Design of Unitary Space-Time Codes from Representations of $SU(2)$

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Abstract

We explicitly construct an irreducible four-dimensional unitary representation of the Lie group $SU(2)$ and use it for the construction of high-rate unitary space-time codes for four transmit antennas. The tools we use are invariant integration on the group to unitarize the representation, and dense spherical codes on the three-dimensional sphere. Our construction calls for the design of such spherical codes in which the angle between any two points is well separated from 120 degrees. We give a partial solution to this restricted design problem and use numerical optimization techniques to optimize our solution.

1 Introduction

It is well-known that multiple antenna links promise very high data rates at very low error probabilities [1, 2]. The theory is in a rather satisfactory level for fixed wireless links in which the fading channel coefficients are known to the sender and the receiver. However, for mobile applications in which the channel changes very rapidly the situation is far less understood, both from an information theoretic and a code design point of view.

In [3], and independently in [4] the authors introduce a differential transmission scheme which is well-suited for mobile communication. The signals transmitted are modulated through unitary $n \times n$-matrices. For this modulation scheme, the authors derive upper bounds on the pairwise probability of error of the maximum likelihood decoder under the assumptions that the fading coefficients as well as the noise are statistically independent complex normally distributed random variables. As it turns out, if the SNR, the number of receiving antennas, and the number of transmitting antennas are fixed, then the pairwise probability of error decays inversely exponentially with the *diversity product* of the code. Recall that the *diversity distance* between two complex $n \times n$-matrices A and B is defined as $\frac{1}{2}|\det(A-B)|^{1/n}$. The diversity product $\zeta(\mathcal{V})$ of a set $\mathcal{V}$ of L unitary $n \times n$-matrices $V_1, \ldots, V_L$ is then the minimal diversity distance, i.e., [1]

$$\zeta(\mathcal{V}) := \frac{1}{2} \min_{i \neq j} |\det(V_i - V_j)|^{1/n}.$$

The set $\mathcal{V}$ is also called a *unitary space-time code.* The *code design problem* is thus the following: given a minimal diversity product ζ and n, construct a set $\mathcal{V}$ of unitary $n \times n$-matrices having as many elements as possible such that $\zeta(\mathcal{V}) \geq \zeta$.

Despite various efforts the code design problem is still in its infancy, especially for high rate codes. In particular, we don't know any upper bound for the maximum number of elements of a set with a prescribed minimum diversity product. What we do know can be summarized as follows: in [3] the authors construct unitary space-time codes which form a cyclic group under matrix multiplication. At around the same time, [5] used orthogonal designs introduced earlier by Alamouti [6] to design space-time codes for two transmit antennas. In a later paper [7] the authors realized the connection between the code design problem for two transmit antennas and the problem of designing spherical codes on the three-dimensional unity sphere in the four-dimensional space. Moreover, [7] classified all finite sets of unitary matrices that have a nonzero diversity product and form a group under matrix multiplication. (We remark that Hughes [4, 8] independently classified such groups of order a power of 2.) Simulation results for groups that have zero diversity product were given later in [9]. Some more examples of designing codes based on generalized orthogonal designs can be found in [10].

In this paper, we will continue the spirit of [7] in a different direction: instead of using representations of finite groups, we will use representations of certain compact Lie groups. The specific example in this paper is the Lie group $SU(2)$ which is the group of 2×2-unitary matrices of determinant one, but many of the techniques can be applied to other types of Lie groups as well. The paper is motivated by a recent result of Hassibi and Khorrami [11]: they prove that the only fixed-point-free Lie groups are the groups $U(1)$ (the complex unit circle) and $SU(2)$. (Recall that a Lie group G is a differentiable manifold which is a group and in which the group multiplication is continuous.)

This negative result can be turned positive in the following way: could we actually construct

[1]The same relationship, albeit with different constants, holds also if the channel is known.

subsets of Lie groups that have positive (and in fact good) diversity products? The key to a solution to this problem is the use of representations of Lie groups. By the well-known theorem of Peter-Weyl [12, Theorem 3.1], any irreducible representation of a compact Lie group is unitary and finite dimensional. For this reason, we will concentrate on compact Lie groups right away.

