Abstract

A complete set of $N+1$ mutually unbiased bases (MUBs) forms a convex polytope in the $N^2-1$ dimensional space of $N \times N$ Hermitian matrices of unit trace. As a geometrical object such a polytope exists for all values of $N$, while it is unknown whether it can be made to lie within the body of density matrices unless $N = p^k$, where $p$ is prime. We investigate the polytope in order to see if some values of $N$ are geometrically singled out. One such feature is found: It is possible to select $N^2$ facets in such a way that their centers form a regular simplex if and only if there exists an affine plane of order $N$. Affine planes of order $N$ are known to exist if $N = p^k$; perhaps they do not exist otherwise. However, the link to the existence of MUBs—if any—remains to be found.
I. Introduction

Lately there has been an increase of interest in *mutually unbiased bases*—MUBs for short—in relation to quantum foundations and quantum information. Two orthonormal bases \(\{|e_i\}\) and \(\{|f_i\}\) in Hilbert space \(\mathcal{H}^N\) are said to be mutually unbiased if, for all \(i, j\),

\[
|\langle e_i | f_j \rangle|^2 = \frac{1}{N}.
\]  

(1)

Complete knowledge of the observable corresponding to one of the bases implies total ignorance about the outcome of a measurement in the other basis. This is a finite dimensional analogy to the complementarity of position and momentum in the continuous case.

One of the main features about MUBs was proved in the late eighties by Wootters and Fields \[1\]. It has to do with optimal state determination of mixed quantum states. If one wants to determine the \(N^2 - 1\) parameters of an \(N \times N\) density matrix, using von Neumann measurements, one needs \(N + 1\) different observables. The statistical errors in the determination are minimized if one chooses observables corresponding to bases that are all mutually unbiased. It was seen (and will be seen later in this paper) that this number of MUBs is the most there can exist; thus \(N + 1\) MUBs are called a complete set of MUBs. But, in spite of efforts that have been made, it is not known if it is possible in general to have a complete set of MUBs.

Ivanović \[2\] has found complete sets of MUBs for prime dimensions, \(N = p\). His construction was generalized by Wootters and Fields \[1\] to prime power dimensions, \(N = p^k\). There the existence of finite fields with \(p^k\) elements is crucial, and further generalizations are difficult to find since no other finite fields exists. One conjecture is that it is not possible to have a complete set of MUBs unless the dimension is a prime power. Using the construction for prime power dimensions one can find \(\min\{p_1^{k_1}, \ldots, p_r^{k_r}\} + 1\) MUBs in the dimension \(N = p_1^{k_1} \cdots p_r^{k_r}\), where the \(p_i\)'s are all distinct prime numbers \[3\] (see also \[4, 5\]). This gives a lower bound on the maximal number of MUBs. But recently it was proved that one at least sometimes can have more than this \[6\]: this is for certain square dimensions.

In this paper we observe that a complete set of MUBs forms a convex polytope in the set of Hermitian \(N \times N\) matrices of unit trace. In fact, as a convex body such a polytope exists regardless of whether the MUBs exist or not. The details are explained in section II, and result in a reformulation of the question of the existence of a complete set of MUBs. In section III we turn our attention to the relation between MUBs and finite affine planes.
This connection is central to Wootters’ suggestion as to how the MUBs can be used, namely, to perform state tomography using a Wigner function defined on finite affine planes of order $N$ (see also [9] for an accessible introduction of the main ideas). We find an elegant condition, using the language introduced in section II, that tells us exactly how the affine planes enter the game. More precisely, we show that an affine plane of order $N$ exists if and only if a regular simplex can be inscribed in our polytope in a certain way. On the face of it, this has nothing to do with the existence of MUBs. In section IV we return to the question of when a complete set of MUBs can be associated to the polytope; in particular we investigate whether either the polytope or the set of density matrices is “skew” in some sense. We conclude in section V with a summary.

II. The complementarity polytope

Instead of looking at state vectors we will study how the MUB states sit in the set of density matrices. This is the subset of positive matrices, in the set of Hermitian matrices with unit trace. If distances squared between two matrices are defined by

$$D^2(A, B) = \frac{1}{2} \text{Tr}(A - B)^2,$$

then the set of Hermitian matrices with unit trace form an $N^2 - 1$ dimensional Euclidean space. Choosing the matrix

$$\rho_* = \frac{1}{N} \mathbb{I}$$

as the origin, this is a vector space, with scalar product

$$\langle A, B \rangle = \frac{1}{4} \left[D^2(A + B, \rho_*) - D^2(A - B, \rho_*)\right] = \frac{1}{2} \left[\text{Tr}AB - \frac{1}{N}\right].$$

Thus two matrices are orthogonal if $\text{Tr}AB = 1/N$.

