Quaternionic equiangular lines

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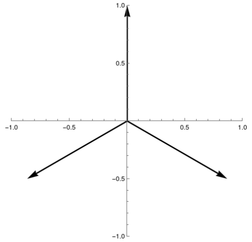
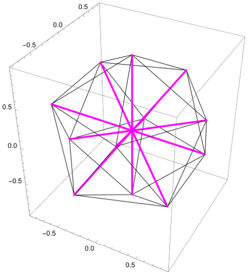
Introduction

The unit vectors $\Phi = (f_r)_{r=1}^{n}$ in $\mathcal{H}$ are called **equiangular** if the angles between them are constant, i.e.

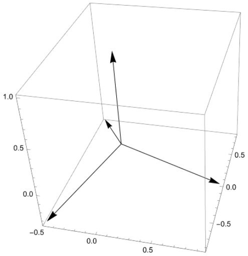
$$|\langle f_r | f_s \rangle|^2 = \lambda = \cos^2(\theta), \text{ for } r \neq s.$$



(a) $\mathcal{H} = \mathbb{R}^2$



(b) $\mathcal{H} = \mathbb{R}^3$



(c) $\mathcal{H} = \mathbb{C}^2$, using Bloch representation

Figure: Simple examples of maximal configurations of equiangular lines

Number of equiangular lines

Theorem

Suppose $d \geq 2$. Let $\Phi = (f_r)_{r=1}^n \subset \mathbb{F}^d$, where $\mathbb{F}$ is $\mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$, be a sequence of non-parallel unit vectors giving a set of equiangular lines. Then

$$n \leq \begin{cases} \frac{d(d+1)}{2}, & \mathbb{F} = \mathbb{R}; \\ d^2, & \mathbb{F} = \mathbb{C}; \\ 2d^2 - d, & \mathbb{F} = \mathbb{H}. \end{cases}$$

Moreover, when the bound is attained,

$$\lambda = |\langle f_r | f_s \rangle|^2 = \begin{cases} \frac{1}{d+2}, & \mathbb{F} = \mathbb{R}; \\ \frac{1}{d+1}, & \mathbb{F} = \mathbb{C}; \\ \frac{1}{d+\frac{1}{2}}, & \mathbb{F} = \mathbb{H}. \end{cases}$$

Quaternions

Quaternions (1)

- Quaternions were first described by W.R. Hamilton in 1843.
- Motivation: to generalise complex number in order to describe points in three-dimensional space.

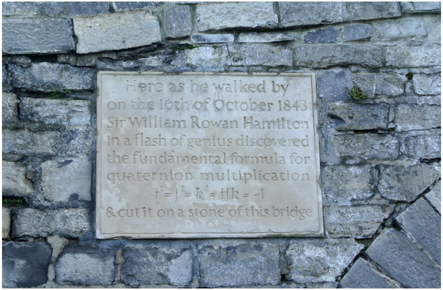


Figure: Plaque concerning quaternions on Broom Bridge, Dublin[1]

[1] Source: https://commons.wikimedia.org/wiki/File:Inscription_on_Broom_Bridge_(Dublin)_regarding_the_discovery_of_Quaternions_multiplication_by_Sir_William_Rowan_Hamilton.jpg

Quaternions (2)

The **quaternions** $\mathbb{H}$ are numbers of the form $q = q_1 + q_2 i + q_3 j + q_4 k$, where $q_1, \ldots, q_4 \in \mathbb{R}$, with addition

$$q + p := (q_1 + p_1) + (q_2 + p_2)i + (q_3 + p_3)j + (q_4 + p_4)k$$

and the non-commutative multiplication is given by

$$i^2 = j^2 = k^2 = ijk = -1.$$

From this equations, we can derive

$$\begin{array}{lll} ij = k, & jk = i, & ki = j, \\ ji = -k, & kj = -i, & ik = -j. \end{array}$$

Hence, $q = (q_1 + q_2 i) + (q_3 + q_4 i)j$.