In this paper, we will investigate the four-dimensional irreducible representation of $SU(2)$. With respect to standard bases this representation is not unitary. However, by the Peter-Weyl theorem it is equivalent to a unitary representation. To compute the latter, we need to use invariant integration on the group $SU(2)$. This is done in the appendices A and B. It turns out that the eigenvalues of this representation are ζ, ζ^3 and their inverses if the representation is evaluated at an element with eigenvalues ζ and ζ^{-1}. Obviously, the representation is not fixed-point-free, since it maps third roots of unity to the identity element. However, if we can avoid the third roots of unity, we can make the representation fixed-point-free, at least on a subset of $SU(2)$. An analysis of this representation reveals that it leads to a good four-dimensional space-time code if, under the identification of $SU(2)$ with the three dimensional unity sphere $\mathbb{S}^3$, the points are not too close and no two points have an angle which is close to $2\pi/3$ (see Section 3). The task at hand is then the construction of such sets on $\mathbb{S}^3$. To obtain such a set, we start from a good spherical code on $\mathbb{S}^3$. Then we identify a large connected region of $\mathbb{S}^3$ for which the scalar product of any two points is larger than $-1/2$ by some fixed amount. The set of points of $\mathbb{S}^3$ at which the representation is evaluated is then the intersection of this region with the original spherical code.

Using a numerical optimization procedure discussed in Appendix C, we construct in Section 3 codes for four transmit antennas for which the diversity product is roughly $\sqrt{6\epsilon}/2$ starting from a spherical code in which all scalar products are less than $1 - \epsilon$.

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2 A four-dimensional representation of $SU(2)$

A finite dimensional complex representation of a group G is an action of G on a finite dimensional complex vector space V. Because of the properties of the group action, any element of the group can then be regarded as an automorphism of the vector space. Therefore, the group G can be embedded into $\mathrm{GL}(V)$, the group of automorphisms of V. Fixing the bases in V results in representing elements of G as invertible matrices (hence the name representation). In this section we will introduce a four-dimensional (in fact, the only four-dimensional irreducible) representation of the Lie group $SU(2)$ and study some of its properties.

Let V be the complex vector space of homogeneous bivariate polynomials of degree 3. The group $SU(2)$ acts on V in the following manner:

$$\begin{pmatrix} a & b \\ -\bar{b} & \bar{a} \end{pmatrix} f(x,y) = f(ax+by, -\bar{b}x+\bar{a}y).$$

Writing this action in terms of the standard basis x^3, x^2y, x^2, y^3 of V, we see that the representation matrix of this action is given by

$$\Delta\begin{pmatrix} a & b \\ -\bar{b} & \bar{a} \end{pmatrix} = \begin{pmatrix} a^3 & 3a^2b & 3ab^2 & b^3 \\ -a^2\bar{b} & a(|a|^2-2|b|^2) & b(2|a|^2-|b|^2) & \bar{a}b^2 \\ a\bar{b}^2 & \bar{b}(|b|^2-2|a|^2) & \bar{a}(2|b|^2-|a|^2) & b\bar{a}^2 \\ -\bar{b}^3 & 3\bar{b}^2a & -3\bar{b}\bar{a}^2 & \bar{a}^3 \end{pmatrix}. \tag{1}$$

It is well-known that the representation Δ is irreducible [12].

The eigenvalues of $\Delta(g)$ are easy to determine.

Proposition 1. *Suppose that $g \in SU(2)$ has the eigenvalues η and $\bar{\eta}$. Then the eigenvalues of $\Delta(g)$ are $\eta, \bar{\eta}, \eta^3, \bar{\eta}^3$.*

Proof. The matrix $g \in SU(2)$ is conjugate to a diagonal matrix D with diagonal entries η and $\bar{\eta}$. Since Δ is a representation, it respects conjugation, the eigenvalues of $\Delta(g)$ are the same as the eigenvalues of $\Delta(D)$. The latter are computed explicitly from (1) to be $\eta^3, \eta, \bar{\eta}$, and $\bar{\eta}^3$. $\square$

Note that with respect to the canonical basis x^3, x^2y, xy^2, y^3 the representation Δ is *not* unitary. However, the right choice of the basis makes Δ unitary. In fact, Appendix B shows that the equivalent representation

$$R\begin{pmatrix} a & b \\ -\bar{b} & \bar{a} \end{pmatrix} = \begin{pmatrix} a^3 & \sqrt{3}a^2b & \sqrt{3}ab^2 & b^3 \\ -\sqrt{3}a^2\bar{b} & a(|a|^2-2|b|^2) & b(2|a|^2-|b|^2) & \sqrt{3}\bar{a}b^2 \\ \sqrt{3}a\bar{b}^2 & \bar{b}(|b|^2-2|a|^2) & \bar{a}(2|b|^2-|a|^2) & \sqrt{3}b\bar{a}^2 \\ -\bar{b}^3 & \sqrt{3}\,\bar{b}^2a & -\sqrt{3}\,\bar{b}\bar{a}^2 & \bar{a}^3 \end{pmatrix} \tag{2}$$

is unitary. The method to derive this result is the use of invariant integration on $SU(2)$ which is briefly recalled in Appendix A.