The pure states $|\Psi\rangle$ are now the projectors $P = |\Psi\rangle\langle\Psi|$, sitting on a sphere centered at the origin and with radius $\sqrt{(N - 1)/2N}$. This is the outsphere of the set of density matrices, which in itself is the convex hull of the projectors.

The projectors corresponding to two states from an ON-basis in Hilbert space sit at unit distance from each other. Therefore a full basis $\{P_k^{(i)}\}, k =$
1, . . . , N, forms a regular simplex in an \( N - 1 \) dimensional subspace. This statement follows from equation (2) and the equation

\[
\Tr P^{(l)}_k P^{(l')}_{k'} = 0 \quad k \neq k'.
\tag{5}
\]

This kind of simplex will sometimes, for clarification, be called a P-simplex, since we will later encounter other simplicies. Now assume that we have several bases \( \{ P^{(l)}_k \} \), where \( l \) labels the basis and \( k \) the state in that basis, which are mutually unbiased with each other. Then (from eq. (1))

\[
\Tr P^{(l)}_k P^{(l')}_{k'} = \frac{1}{N} \quad l \neq l'.
\tag{6}
\]

This means that projectors belonging to different MUBs are orthogonal. Thus the simplices from different MUBs sit in orthogonal subspaces. Every subspace has dimension \( N - 1 \) and the full dimension of the space of density matrices is \( N^2 - 1 \), so the maximum number of MUBs is \( N + 1 \). Such a set is called a complete set of MUBs.

If we have a complete set of MUBs, their \( N(N+1) \) states defines a convex polytope—the complementarity polytope—in our \( N^2 - 1 \) dimensional space. But it is possible to have a complementarity polytope for any \( N \). Just take \( N + 1 \) regular simplices, each with \( N \) corners at unit distance from each other. Let the simplices sit in orthogonal subspaces, and centered at the origin. The complementarity polytope is the convex hull of the \( N(N+1) \) corners of these P-simplices. However, it will not be true in general that the corners are matrices with non-negative spectrum, that is that they are density matrices. The question of the existence of a complete set of MUBs can now be reformulated: Is it possible to arrange the complementarity polytope so that it is a subset of the set of density matrices? We need to somehow rotate the polytope in such a way that all its corners coincide with pure states. By construction the corners automatically lie on the outsphere of the set of density matrices, but generally not at pure states, since the pure states only constitute a small subset of the sphere (a \( 2N - 2 \) dimensional subset of the \( N^2 - 2 \) dimensional sphere; the numbers match only for \( N = 2 \)). Also when the corners of the polytope do not correspond to density matrices, we will denote them \( P^{(l)}_k \)—they still obey equations (5) and (6)—or sometimes \( P_\omega \), with a collective index \( \omega \) that runs between 1 and \( N(N + 1) \).

So the complementarity polytope exists for all \( N \). It is a distinct possibility that a complete set of MUBs does not exist when \( N \neq p^k \). If this is true something should happen for these \( N \), either with the polytope or with the set of density matrices. Something that makes it impossible to rotate
the polytope so that it fits in the set of density matrices. Is it possible to understand why? Now we will go on and study the complementarity polytope, to see if we can get any clues.

We will work in the space of matrices with \( \text{Tr} M = 1 \). When studying the polytope we need distances, and that means traces like \( \text{Tr} M^2 \) and \( \text{Tr} M_1 M_2 \). In quantum mechanics, on the other hand, the matrices should be positive, \( M \geq 0 \), to describe states. To assure this the full spectrum is needed, and therefore knowledge about \( \text{Tr} M \) and \( \text{Tr} M^2 \) is not enough. Also the traces \( \text{Tr} M^3, \ldots, \text{Tr} M^N \) are needed to derive the eigenvalues. The requirements coincide for two by two matrices, and then it is trivial to fit the polytope in the set of density matrices (i.e. the Bloch ball).

