume that there is an index u such that $\theta_{u+1} - \theta_u \geq \pi$, we want to derive a contradiction.

Since $\theta_{u+1} - \theta_u \geq \pi$ and $0 \leq \theta_u \leq \theta_{u+1} < 2\pi$, we have $\theta_u \leq \pi \leq \theta_{u+1}$. Let us consider a new constellation $\{\hat{A}_1, \cdots, \hat{A}_u, -\hat{A}_{u+1}, \cdots, -\hat{A}_L\} \subseteq \mathbf{SU}(2)$. We want to show that this new constellation on $\mathbf{S}^3$ has the minimum Euclidean distance $\sqrt{d_L}$.

For $i < j \leq u$, $0 \leq \theta_i \leq \theta_j \leq \theta_u \leq \pi$, hence $\theta_j - \theta_i \leq \pi$. By Lemma 2,

$$\det(\hat{A}_i - \hat{A}_j) = |\det(A_i - A_j)| + 4\sin^2((\theta_i - \theta_j)/4) \geq d_L > 2.$$

For $i > j \geq u+1$, since $\theta_{u+1} \geq \pi$, we have $\theta_i - \theta_j \leq \pi$. Therefore, by Lemma 2, we have

$$\det(-\hat{A}_i - (-\hat{A}_j)) = \det(\hat{A}_i - \hat{A}_j) = |\det(A_i - A_j)| + 4\sin^2((\theta_i - \theta_j)/4) \geq d_L > 2.$$

For $i \leq u < u+1 \leq j$, since $\theta_j - \theta_i \geq \theta_{u+1} - \theta_u \geq \pi$, by Lemma 2 we have

$$\det(\hat{A}_j - \hat{A}_i) = 4\sin^2((\theta_j - \theta_i)/4) - |\det(A_j - A_i)|.$$

Note that $\det(-\hat{A}_j - \hat{A}_i) = 4 - \det(\hat{A}_j - \hat{A}_i)$. Thus,

$$\det(-\hat{A}_j - \hat{A}_i) = 4 - 4\sin^2((\theta_j - \theta_i)/4) + |\det(A_j - A_i)| \geq |\det(A_j - A_i)| \geq d_L.$$

Therefore, using (4) we have shown that the minimum Euclidean distance of the points $\{\hat{A}_1, \cdots, \hat{A}_u, -\hat{A}_{u+1}, -\hat{A}_L\}$ on $\mathbf{S}^3$ is greater than $\sqrt{d_L} > \sqrt{2}$. This contradicts with the fact that, when $L \geq 6$, the maximal minimum distance of L-point packing on the sphere $\mathbf{S}^3$ is $\sqrt{2}$ from the packing theory [20]. **q.e.d.**

Proof of Lemma 4

We only prove the case of $L = 4$ and the other cases can be similarly proved.

We first prove that there exists t, $1 \le t \le 4$, such that $\|\mathbf{P}_0 - \mathbf{P}_t\|^2 \le 2 + 2\sqrt{1 - 3d/8}$. Since an orthogonal transformation does not change the distance between any two points, without loss of generality, we may assume $\mathbf{P}_0 = (1, 0, 0, 0)$. Let $\mathbf{P}_i = (a_i, b_i, c_i, e_i)$. Then, $\|\mathbf{P}_j - \mathbf{P}_0\|^2 = 2 - 2a_j$.

We may assume that $a_i \neq 1, -1$. In fact, if $a_i = 1$, we let $t = i$, which is because $\|\mathbf{P}_t - \mathbf{P}_0\|^2 = 0 < 2 + 2\sqrt{1 - 3d/8}$. If $a_i = -1$, then $\|\mathbf{P}_i - \mathbf{P}_0\|^2 = 4$. Let $t \neq i$ and we have

$$\begin{aligned}\|\mathbf{P}_t - \mathbf{P}_0\|^2 &= 2 - 2a_t = 4 - (2 + 2a_t) = 4 - \|\mathbf{P}_t - \mathbf{P}_i\|^2 \\ &\le 4 - d \le 2 + 2\sqrt{1 - 3d/8},\end{aligned}$$

where the third equality is from the assumption $a_i = -1$, and the first inequality is from the assumption $\|\mathbf{P}_t - \mathbf{P}_i\|^2 \ge d$.

We next derive a contradiction by assuming $\|\mathbf{P}_i - \mathbf{P}_0\|^2 > 2 + 2\sqrt{1 - 3d/8}$ for $i = 1, 2, 3, 4$. Since $\|\mathbf{P}_i - \mathbf{P}_0\|^2 = 2 - 2a_i$, we have

$$a_i < -\sqrt{1 - 3d/8}. \tag{19}$$

On the other hand, since $\|\mathbf{P}_i - \mathbf{P}_j\|^2 \ge d$, we have

$$2 - 2a_ia_j + (\|\mathbf{b}_i - \mathbf{b}_j\|^2 - 2)r_ir_j \ge d,$$

where $r_i, r_j, \mathbf{b}_i, \mathbf{b}_j$ are the same as those described in (11)-(13) in the proof of Theorem 1. Since $a_i, a_j \neq 1$ or -1, we have $r_i, r_j > 0$. Therefore, we obtain

$$\|\mathbf{b}_i - \mathbf{b}_j\|^2 \ge 2 + \frac{d - 2 + 2a_ia_j}{r_ir_j}, \quad i, j = 1, 2, 3, 4, i \neq j. \tag{20}$$

From (19), we know that $a_j \le 0$. It is not hard to check that, on interval $(-1, 0]$, the right hand side of (20) is strictly decreasing for a_i and a_j. Therefore, by using (19), we obtain

$$\begin{aligned}\|\mathbf{b}_i - \mathbf{b}_j\|^2 &\ge 2 + \frac{d - 2 + 2a_ia_j}{r_ir_j} \\ &> 2 + \frac{d - 2 + 2(1 - 3d/8)}{1 - (1 - 3d/8)} = 8/3, \quad i, j = 1, 2, 3, 4, i \neq j.\end{aligned} \tag{21}$$

Clearly, (21) contradicts with the result of 4-point packing on $\mathbf{S}^2$. This proves that there exists a $t \in \{1, 2, 3, 4\}$ such that

$$\|\mathbf{P}_0 - \mathbf{P}_t\|^2 \le 2 + 2\sqrt{1 - 3d/8}.$$

We next prove that there exists an $s \in \{1, 2, 3, 4\}$ such that

$$\|\mathbf{P}_0 - \mathbf{P}_s\|^2 \ge 2 - 2\sqrt{1 - 3d/8}. \tag{22}$$

To do so, let us consider point $-\mathbf{P}_0$. By the above result, there exists an $s \in \{1,2,3,4\}$ such that

$$\| - \mathbf{P}_0 - \mathbf{P}_s\|^2 \leq 2 + 2\sqrt{1 - 3d/8}.$$

Since

$$\| - \mathbf{P}_0 - \mathbf{P}_s\|^2 = 2 + 2a_s = 4 - (2 - 2a_s) = 4 - \|\mathbf{P}_0 - \mathbf{P}_s\|^2,$$

we obtain

$$4 - \|\mathbf{P}_0 - \mathbf{P}_s\|^2 \leq 2 + 2\sqrt{1 - 3d/8},$$

or

$$\|\mathbf{P}_0 - \mathbf{P}_s\|^2 \geq 2 - 2\sqrt{1 - 3d/8}.$$

q.e.d.

Proof of Lemma 6

Let $\hat{A}_j = (a_j, b_j, c_j, e_j)$ for $j = 1,2,3$. We want to convert these three 4-dimensional unit vectors equivalently into three 3-dimensional unit vectors by employing orthogonal transformations. We may first assume $\hat{A}_1 = I$. By using a rotation

$$\begin{pmatrix} 1 & 0 \\ 0 & R \end{pmatrix}$$

on $\mathbf{S}^3$, we can assume $\hat{A}_2 = (a_2, r_2, 0, 0)$, where R is a 3×3 orthogonal matrix, and $r_2 = \sqrt{1 - a_2^2}$. Similarly, using a rotation

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & T \end{pmatrix}$$

on $\mathbf{S}^3$, we can assume $\hat{A}_3 = (a_3, r_3, c_3, 0)$, where T is a 2×2 orthogonal matrix. Thus, after normalizations, we may assume $\hat{A}_1, \hat{A}_2, \hat{A}_3$ of the following forms:

$$\hat{A}_1 = (1,0,0,0), \quad \hat{A}_2 = (a_2, r_2, 0, 0), \quad \hat{A}_3 = (a_3, b_3, c_3, 0),$$

which are equivalent to three 3-dimensional vectors on the 2-dimensional sphere $\mathbf{S}^2$. Furthermore, we may assume $\theta_1 = 0$.

Because $\theta_3 - \theta_1 \leq \pi$ and $0 = \theta_1 \leq \theta_2 \leq \theta_3$, it is obvious that $\theta_2, \theta_3 \leq \pi$ and $\theta_3 - \theta_2 \leq \pi$. Therefore, by Lemma 2 and the condition $|\det(A_i - A_j)| \geq d_6$, we have

$$\det(\hat{A}_i - \hat{A}_j) \geq d_6 + 4\sin^2((\theta_i - \theta_j)/4), \quad 1 \leq i < j \leq 3. \tag{23}$$

From (23), we have $\det(\hat{A}_1 - \hat{A}_2) > 2$, $\det(\hat{A}_1 - \hat{A}_3) > 2$, and $\det(\hat{A}_3 - \hat{A}_2) > 2$. This means that the points $\hat{A}_2, \hat{A}_3$ are on the different half sphere from the point $\hat{A}_1$.