Quaternions (3)

- Let $q = q_1 + q_2 i + q_3 j + q_4 k \in \mathbb{H}$,
  - The **conjugate** is $\overline{q} \coloneqq q_1 - q_2 i - q_3 j - q_4 k$,
  - The **norm** is $|q| \coloneqq \sqrt{q\overline{q}} = \sqrt{q_1^2 + q_2^2 + q_3^2 + q_4^2}$,
  - The **real part** is $\mathrm{Re}(q) \coloneqq q_1$.
- Quaternions form a non-commutative field and the inverse of $q \neq 0$ is

$$q^{-1} = \frac{\overline{q}}{|q|^2}.$$

- Quaternions can be represented with Pauli matrices, e.g.

$$1 \mapsto I,\ i \mapsto -i\sigma_x,\ j \mapsto -i\sigma_y,\ k \mapsto -i\sigma_z.$$

Quaternionic vector spaces

- Due to noncommutativity, we must distinguish between scalar multiplication from the left or the right when generalising vector spaces to non-commutative fields.
- Further, we consider only multiplication from the right and finite-dimensional quaternionic vector spaces.
- A $\mathbb{H}$-linear map between such vector spaces, $A : \mathcal{V} \to \mathcal{W}$, satisfies

$$A(v_1 q_1 + v_2 q_2) = A(v_1) q_1 + A(v_2) q_2$$

  for any $v_1, v_2 \in \mathcal{V}$ and $q_1, q_2 \in \mathbb{H}$.
- Linear maps can be represented by matrices.
- **Trace** of a quaternionic matrix is defined as

$$\mathrm{Tr}(A) := \mathrm{Re}\left(\sum_{t=1}^{d} A_{tt}\right).$$

Inner products

Let $\mathcal{V}$ be a quaternionic vector space.

- An inner product on $\mathcal{V}$ can be introduced as a map $\langle\cdot|\cdot\rangle : \mathcal{V} \times \mathcal{V} \to \mathbb{H}$, which is conjugate symmetric, $\mathbb{H}$-linear in the second variable and positive definite.
- For any $v, w \in \mathcal{V}$ and $q_1, q_2 \in \mathbb{H}$,

$$\langle vq_1|wq_2\rangle = \overline{q}_1\langle v|w\rangle q_2.$$

- The prototypical example is $\mathbb{H}^d$ with the inner product

$$\langle v|w\rangle := \sum_{r=1}^{d} \overline{v}_r w_r.$$

- $(\mathcal{V}, \langle\cdot|\cdot\rangle)$ is a called a **quaternionic Hilbert space**.
- The notion of adjoint operator and the classes of self-adjoint (Hermitian), positive semidefinite and unitary operators are defined analogously to the complex case.

Context: quaternionic quantum mechanics

Standard quantum mechanics

- In quantum mechanics, the **state space** is the set of density matrices,

$$\mathcal{S}(\mathcal{H}) = \{\rho \in \mathcal{L}_s(\mathcal{H}) : \rho \geq 0, \operatorname{tr} \rho = 1\},$$

  where $\mathcal{H} \simeq \mathbb{C}^d$ is a complex Hilbert space.

- **Observables** are given by POVMs: (finite) collections of **effects**, $\Pi = (\Pi_\omega)_{\omega \in \Omega}$, where $\Pi_\omega \in \mathcal{L}_s(\mathcal{H})$, $\Pi_\omega \geq 0$, such that

$$\sum_{\omega \in \Omega} \Pi_\omega = I,$$

  where Ω is the set of possible outcomes.