For \( N = 2 \) the complementarity polytope is an octahedron (figure 1). Schematically we can think of it as three one dimensional orthogonal P-simplices, like \( \bullet \bullet \bullet \). When \( N = 3 \) we have four totally orthogonal triangles, \( \triangle \triangle \triangle \triangle \), when \( N = 4 \) we have five tetrahedra, \( \square \square \square \square \), and so on for any \( N \). All the edges in the polytope are extremal, except when \( N = 2 \). A face of the polytope is obtained as the convex hull of a set of corners, where—to ensure that the face really belongs to the boundary of the polytope—at least one corner from each P-simplex is not included. We will be interested in the faces formed by taking exactly one corner \( P_\omega \) from each P-simplex (in the case \( N = 3 \) this is for example \( \Delta \Delta \Delta \Delta \)). There are \( N^{N+1} \) such faces and these faces are themselves \( N \) dimensional regular simplices. We call them point faces (in the next section, we will see that they are related to Wootters' phase points \( \mathbb{S} \)). To each point face \( \alpha \) we will
associate a "point face operator"

$$A_{\alpha} = \rho* + \sum_{P_{\omega} \in \alpha} (P_{\omega} - \rho*) = \sum_{P_{\omega} \in \alpha} P_{\omega} - \mathbb{1} .$$  \hspace{1cm} (7)

For these operators we have

$$\text{Tr}A_{\alpha} = 1 \quad \text{and} \quad \text{Tr}A_{\alpha}^2 = N .$$  \hspace{1cm} (8)

The second equality follows from

$$(A_{\alpha} + \mathbb{1})^2 = (\sum_{P_{\omega} \in \alpha} P_{\omega})^2 = \sum_{P_{\omega} \in \alpha} P_{\omega}^2 + \sum_{P_{\omega} \in \alpha} \sum_{P_{\omega}' \neq P_{\omega}} P_{\omega}P_{\omega}'$$  \hspace{1cm} (9)

$$\Rightarrow \text{Tr}A_{\alpha}^2 + 2 + N = (N+1) + (N+1)N \frac{1}{N} \quad \iff \quad \text{Tr}A_{\alpha}^2 = N .$$

In our vector space a point face operator $A_{\alpha}$ corresponds to a point on the ray from the origin through the center of the point face. If continued in the other direction, this ray hits the center of a facet, i.e. a face of dimension $N^2 - 2$. This facet is the convex hull of the corners not included in the point face (like $\triangle \cdot \cdot \triangle \cdot \cdot \triangle \cdot \cdot \triangle \cdot \cdot$). Hence point faces and facets are in one-to-one correspondence, and they are placed opposite to each other at the boundary of the polytope. The case $N = 2$ is special since its point faces are facets, and conversely.

Every point face operator defines a set of parallel hyperplanes through the equation

$$\text{Tr}\rho A_{\alpha} = \text{constant} ,$$  \hspace{1cm} (10)

where $\rho$ belongs to the set of Hermitian matrices of unit trace. The facet lies in that hyperplane where the constant is zero, and the point face where it is one (figure 2). We could have chosen the point face operator $A_{\alpha}$ somewhere else on the ray, which would just have given us other constants than zero and one at the faces. The choice we made for $A_{\alpha}$ is in accordance with Wotters' phase point operators [8]. All corners lies in the hyperplanes with
either $\text{Tr}\rho A_\alpha = 0$ or $\text{Tr}\rho A_\alpha = 1$. Thus all points in the polytope have $0 \leq \text{Tr}\rho A_\alpha \leq 1$. Note that this observation provides the formal proof that the faces really are faces, that is that they consist of points belonging to the boundary of the polytope. Note also that this very way of characterizing the facets of the polytope was used by Galvão [10], although he expressed it a little differently—his statement is that the discrete Wigner function, defined by Wootters [8], vanishes on facets of the polytope.

III. The affine planes

The discrete Wigner function used by Wootters [7, 8] is defined by equation (10)—the constant is the Wigner function $\alpha$-component for the matrix $\rho$—for a selected subset of $N^2$ face point operators. Thinking about this construction from the point of view of the complementarity polytope, we encounter a rather striking geometrical fact. The idea is to ask whether it is possible to inscribe a regular simplex—call it an $A$-simplex—in the complementarity polytope, in such a way that its $N^2$ corners sit at the centers of $N^2$ selected facets. We will turn this into a combinatorial problem, that has a solution if and only if there exists a finite affine plane of order $N$. Wootters’ discrete Wigner function lives on such an affine plane. But it is known that affine planes do not exist for certain values of $N$, so we have found a geometrical property of the polytope that definitely singles out certain values of $N$ for special attention. The argument relies on some elementary facts taken from the branch of combinatorics that deals with finite affine planes, Latin squares, and so on. A readable introduction that contains all we need is the book by Bennett [11].