Let O be the original point of coordinates and γ_{12} be the angle $\angle A_1OA_2$, γ_{13} be the angle $\angle A_1OA_3$. Then,

$$\begin{aligned} 2-2\cos(\gamma_{12}) &= \det(\hat{A}_1-\hat{A}_2) \geq d_6+4\sin^2(\theta_2/4), && (24)\\ 2-2\cos(\gamma_{13}) &= \det(\hat{A}_1-\hat{A}_3) \geq d_6+4\sin^2(\theta_3/4), && (25)\end{aligned}$$

Clearly, when $\hat{A}_1,\hat{A}_2,\hat{A}_3$ are on the same circle, the distance between $\hat{A}_2$ and $\hat{A}_3$ achieves the maximum. Therefore,

$$\det(\hat{A}_2-\hat{A}_3) \leq 2-2\cos(2\pi-\gamma_{12}-\gamma_{13}) = 2-2\cos(\gamma_{12}+\gamma_{13}).$$

Applying (23) for $i=2$ and $j=3$, we get that

$$d_6+4\sin^2((\theta_3-\theta_2)/4) \leq 2-2\cos(\gamma_{12}+\gamma_{13}).$$

That is

$$d_6/2+\cos(\gamma_{12}+\gamma_{13}) \leq \cos((\theta_3-\theta_2)/2). \tag{26}$$

From (24),(25), we have $\gamma_{12} \geq \arccos(\cos(\theta_2/2)-d_6/2)$ and $\gamma_{13} \geq \arccos(\cos(\theta_3/2)-d_6/2)$. But from (26), noticing that $\pi \leq \gamma_{12}+\gamma_{13} \leq 2\pi$, we have $\gamma_{12}+\gamma_{13} \leq \pi+\arccos(d_6/2-\cos((\theta_3-\theta_2)/2))$. Hence,

$$\begin{aligned}&\pi+\arccos(d_6/2-\cos((\theta_3-\theta_2)/2))\\ &\quad -\arccos(\cos(\theta_2/2)-d_6/2)-\arccos(\cos(\theta_3/2)-d_6/2) \geq 0.\end{aligned} \tag{27}$$

We can check that the left hand side of (27), is decreasing for d_6. By condition $d_6 \geq \sqrt{22}-5/2$, we then have

$$\begin{aligned}&\pi+\arccos((\sqrt{22}-5/2)/2-\cos((\theta_3-\theta_2)/2))\\ &\quad -\arccos(\cos(\theta_2/2)-(\sqrt{22}-5/2)/2)-\arccos(\cos(\theta_3/2)-(\sqrt{22}-5/2)/2) \geq 0.\end{aligned} \tag{28}$$

Assume $\theta_3 > 5\pi/6$, we want to derive a contradiction. In fact, by investigating the left hand side of (28), we find that it is decreasing for θ_3. Therefore, we have

$$\begin{aligned}&\pi+\arccos((\sqrt{22}-5/2)/2-\cos((5\pi/6-\theta_2)/2))\\ &\quad -\arccos(\cos(\theta_2/2)-(\sqrt{22}-5/2)/2)-\arccos(\cos(5\pi/12)-(\sqrt{22}-5/2)/2) \geq 0,\end{aligned} \tag{29}$$

which is impossible since the maximum of the left hand side of (29) for $\theta_2 \in [0,\pi]$ is less than -0.02. Therefore, the lemma is proved. **q.e.d**

Proof of Lemma 7

Let

$$f(x) = 2\sin(\arccos(a+d/2)/2) - \frac{x-\cos(\arccos(d/2+x)+\arccos(d/2+a))-d/2}{\cos(\arccos(-a)/2)} - d.$$

Then, to prove the lemma, it is enough to prove that $f(x) \geq 0$ for $-1 < x \leq 1 - d/2$. Obviously, $f(x)$ is an infinitely differentiable function in the interval $(-1, 1 - d/2)$. Moreover, its derivative is

$$f'(x) = -\frac{\sqrt{1-(d/2+x)^2} - \sin(\arccos(d/2+x) + \arccos(d/2+a))}{\sqrt{1-(d/2+x)^2}\cos(\arccos(-a)/2)}.$$

Hence, equation $f'(x) = 0$ becomes

$$\sin(\arccos(d/2+x) + \arccos(d/2+a)) = \sin(\arccos(d/2+x)).$$

Since $\arccos(d/2+x) + \arccos(d/2+a) \geq \pi/2$ and $\arccos(d/2+x) < \pi/2$, the *unique* solution x_0 of the equation $f'(x) = 0$ satisfies

$$\arccos(d/2+x_0) + \arccos(d/2+a) = \pi - \arccos(d/2+x_0).$$

Hence,

$$x_0 = \sin(\arccos(d/2+a)/2) - d/2.$$

The second derivative of $f(x)$ at x_0 is

$$f''(x_0) = \frac{2\sin(\arccos(d/2+a)/2)}{\cos^2(\arccos(d/2+a)/2)\cos(\arccos(-a)/2)} > 0.$$

Thus, we have shown that, the equation $f'(x) = 0$ has unique solution x_0 in the interval $(-1, 1-d/2)$ and $f''(x_0) > 0$. Therefore, $f(x_0)$ is the minimum value of $f(x)$ in this interval, that is, $f(x) \geq f(x_0)$ for $x \in (-1, 1-d/2)$. On the other hand,

$$f(x_0) = \frac{(1-\cos(\arccos(-a)/2))(d - 2\sin(\arccos(d/2+a)/2))}{\cos(\arccos(-a)/2)} \geq 0,$$

where the inequality comes from the assumption $d > 2$ and $a \leq 1 - d/2 < 0$. This proves that, when $b \in (-1, 1-d/2)$, we have $f(b) \geq 0$. If $b = 1 - d/2$, then we have $\arccos(d/2+b) = 0$, which implies $\arccos(d/2+b) + \arccos(d/2+a) = \arccos(d/2+a) \leq \pi/2$ that contradicts with the condition. This shows that $b \neq 1 - d/2$ in the lemma. Therefore, we have proved the lemma. **q.e.d.**

Proof of Proposition 2

We denote $\mathcal{G} = \{A_1, \cdots, A_6\}$ and inherit the previous notations (a_i, b_i, c_i, e_i) for $\hat{A}_i, i = 1, \cdots, 6$, and assume that $\hat{A}_5 = I$. Since for $1 \leq j \leq 4$ and $j = 6$, $|\theta_5 - \theta_j| \leq \pi$, from Lemma 2,

$$2 < d_6 \leq |\det(A_5 - A_j)| = 2 - 2a_j - 4\sin^2((\theta_5 - \theta_j)/4). \tag{30}$$

This implies $a_j \leq \cos((\theta_5 - \theta_j)/2) - d_6/2 \leq 1 - d_6/2 < 0$ for $j = 1, 2, \cdots, 6$.

We divide the proof of this proposition into two cases according to the number a_6: one is $a_6 = -1$ and the other is $a_6 > -1$.

Case 1 $a_6 = -1$.

Since $a_6 = -1$, we have $\hat{A}_6 = (-1, 0, 0, 0)$. If there exists a $j \in \{1, 2, 3\}$ such that $a_j = -1$, then $b_j = c_j = e_j = 0$ and $\det(\hat{A}_4 - \hat{A}_j) = 2 + 2a_4$. Thus, from Lemma 2 we have

$$\begin{aligned} 2 < d_6 \leq |\det(A_4 - A_j)| &= \det(\hat{A}_4 - \hat{A}_j) - 4\sin^2((\theta_4 - \theta_j)/4) \\ &= 2\cos((\theta_4 - \theta_j)/2) + 2a_4, \end{aligned}$$

which contradicts with the fact $a_4 < 0$. Hence, $a_j > -1$ for $j = 1, 2, 3$. Similarly, we can prove $a_4 > -1$. Therefore, $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3, \mathbf{b}_4$ are well-defined in (11) and belong to $\mathbf{S}^2$.

From the result of [11], the optimal determinant for 5 unitary matrices is 12/5, so we have $d_6 \leq 12/5 = 2.4$. We next show that there exists at least one a_j for $j \in \{1, 2, 3, 4\}$ such that $a_j \geq -\sqrt{1 - 3d_6/8}$. Otherwise, assume, for all $j \in \{1, 2, 3, 4\}$, $a_j < -\sqrt{1 - 3d_6/8}$. Then, from the optimal constellation conditions, we have

$$d_6 \leq \det(\hat{A}_i - \hat{A}_j) - 4\sin^2((\theta_i - \theta_j)/4) \leq \det(\hat{A}_i - \hat{A}_j).$$

Using (13), we obtain

$$\begin{aligned} \|\mathbf{b}_i - \mathbf{b}_j\|^2 &\geq 2 + \frac{d_6 - 2 + 2a_i a_j}{r_i r_j} \\ &> 2 + \frac{d_6 - 2 + 2(-\sqrt{1 - 3d_6/8})^2}{(1 - (-\sqrt{1 - 3d_6/8})^2)} = \frac{8}{3}. \end{aligned}$$

where the second inequality is from the assumption $a_i, a_j < -\sqrt{1 - 3d_6/8}$ and the fact that the right hand side of the first inequality above is decreasing for $1 < a_i, a_j < 0$. Therefore,

$$\sum_{1 \leq i < j \leq 4} \|\mathbf{b}_i - \mathbf{b}_j\|^2 > 6 \times \frac{8}{3} = 16,$$

which contradicts with the result in Lemma 5. Thus, we have proven that there exists an a_j, $j \in \{1, 2, 3, 4\}$, such that $a_j \geq -\sqrt{1 - 3d_6/8}$.

Since $a_6 = -1$ and $\theta_6 - \theta_j \geq \pi$, from Lemma 2 we have

$$\begin{aligned} d_6 &\leq |\det(A_6 - A_j)| = 4\sin^2((\theta_6 - \theta_j)/4) - \det(\hat{A}_6 - \hat{A}_j) \\ &= 4\sin^2((\theta_6 - \theta_j)/4) - (2 + 2a_j) \\ &\leq -2\cos((\theta_6 - \theta_j)/2) + 2\sqrt{1 - 3d_6/8}, \end{aligned}$$

which implies

$$\cos((\theta_6 - \theta_j)/2) \leq \sqrt{1 - 3d_6/8} - d_6/2. \tag{31}$$

On the other hand, from $|\det(A_6 - A_5)| \geq d_6$, i.e.,

$$d_6 \leq \det(\hat{A}_6 - \hat{A}_5) - 4\sin^2((\theta_6 - \theta_5)/4) = 2 + 2 - 4\sin^2((\theta_6 - \theta_5)/4),$$

we have

$$\cos((\theta_6-\theta_5)/2) \geq d_6/2-1. \qquad (32)$$

Similarly, from $|\det(A_5-A_j)| \geq d_6$ and $\theta_5-\theta_j \leq \pi$, we have

$$d_6 \leq |\det(A_5-A_j)| = \det(\hat{A}_5-\hat{A}_j)-4\sin^2((\theta_5-\theta_j)/4) = 2-2a_j-4\sin^2((\theta_5-\theta_j)/4),$$

which implies

$$\cos((\theta_5-\theta_j)/2) \geq d_6/2+a_j \geq d_6/2-\sqrt{1-3d_6/8}. \qquad (33)$$

Since (31), (32), and (33) have the same forms as the ones of (15), (17), and (18), we can use the same technique used in the proof of Case (iii) when $p=4$ in the proof of Theorem 1 as follows. From (31) and (33), we have

$$\theta_6-\theta_j \geq 2\arccos(\sqrt{1-3d_6/8}-d_6/2) \quad \text{and} \quad \theta_5-\theta_j \leq 2\arccos(d_6/2-\sqrt{1-3d_6/8}).$$

Hence,

$$\begin{aligned}\theta_6-\theta_5 &\geq 2\arccos(\sqrt{1-3d_6/8}-d_6/2)-2\arccos(d_6/2-\sqrt{1-3d_6/8})\\ &= 2\pi-4\arccos(d_6/2-\sqrt{1-3d_6/8}).\end{aligned}$$

From (32), we have $\theta_6-\theta_5 \leq 2\arccos(d_6/2-1)$. Therefore,

$$2\pi-4\arccos(d_6/2-\sqrt{1-3d_6/8}) \leq 2\arccos(d_6/2-1),$$

which implies $d_6 \leq -5/2+\sqrt{22}$.