3 Construction of space-time codes from restricted spherical codes on $\mathbb{S}^3$

In view of the results of the previous section, A subset $\mathcal{V}$ of $SU(2)$ gives rise to a good four-dimensional space-time code if for any two matrices A and B in $\mathcal{V}$ the eigenvalues of AB^* are bounded away from the third roots of unity. In this section, we give a construction of such matrices. Our starting point is the identification of $SU(2)$ as $\mathbb{S}^3$, the three-dimensional sphere embedded in $\mathbb{R}^4$. This well-known identification is as follows: any element A in $SU(2)$ can be written as

$$A = \begin{pmatrix} a & b \\ -\overline{b} & \overline{a} \end{pmatrix}$$

with $|a|^2+|b|^2 = 1$. The mapping which takes A to the point $(\mathrm{Re}(a), \mathrm{Im}(a), \mathrm{Re}(b), \mathrm{Im}(b))$ is easily seen to be an isomorphism of the topological space $\mathbb{S}^3$ endowed with the Euclidean norm, and the space $SU(2)$ endowed with the distance function $\mathrm{dist}(A, B) := |\det(A - B)|$. Under this identification, the code design problem for $SU(2)$ translates into the design of good spherical codes on $\mathbb{S}^3$, see also [7].

It is further easily seen that the eigenvalues of the matrix A are the roots of the quadratic $X^2 - 2\mathrm{Re}(a)X + 1$. Let

$$B = \begin{pmatrix} c & d \\ -\overline{d} & \overline{c} \end{pmatrix}.$$

Then we have

$$AB^* = \begin{pmatrix} a\overline{c} + b\overline{d} & -ac + bd \\ -\overline{bd} + \overline{ac} & \overline{a}c + \overline{b}d \end{pmatrix}.$$

Hence, the eigenvalues of AB^* are the roots of the quadratic $X^2 - 2\mathrm{Re}(a\overline{c} + b\overline{d}) + 1$. Abusing the notation and identifying A and B with the points $A = (a_1, \ldots, a_4)$ and $B = (b_1, \ldots, b_4)$ on $\mathbb{S}^3$, we see that the eigenvalues of AB^* are roots of $X^2 - 2\langle A, B\rangle X + 1$, where $\langle \cdot, \cdot \rangle$ is the standard dot-product in $\mathbb{R}^4$.

Theorem 1. *Let $\mathcal{V}$ be a finite subset of $SU(2)$ with the property that for any A, B in $\mathcal{V}$, $A \neq B$, we* *have that $1-r \geq \varepsilon$ and $-4r^3+3r+1 \geq \delta$, where $r = \langle A, B\rangle$ under the identification of $SU(2)$ with $\mathbb{S}^3$. Then*

$$\zeta(R(\mathcal{V})) \geq \frac{\sqrt[4]{4\varepsilon\delta}}{2},$$

where R is the irreducible four-dimensional representation of $SU(2)$ defined in Section 2.

Proof. Let η and $\overline{\eta}$ be the eigenvalues of AB^*. Then the eigenvalues of $R(AB^*)$ are, by Proposition 1 equal to $\eta, \overline{\eta}, \eta^3, \overline{\eta}^3$, and hence the diversity distance between $R(A)$ and $R(B)$ equals

$$\frac{1}{2}|(1-\eta)(1-\overline{\eta})|^{1/4}|(1-\eta^3)(1-\overline{\eta}^3)|^{1/4} = \frac{1}{2}|2-(\eta+\overline{\eta})|^{1/4}|2-(\eta^3+\overline{\eta}^3)|^{1/4}.$$

Let $r = \langle A, B\rangle$. As was shown above, η and $\overline{\eta}$ are the roots of the quadratic $X^2 - 2rX + 1$. Hence,

$$|2-(\eta+\overline{\eta})| = 2|1-r| \geq 2\varepsilon.$$

Further, $\eta^3 + \overline{\eta}^3 = (\eta+\overline{\eta})^3 - 3(\eta+\overline{\eta}) = 2r(4r^2-3)$. So,

$$|2-(\eta^3+\overline{\eta}^3)| = 2|-4r^3+3r+1| \geq 2\delta.$$

The assertion now follows. □

We call a spherical code C on $\mathbb{S}^3$ an (ε, δ, c)-*restricted* code if for all $x, y \in C$ we have that $1 - \langle x, y\rangle \geq \varepsilon$ and $|\langle x, y\rangle - c| \geq \delta$. In other words, the elements of C avoid certain angles. An immediate corollary to the pervious result is then