The question we will actually discuss is whether it is possible to select $N^2$ of the matrices $A_\alpha$, such that they form an $A$-simplex. Since these matrices lie on rays through the centers of the facets, at a fixed distance from $\rho_*$, this question is equivalent to the question as phrased above. These matrices will form a regular simplex if and only if

$$\text{Tr}A_\alpha A_\beta = N\delta_{\alpha\beta}.$$  

(11)

This follows from the ratio $R_{N^2-1}^2/L^2 = (N^2 - 1)/(2N^2)$ for simplicies (see eq. [13]). The radius of the $A$-simplex’ outsphere should be $R_{N^2-1} = D(A_\alpha, \rho_*)$ and the side length $L = D(A_\alpha, A_\beta)$. From this point on the index $\alpha$ is restricted to run from 1 to $N^2$. Observe that the matrices form an orthogonal basis in the space of Hermitian matrices of order $N$, i.e. in the Lie algebra of $U(N)$, albeit an unconventional one since they all have unit trace.
To see how the requirement (11) can be met, we modify equation (9) appropriately:

$$\text{Tr}A_\alpha A_\beta + 2 + N = \text{Tr} \sum_{P_\omega \in \alpha} P_\omega \sum_{P_\omega \in \beta} P_\omega.$$  \hspace{1cm} (12)

Now we must choose the two sets of projectors $P_\omega$ that should span the point faces $\alpha$ and $\beta$, such that the right hand side yields $2 + N$ (when $\alpha \neq \beta$). There are $N + 1$ terms where the two $P_\omega$s come from the same $P$-simplex. Such a term is zero, according to equation (5), unless we have the same choice of $P_\omega$. Then it equals one ($\text{Tr} P_\omega^2 = 1$). The remaining $N(N + 1)$ terms, where the $P_\omega$s come from different $P$-simplices, equal $1/N$, as in equation (6), giving the sum $N + 1$. Then we see that what we need is to choose exactly one common projector $P_\omega$ in the sets spanning point faces $\alpha$ and $\beta$. And this must be done for every pair of the $N^2$ matrices that would give us an $A$-simplex. Hence we have a combinatorial problem on our hands, and indeed a well known combinatorial problem, as we will now proceed to show.

Order the point face operators in an $N \times N$ array. Let each point face operator be represented by $N + 1$ $P$-simplices, from which exactly one out of $N$ corners is selected. In every column, the choice of corner from the first simplex is the same, and in every row, the choice of corner from the second simplex is the same. We illustrate this first step of the construction for $N = 3$:

$$\begin{array}{cccc}
\Delta & \Delta & \Delta & \Delta \\
\Delta & \Delta & \Delta & \Delta \\
\Delta & \Delta & \Delta & \Delta
\end{array}$$

Now we must make choices of corners from the third simplex so that a given choice occurs exactly once in every column and exactly once in every row. If we think of the $N$ corners of a $P$-simplex as letters in an alphabet of $N$ letters, we realize that our problem is equivalent to that of finding a Latin square. Latin squares of order $N$ always exist, and indeed there are many Latin squares. Altogether we need $N - 1$ Latin squares for the choices in the remaining simplices. They have to obey consistency conditions that arise already when we turn to the fourth simplex. Consider the pair of choices made from the third and fourth simplex. There are $N^2$ such pairs altogether, and they are not allowed to occur more than once in the array—if
they did, two different face point operators would have more than one \( P_\omega \) in common. This means that the third and fourth simplex must define a pair of orthogonal Latin squares, where two Latin squares are said to be orthogonal if every pair of letters, one from each Latin square, defines a unique position in the array. The same goes for every pair of the \( N - 1 \) Latin squares that we are trying to construct, so altogether we need \( N - 1 \) mutually orthogonal Latin squares. One can convince oneself that these choices will give exactly one corner in common for every pair of point faces, as is required.