Case 2 $a_6 > -1$.

The main idea of the following proof of this case is to construct a new constellation, $\mathcal{G}^{**}$, that also has the diversity product d_6 and satisfies the conditions of Case 1. To do so, we first take some rotations and duals of $\mathcal{G}$ to generate a constellation $\mathcal{G}''$. Using $\mathcal{G}''$ and $\mathcal{G}$, we can obtain a desired $\mathcal{G}^{**}$. We next divide the proof into three steps. The first step is to diagonalize matrix $\hat{A}_6$ without altering $\hat{A}_5 = I$ and other properties and to establish an equality on a_6. The second step is to construct a constellation $\mathcal{G}''$ through rotations and duals of $\mathcal{G}$. The third one is to construct $\mathcal{G}^{**}$.

Step 1. Diagonalization of $\hat{A}_6$ and an equality on a_6

Since $a_6 > -1$, vector $\mathbf{b}_6$ is a well-defined point on the sphere $\mathbf{S}^2$. Then, there exists a real-valued rotation T on $\mathbf{S}^2$ such that $\mathbf{b}_6 \cdot T = (1,0,0)$. Let

$$Q = \begin{pmatrix} 1 & 0 \\ 0 & T \end{pmatrix}.$$

Then, Q is an orthogonal matrix and

$$\begin{aligned}(a_6,b_6,c_6,e_6)\cdot Q &= (a_6,(b_6,c_6,e_6)\cdot T) = (a_6, r_6(b_6/r_6, c_6/r_6, e_6/r_6)\cdot T)\\ &= (a_6, r_6\mathbf{b}_6\cdot T) = (a_6, r_6, 0, 0),\end{aligned}$$

and $(1,0,0,0)\cdot Q=(1,0,0,0)$, where $r_6=\sqrt{1-a_6^2}$. If we let

$$(\tilde{a}_j,\tilde{b}_j,\tilde{c}_j,\tilde{e}_j)=(a_j,b_j,c_j,e_j)\cdot Q,\ \ 1\le j\le 6,$$

then, these points are on the unit sphere $\mathbf{S}^3$. By using the mapping i^{-1} defined in Section 2, we obtain six 2×2 unitary matrices belonging to $\mathbf{SU}(2)$. Denote these matrices by $\tilde{\hat{A}}_j$ for $1\le j\le 6$. Then, $\tilde{\hat{A}}_5=I$ and

$$\tilde{\hat{A}}_6=\begin{pmatrix} a_6+jr_6 & 0\\ 0 & a_6-jr_6\end{pmatrix},$$

which is diagonal. Furthermore, since Q is an orthogonal matrix, we have

$$\begin{aligned}\det(\tilde{\hat{A}}_i-\tilde{\hat{A}}_j) &= \|i(\tilde{\hat{A}}_i)-i(\tilde{\hat{A}}_j)\|^2=\|i(\hat{A}_i)-i(\hat{A}_j)\|^2\\ &= \det(\hat{A}_i-\hat{A}_j),\quad 1\le i<j\le 6,\end{aligned}$$

where the first equality is from (8), and the second equality is from the fact that Q is orthogonal, and the last equality is also from (8). Set $\tilde{A}_j=e^{j\theta_j/2}\tilde{\hat{A}}_j$ for $1\le j\le 6$. Then, by Corollary 1,

$$\det(\tilde{A}_i-\tilde{A}_j)=\det(A_i-A_j),\quad 1\le i<j\le 6.$$

Thus, we have obtained a constellation that has diversity product d_6 but $\tilde{\hat{A}}_5=I$ and $\tilde{\hat{A}}_6$ is diagonal. Therefore, in the following proof, we assume the constellation $\mathcal{G}$ has the property: $\hat{A}_5=I$ and $\hat{A}_6$ has the above diagonal form.

We now establish an equality on a_6. According to the relationships among the angles, the following inequality are clear by using the optimality conditions and Corollary 1:

$$\begin{aligned} d_6 &\le |\det(A_6-A_j)|=4\sin^2((\theta_6-\theta_j)/4)-\det(\hat{A}_6-\hat{A}_j),\quad j=1,2,3,4, &(34)\\ d_6 &\le |\det(A_5-A_j)|=\det(\hat{A}_5-\hat{A}_j)-4\sin^2((\theta_5-\theta_j)/4)\\ &= 2-2a_j-4\sin^2((\theta_5-\theta_j)/4)=2\cos((\theta_5-\theta_j)/2)-2a_j,\quad j=1,2,3,4, &(35)\\ d_6 &\le |\det(A_6-A_5)|=\det(\hat{A}_6-\hat{A}_5)-4\sin^2((\theta_6-\theta_5)/4)\\ &= 2-2a_6-4\sin^2((\theta_6-\theta_5)/4)=2\cos((\theta_6-\theta_5)/2)-2a_6. &(36)\end{aligned}$$

Furthermore, we may assume the equality holds in (36), i.e.,

$$\begin{aligned} d_6 &= |\det(A_6-A_5)|=\det(\hat{A}_6-\hat{A}_5)-4\sin^2((\theta_6-\theta_5)/4)\\ &= 2-2a_6-4\sin^2((\theta_6-\theta_5)/4)=2\cos((\theta_6-\theta_5)/2)-2a_6. \qquad (37)\end{aligned}$$

In fact, if

$$d_6<\det(\hat{A}_6-\hat{A}_5)-4\sin^2((\theta_6-\theta_5)/4)=2-2a_6-4\sin^2((\theta_6-\theta_5)/4)=2\cos((\theta_6-\theta_5)/2)-2a_6,$$

then,

$$d_6/2+a_6<\cos((\theta_6-\theta_5)/2)\le 1.$$

Since $d_6 > 2$ and $a_6 > -1$, we have $d_6/2+a_6 > 0$. Therefore, $0 \le \arccos(d_6/2+a_6) < \pi/2$ is well-defined. Let $\theta_6' = \theta_5 + 2\arccos(d_6/2 + a_6)$. Then $0 \le \theta_6' - \theta_5 < \pi$, $\theta_6' < 2\pi$ (due to the assumption $\theta_5 \le \pi$), and

$$\cos((\theta_6' - \theta_5)/2) = \frac{d_6}{2} + a_6 < \cos((\theta_6 - \theta_5)/2).$$

Therefore, $\theta_6' > \theta_6$. Let $A_6' = e^{j\theta_6'/2}\hat{A}_6$. Clearly,

$$\begin{aligned} |\det(A_6' - A_5)| &= \det(\hat{A}_6 - \hat{A}_5) - 4\sin^2((\theta_6' - \theta_5)/4) \\ &= -2a_6 + 2\cos((\theta_6' - \theta_5)/2) = -2a_6 + 2(d_6/2 + a_6) = d_6 \end{aligned}$$

On the other hand, for $j = 1, 2, 3, 4$, $\theta_6' - \theta_j > \theta_6 - \theta_j \ge \pi$, and hence,

$$\begin{aligned} |\det(A_6' - A_j)| &= 4\sin^2((\theta_6' - \theta_j)/4) - \det(\hat{A}_6 - \hat{A}_j) \\ &> 4\sin^2((\theta_6 - \theta_j)/4) - \det(\hat{A}_6 - \hat{A}_j) \ge d_6. \end{aligned}$$

Therefore, $\{A_1, \cdots, A_5, A_6'\}$ is also an optimal design with $d_6 = \det(\hat{A}_6 - \hat{A}_5) - 4\sin^2((\theta_6' - \theta_5)/4)$ and $\hat{A}_6' = \hat{A}_6$. Thus, in the following proof of this proposition, we assume (37) holds. From (37), we obtain

$$a_6 = \cos((\theta_6 - \theta_5)/2) - d_6/2. \tag{38}$$

Step 2. Rotations and duals of $\mathcal{G}$.

Let us first make a rotation of angle $-\theta_4$ to $\mathcal{G}$ to generate a new constellation. Denote this new constellation as $\mathcal{G}^*$, i.e., we define $\mathcal{G}^* = \{A_1^*, A_2^*, A_3^*, A_4^*, A_5^*, A_6^*\}$ where $A_j^* = e^{-j\theta_4/2}A_j$. For $j = 1, 2, 3$, $A_j^* \in \mathbf{SU}(2, 2\pi - (\theta_4 - \theta_j))$, and for $j = 4, 5, 6$, $A_j^* \in \mathbf{SU}(2, (\theta_j - \theta_4))$. Therefore,

$$\{\hat{A}_1^*, \hat{A}_2^*, \hat{A}_3^*, \hat{A}_4^*, \hat{A}_5^*, \hat{A}_6^*\} = \{-\hat{A}_1, -\hat{A}_2, -\hat{A}_3, \hat{A}_4, \hat{A}_5, \hat{A}_6\},$$

and

$$\{\theta_1^*, \theta_2^*, \theta_3^*, \theta_4^*, \theta_5^*, \theta_6^*\} = \{2\pi - \theta_4, 2\pi - (\theta_4 - \theta_2), 2\pi - (\theta_4 - \theta_3),\ \ 0,\ \ \theta_5 - \theta_4, \theta_6 - \theta_4\}.$$

Note that $\theta_4^* = 0$ and $\hat{A}_4^* \in \mathbf{SU}(2)$.