Corollary 1. *Let C be an $(\varepsilon, \delta, -1/2)$-restricted code. Then $\zeta(R(C)) \geq \sqrt[4]{4\varepsilon\delta}/2$, where C is regarded as a subset of $SU(2)$.*

How can we construct a $(\varepsilon, \delta, -1/2)$-restricted code? We will describe one simple method in the following. We start with a spherical code S in which any two elements have a scalar product which is at least ε. Constructions for such codes are well-known, see, e.g. [13]. What we want to do is to "cut out" from $\mathbb{S}^3$ a region Σ in which any two elements have a scalar product which is at least $-1/2+\delta$. Then the code C is just the intersection of the region with S. If the spherical code C is good, then it is likely to be "well-distributed", i.e., that any large enough subset of the sphere contains a number of elements of S which is proportional to its volume (with respect to the volume of $\mathbb{S}^3$). Hence, we expect that the number of elements of C is roughly equal to $\mathrm{vol}(\Sigma)|S|/\mathrm{vol}(\mathbb{S}^3)$, where $\mathrm{vol}(X)$ is the volume of the three-dimensional manifold X.

Using an optimization technique that we describe in Appendix C, we can show the following.

Proposition 2. *Let Σ be the subset of $\mathbb{S}^3$ defined by*

$$\begin{aligned}\Sigma \;:=\; & \Big\{ \Big(\cos(\varphi)\cos(\psi)\cos(\theta), \sin(\varphi)\cos(\psi)\cos(\theta), \sin(\psi)\cos(\theta), \sin(\theta) \Big) \;\Big| \\ & \quad 0 \le \varphi \le 1.8174, -0.319 \le \psi \le \frac{\pi}{2}, -0.3467 \le \theta \le \frac{\pi}{2} \Big\}.\end{aligned}$$

Then $\mathrm{vol}(\Sigma)/\mathrm{vol}(\mathbb{S}^3) > 0.135$ *and any two points in* Σ *have a scalar product which is at most* -0.4985.

Proof. See Appendix C. □

This gives us the following result.

Corollary 2. *Let S be a spherical code in which $\langle x, y \rangle \le 1 - \varepsilon$ for all x and y in the code, and let $\mathcal{V} = S \cap \Sigma$. Then for small ε we have*

$$\zeta(R(\mathcal{V})) \ge \frac{\sqrt[4]{4\varepsilon(9\varepsilon - 12\varepsilon^2 + 4\varepsilon^3)}}{2}$$

Proof. For any two points x, y in $\mathcal{V}$ we have $-0.4985 \le \langle x, y \rangle \le 1 - \varepsilon$ by construction of the set $\mathcal{V}$. Let ε be small enough so that 9ε is smaller than the value of the polynomial $-4r^3 + 3r + 1$ at -0.4985. Then for r between -0.4985 and $1 - \varepsilon$ the value of $-4r^3 + 3r + 1$ is at least its value at $1 - \varepsilon$ which is $9\varepsilon - 12\varepsilon^2 + 4\varepsilon^3$. The assertion now follows from Theorem 1. □

4 Conclusion

In this paper we showed how to use the irreducible four-dimensional representation of $SU(2)$ to construct a family of space-time codes for four transmit antennas. The combinatorial properties of the representation lead to a very non-obvious embedding of $SU(2)$ into $SU(4)$. The unitarization of the representation is done via invariant integration on the group $SU(2)$. The code design problem then reduces to the design of certain restricted spherical codes. We gave a partial solution to this problem by reducing it to a certain optimization problem on the three-dimensional unit sphere.

The results of this paper can be extended to various other compact Lie groups. The fact that all irreducible representations of these groups are unitary and finite dimensional, and the fact that most arithmetic data about these representations are known (e.g., the weights, see [12, Chap. VI]) make these groups ideal candidates for the design of very high rate space-time codes. We hope that this note sparks the interest of the community in this very fruitful area of research.

References

[1] I. E. Telatar, "Capacity of multi-antenna gaussian channels," tech. rep., Bell Laboratories, Lucent Technologies, 1995.