For \( N = 3 \), the finished construction looks as follows:

\[
\begin{array}{cccc}
\triangle & \triangle & \triangle & \triangle \\
\triangle & \triangle & \triangle & \triangle \\
\triangle & \triangle & \triangle & \triangle \\
\end{array}
\]

The conclusion is that our problem of inscribing a regular simplex (an A-simplex) into the Complementarity Polytope is equivalent to that of finding \( N - 1 \) mutually orthogonal Latin squares. But the latter problem is in its turn equivalent to that of defining a finite affine plane of order \( N \). These are combinatorial structures containing \( N^2 \) points and \( N + 1 \) pencils of \( N \) parallel lines each. (In the original quantum mechanics references, these are called “foliations” [7] or “striations” [8]. However, “pencils” seems to be more standard [11].) Each of the lines contains \( N \) points. Setting two of the pencils aside in order to define an array of \( N^2 \) points, the axioms that define an affine plane will require the final \( N - 1 \) pencils to form mutually orthogonal Latin squares. Hence we have proved that our problem is equivalent to that of defining an affine plane of order \( N \).

We have also set up a one-to-one correspondence between the P-simplices that define the Complementarity Polytope, on the one hand, and the pencils of parallel lines in an affine plane on the other. This extends to a one-to-one correspondence between the corners of our polytope and the lines of the affine plane. The points of the latter correspond to a very special collection of \( N^2 \) facets of the polytope. This should be obvious to readers familiar with finite affine planes, but it is instructive to see how it goes for \( N = 3 \). In an affine plane, two points always determine a line. As an example, the pair of points represented by \( \triangle \triangle \triangle \triangle \) and \( \triangle \triangle \triangle \triangle \) (these are two point faces, belonging to the particular set of point faces that we have listed in our array) uniquely determine the line \( \triangle \triangle \triangle \) (this is the only corner of the polytope that belongs to both faces). Also a pair of lines, such as \( \triangle \triangle \triangle \) and \( \triangle \triangle \triangle \), uniquely determine a point, in this case \( \triangle \triangle \triangle \) (since
this is the only point face in our array that contains this particular pair of corners. In the latter case we must make an exception if we pick two corners from the same P-simplex; an example would be $\triangle \triangle \triangle$ and $\triangle \triangle \triangle$. They represent lines coming from the same pencil of parallel lines.

About the existence of affine planes, the following is known: Affine planes of order $N$ do exist if $N = p^k$, where $p$ is a prime number. They do not exist if $N = 4k + 1$ or $N = 4k + 2$, unless possibly when $N$ is the sum of two squares (a statement known as the Bruck-Ryser theorem). They do not exist if $N = 10$ (this case has been settled by state-of-the-art modern computers). All other cases, beginning with $N = 12$, are open (so much for today’s computers). Concerning the cases where affine planes exist, we observe that they can be constructed using ordinary vector space methods, if the scalar numbers employed are taken from finite number fields. This option is open only if $N = p^k$, but examples of affine planes that do not arise in this way are known—thus, for $N = 9$, four nonisomorphic affine planes are known, only one of which can be coordinatized by a field. However, all examples so far constructed have $N = p^k$.

It will not have escaped the reader that we have not explained to what extent the question of the existence of an affine plane has anything to do with the question of the existence of a complete set of MUBs. We will make some comments on this issue in the concluding section—but no explanation will be forthcoming.

IV. Is there some strangeness in the proportions?

We have two convex bodies in dimension $N^2 - 1$: the set of density matrices and the complementarity polytope. Now we study some more geometrical facts about these sets.

Let us derive the volume of the complementarity polytope. In every $N - 1$ dimensional subspace containing a P-simplex, the coordinates of the $N$ corners are given by the vectors

\[
\begin{bmatrix}
-r_1 \\
-r_2 \\
-r_3 \\
\vdots \\
-r_{N-1}
\end{bmatrix}
\begin{bmatrix}
R_1 \\
-r_2 \\
-r_3 \\
\vdots \\
-r_{N-1}
\end{bmatrix}
\begin{bmatrix}
0 \\
R_2 \\
-r_3 \\
\vdots \\
-r_{N-1}
\end{bmatrix}
\begin{bmatrix}
0 \\
0 \\
0 \\
\vdots \\
0
\end{bmatrix}
\begin{bmatrix}
0 \\
R_{N-2} \\
-R_{N-1} \\
0 \\
R_{N-1}
\end{bmatrix}
\]

(13)

where $r_n = 1/\sqrt{2n(n+1)}$ and $R_n = nr_n$ are the radii of the inscribed and the circumscribed spheres of an $n$ dimensional simplex. From this we get
the $N(N+1)$ vectors for the corners of the polytope, in the full $N^2 - 1$ dimensional space. The polytope consists of cones with the facets as their bases. If we choose $N-1$ vectors from each P-simplex—this can be done by discarding the first of the vectors above (in eq. (13))—we get $N^2 - 1$ vectors such that they span a cone with a facet as its base. The volume of the cone is found from the determinant of the spanning vectors, and the volume of the polytope by multiplying with the number of facets, $N^{N+1}$:

$$V_{\text{polytope}} = N^{N+1} \frac{1}{(N^2 - 1)!} (R_1 R_2 \cdots R_{N-1})^{N+1} = \frac{\sqrt{N}^{N+1}}{(N^2 - 1)!\sqrt{2^{N^2-1}}}.$$  