We next consider the dual of $\mathcal{G}^*$ and denote this dual as $\tilde{\mathcal{G}^*}$, i.e.,

$$\tilde{\mathcal{G}^*} = \{\tilde{A}_1^*, \tilde{A}_2^*, \tilde{A}_3^*, \tilde{A}_4^*, \tilde{A}_5^*, \tilde{A}_6^*\},$$

where $\tilde{A}_j^*$ is the dual of A_j^*. By the definition of dual, we have

$$\begin{aligned} \{\hat{\tilde{A}}_1^*, \hat{\tilde{A}}_2^*, \hat{\tilde{A}}_3^*, \hat{\tilde{A}}_4^*, \hat{\tilde{A}}_5^*, \hat{\tilde{A}}_6^*\} &= \{-\hat{A}_1^*, -\hat{A}_2^*, -\hat{A}_3^*, \hat{A}_4, -\hat{A}_5^*, -\hat{A}_6^*\} \\ &= \{\hat{A}_1, \hat{A}_2, \hat{A}_3, \hat{A}_4, -\hat{A}_5, -\hat{A}_6\} \end{aligned}$$

and their corresponding angles

$$\begin{aligned} \{\tilde{\theta}_1^*, \tilde{\theta}_2^*, \tilde{\theta}_3^*, \tilde{\theta}_4^*, \tilde{\theta}_5^*, \tilde{\theta}_6^*\} &= \{2\pi - \theta_1^*, 2\pi - \theta_2^*, 2\pi - \theta_3^*, \theta_4^*, 2\pi - \theta_5^*, 2\pi - \theta_6^*\} \\ &= \{\theta_4, \theta_4 - \theta_2, \theta_4 - \theta_3,\ \ 0,\ \ 2\pi - (\theta_5 - \theta_4), 2\pi - (\theta_6 - \theta_4)\}. \end{aligned}$$

Notice that in $\tilde{\mathcal{G}}^*$, $\tilde{\theta}_4^* = 0$, i.e., $\tilde{A}_4^* \in \mathbf{SU}(2)$. To have the right order of angles, we rearrange the order of $\tilde{\mathcal{G}}^*$ as follows. Let

$$A_1' = \tilde{A}_4^*, A_2' = \tilde{A}_3^*, A_3' = \tilde{A}_2^*, A_4' = \tilde{A}_1^*, A_5' = \tilde{A}_6^*, A_6' = \tilde{A}_5^*,$$

If we write $A_j' = e^{j\theta_j'/2}\hat{A}_j' \in \mathbf{SU}(2, \theta_j')$, then

$$\begin{aligned}\{\hat{A}_1', \hat{A}_2', \hat{A}_3', \hat{A}_4', \hat{A}_5', \hat{A}_6'\} &= \{\hat{\tilde{A}}_4^*, \hat{\tilde{A}}_3^*, \hat{\tilde{A}}_2^*, \hat{\tilde{A}}_1^*, \hat{\tilde{A}}_6^*, \hat{\tilde{A}}_5^*\} \\ &= \{\hat{A}_4, \hat{A}_3, \hat{A}_2, \hat{A}_1, -\hat{A}_6, -\hat{A}_5\},\end{aligned}$$

and

$$\begin{aligned}\{\theta_1', \theta_2', \theta_3', \theta_4', \theta_5', \theta_6'\} &= \{\tilde{\theta}_4^*, \tilde{\theta}_3^*, \tilde{\theta}_2^*, \tilde{\theta}_1^*, \tilde{\theta}_6^*, \tilde{\theta}_5^*\} \\ &= \{0, \theta_4 - \theta_3, \theta_4 - \theta_2, \theta_4, 2\pi - (\theta_6 - \theta_4), 2\pi - (\theta_5 - \theta_4)\}.\end{aligned}$$

It is clear that

$$0 = \theta_1' \le \theta_2' \le \theta_3' \le \theta_4' \le \theta_5' \le \theta_6' < 2\pi,$$

and

$$\theta_6' \ge \pi, \;\; \theta_5' \le \pi, \;\; \theta_6' - \theta_4' \ge \pi.$$

This means that the conditions on $\{\theta_1', \theta_2', \cdots, \theta_6'\}$ are the same as those on $\{\theta_1, \theta_2, \cdots, \theta_6\}$. Therefore, constellation $\{A_j'\}$ has the same properties as $\{A_j\}$ does if they have the same normalizations on their projections $\{\hat{A}_j'\}$ as $\{A_j\}$ do, namely $\hat{A}_5' = I$ and $\hat{A}_6'$ is diagonal. It is assumed that $\hat{A}_5 = I$. We now want to convert $\hat{A}'_5$ to I. Because $\hat{A}_5' = -\hat{A}_6$, we multiply $-\hat{A}_6^H$ to $\{A_1', \cdots, A_6'\}$ from the left and the resultant constellation is denoted by $\{A_1'', \cdots, A_6''\} \triangleq \mathcal{G}''$. If we let $A_j'' = e^{j\theta_j''/2}\hat{A}_j''$, then we have

$$\begin{aligned}\{\hat{A}_1'', \hat{A}_2'', \hat{A}_3'', \hat{A}_4'', \hat{A}_5'', \hat{A}_6''\} &= \{-\hat{A}_6^H\hat{A}_1', -\hat{A}_6^H\hat{A}_2', -\hat{A}_6^H\hat{A}_3', -\hat{A}_6^H\hat{A}_4', -\hat{A}_6^H\hat{A}_5', -\hat{A}_6^H\hat{A}_6'\} \\ &= \{-\hat{A}_6^H\hat{A}_4, -\hat{A}_6^H\hat{A}_3, -\hat{A}_6^H\hat{A}_2, -\hat{A}_6^H\hat{A}_1, I, \hat{A}_6^H\}\end{aligned} \tag{39}$$

and

$$\begin{aligned}\{\theta_1'', \theta_2'', \theta_3'', \theta_4'', \theta_5'', \theta_6''\} &= \{\theta_1', \theta_2', \theta_3', \theta_4', \theta_5', \theta_6'\} \\ &= \{0, \theta_4 - \theta_3, \theta_4 - \theta_2, \theta_4, 2\pi - (\theta_6 - \theta_4), 2\pi - (\theta_5 - \theta_4)\},\end{aligned} \tag{40}$$

from which one can see that $\hat{A}_5'' = I$ and $\hat{A}_6''$ is diagonal since $\hat{A}_6^H$ is diagonal. Therefore, constellation $\mathcal{G}''$ has the same properties as $\mathcal{G}$ does. Additionally, from (39), we have $a_5'' = 1$ and $a_6'' = a_6$.

Since $\mathcal{G}''$ has the same angle relationships as those of $\mathcal{G}$, inequalities (34)-(36) are also true if a_j is replaced by a_j'', and θ_j is replaced by θ_j''. Furthermore, since $\theta_6 - \theta_5 = \theta_6'' - \theta_5''$ and $a_6'' = a_6$, equalities (37) and (38) hold for $\mathcal{G}''$.

We next establish some relationships between a_j and a_j'' for $j = 1, 2, 3, 4$.

Let $\alpha = \arccos(-a_6)$. Then $0 \le \alpha < \pi/2$ because $a_6 < 0$. From the form of $\hat{A}_6$ in Step 1, we have

$$\hat{A}_6 = \begin{pmatrix} -\cos\alpha + j\sin\alpha & 0 \\ 0 & -\cos\alpha - j\sin\alpha \end{pmatrix}.$$

Going back to (39), we obtain, for $j = 1, 2, 3, 4$,

$$\begin{aligned} &\begin{pmatrix} a''_j + jb''_j & c''_j + jd''_j \\ -c''_j + jd''_j & a''_j - jb''_j \end{pmatrix} \\ &\quad = \begin{pmatrix} \cos\alpha + j\sin\alpha & 0 \\ 0 & \cos\alpha - j\sin\alpha \end{pmatrix} \begin{pmatrix} a_{4-j+1} + jb_{4-j+1} & c_{4-j+1} + je_{4-j+1} \\ -c_{4-j+1} + je_{4-j+1} & a_{4-j+1} - jb_{4-j+1} \end{pmatrix}. \end{aligned}$$

In other words,

$$\begin{pmatrix} a''_j \\ b''_j \\ c''_j \\ d''_j \end{pmatrix} = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 & 0 \\ \sin\alpha & \cos\alpha & 0 & 0 \\ 0 & 0 & \cos\alpha & -\sin\alpha \\ 0 & 0 & \sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} a_{4-j+1} \\ b_{4-j+1} \\ c_{4-j+1} \\ e_{4-j+1} \end{pmatrix}, \quad j = 1, 2, 3, 4. \tag{41}$$

We need more relationships between coefficients a_j and a''_j for $j = 1, 2, 3, 4$. For $j = 1, 2, 3, 4$, from (35), we have

$$\theta_5 - \theta_j \le 2\arccos(d_6/2 + a_j).$$

By (40), we obtain $\theta''_6 - \theta''_{4-j+1} = 2\pi - (\theta_5 - \theta_j)$. Hence

$$\theta''_6 - \theta''_{4-j+1} \ge 2\pi - 2\arccos(d_6/2 + a_j).$$

Therefore,

$$\theta''_6 - \theta''_5 \ge 2\pi - 2\arccos(d_6/2 + a_j) - (\theta''_5 - \theta''_{4-j+1}). \tag{42}$$

Since (38) holds also for $\mathcal{G}''$, the left hand side of (42) is equal to

$$2\arccos(d_6/2 + a''_6) = 2\arccos(d_6/2 + a_6).$$

For the right hand side of (42), since

$$\begin{aligned} d_6 &\le |\det(A''_5 - A''_{4-j+1})| = \det(\hat{A}''_5 - \hat{A}''_{4-j+1}) - 4\sin^2((\theta''_5 - \theta''_{4-j+1})/4) \\ &= 2 - 2a''_{4-j+1} - 4\sin^2((\theta''_5 - \theta''_{4-j+1})/4), \end{aligned}$$

i.e.,

$$\theta''_5 - \theta''_{4-j+1} \le 2\arccos(d_6/2 + a''_{4-j+1}).$$

Hence, (42) can be changed into

$$\arccos(d_6/2 + a''_{4-j+1}) \ge \pi - \arccos(d_6/2 + a_j) - \arccos(d_6/2 + a_6). \tag{43}$$

Or equivalently,

$$a''_{4-j+1} \leq -\cos\left(\arccos(d_6/2 + a_j) + \arccos(d_6/2 + a_6)\right) - d_6/2 < 0, \tag{44}$$

where the second inequality is from $d_6 > 2$. Properties (41), (43), and (44) are important for the following proof, which provides us some relationships between a_j and a''_{4-j} through a_6 and d_6.

Step 3. Construction of a new constellation $\mathcal{G}^{**}$ that satisfies Case 1.