[2] G. J. Foschini, "Layered space-time architecture for wireless communication in a fading environment when using multi-element antennas," *Bell Labs. Tech. J.*, vol. 1, no. 2, pp. 41–59, 1996.

[3] B. Hochwald and W. Sweldens, "Differential unitary space time modulation," tech. rep., Bell Laboratories, Lucent Technologies, Mar. 1999. Also submitted to *IEEE Trans. Comm.* Downloadable from `http://mars.bell-labs.com`.

[4] B. Hughes, "Differential space-time modulation," *submitted to IEEE Trans. Info. Theory*, 1999.

[5] V. Tarokh and H. Jafarkhani, "A differential detection scheme for transmit diversity," *to appear in J. Sel. Area Comm.*, 2000.

[6] S. M. Alamouti, "A simple transmitter diversity scheme for wireless communications," *IEEE J. Sel. Area Comm.*, pp. 1451–1458, 1998.

[7] B. Hassibi, B. Hochwald, A. Shokrollahi, and W. Sweldens, "Representation theory for high-rate multiple-antenna code design," tech. rep., Bell Laboratories, Lucent Technologies, 2000. Downloadable from `http://mars.bell-labs.com`.

[8] B. Hughes, "Optimal space-time constellations from groups," *submitted to IEEE Trans. Info. Theory*, 2000.

[9] A. Shokrollahi, “Computing the performance of space time group codes from their character table,” 2000. Tech. Rep., Bell Laboratories, Lucent Technologies. Downloadable from `http://mars.bell-labs.com`.

[10] H. Jafarkhani and V. Tarokh, “Multiple transmit antenna differential detection from generalized orthogonal designs,” 2000. Preprint, AT&T.

[11] B. Hassibi and M. Khorrami Unpublished manuscript, 2000.

[12] T. Bröcker and T. tom Dieck, *Representations of Compact Lie Groups.* No. 98 in Graduate Texts in Mathematics, Springer Verlag, New York, 1985.

[13] J. Hamkins and K. Zeger, “Asymptotically dense spherical codes,” *IEEE Trans. Info. Theory*, vol. 43, pp. 1774–1798, 1997.

[14] K. Price and R. Storn, “Differential evolution - a simple and efficient heuristic for global optimization over continuous spaces,” *Journal of Global Optimization*, vol. 11, pp. 341–359, 1997.

[15] A. Shokrollahi and R. Storn, “Design of efficient erasure codes with differential evolution,” in *Proceedings of ISIT'00*, p. 5, 2000.

A Invariant integration on $SU(2)$

Our aim in this section is to derive the *invariant integration* on $SU(2)$, i.e, a measure $\mathrm{d}g$ on $SU(2)$ with the property that for all functions f defined on $SU(2)$ and all $h \in SU(2)$ we have

$$\int_{SU(2)} f(g)\ \mathrm{d}g = \int_{SU(2)} f(gh)\ \mathrm{d}g.$$

The clue is the identification of $SU(2)$ with the sphere $\mathbb{S}^3$. We claim that under this identification, the standard measure of $\mathbb{R}^4$ is invariant under multiplication by a fixed element of $SU(2)$. To see this, let A be a generic matrix corresponding to the point $[A_1, \ldots, A_4]$ on $\mathbb{S}^3$, and let H be a fixed matrix corresponding to the point $[h_1, \ldots, h_4]$. Then AH corresponds to the point

$$AH = \begin{array}{l} [A_1\,h_1 - A_2\,h_2 - A_3\,h_3 - A_4\,h_4, A_1\,h_2 + A_2\,h_1 + A_3\,h_4 - A_4\,h_3, \\ A_1\,h_3 - A_2\,h_4 + A_3\,h_1 + A_4\,h_2, -A_3\,h_2 + A_4\,h_1 + A_1\,h_4 + A_2\,h_3]. \end{array}$$

This transformation changes the variables $A_1, \ldots, A_4$, and the variable change is given by the matrix

$$\begin{bmatrix} h_1 & h_2 & h_3 & h_4 \\ -h_2 & h_1 & -h_4 & h_3 \\ -h_3 & h_4 & h_1 & -h_2 \\ -h_4 & -h_3 & h_2 & h_1 \end{bmatrix},$$

whose determinant is

$$\left(h_1{}^2 + h_2{}^2 + h_3{}^2 + h_4{}^2\right)^2 = 1.$$

Therefore, right multiplication with elements of $SU(2)$ leaves the standard measure on $\mathbb{S}^3$ invariant. Hence,

$$\int_{SU(2)} f(g)\ \mathrm{d}g = \int_{\mathbb{S}^3} f(x)\ \mathrm{d}x. \tag{3}$$