How does this volume compare to the volume of the set of density matrices? This second volume is given by [12]

$$V_\rho = \frac{\sqrt{N} \pi^{N(N-1)/2}}{\sqrt{2} \pi^{N-1}} \frac{1! \cdot 2! \cdot 3! \cdots (N-1)!}{(N^2 - 1)!}.$$  

(A factor $1/\sqrt{2}$ for every dimension is included, to adjust for our different conventions in the definition of distance.) Hence, the ratio between the volumes of the polytope and the set of density matrices is

$$\frac{V_{\text{polytope}}}{V_\rho} = \frac{\sqrt{N}^N}{\sqrt{2} \pi^{N(N-1)/2} \cdot 1! \cdot 2! \cdots (N-1)!}.$$  

For $N = 2$ we get $V_{\text{polytope}} = 1/6$ and $V_\rho = \pi/6$, as we should for an octahedron and the Bloch ball, and $V_{\text{polytope}}/V_\rho = 1/\pi$. The fraction $V_{\text{polytope}}/V_\rho$ is less than one and decreases rapidly with the dimension $N$—a reasonable result remembering that most of the volume in a higher dimensional ball lies near the surface: The set of density matrices touches the circumscribed sphere at all the pure states, but the polytope only at its corners. Also, the inscribed sphere of the set of density matrices has a larger radius than the inscribed sphere of the polytope. So the volume of the polytope is certainly not too large to be included in the set of density matrices. But this doesn’t say much about whether the polytope fits inside the set of density matrices or not.

We also compute the radius of the insphere and the area of the polytope. We can get a point on the insphere of the polytope as an equal weight convex combination of points on the inspheres of the P-simplices, one from each simplex. The radius of the insphere of a simplex in $N-1$ dimensions is $r_{N-1} = 1/\sqrt{2N(N-1)}$. The radius $r_{\text{in}}$ of the insphere of the whole
polytope, built of \( N + 1 \) simplices, is then (by Pythagoras’ theorem and remembering that the P-simplices are totally orthogonal)

\[
    r_{in} = \sqrt{(N + 1) \left( \frac{r_{N-1}}{N + 1} \right)^2} = \frac{1}{\sqrt{2N(N^2 - 1)}}. \tag{17}
\]

The area of the polytope is the \((N^2 - 2\) dimensional) area of its facets. This is, again, the bases of the cones building up the polytope. The height of the cones is the radius \( r_{in} \). Using \( V_{\text{cone}} = A_{\text{base}} r_{in} / \text{dim}(\text{cone}) \) we get

\[
    \frac{A_{\text{polytope}}}{V_{\text{polytope}}} = \frac{\text{dim}(\text{polytope})}{r_{in}} = \sqrt{2N(N^2 - 1)(N^2 - 1)} \tag{18}
\]

and

\[
    A_{\text{polytope}} = \frac{\sqrt{N^{N+2}} \sqrt{N^2 - 1}}{(N^2 - 1)! \sqrt{2^{N^2 - 2}}} \tag{19}
\]

Multiplying equation (18) with the radius of the outsphere, \( R = R_{N-1} = \sqrt{N - 1}/\sqrt{2N} \), to fix the scale, we then compare with the set of density matrices:

\[
    R \frac{A_{\text{polytope}}}{V_{\text{polytope}}} = (N - 1)^{\frac{3}{2}} (N^2 - 1)^{\frac{3}{2}}, \quad R \frac{A_{\{\rho\}}}{V_{\{\rho\}}} = (N - 1)(N^2 - 1). \tag{20}
\]

Asymptotically, this ratio behaves like \((\text{dimension})^{7/4}\) for the polytope, and like \((\text{dimension})^{3/2}\) for the set of density matrices. The latter value of the exponent happens to coincide with that for hypercubes, while regular simplices behave like \((\text{dimension})^{2}\). So the polytope is closer to the simplex—but we can see nothing that singles out some particular values of \( N \).