Let $\beta = \alpha/2$. Let $\theta_j^{**} = \theta_4/2$ for $j = 1, 2, 3, 4$, and let $\theta_5^{**} = (\theta_5 + \theta''_5)/2$, $\theta_6^{**} = (\theta_6 + \theta''_6)/2$. Let $\hat{A}_5^{**} = I$ and $\hat{A}_6^{**} = -I$. Define, for $j = 1, 2, 3, 4$,

$$\begin{pmatrix} a_j^{**} \\ b_j^{**} \\ c_j^{**} \\ d_j^{**} \end{pmatrix} = \begin{pmatrix} \cos\beta & -\sin\beta & 0 & 0 \\ \sin\beta & \cos\beta & 0 & 0 \\ 0 & 0 & \cos\beta & -\sin\beta \\ 0 & 0 & \sin\beta & \cos\beta \end{pmatrix} \begin{pmatrix} a_j \\ b_j \\ c_j \\ e_j \end{pmatrix}. \tag{45}$$

and

$$\hat{A}_j^{**} = i^{-1}((a_j^{**}, b_j^{**}, c_j^{**}, d_j^{**})), \tag{46}$$

where i is the isomorphic mapping defined in Section 2. From (45), we know that $\hat{A}_j^{**}$, $j = 1, 2, 3, 4$, are on $\mathbf{S}^3$. Thus, we can view $\hat{A}_j^{**}$ as unitary matrices in $\mathbf{SU}(2)$. Furthermore, from (45), we have $\det(\hat{A}_i^{**} - \hat{A}_j^{**}) = \det(\hat{A}_i - \hat{A}_j)$.

$\mathcal{G}^{**}$ is defined as follows:

$$A_6^{**} = e^{j\theta_6^{**}/2}(-I),\ A_5^{**} = e^{j\theta_5^{**}/2} I,\ A_j^{**} = e^{j\theta_j^{**}/2}\hat{A}_j^{**},\ \ j = 1, 2, 3, 4. \tag{47}$$

We next show that the diversity product of this new constellation $\mathcal{G}^{**}$ is d_6, i.e., we show $|\det(A_i^{**} - A_j^{**})| \geq d_6$ for $1 \leq i < j \leq 6$.

From the definition of $\mathcal{G}^{**}$, we have

$$\theta_6^{**} = (2\pi - \theta_5 + \theta_4 + \theta_6)/2, \quad \theta_5^{**} = (2\pi - \theta_6 + \theta_4 + \theta_5)/2, \tag{48}$$

$$(\theta_6^{**} - \theta_j^{**}) + (\theta_5^{**} - \theta_j^{**}) = 2\pi, \ \ j = 1, 2, 3, 4. \tag{49}$$

For $1 \leq i < j \leq 4$, from (45) and $\theta_i^{**} = \theta_j^{**} = \theta_4/2$, we have

$$\begin{aligned} |\det(A_i^{**} - A_j^{**})| &= \det(\hat{A}_i^{**} - \hat{A}_j^{**}) = \det(\hat{A}_i - \hat{A}_j) \\ &\geq d_6 + 4\sin^2((\theta_i - \theta_j)/4) \geq d_6, \end{aligned} \tag{50}$$

where the first inequality is from the conditions of $\mathcal{G}$. For $|\det(A_6^{**} - A_5^{**})|$, we have

$$\begin{aligned} |\det(A_6^{**} - A_5^{**})| &= \det(-I - I) - 4\sin^2((\theta_6^{**} - \theta_5^{**})/4) = 2 + 2\cos((\theta_6^{**} - \theta_5^{**})/2) \\ &= 2 + 2\cos((\theta_6 - \theta_5)/2) = 2 + 2\cos(\arccos(d_6/2 + a_6)) \\ &= 2 + 2a_6 + d_6 \geq d_6, \end{aligned} \tag{51}$$

where the third equality is from the definitions of θ_6^{**} and θ_5^{**}, and the forth equality is from (38).

For $j = 1, 2, 3, 4$, from Corollary 1 we have

$$\begin{aligned}
|\det(A_6^{**} - A_j^{**})| &= |4\sin^2((\theta_6^{**} - \theta_j^{**})/4) - \det(-I - \hat{A}_j^{**})| \\
&= |4\sin^2((\theta_6^{**} - \theta_j^{**})/4) - 4 + \det(I - \hat{A}_j^{**})| \\
&= |-2 - 2\cos((\theta_6^{**} - \theta_j^{**})/2) + \det(I - \hat{A}_j^{**})| \\
&= |-2 + 2\cos((\theta_5^{**} - \theta_j^{**})/2) + \det(I - \hat{A}_j^{**})| \\
&= |-4\sin^2((\theta_5^{**} - \theta_j^{**})/4) + \det(I - \hat{A}_j^{**})| \\
&= |\det(A_5^{**} - A_j^{**})|, \qquad (52)
\end{aligned}$$

where the forth equality is from (49). Therefore, we now only need to show $|\det(A_5^{**} - A_j^{**})| \geq d_6$.

Since

$$\begin{aligned}
|\det(A_5^{**} - A_j^{**})| &= |\det(I - \hat{A}_j^{**}) - 4\sin^2((\theta_5^{**} - \theta_j^{**})/4)| \\
&= |2\cos((\theta_5^{**} - \theta_j^{**})/2) - 2a_j^{**}| \\
&= |2\cos((2\pi - \theta_6 + \theta_5)/4) - 2a_j^{**}| = |2\sin((\theta_6 - \theta_5)/4) - 2a_j^{**}| \\
&= |2\sin(\arccos(a_6 + d_6/2)/2) - 2a_j^{**}|, \qquad (53)
\end{aligned}$$

we need to estimate coefficients a_j^{**}. From (41), we have

$$a''_{4-j+1} = \cos(\alpha)a_j - \sin(\alpha)b_j.$$

On the other hand, from (45), we have

$$a_j^{**} = \cos(\beta)a_j - \sin(\beta)b_j.$$

By noticing that $\beta = \alpha/2$, we obtain

$$a_j^{**} = \frac{a_j + a''_{4-j+1}}{2\cos\beta} = \frac{a_j + a''_{4-j+1}}{2\cos(\arccos(-a_6)/2)} < 0, \qquad (54)$$

where the second equality is from $\beta = \alpha/2 = \arccos(-a_6)/2$ and the last inequality is from the fact that $a_j < 0$ proved in the beginning of this proof and (44). Since $0 \leq \arccos(x) \leq \pi$, we have

$$2\sin(\arccos(a_6 + d_6/2)/2) - 2a_j^{**} > 0.$$

Thus, going back to (53), we have

$$|\det(A_5^{**} - A_j^{**})| = 2\sin(\arccos(a_6 + d_6/2)/2) - \frac{a_j + a''_{4-j+1}}{\cos(\arccos(-a_6)/2)}. \qquad (55)$$

But from (44),

$$a''_{4-j+1} \leq -\cos(\arccos(d_6/2 + a_j) + \arccos(d_6/2 + a_6)) - d_6/2.$$

From this estimate and the fact that $\cos(\arccos(-a_6)/2) > 0$ due to $-1 < a_6 < 0$, (55) becomes

$$|\det(A_5^{**} - A_j^{**})| \geq 2\sin(\arccos(a_6 + d_6/2)/2) - \frac{a_j - \cos(\arccos(d_6/2 + a_j) + \arccos(d_6/2 + a_6)) - d_6/2}{\cos(\arccos(-a_6)/2)}. \quad (56)$$

From (35), (38), and $\theta_6 - \theta_j \geq \pi$ for $j = 1, 2, 3, 4$, we have

$$\arccos(d_6/2 + a_j) + \arccos(d_6/2 + a_6) \geq (\theta_5 - \theta_j)/2 + (\theta_6 - \theta_5)/2 = (\theta_6 - \theta_j)/2 \geq \pi/2.$$

Since $-1 < a_6, a_j \leq 1 - d_6/2$ and $2 < d_6 \leq 2.4$, by Lemma 7, the right hand side of (56) is greater than or equal to d_6. Therefore, we have

$$|\det(A_5^{**} - A_j^{**})| \geq d_6. \quad (57)$$

From (50), (51), (52), and (57), we have proved that $\mathcal{G}^{**}$ has diversity product d_6. Furthermore, $a_6^{**} = -1$ and $\theta_j^{**} = \theta_4/2$ for $j = 1, 2, 3, 4$. If we rotate $\mathcal{G}^{**}$ by angle $-\theta_4/2$, we obtain $\theta_1^{**} = 0$. Then, the rotated constellation satisfies the conditions on Case 1 of this proof and therefore, we have the result $d_6 \leq \sqrt{22} - 5/2$. **q.e.d.**

As a remark, from the last part of the above proof, one can see that after the rotation of angle $-\theta_4/2$ of the new constellation $\mathcal{G}^{**}$, the first four $\theta_j^{**} = 0$ for $j = 1, 2, 3, 4$. Thus, it corresponds to $p = 4$ and is back to the case (iii) in the main proof of Theorem 1, which also proves $d_6 \leq \sqrt{22} - 5/2$.

Proof of Proposition 3

Since $0 \leq \theta_j \leq \pi$ for $1 \leq j \leq 5$, we have $|\theta_i - \theta_j| \leq \pi$ for $1 \leq i < j \leq 4$ and therefore, from Lemma 2, $|\det(A_i - A_j)| = \det(\hat{A}_i - \hat{A}_j) - 4\sin^2((\theta_i - \theta_j)/4)$, hence,

$$\|\mathbf{b}_i - \mathbf{b}_j\|^2 \geq 2 + \frac{d_6 - 2\cos((\theta_i - \theta_j)/2) + 2a_i a_j}{r_i r_j}, \quad 1 \leq i < j \leq 4, \quad (58)$$

where $\mathbf{b}_l$ and r_l are described in (11)-(13). To prove this proposition, we next estimate the above lower bounds for $\|\mathbf{b}_i - \mathbf{b}_j\|$ for $1 \leq i < j \leq 4$ under the assumption of $d_6 \geq -5/2 + \sqrt{22}$ such that the inequality in Lemma 5 for these 4-points on the sphere $\mathbf{S}^2$ is violated. To do so, we estimate lower bounds on $|\theta_i - \theta_j|$ and upper bounds on a_j in the following.