Note that the right hand integral is a surface integral. In general, if a surface in the four-dimensional space is given by the equation $u = F(x, y, z)$ for (x, y, z) in the domain D, then the surface integral is given by

$$\int_{(x,y,z)\in D} \sqrt{1 + \left(\frac{\partial F}{\partial x}\right)^2 + \left(\frac{\partial F}{\partial y}\right)^2 + \left(\frac{\partial F}{\partial z}\right)^2}\, f(x, y, z, F(x, y, z))\ \mathrm{d}x\ \mathrm{d}y\ \mathrm{d}z.$$

In our case $F(x, y, z) = \pm\sqrt{1 - x^2 - y^2 - z^2}$ and $\partial F/\partial x = \mp x/\sqrt{1 - x^2 - y^2 - z^2}$. (Similarly for y and z.) We choose one of the signs, keeping in mind that then the value of the integral has to be doubled. So, the right hand integral in (3) is

$$2\int_{\mathbb{S}^3} \frac{1}{\sqrt{1 - x^2 - y^2 - z^2}} f(x, y, z, \sqrt{1 - x^2 - y^2 - z^2})\ \mathrm{d}x\ \mathrm{d}y\ \mathrm{d}z.$$

To evaluate this integral, we will use the Eulerian angles, i.e., the parametrization

$$\begin{aligned} x &= \cos(\varphi)\cos(\psi)\cos(\theta), & y &= \sin(\varphi)\cos(\psi)\cos(\theta), \\ z &= \sin(\psi)\cos(\theta), & u &= \sin(\theta). \end{aligned}$$

Since by our choice of the signs u is positive, θ runs over the interval $[0, \pi]$. Similarly, ψ runs over the interval $[-\pi/2, \pi/2]$, and φ runs over the interval $[0, \pi]$.The matrix describing the change of variables is

$$\begin{bmatrix} -\sin(\varphi)\cos(\psi)\cos(\theta) & -\cos(\varphi)\sin(\psi)\cos(\theta) & -\cos(\varphi)\cos(\psi)\sin(\theta) \\ \cos(\varphi)\cos(\psi)\cos(\theta) & -\sin(\varphi)\sin(\psi)\cos(\theta) & -\sin(\varphi)\cos(\psi)\sin(\theta) \\ 0 & \cos(\psi)\cos(\theta) & -\sin(\psi)\sin(\theta) \end{bmatrix},$$

and its determinant is easily computed to be $-\cos(\psi)\cos(\theta)^2\sin(\theta)$. Further, $\sqrt{1-x^2-y^2-z^2} = \sin(\theta)$. Hence, the integral on the right hand side of (3) equals

$$2\int_0^{\pi}\int_0^{\pi}\int_0^{\pi} f(x,y,z,u)\cos(\psi)\cos(\theta)^2 \,\mathrm{d}\theta\,\mathrm{d}\psi\,\mathrm{d}\varphi, \tag{4}$$

where x, y, z, u are the functions described above.

B Unitarizing the Representation Δ

Let Δ be the representation of $SU(2)$ defined in (1), and let $\langle\cdot,\cdot\rangle$ denote the standard Hermitian bilinear form on $\mathbb{C}^4$. That is, $\langle x, y\rangle = y^*x$, where y^* is the Hermitian conjugate of y. The representation Δ is not unitary with respect to this bilinear form. In this section, we construct a real positive definite symmetric matrix A such that $\Delta(g)$ is unitary with respect to the new bilinear form $\langle\langle x, y\rangle\rangle := y^*Ax$. Let T be a matrix such that $T^*T = A$. Then the equivalent representation R given as $R(g) := T\Delta(g)T^{-1}$ is unitary with respect to the standard Hermitian scalar product. Indeed, we have

$$\begin{aligned} \langle R(g)x, R(g)y\rangle &= y^*R(g)^*R(g)x \\ &= y^*T^{-*}\Delta(g)^*T^*T\Delta(g)T^{-1}x \\ &= y^*T^{-*}\Delta(g)^*A\Delta(g)T^{-1}x \\ &= y^*T^{-*}AT^{-1}x \qquad \text{(since } \Delta(g) \text{ is unitary for } \langle\langle\cdot,\cdot\rangle\rangle) \\ &= y^*x \\ &= \langle x, y\rangle. \end{aligned}$$