One thing that characterizes convex bodies is their largest inscribed ellipsoid. For example whether this ellipsoid turns out to be a ball (corresponding to the insphere) or not. If it is not a ball the body is kind of stretched or flattened in some directions. Here we can rely on a useful theorem due to Fritz John[13].

**John’s theorem:**

The ball \( B \) is the ellipsoid of maximal volume that can be contained in a convex body \( K \) if and only if: \( B \in K \) and there exist vectors \( \{u_i\}_i^m \) at the boundary of both \( B \) and \( K \), and a set of positive numbers \( \{c_i\}_i^m \), such that

\[
    (i) \quad \sum_{i=1}^m c_i u_i = 0 \quad \text{and} \quad (ii) \quad \sum_{i=1}^m c_i u_i \otimes u_i = 1. \tag{21}
\]
These conditions correspond to the possibility to have masses $c_i$ at some points $u_i$ where the sphere touches the boundary of the convex body, such that the center of mass is at the center of the sphere, and such that the inertia tensor is the identity.

Are the inspheres of the set of density matrices and of the complementarity polytope the largest inscribed ellipsoids?

Let’s start with the density matrices. In those dimensions where we can find a complete set of $N + 1$ MUBs, look at the corresponding P-simplices. The insphere of the set of density matrices has the same radius as the inspheres of the simplices [14]. Anti-parallel to the vectors for the $N$ corners of each simplex there are vectors corresponding to the points where the insphere touches the boundary—call them $e_k^{(l)}$, where $l = 1, \ldots, N + 1$ labels the simplices and $k = 1, \ldots, N$ labels the different vectors in each simplex (figure 3). Then

$$
\sum_{k=1}^{N} e_k^{(l)} = 0 \quad \text{hence} \quad \sum_{l=1}^{N+1} \sum_{k=1}^{N} e_k^{(l)} = 0 ,
$$

and the first condition in the theorem is fulfilled (for $c_i = c$, any constant).

In the second condition, for every simplex, the sum over $k$ gives the identity (times a factor) in the $N - 1$ dimensional subspace of the simplex. And then the sum over $l$ gives the identity in the full $(N+1)(N-1)$ dimensional space:

$$
\sum_{k=1}^{N} e_k^{(l)} \otimes e_k^{(l)} \propto 1_{N-1} \quad \text{hence} \quad \sum_{l=1}^{N+1} \sum_{k=1}^{N} e_k^{(l)} \otimes e_k^{(l)} \propto 1_{N^2-1} .
$$

Thereby we have proved that the insphere of the set of density matrices is the largest inscribed ellipsoid, when we have a complete set of MUBs.
What can we say about the largest ellipsoid in the set of density matrices, without using a complete set of MUBs? We are looking for points that fulfill John’s theorem. These points should lie at the insphere and at the boundary. The possible points are those that sit opposite to the pure states. (The innermost states at the boundary have spectrum $(0, 1/N, \ldots, 1/N)$ and lie opposite to the states with spectrum $(1, 0, \ldots, 0)$, i.e. the pure states, lying at the circumscribed sphere.) Thus we can look at the pure states $|\Psi\rangle$ instead (in the theorem it only corresponds to a change of the constants $c_i$, by a factor).

A vector $u$ corresponds to a density matrix $|\Psi\rangle\langle\Psi|$. The first condition (in eq. (21)) becomes

$$\sum_i c_i |\Psi_i\rangle\langle\Psi_i| \propto I_N .$$

This is the condition that the set of projectors $\{|\Psi_i\rangle\langle\Psi_i|\}$ form a POVM (with one dimensional projectors as its element). A first requirement from the second condition,

$$\sum_i c_i u_i \otimes u_i = I_{N^2-1} ,$$

is that the states must span the whole space of density matrices. Since $u_i \otimes u_i$ is a projector of rank one, we must have at least $N^2 - 1$ vectors $u_i$. But if we have only $N^2 - 1$ vectors, they have to be linearly independent and the first condition can not be fulfilled. Therefore we must have at least $N^2$ vectors. One set of vectors that would suit us—if they can be found among the pure states—is a set of vectors spanning an $N^2 - 1$ dimensional regular simplex (then all $c_i = c$, a constant). This is exactly what have been called a symmetric informationally complete POVM (SIC-POVM). These have been found in dimensions $N = 1, 3, 4, 5$ [3,15] and 6 [16], and it has been conjectured that they exist in all dimensions (based on numerical solutions up to $N = 45$ [15]). Thus, if there exists a SIC-POVM, then there is no larger inscribed ellipsoid in the set of density matrices than the insphere. It is interesting to note that a SIC-POVM is found also for the case $N = 6 = 2 \cdot 3$—an $N$ which is not a power of a prime.