(i). Upper bound on a_1

Similar to the proof of Proposition 2, we can assume that $\hat{A}_5 = I$. Then

$$d_6 \leq |\det(A_6 - A_j)| = 4\sin^2((\theta_6 - \theta_j)/4) - \det(\hat{A}_6 - \hat{A}_j), \quad j = 1, 2, 3. \quad (59)$$

$$\begin{aligned} d_6 &\leq |\det(A_6 - A_5)| = \det(\hat{A}_6 - \hat{A}_5) - 4\sin^2((\theta_6 - \theta_5)/4) \\ &= 2 - 2a_6 - 4\sin^2((\theta_6 - \theta_5)/4) = 2\cos((\theta_6 - \theta_5)/2) - 2a_6. \quad (60) \end{aligned}$$

$$\begin{aligned} d_6 &\leq |\det(A_5 - A_j)| = \det(\hat{A}_5 - \hat{A}_j) - 4\sin^2((\theta_5 - \theta_j)/4) \\ &= 2 - 2a_j - 4\sin^2((\theta_5 - \theta_j)/4) = 2\cos((\theta_5 - \theta_j)/2) - 2a_j, \quad j = 1, 2, 3, 4. \quad (61) \end{aligned}$$

From (61), we have that $a_1 \le \cos(\theta_5/2) - d_6/2$. Hence, to have an upper bound, it is enough to have a lower bound on θ_5. For $1 \le i \ne j \le 3$, $|\theta_i - \theta_j| \le \pi$. Thus, by Lemma 2,

$$\det(\hat{A}_i - \hat{A}_j) \ge |\det(A_i - A_j)| \ge d_6.$$

Thus, by Lemma 4, there exists $s \in \{1,2,3\}$ such that

$$\det(\hat{A}_6 - \hat{A}_s) \ge 2 - 2\sqrt{1 - d_6/3}.$$

Combining this with (59) we have

$$d_6 \le 4\sin^2((\theta_6 - \theta_s)/4) - (2 - 2\sqrt{1 - d_6/3}),$$

or

$$\theta_6 - \theta_s \ge 2\arccos(-d_6/2 + \sqrt{1 - d_6/3}).$$

Therefore,

$$\theta_6 \ge 2\arccos(-d_6/2 + \sqrt{1 - d_6/3}). \tag{62}$$

Similarly, by considering $\hat{A}_6$ with $\{\hat{A}_4, \hat{A}_5\}$ and Lemma 4, there exists $u \in \{4,5\}$ such that

$$\det(\hat{A}_6 - \hat{A}_u) \le 2 + 2\sqrt{1 - d_6/4},$$

Since $0 \le \theta_6 - \theta_u \le \pi$, we have

$$d_6 \le \det(\hat{A}_6 - \hat{A}_u) - 4\sin^2((\theta_6 - \theta_u)/4) \le 2 + 2\sqrt{1 - d_6/4} - 4\sin^2((\theta_6 - \theta_u)/4),$$

which implies

$$\theta_6 - \theta_u \le 2\arccos(d_6/2 - \sqrt{1 - d_6/4}).$$

Since $\theta_4 < \theta_5$ and $u \in \{4,5\}$, we have

$$\theta_6 - \theta_5 \le 2\arccos(d_6/2 - \sqrt{1 - d_6/4}). \tag{63}$$

From (62) and (63), we have

$$\theta_5 \ge 2\arccos(-d_6/2 + \sqrt{1 - d_6/3}) - 2\arccos(d_6/2 - \sqrt{1 - d_6/4}). \tag{64}$$

On the other hand, from (61) for $j = 1$, we have

$$d_6 \le 2 - 2a_1 - 4\sin^2(\theta_5/4) = 2\cos(\theta_5/2) - 2a_1,$$

i.e.,

$$a_1 \le \cos(\theta_5/2) - d_6/2.$$

Thus, by combining with (64), we obtain an estimation of a_1 as follows:

$$a_1 \leq \cos\left(\arccos(-d_6/2+\sqrt{1-d_6/3}) - \arccos(d_6/2-\sqrt{1-d_6/4})\right) - d_6/2.$$

Note that $d_6 \geq \sqrt{22}-5/2$. Therefore, from the above estimate we have

$$a_1 \leq -0.5975. \tag{65}$$

(ii). Upper bound on a_2

It is similar to (i). By considering $\hat{A}_6$ with $\{\hat{A}_2, \hat{A}_3\}$ and Lemma 4, there exists $v \in \{2,3\}$ such that

$$\det(\hat{A}_6 - \hat{A}_v) \geq 2 - 2\sqrt{1-d_6/4}.$$

From (59) for $j = v$, we have

$$d_6 \leq 4\sin^2((\theta_6-\theta_v)/4) - \det(\hat{A}_6 - \hat{A}_v) \leq 4\sin^2((\theta_6-\theta_v)/4) - (2-2\sqrt{1-d_6/4}).$$

Therefore,

$$\theta_6 - \theta_v \geq 2\arccos(-d_6/2+\sqrt{1-d_6/4}).$$

Since $\theta_2 \leq \theta_3$ and $v \in \{2,3\}$, we have

$$\theta_6 - \theta_2 \geq 2\arccos(-d_6/2+\sqrt{1-d_6/4}).$$

Using $\theta_6 - \theta_2 = \theta_6 - \theta_5 + \theta_5 - \theta_2$ and (63), we have

$$\theta_5 - \theta_2 \geq 2\arccos(-d_6/2+\sqrt{1-d_6/4}) - 2\arccos(d_6/2-\sqrt{1-d_6/4}).$$

On the other hand, from (61) for $j = 2$, we have $a_2 + d_6/2 \leq \cos((\theta_5-\theta_2)/2)$. Therefore,

$$a_2 \leq \cos\left(\arccos(-d_6/2+\sqrt{1-d_6/4}) - \arccos(d_6/2-\sqrt{1-d_6/4})\right) - d_6/2.$$

Thus, from $d_6 \geq \sqrt{22}-5/2$, we have

$$a_2 \leq -0.4524. \tag{66}$$

(iii). Upper bound on a_3

It is not hard to see that matrices

$$\{\hat{A}_6, e^{j(2\pi-\theta_6)/2}(-\hat{A}_1), e^{j(2\pi-\theta_6+\theta_3)/2}(-\hat{A}_3)\}$$

satisfies the conditions of Lemma 6. Thus, by Lemma 6 we have $2\pi - \theta_6 + \theta_3 \leq 5\pi/6$, i.e.,

$$\theta_6 - \theta_3 \geq 2\pi - 5\pi/6 = 7\pi/6.$$

Hence,

$$\theta_5 - \theta_3 = \theta_6 - \theta_3 - (\theta_6 - \theta_5) \geq 7\pi/6 - 2\arccos(d_6/2 - \sqrt{1 - d_6/4}),$$

where the inequality is from (63). From (61), we have $a_3 \leq \cos((\theta_5 - \theta_3)/2) - d_6/2$. Therefore,

$$a_3 \leq \cos(7\pi/12 - \arccos(d_6/2 - \sqrt{1 - d_6/4})) - d_6/2.$$

Using the fact $d_6 \geq \sqrt{22} - 5/2$, we obtain

$$a_3 \leq -0.3292. \tag{67}$$

(vi). Upper bound on a_4 and lower bound on θ_4

From (61), we have $a_4 \leq \cos((\theta_5 - \theta_4)/2) - d_6/2 \leq 1 - d_6/2$. The assumption $d_6 \geq \sqrt{22} - 5/2$ implies

$$a_4 \leq -0.0952. \tag{68}$$

Since $\{A_4, A_5, A_6\}$ satisfies the conditions of Lemma 6, we have $\theta_6 - \theta_4 \leq 5\pi/6$. By using (62), we obtain

$$\theta_4 \geq 2\arccos(-d_6/2 + \sqrt{1 - d_6/3}) - 5\pi/6.$$

From $d_6 \geq \sqrt{22} - 5/2$, we have

$$\theta_4 \geq 100.3010^\circ. \tag{69}$$

(v). Lower Bounds on $\|\mathbf{b}_i - \mathbf{b}_j\|^2$ for $1 \leq i < j \leq 4$

We now apply the estimates in (65), (66), (67), (68), and (69) to estimate some lower bounds of $\|\mathbf{b}_i - \mathbf{b}_j\|$ for $1 \leq i \neq j \leq 4$ through (58).

For $1 \leq i < j \leq 4$ and $(i, j) \neq (1, 4)$, we have

$$\begin{aligned} \|\mathbf{b}_i - \mathbf{b}_j\|^2 &\geq 2 + \frac{d_6 - 2\cos((\theta_i - \theta_j)/2) + 2a_i a_j}{\sqrt{1 - a_i^2}\sqrt{1 - a_j^2}} \\ &\geq 2 + \frac{\sqrt{22} - 5/2 - 2 + 2a_i a_j}{\sqrt{1 - a_i^2}\sqrt{1 - a_j^2}}. \end{aligned}$$

Since the right hand side of the above inequality is decreasing for $-1 < a_i, a_j < 0$, by using (65), (66), (67), and (68), we obtain

$$\begin{aligned} &\|\mathbf{b}_1 - \mathbf{b}_2\|^2 \geq 3.0223, \quad \|\mathbf{b}_1 - \mathbf{b}_3\|^2 \geq 2.7710, \quad \|\mathbf{b}_2 - \mathbf{b}_3\|^2 \geq 2.5798, \\ &\|\mathbf{b}_2 - \mathbf{b}_4\|^2 \geq 2.3115, \quad \|\mathbf{b}_3 - \mathbf{b}_4\|^2 \geq 2.2693. \end{aligned}$$

For $\|\mathbf{b}_1 - \mathbf{b}_4\|^2$, we have

$$\begin{aligned} \|\mathbf{b}_1 - \mathbf{b}_4\|^2 &\geq 2 + \frac{d_6 - 2\cos(\theta_4/2) + 2a_1 a_4}{\sqrt{1 - a_1^2}\sqrt{1 - a_4^2}} \\ &\geq 2 + \frac{\sqrt{22} - 5/2 - 2\cos(100.3010^\circ/2) + 2a_1 a_4}{\sqrt{1 - a_1^2}\sqrt{1 - a_4^2}} \geq 3.2811. \end{aligned}$$

Therefore,

$$\sum_{1\le i<j\le 4} \|\mathbf{b}_i - \mathbf{b}_j\|^2 \ge 16.2350 > 16,$$

which contradicts with Lemma 5. This proves the proposition. **q.e.d.**

Proof of Proposition 4

We also divide this proof into several cases according to the angle θ_5.