The construction of the bilinear form $\langle\langle\cdot,\cdot\rangle\rangle$ is well-known and uses the invariant integral on $SU(2)$:

$$\langle\langle x,y\rangle\rangle := \int_{SU(2)} y^*\Delta(g)^*\Delta(g)x \; \mathrm{d}g. \tag{5}$$

This form is indeed invariant under $\Delta(SU(2))$: for all $h \in SU(2)$ we have

$$\begin{aligned}
\langle\langle \Delta(h)x, \Delta(h)y\rangle\rangle &= \int_{SU(2)} y^*\Delta(h)^*\Delta(g)^*\Delta(g)\Delta(h)x \; \mathrm{d}g \\
&= \int_{SU(2)} y^*\Delta(h)^*\Delta(g)^*\Delta(g)\Delta(h)x \; \mathrm{d}g \\
&= \int_{SU(2)} y^*\Delta(gh)^*\Delta(gh)x \; \mathrm{d}g \qquad \text{(since } \Delta \text{ is a representation)} \\
&= \int_{SU(2)} y^*\Delta(g)^*\Delta(g)x \; \mathrm{d}g \qquad \text{(because of invariant integration)} \\
&= \langle x,y\rangle.
\end{aligned}$$

A small calculation shows that $\langle\langle x,y\rangle\rangle = y^*Ax$, where $A = (a_{ij})$ with

$$a_{ij} = \int_{SU(2)} \Big(\Delta(g)^*\Delta(g)\Big)_{ij} \; \mathrm{d}g.$$

The computation of the a_{ij} is rather lengthy. We exemplify it in the case of a_{11}. Let

$$g = \begin{pmatrix} a & b \\ -\overline{b} & \overline{a} \end{pmatrix}.$$

Then we have

$$a_{11} = \Big(\Delta(g)^*\Delta(g)\Big)_{11} = (a_1^2 + b_1^2)^2 + (a_2^2 + b_2^2)^2.$$

Using the invariant integral of (5), we obtain

$$a_{11} = 2\int_0^{\pi}\int_{-\pi/2}^{\pi/2}\int_0^{\pi} 2\cos(\psi)^5\cos(\theta)^6 - 2\,\cos(\psi)^3\cos(\theta)^4 + \cos(\psi)\cos(\theta)^2 \; \mathrm{d}\theta\;\mathrm{d}\psi\;\mathrm{d}\varphi = \frac{4}{3}\pi^2.$$

Doing the calculations for all the a_{ij} gives

$$A = 4\pi^2 \begin{pmatrix} \frac{1}{3} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \frac{1}{3} \end{pmatrix}.$$

A square root of A is easy to compute. The equivalent unitary representation R is then given by

$$R\begin{pmatrix} a & b \\ -\overline{b} & \overline{a} \end{pmatrix} = \begin{pmatrix} a^3 & \sqrt{3}a^2b & \sqrt{3}ab^2 & b^3 \\ -\sqrt{3}a^2\overline{b} & a(|a|^2 - 2|b|^2) & b(2|a|^2 - |b|^2) & \sqrt{3}\overline{a}b^2 \\ \sqrt{3}a\overline{b}^2 & \overline{b}(|b|^2 - 2|a|^2) & \overline{a}(2|b|^2 - |a|^2) & \sqrt{3}b\overline{a}^2 \\ -\overline{b}^3 & \sqrt{3}\,\overline{b}^2 a & -\sqrt{3}\,\overline{b}\overline{a}^2 & \overline{a}^3 \end{pmatrix}.$$

C Restricted spherical codes

Proposition 3. *Suppose that $0 \le b \le \pi/2$, and that $\alpha < 0$. Then, for $-b \le x, y \le \pi/2$ the minimum of the function $\alpha\cos(x)\cos(y) + \sin(x)\sin(y)$ is*

$$-\sqrt{\alpha^2\cos(b)^2 + \sin(b)^2}.$$

Proof. We study $f(x) = \alpha\cos(x)\cos(y)+\sin(x)\sin(y)$ as a function of x in the interval $-b \le x \le \pi/2$. As such, it has a local minimum at x_0 with $\tan(x_0) = \tan(y)/alpha$, as is easily seen by differentiation. Further, the function is monotonically increasing for $x \ge x_0$, and monotonically decreasing for $x \le x_0$. The value of $f(x)$ at x_0 is easily computed to be $-\sqrt{\alpha^2\cos(y)^2 + \sin(y)^2}$.

Suppose that $y < 0$. Then $x_0 > 0$ since $\alpha < 0$. In particular, $x_0 > -b$, and the minimal value of $f(x)$ is $-\sqrt{\alpha^2\cos(y)^2 + \sin(y)^2}$. The minimal value of this expression for $y < 0$ is $-\sqrt{\alpha^2\cos(b)^2 + \sin(b)^2}$.