- Probability of obtaining an outcome $\omega \in \Omega$, if the state before the measurement was $\rho \in \mathcal{S}(\mathcal{H})$, is given by the **Born rule**,

$$p_\omega(\rho) = \operatorname{Tr}(\rho \Pi_\omega).$$

SIC-POVMs

- A **SIC-POVM** is a POVM $\Pi = (\Pi_\omega)_{\omega=1}^{d^2}$, where $\Pi_\omega = \frac{1}{d}|\phi_\omega\rangle\langle\phi_\omega|$ for some unit vectors $|\phi_\omega\rangle \in \mathcal{H}$ such that

$$|\langle\phi_\omega|\phi_\omega\rangle|^2 = \frac{1}{d+1}, \tag{1}$$

  which means that the complex lines given by $|\phi_\omega\rangle$ are **equiangular**.
- The existence of SIC-POVMs in arbitary dimension (Zauner's conjecture[2]) remains an open problem.
- The existence of SIC-POVM in dimension d is equivalent to the existence of d^2 equiangular lines in $\mathbb{C}^d$.

[2] Zauner (1999).

States

- The **quaternionic quantum state** is described by $\rho \in \mathcal{L}_s(\mathcal{H})$ satisfying $\rho \geq 0$ and $\operatorname{Tr} \rho = 1$, where $\mathcal{H}$ is a quaternionic Hilbert space.
- The set of states is convex.
- Its extreme points (pure states) are rank-1 projections, i.e. those states which satisfy $\rho^2 = \rho$.
- $A \in \mathcal{L}_s(\mathcal{H})$ is a pure quaternionic quantum state if and only if

$$\operatorname{Tr}(A^2) = \operatorname{Tr}(A^3) = 1.$$

Measurements

- An **observable** with the set of outcomes Ω is described by a **quaternionic POVM**: a collection of **effects** $\Pi = (\Pi_\omega)_{\omega \in \Omega}$, $\Pi_\omega \in \mathcal{L}_s(\mathcal{H})$, $\Pi_\omega \geq 0$, such that

$$\sum_{\omega \in \Omega} \Pi_\omega = I.$$

- The set of quaternionic POVMs is convex.
- Probability of obtaining an outcome $\omega \in \Omega$ in the measurement Π, performed on a physical system whose state is described by ρ is

$$p_\omega(\rho) = \mathrm{Tr}(\rho \Pi_\omega).$$

Equiangular lines

Equiangularity

- The unit vectors $\Phi = (f_r)_{r=1}^n$ in $\mathcal{H}$ are called **equiangular** if the angles between them are constant, i.e.

$$|\langle f_r | f_s \rangle|^2 = \lambda = \cos^2(\theta), \text{ for } r \neq s.$$

- Examples: orthonormal bases, vertices of regular simplex.
- For equiangular vectors we obtain (using the variational characterisation) the inequality

$$\lambda \geq \frac{n-d}{d(n-1)},$$

where $d = \dim \mathcal{H}$.

Number of equiangular lines

The set of self-adjoint operators $\mathcal{L}_s(\mathcal{H})$ is a real vector space.

Theorem

Suppose $d \geq 2$. Let $\Phi = (f_r)_{r=1}^n \subset \mathbb{F}^d$, where $\mathbb{F}$ is $\mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$, be a sequence of non-parallel unit vectors giving a set of equiangular lines. The orthogonal projections $P_r : f \mapsto f_r \langle f_r | f \rangle$ are $\mathbb{R}$-linearly independent, hence

$$n \leq \begin{cases} \frac{d(d+1)}{2}, & \mathbb{F} = \mathbb{R}; \\ d^2, & \mathbb{F} = \mathbb{C}; \\ 2d^2 - d, & \mathbb{F} = \mathbb{H}. \end{cases}$$

with equality if and only if $(P_j)_{j=1}^n$ is a basis for $\mathcal{L}_s(\mathcal{H})$. In such case,

$$\lambda = |\langle f_r | f_s \rangle|^2 = \begin{cases} \frac{1}{d+2}, & \mathbb{F} = \mathbb{R}; \\ \frac{1}{d+1}, & \mathbb{F} = \mathbb{C}; \\ \frac{1}{d+\frac{1}{2}}, & \mathbb{F} = \mathbb{H}. \end{cases}$$