Just one more comment on John’s theorem and density matrices. There could be many other ways to fulfill the conditions, than using a SIC-POVM, since we can use more vectors $u_i$ and we have the freedom to use different weights $c_i$. Altogether we find it probable that the largest ellipsoid in the set of density matrices is always a ball.

Now we turn to the complementarity polytope. The points at which the insphere of the polytope touches the boundary are convex combinations of
vectors $e_k^{(l)}$, one from each of the $N + 1$ P-simplices:

$$u_{k_1, \ldots, k_N} = \frac{1}{N+1} \sum_{l=1}^{N+1} e_k^{(l)},$$  \hspace{1cm} (26)

for every combination of values of $k_1, \ldots, k_N$.

Since the sum over the vectors $e_k^{(l)}$ for each simplex (given $l$) is zero, the sum over all vectors $u_{k_1, \ldots, k_N}$ will also be zero, thus the first condition in the theorem is fulfilled (for $c_i = c$ any constant).

What about the second condition?

$$\sum_{k_1, \ldots, k_N} u_{k_1, \ldots, k_N} \otimes u_{k_1, \ldots, k_N} \propto \sum_{k_1, \ldots, k_N}^{N+1} \sum_{l=1}^{N+1} e_k^{(l)} \otimes e_k^{(l')}$$  \hspace{1cm} (27)

First look at the terms where $l \neq l'$, and for a given $l = L$.

$$\sum_{k_1, \ldots, k_N} e_{k_L}^{(L)} \otimes \sum_{l=l'}_{l \neq L} e_{k_{l'}}^{(l')} = \left( \sum_{k_1, \ldots, k_{L-1}} e_{k_L}^{(L)} \right) \otimes \left( \sum_{l=l'}_{k_{L+1}, \ldots, k_N} \sum_{l' \neq L} e_{k_{l'}}^{(l')} \right) = 0$$  \hspace{1cm} (28)

This is zero since the first factor, the sum over the vectors for one P-simplex, is zero. Then all that is left are the terms where $l = l'$:

$$\sum_{k_1, \ldots, k_N}^{N+1} e_{k_l}^{(l)} \otimes e_{k_l}^{(l')} = \sum_{l=1}^{N+1} \sum_{k_1, \ldots, k_{L-1}} e_k^{(l)} \otimes e_k^{(l')} \propto I_{N^2-1}$$  \hspace{1cm} (29)

as in equation (23). Thus the second condition of the theorem is fulfilled, and the insphere is the largest ellipsoid that can be inscribed in the polytope. In this sense, neither the set of density matrices nor the complementarity polytope is “skew”.

V. Conclusions

The Complementarity Polytope exists in any vector space of dimension $N^2 - 1$. The question whether a complete set of $N+1$ MUBs exists has been much discussed recently; in addition to the references that we have already given, see refs. [17, 18, 19, 20]. It is equivalent to the question whether the Complementarity Polytope can be inscribed in the convex body of density matrices. If this is indeed possible only for some special values of $N$, say $N = p^k$ where $p$ is prime, then it seems to us that one can reasonably expect
to find some strangeness in the proportions of, either the body of density matrices, or the Complementarity Polytope, for these values of $N$. We have examined the latter in section IV, with regard to its volume, area and the shape of the maximal inscribed ellipsoid, but we were unable to put our finger on any peculiarities. The prime factorization of $N$ does not appear in these calculations at all. In section III we did find a peculiarity, namely that a regular simplex can be inscribed in the polytope (with its corners sitting at the midpoints of $N^2$ selected facets) if and only if an affine plane of order $N$ exists. This condition excludes an infinite number of non-prime values of $N$, but unfortunately we are unable to see what, exactly, this has to do with the existence of MUBs. What we do know is that an affine plane coordinatized by a field can be used to derive the existence of MUBS \[8\], but we do not know anything about the converse.

It remains possible that there is a connection between the existence of affine planes and the existence of MUBs [21]. In fact, as noted by Zauner [3], it looks suspicious that only 3 MUBs have been found for $N = 6$, where it is known to be impossible to find a single pair of orthogonal Latin squares. Therefore we believe that our underlying idea is sound, that the translation of the affine plane question into a geometric question about the Complementarity Polytope is interesting, and that further investigation of the latter may bear fruit.

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