Suppose now that $y > 0$. Since $\alpha < 0$, $x_0 < 0$. If $x_0 > -b$, then the minimal value of $f(x)$ in the interval $[-b, \pi/2]$ is again $-\sqrt{\alpha^2\cos(b)^2 + \sin(b)^2}$, by the same reasoning as above. However, if $x_0 \le -b$, then by the monotonicity properties of $f(x)$ its minimal value is $f(-b)$ which is $\alpha\cos(b)\cos(y) - \sin(b)\sin(y)$. Regard this as a function of y. Again, taking derivatives, we see that its minimal value is $-\sqrt{\alpha^2\cos(b)^2+\sin(b)^2}$ which is achieved at y_0 such that $\tan(y_0) = -\tan(b)/\alpha$. y_0 is in the domain of $f(x)$, so that the minimal value of $f(x)$ is indeed as claimed in the proposition. $\square$

Proposition 4. *Let a, b, c be positive real numbers with $\pi/2 \le a \le \pi$, $b, c \le \pi/2$. Further, let $\Sigma_{a,b,c}$ be the subset of $\mathbb{S}^3$ defined as*

$$\Sigma_{a,b,c} := \Big\{\Big(\cos(\varphi)\cos(\psi)\cos(\theta), \sin(\varphi)\cos(\psi)\cos(\theta), \sin(\psi)\cos(\theta), \sin(\theta)\Big) \ \Big| \ 0 \le \varphi \le a, -b \le \psi \le \frac{\pi}{2}, -c \le \theta \le \frac{\pi}{2}\Big\}.$$

Then the minimal value of $\langle x, y\rangle$ for $x, y \in \Sigma_{a,b}$ is

$$-\sqrt{\sin(c)^2 + \Big(\sin(b)^2 + \cos(a)^2\cos(b)^2\Big)\cos(c)^2}, \tag{6}$$

and the volume of $\Sigma_{a,b,c}$ is

$$\mathrm{vol}\Big(\Sigma_{a,b,c}\Big) = a\Big(1+\sin(b)\Big)\left(\frac{\pi}{4} + \frac{1}{2}\cos(c)\sin(c) + \frac{1}{2}c\right). \tag{7}$$

Proof. Let x and y be two points in $\Sigma_{a,b,c}$ that correspond to the angles φ, ψ, θ and φ', ψ', θ', respectively. A calculation shows that

$$\langle x, y\rangle = \alpha\cos(\theta)\cos(\theta') + \sin(\theta)\sin(\theta'),$$

where

$$\alpha = \cos(\varphi-\varphi')\cos(\psi)\cos(\psi') + \sin(\psi)\sin(\psi').$$

$\langle x, y\rangle$ is a monotonically decreasing function of α, hence its minimum value is attained when α is minimal, and in that case the minimal value is $-\sqrt{\alpha^2\cos(c)^2+\sin(c)^2}$ by Proposition 3, assuming that the minimal value of α is negative. The minimal value of α is, by the same reasoning, attained when $\cos(\varphi-\varphi')$ is minimal. The minimum value of this expression is $\cos(a)$, as can be easily seen. Since $\pi/2 \le a \le \pi$, this value is negative, and so the minimal value of α is, by Proposition 4, equal to $-\sqrt{\cos(a)^2\cos(b)^2+\sin(b)^2}$, which is negative. Combining these results, we see that the minimal value of $\langle x, y\rangle$ is indeed what we claim it to be.

The computation of the volume of $\Sigma_{a,b,c}$ is rather trivial, and is obtained from the computation of the surface integral of the sphere using the spherical coordinates (see also Appendix A). Indeed, we have

$$\mathrm{vol}(\Sigma_{a,b,c}) = \int_0^a \int_{-b}^{\pi/2} \int_{-c}^{\pi/2} \cos(\theta)^2 \cos(\psi)\ \mathrm{d}\theta\ \mathrm{d}\psi\ \mathrm{d}\varphi.$$

A standard calculation reveals the result. □

Proposition 2 follows now by a straightforward calculation. Indeed, the specific numbers there were obtained via an optimization procedure: maximize the volume of $\Sigma_{a,b,c}$ as given in 7 under the constraint that 6 is larger than $-1/2$. There are various ways for running the optimization. We opted to choose the differential evolution technique [14] which has proved a powerful tool in many other areas [15].