Real case

- The upper bound on the number of equiangular lines in $\mathbb{R}^d$ is $\frac{d(d+1)}{2}$.
- This bound is attained for $d = 2, 3, 7, 23$.
- It is believed that these are the only dimensions for which the bound is attained.
- The maximal number of equiangular lines in $\mathbb{R}^4$ is 6.
- The maximal number of equiangular lines in $\mathbb{R}^5$ is 10.
- The exact value of the maximal number of equiangular lines in $\mathbb{R}^d$ is known for $d = 2, \ldots, 17$ and $d = 21, 22, 23$ (as of Jan 2024).
- In $\mathbb{R}^{18}$, there are at most 59 equiangular lines[3].

[3] Greeves, Syatriadi (2024).

Complex case

- Zauner conjectured[4] that for every dimension d, there exists a set of d^2 equiangular lines in $\mathbb{C}^d$.
- The conjecture is believed to be true, although it remains an open problem.
- Analytical solutions have been found for every d up to 53 and for some higher dimensions up to $d = 5799$ (as of March 2025).
- Numerical solutions are known up to $d = 193$ with sporadic results up to $d = 39604$ (as of March 2025).
- All known sets of d^2 equiangular lines are orbits of the Weyl-Heisenberg group, with the exception of the Hoggar[5] lines in $\mathbb{C}^8$.

[4] Zauner (1999).
[5] Hoggar (1978).

Quaternionic case (1)

- The upper bound on the number of equiangular lines in $\mathbb{H}^d$ is $2d^2 - d$.
- The existence of 6 equiangular lines in $\mathbb{H}^2$ has been proved[6].
- The existence of 15 equiangular lines in $\mathbb{H}^3$ has been proved[7].

[6] Fard (2008), independently by Et-Taoui (2020).

[7] Cohn, Kumar, Minton (2016).

Quaternionic case (2)

Maximal configuration of equiangular lines in $\mathbb{H}^2$ is[8]:

$$f_1 = \begin{pmatrix} \alpha + \beta i + \frac{1}{4}j + \gamma k \\ \delta \end{pmatrix}, \quad f_2 = \begin{pmatrix} -\alpha + \beta i + \frac{1}{4}j + \gamma k \\ \delta \end{pmatrix},$$

$$f_3 = \begin{pmatrix} -2\beta i + \frac{1}{4}j + \gamma k \\ \delta \end{pmatrix}, \quad f_4 = \begin{pmatrix} -\frac{3}{4}j + \gamma k \\ \delta \end{pmatrix},$$

$$f_5 = \begin{pmatrix} -\gamma k \\ \delta \end{pmatrix}, \quad f_6 = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

where $\alpha = \frac{\sqrt{6}}{4}, \beta = \frac{\sqrt{2}}{4}, \gamma = \frac{\sqrt{15}}{20}, \delta = \sqrt{\frac{2}{5}}$.

[8] Fard (2008).

Quaternionic case (3)

- Numerical calculations[9] suggest that for $\mathbb{H}^4$, this bound is not attained.
- It is believed[10] that the number of equiangular lines in $\mathbb{H}^d$ is rarely maximal, i.e. $2d^2 - d$.

It was conjectured by Waldron[11] that:

Conjecture

The maximal number of quaternionic equiangular lines in $\mathbb{H}^d$ is strictly larger than the maximal number of complex equiangular lines in $\mathbb{C}^d$ for each $d \geq 2$.

[9] Cohn, Kumar, Minton (2016).
[10] Waldron (2025).
[11] Waldron (2025).

Quaternionic reflections

- A quaternionic reflection is a unitary map $A \in U(\mathbb{H}^d)$, $A \neq I$, which fixes a subspace of dimension $d-1$ in $\mathbb{H}^d$, i.e. $\mathrm{rank}(I-A) = d-1$.
- A group generated by quaternionic reflections is called a quaternionic reflection group.