Case 1 $\theta_5 - \theta_3 \ge \pi$

Let

$$\begin{aligned} A_1' &= e^{-j\theta_5/2}A_5 = \hat{A}_5, & A_2' &= e^{-j\theta_5/2}A_6 = e^{j(\theta_6-\theta_5)/2}\hat{A}_6, \\ A_3' &= e^{-j\theta_5/2}A_1 = e^{j(2\pi-\theta_5)/2}(-\hat{A}_1), & A_4' &= e^{-j\theta_5/2}A_2 = e^{j(2\pi-\theta_5+\theta_2)/2}(-\hat{A}_2), \\ A_5' &= e^{-j\theta_5/2}A_3 = e^{j(2\pi-\theta_5+\theta_3)/2}(-\hat{A}_3), & A_6' &= e^{-j\theta_5/2}A_4 = e^{j(2\pi-\theta_5+\theta_4)/2}(-\hat{A}_4). \end{aligned}$$

Then, constellation $\{A_1', A_2', \cdots, A_6'\}$ satisfies the conditions of Case I in the proof of Theorem 1 and therefore, we have the result in this case.

Case 2 $\theta_5 - \theta_3 \le \pi$ **and** $\theta_5 - \theta_2 \ge \pi$

Without loss of generality, we assume that $\hat{A}_4 = I$. Assume $d_6 \ge -5/2 + \sqrt{22}$. We divide this proof into two steps. Step 1 is to estimate angles θ_j for $j = 2, 3, 4, 5, 6$. Step 2 is to use these estimations to induce a contradiction. Let us begin with Step 1.

Step 1. Estimations on the angles θ_j for $j = 2, 3, 4, 5, 6$

Since sets of matrices $\{A_4, A_5, A_6\}$, $\{A_3, A_4, A_5\}$, and $\{A_1, A_2, A_4\}$ all satisfy the conditions of Lemma 6, from Lemma 6 we have

$$\theta_6 - \theta_4 \le 5\pi/6, \quad \theta_5 - \theta_3 \le 5\pi/6, \quad \theta_4 \le 5\pi/6. \tag{70}$$

We now estimate these angles in more details. First, from the above, we have

$$\theta_6 = (\theta_6 - \theta_4) + \theta_4 \le 5\pi/6 + 5\pi/6 = 5\pi/3. \tag{71}$$

We next estimate some lower bounds on θ_j for $j = 3, 4, 5, 6$.

Similar to the proof of Proposition 3, by considering $\hat{A}_5$ with $\{\hat{A}_1, \hat{A}_2\}$ and $\det(\hat{A}_1 - \hat{A}_2) \ge d_6$, by Lemma 4, there exists a t, $t \in \{1, 2\}$, such that

$$\det(\hat{A}_5 - \hat{A}_t) \ge 2 - 2\sqrt{1 - d_6/4}.$$

Since $\theta_5 - \theta_t \ge \pi$, we obtain

$$\begin{aligned} d_6 &\le |\det(A_5 - A_t)| \le 4\sin^2((\theta_5 - \theta_t)/4) - \det(\hat{A}_5 - \hat{A}_t) \\ &\le 4\sin^2((\theta_5 - \theta_t)/4) - (2 - 2\sqrt{1 - d_6/4}) \\ &= -2\cos((\theta_5 - \theta_t)/2) + 2\sqrt{1 - d_6/4}. \end{aligned}$$

Hence,

$$\theta_5 - \theta_t \geq 2\arccos(-d_6/2 + \sqrt{1 - d_6/4}).$$

Thus,

$$\theta_5 \geq 2\arccos(-d_6/2 + \sqrt{1 - d_6/4}) \triangleq \beta_5. \tag{72}$$

Since $d_6 \geq \sqrt{22} - 5/2$, (72) implies

$$\theta_5 \geq \beta_5 > 229.9981^\circ. \tag{73}$$

From (70), i.e., $\theta_5 - \theta_3 \leq 5\pi/6$, we have

$$\theta_3 \geq 2\arccos(-d_6/2 + \sqrt{1 - d_6/4}) - 5\pi/6 = \beta_5 - 5\pi/6 \triangleq \beta_3. \tag{74}$$

Hence,

$$\theta_3 > 79.9981^\circ. \tag{75}$$

To have lower bounds on θ_6 and θ_4, we consider three matrices

$$\{B_1, B_2, B_3\} \triangleq \{\hat{A}_6,\ e^{j(2\pi - \theta_6)/2}(-\hat{A}_1),\ e^{j(2\pi - \theta_6 + \theta_3)/2}(-\hat{A}_3)\}.$$

We first claim that these three matrices satisfy the condition of Lemma 6. In fact, since $\theta_6 - \theta_3 \geq \pi$, we have $2\pi - \theta_6 + \theta_3 \leq \pi$. On the other hand,

$$\begin{aligned} e^{\theta_6/2} \cdot \{B_1, B_2, B_3\} &= e^{\theta_6/2} \cdot \left\{\hat{A}_6,\ e^{j(2\pi - \theta_6)/2}(-\hat{A}_1),\ e^{j(2\pi - \theta_6 + \theta_3)/2}(-\hat{A}_3)\right\} \\ &= \left\{e^{\theta_6/2}\hat{A}_6,\ e^{2\pi/2}(-\hat{A}_1),\ e^{(2\pi + \theta_3)/2}(-\hat{A}_3)\right\} \\ &= \{A_6, A_1, A_3\}, \end{aligned}$$

i.e.,

$$\{B_1, B_2, B_3\} = e^{-j\theta_6/2}\{A_6, A_1, A_3\}.$$

Therefore,

$$|\det(B_i - B_j)| \geq d_6 \geq \sqrt{22} - 5/2, \quad \text{for } 1 \leq i \neq j \leq 3.$$

By Lemma 6, we have

$$2\pi - \theta_6 + \theta_3 \leq 5\pi/6. \tag{76}$$

Results (71) and (76) imply

$$\theta_3 \leq \pi/2 = 90^\circ. \tag{77}$$

Results (75) and (76) imply

$$\theta_6 \geq 289.9981^\circ. \tag{78}$$

By (70), $\theta_4 \geq \theta_6 - 150^\circ$, hence,

$$\theta_4 \geq 289.9981^\circ - 150^\circ = 139.9981^\circ. \tag{79}$$

We next estimate an upper bound on θ_2. From (70) and (77), we have

$$\theta_5 \leq 150^\circ + \theta_3 \leq 240^\circ. \tag{80}$$

Consider

$$\{B_1', B_2', B_3'\} \triangleq \left\{\hat{A}_5,\ e^{j(2\pi-\theta_5)/2}(-\hat{A}_1),\ e^{j(2\pi-\theta_5+\theta_2)/2}(-\hat{A}_2)\right\}.$$

Similar to the previous B_i, $\{B_1', B_2', B_3'\}$ satisfies the conditions of Lemma 6. Therefore,

$$2\pi - \theta_5 + \theta_2 \leq 150^\circ. \tag{81}$$

Using (80) and (81), we obtain

$$\theta_2 \leq 30^\circ. \tag{82}$$

Using this estimate and (79) and (77), we obtain

$$\theta_4 - \theta_2 \geq 139.9981^\circ - 30^\circ = 109.9981^\circ,\ \ \theta_3 - \theta_2 \geq 79.9981^\circ - 30^\circ = 49.9981^\circ. \tag{83}$$

Step 2. Estimations on $\det(\hat{A}_i - \hat{A}_j)$ for $1 \leq i < j \leq 4$.

For $1 \leq i < j \leq 4$, since $\theta_j - \theta_i \leq \pi$, we have

$$\sqrt{22} - 5/2 \leq d_6 \leq |\det(A_i - A_j)| \leq \det(\hat{A}_i - \hat{A}_j) - 4\sin^2((\theta_j - \theta_i)/4).$$

Therefore,

$$\det(\hat{A}_i - \hat{A}_j) \geq \sqrt{22} - 5/2 + 4\sin^2((\theta_j - \theta_i)/4). \tag{84}$$

Using (74), (79), (83), and (84), we have

$$\begin{aligned}
\det(\hat{A}_4 - \hat{A}_1) &\geq \sqrt{22} - 5/2 + 4\sin^2(\theta_4/4) \\
&\geq \sqrt{22} - 5/2 + 4\sin^2(139.9981^\circ/4) > 3.5063, \\
\det(\hat{A}_4 - \hat{A}_2) &\geq \sqrt{22} - 5/2 + 4\sin^2((\theta_4 - \theta_2)/4) \\
&\geq \sqrt{22} - 5/2 + 4\sin^2(109.9981^\circ/4) > 3.0432, \\
\det(\hat{A}_4 - \hat{A}_3) &\geq \sqrt{22} - 5/2 + 4\sin^2((\theta_4 - \theta_3)/4) \\
&\geq \sqrt{22} - 5/2 + 4\sin^2((139.9981^\circ - 90^\circ)/4) > 2.3777, \\
\det(\hat{A}_3 - \hat{A}_2) &\geq \sqrt{22} - 5/2 + 4\sin^2((\theta_3 - \theta_2)/4) \\
&\geq \sqrt{22} - 5/2 + 4\sin^2(49.9981^\circ/4) > 2.3777, \\
\det(\hat{A}_3 - \hat{A}_1) &\geq \sqrt{22} - 5/2 + 4\sin^2(\theta_3/4) \\
&\geq \sqrt{22} - 5/2 + 4\sin^2(79.9981^\circ/4) > 2.6583, \\
\det(\hat{A}_2 - \hat{A}_1) &\geq \sqrt{22} - 5/2 > 2.1904.
\end{aligned}$$

Therefore,

$$\sum_{1 \leq i < j \leq 4} \det(\hat{A}_i - \hat{A}_j) > 16.1536 > 16,$$

which contradicts with Lemma 5. Therefore, we have the result in this case.

Case 3 $\theta_5 - \theta_3 \leq \pi$ **and** $\theta_5 - \theta_2 \leq \pi$

Let

$$A'_j = e^{-j\theta_2/2} A_{j+1}, \ \text{ for } \ j = 1, 2, 3, 4, 5,$$

and

$$A'_6 = e^{-j\theta_2/2} A_1 = e^{j(2\pi - \theta_2)/2} \hat{A}_1.$$

Then the new constellation $\{A'_1, A'_2, \cdots, A'_6\}$ satisfies the conditions of the above Case 2. Thus, we have proved the proposition. **q.e.d**

Proof of Proposition 5

We divide this proof into two cases according to angle θ_5.

Case 1 $\theta_5 - \theta_2 \geq \pi$

In this case, without loss of generality, we assume $\hat{A}_3 = I$. Assume $d_6 \geq -5/2 + \sqrt{22}$. We want to derive a contradiction.