Quaternionic case (4)

- The maximal set of six equiangular lines in $\mathbb{H}^2$ was obtained as the solution to the system[12]

$$|\langle f_r|f_s\rangle|^2 = \frac{2}{5}, \quad r \neq s, \quad |\langle f_r|f_r\rangle|^2 = 1,$$

where $f_r = z_r + w_r j$, $z_r, w_r \in \mathbb{C}^2$.

- They are an orbit of the quaternionic reflection group H_{720} of order 720 and its subgroup of order 24.
- Each of the lines is fixed by a subgroup of H_{720} of order 120.
- Method: start with a given quaternionic reflection group and find the associated set of highly symmetric lines.

[12] Et-Taoui (2020).

Tight frames

Let $\mathcal{H}$ be a finite-dimensional Hilbert space over $\mathbb{F}$, which is $\mathbb{R}$, $\mathbb{C}$ or $\mathbb{H}$ and $d := \dim \mathcal{H}$.

- A frame is a sequence of vectors $(f_r)_{r=1}^n$ for which there exist $0 < A < B$ such that for every $f \in \mathcal{H}$,

$$A\|f\|^2 \leq \sum_{r=1}^{n} |\langle f|f_r\rangle|^2 \leq B\|f\|^2.$$

- A frame is called a tight frame if $A = B$ is possible.
- Equivalently, every $f \in \mathcal{H}$ can be expanded as $f = \frac{1}{A}\sum_{r=1}^{d} f_r\langle f_r|f\rangle$.
- Variational characterisation: if $(f_r)_{j=1}^n$ are vectors in $\mathcal{H}$, not all zero, then

$$v(\Phi) := \sum_{r=1}^{n}\sum_{s=1}^{n} |\langle f_r|f_s\rangle|^2 - \frac{1}{d}(\sum_{r=1}^{n} \|f_r\|^2)^2 \geq 0$$

  with equality if and only if $(f_r)_{r=1}^n$ is a tight frame.

Tight equiangular lines (1)

- The equiangular unit vectors $\Phi = (f_r)_{r=1}^n$ are called **tight equiangular**, if Φ is a tight frame.
- For equiangular vectors we obtain (using the variational characterisation) the inequality

$$\lambda = |\langle f_r | f_s \rangle|^2 \geq \frac{n-d}{d(n-1)}, \quad r \neq s,$$

  with equality if and only if Φ is a tight frame.
- In $\mathbb{R}^4$, there are no n tight equiangular lines for $n > 5$.
- In $\mathbb{R}^5$, there are no n tight equiangular lines for $n > 11$.

Tight equiangular lines (2)

- Six tight equiangular lines in $\mathbb{H}^4$ exist[13].
- There is[14] a unique (up to projective unitary equivalence) set of n tight equiangular lines in $\mathbb{H}^2$ for $n = 2, \ldots, 6$.

It was conjectured[15] that:

Conjecture

There exists more than d^2 tight equiangular lines in $\mathbb{H}^d$, $d \geq 2$ (confirmed for $d = 2, 3$, otherwise open).

[13] Waldron (2025).
[14] Fard (2008).
[15] Waldron (2025)

Summary

- Quaternions can be used to develop a formalism analogous to quantum theory.
- In analogy to Zauner's conjecture concerning SIC-POVMs, the problem of existence of maximal number of quaternionic equiangular lines can be considered.
- The upper bound on the number of equiangular lines in $\mathbb{H}^d$, namely $2d^2 - d$, is attained for $d = 2, 3$.
- It is believed that the number of equiangular lines in $\mathbb{H}^d$ is rarely maximal.
- It was conjectured by Waldron that the maximal number of equiangular lines is strictly larger in $\mathbb{H}^d$ than in $\mathbb{C}^d$ for every $d \geq 2$.

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