Since $\theta_5 - \theta_j \geq \pi$ for $j = 1, 2$ and $\theta_2 - \theta_1 \leq \pi$, by considering $\hat{A}_5$ with $\{\hat{A}_1, \hat{A}_2\}$ and using the same technique as before, i.e., Lemma 4, there exists $u \in \{1, 2\}$, such that

$$\det(\hat{A}_5 - \hat{A}_u) \geq 2 - 2\sqrt{1 - d_6/4}.$$

Therefore, from the condition $|\det(A_5 - A_u)| \geq d_6$ and $\theta_5 - \theta_u \geq \pi$, we have

$$4\sin^2((\theta_5 - \theta_u)/4) \geq \det(\hat{A}_5 - \hat{A}_u) + d_6 \geq 2 - 2\sqrt{1 - d_6/4} + d_6.$$

Since $\theta_u \geq 0$, we obtain

$$\cos(\theta_5/2) \leq -d_6/2 + \sqrt{1 - d_6/4}. \tag{85}$$

Since $d_6 \geq \sqrt{22} - 5/2$, we obtain

$$\theta_5 \geq \arccos(-d_6/2 + \sqrt{1 - d_6/4}) > 229.9981^\circ. \tag{86}$$

We now rotate $\{A_1, \cdots, A_6\}$ with angle $-\theta_3$: $A'_j = e^{-j\theta_3/2} A_{j+2}$ for $j = 1, 2, 3, 4$, and $A'_5 = e^{-j\theta_3/2} A_1$ and $A'_6 = e^{-j\theta_3/2} A_2$. Then, it is clear that $\{A'_1, \cdots, A'_6\}$ is also an optimal design. Furthermore, $A'_1 \in \mathbf{SU}(2)$ and the angle θ'_j of A'_j is $\theta_{j+2} - \theta_3$ for $j = 1, 2, 3, 4$. For $j = 5$, since $A'_5 = e^{-j\theta_3/2} A_1 = e^{-j\theta_3/2}\hat{A}_1 = e^{j(2\pi - \theta_3)/2}(-\hat{A}_1)$, hence the angle θ'_5 is $2\pi - \theta_3$. Similarly, the angle θ'_6 is $2\pi - \theta_3 + \theta_2$. Also, $\hat{A'}_j = \hat{A}_{j+2}$ for $j = 1, 2, 3, 4$ and $\hat{A'}_5 = -\hat{A}_1$ and $\hat{A'}_6 = -\hat{A}_2$. In summary, we have

$$\{\hat{A}'_1, \hat{A}'_2, \hat{A}'_3, \hat{A}'_4, \hat{A}'_5, \hat{A}'_6\} = \{\hat{A}_3, \hat{A}_4, \hat{A}_5, \hat{A}_6, -\hat{A}_1, -\hat{A}_2\} \tag{87}$$

and

$$\{\theta'_1, \theta'_2, \theta'_3, \theta'_4, \theta'_5, \theta'_6\} = \{0, \theta_4 - \theta_3, \theta_5 - \theta_3, \theta_6 - \theta_3, 2\pi - \theta_3, 2\pi - \theta_3 + \theta_2\}. \tag{88}$$

We now have $0 = \theta'_1 \leq \theta'_4 \leq \pi \leq \theta'_5$. Moreover, $\theta'_6 - \theta'_3 = 2\pi - \theta_3 + \theta_2 - (\theta_5 - \theta_3) = 2\pi - (\theta_5 - \theta_2) \leq \pi$ and $\theta'_6 - \theta'_2 = 2\pi - \theta_3 + \theta_2 - (\theta_4 - \theta_3) = 2\pi - (\theta_4 - \theta_2) \geq \pi$. Furthermore, $\theta'_5 - \theta'_2 = 2\pi - \theta_3 - (\theta_4 - \theta_3) = 2\pi - \theta_4 \geq \pi$. Therefore, the conditions on $\{A'_1, \cdots, A'_6\}$ are the same as those of $\{A_1, \cdots, A_6\}$. Therefore, similar to (85), we have

$$\cos(\theta'_5/2) \leq -d_6/2 + \sqrt{1 - d_6/4}. \tag{89}$$

By the definitions of θ'_5 stated in (88), we obtain

$$\cos(\theta_3/2) \geq d_6/2 - \sqrt{1 - d_6/4}. \tag{90}$$

Therefore,

$$\theta_3 \leq 2\arccos(d_6/2 - \sqrt{1 - d_6/4}). \tag{91}$$

Since $d_6 \geq \sqrt{22} - 5/2$, we obtain

$$\theta_3 \leq 2\arccos(d_6/2 - \sqrt{1 - d_6/4}) < 130.0018^\circ. \tag{92}$$

By combining it with (86), we have

$$\theta_5 - \theta_3 \geq 99.9962^\circ \tag{93}$$

We next consider $\{\hat{A}_3, \hat{A}_4, \hat{A}_5, \hat{A}_6\}$ on the sphere $\mathbf{S^3}$. First, from Lemma 5, we have

$$\sum_{3\le i<j\le 6} \det(\hat{A}_i - \hat{A}_j) \le 16. \tag{94}$$

For $3 \le i < j \le 6$, we have $\theta_j - \theta_i \le \pi$. by using $|\det(A_i - A_j)| \ge d_6$, we have $\det(\hat{A}_i - \hat{A}_j) \ge d_6 + 4\sin^2((\theta_j - \theta_i)/4)$. Therefore,

$$\begin{aligned}
\det(\hat{A}_6 - \hat{A}_5) &\ge d_6 + 4\sin^2((\theta_6 - \theta_5)/4) \ge d_6, && (95)\\
\det(\hat{A}_6 - \hat{A}_4) &\ge d_6 + 4\sin^2((\theta_6 - \theta_4)/4) \ge d_6 + 4\sin^2((\theta_5 - \theta_4)/4), && (96)\\
\det(\hat{A}_6 - \hat{A}_3) &\ge d_6 + 4\sin^2((\theta_6 - \theta_3)/4) \ge d_6 + 4\sin^2((\theta_5 - \theta_3)/4), && (97)\\
\det(\hat{A}_5 - \hat{A}_4) &\ge d_6 + 4\sin^2((\theta_5 - \theta_4)/4), && (98)\\
\det(\hat{A}_5 - \hat{A}_3) &\ge d_6 + 4\sin^2((\theta_5 - \theta_3)/4), && (99)\\
\det(\hat{A}_4 - \hat{A}_3) &\ge d_6 + 4\sin^2((\theta_4 - \theta_3)/4) \ge d_6. && (100)
\end{aligned}$$

Plugging (95)-(100) into (94) we obtain

$$6d_6 + 8\sin^2((\theta_5 - \theta_4)/4) + 8\sin^2((\theta_5 - \theta_3)/4) \le 16.$$

By applying (93) and $d_6 \ge \sqrt{22} - 5/2$ to solve above inequality, we obtain

$$\theta_5 - \theta_4 \le 99.9966^\circ. \tag{101}$$

Since $\{A'_1, \cdots, A'_6\}$ has the same conditions as the ones of $\{A_1, \cdots, A_6\}$, we have

$$\theta'_5 - \theta'_4 \le 99.9966^\circ. \tag{102}$$

By (88), we have $2\pi - \theta_3 - \theta_6 + \theta_3 \le 99.9966^\circ$, hence,

$$\theta_6 \ge 260.0034^\circ. \tag{103}$$

Using (103), we can revise the estimates on $\theta_6 - \theta_4$ and $\theta_6 - \theta_3$. In fact, because $\{A_1, A_2, A_4\}$ satisfies the conditions of Lemma 6, we have

$$\theta_4 \le 5\pi/6 = 150^\circ. \tag{104}$$

Hence,

$$\theta_6 - \theta_4 \ge 110.0034^\circ. \tag{105}$$

For $\theta_6 - \theta_3$, by using (103) and (92) we have

$$\theta_6 - \theta_3 \ge 130.0016^\circ. \tag{106}$$

Similarly, for $\theta_5 - \theta_4$, from (86) and (104), we have

$$\theta_5 - \theta_4 \geq 229.9981^\circ - 150^\circ = 79.9981^\circ. \tag{107}$$

Plugging (105),(106), (107) and (93) into (96), (97), (98) and (99), respectively, we obtain

$$\begin{aligned}
\det(\hat{A}_6 - \hat{A}_4) &\geq d_6 + 4\sin^2((\theta_6 - \theta_4)/4) \geq d_6 + 4\sin^2(110.0034^\circ/4), \\
\det(\hat{A}_6 - \hat{A}_3) &\geq d_6 + 4\sin^2((\theta_6 - \theta_3)/4) \geq d_6 + 4\sin^2(130.0016^\circ/4), \\
\det(\hat{A}_5 - \hat{A}_4) &\geq d_6 + 4\sin^2((\theta_5 - \theta_4)/4) \geq d_6 + 4\sin^2(79.9981^\circ/4), \\
\det(\hat{A}_5 - \hat{A}_3) &\geq d_6 + 4\sin^2((\theta_5 - \theta_3)/4) \geq d_6 + 4\sin^2(99.9962^\circ/4).
\end{aligned}$$

Therefore, using $d_6 \geq \sqrt{22} - 5/2$, we obtain

$$\begin{aligned}
&\det(\hat{A}_6 - \hat{A}_5) \geq 2.1904, \quad \det(\hat{A}_6 - \hat{A}_4) \geq 3.0433, \quad \det(\hat{A}_6 - \hat{A}_3) \geq 3.3452, \\
&\det(\hat{A}_5 - \hat{A}_4) \geq 2.6583, \quad \det(\hat{A}_5 - \hat{A}_3) \geq 2.9047, \quad \det(\hat{A}_4 - \hat{A}_3) \geq 2.1904.
\end{aligned}$$

Therefore,

$$\sum_{3 \leq i < j \leq 6} \det(\hat{A}_j - \hat{A}_i) \geq 16.3323 > 16,$$

which contradicts with (94). Hence, we have the result in this case.

Case 2 $\theta_5 - \theta_2 \leq \pi$

Let

$$A'_j = e^{-j\theta_2/2} A_{j+1}, \quad \text{for } \ j = 1, 2, 3, 4, 5,$$

and

$$A'_6 = e^{-j\theta_2/2} A_1 = e^{j(2\pi - \theta_2)/2} \hat{A}_1.$$

Then, the new constellation $\{A'_1, A'_2, \cdots, A'_6\}$ satisfies the conditions of Proposition 4. Thus, we have proved the proposition. **q.e.d.**

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