Simplices, frames and questions about reality

Helena Granström

July 30, 2009

Simplices, frames and questions about reality

Filosofie licentiatavhandling

Helena Granström

Att presenteras den 14 september 2009, kl. 13.15, rum 306, hus 6,
Matematiska institutionen, Stockholms universitet, Kräftriket.

The two included papers are *Incomplete Kochen-Specker coloring* and *The frame function, on average.*

Abstract

This thesis is centered around mathematical structures of fundamental importance to quantum foundations and quantum information. Its introductory part acquaints the reader with the basics of the general ideas of frames and simplices, as well as with some central quantum mechanical concepts like density matrices and Hilbert spaces.
Article I deals with the question of contextuality in relation to quantum measurement. Using a specific strategy of assigning truth values to state vectors, some aspects of the Kochen-Specker theorem are explored.
In Article II an object called SIC-POVM is studied, more specifically by investigating the behaviour of a function used to measure the closeness of an arbitrary vector set to such a configuration.
In addition to putting the results of these two papers into context, the aim of this thesis is to offer a discussion of the search for connections between the SIC-POVM and so-called MUBs in odd prime dimensions, as well as a brief comment on a structure here introduced as a Kochen-Specker frame; it is shown that the latter plays a part in the proof of Hardy's paradox as well as for an inequality for testing contextuality due to Klyachko et al.

THANK YOU

first of all to Ingemar, for being an extraordinarily hardy supervisor.
And - even though thank you does not suffice to express what I feel for either of them - also to a certain former neighbor and to the man of my life.

Contents

Chapter 1

POVMs and mathematical preliminaries

1.1 Introduction

What makes a mathematical structure interesting? From a physicist's point of view the answer is not so much its intricacy - the simpler the better, really - as its ubiquitousness. The more frequently it turns up in unexpected places, the more inclined one is to consider it important. Just like π, the sphere or the Golden Mean, the configurations encountered in this thesis are of interest because they arise from the formalism in a natural way. What's more, they make out a convergence point for several areas of mathematical physics, tying together subjects as diverse as group theory, algebraic geometry and combinatorics.

A class of objects around which much of this thesis will revolve - POVMs or Positive Operator Valued Measures - constitutes a good starting point for introducing the mathematical concepts necessary to proceed. The POVM is a set of m positive operators $\{P_i\}$ summing to the identity:

$$\sum_{i=1}^{m} P_i = \mathbf{1}, \quad P_i^\dagger = P_i, \quad P_i \geq 0.$$

If the P_i are all rank one projectors, i.e. proportional to $\mid \psi_i\rangle\langle\psi_i \mid$ for some pure state $\mid \psi_i\rangle$ in the Hilbert space $\mathscr{H}$, the POVM is said to be pure. Any non-pure POVM can, however, be taken into pure form by further partitioning of the POVM elements. For this reason, all POVMs will in the following be assumed to be pure, and by an element of the POVM we will interchangeably mean a Hilbert space vector and the operator constructed from it. Remembering that the operator space - here taken to be real and of finite dimension - has Hilbert space structure when equipped with the Hilbert-Schmidt inner product, we can interpret the operators as vectors in this space. The POVM can then be seen as a generalization of an orthonormal basis, in this context referred to as a PVM (Projective Valued Measure), with the criteria of orthogonality and normalization relaxed.

In terms of what goes on in the laboratory, the POVM can be said to represent a generalized notion of measurement. For a measurement setup corresponding to the regular ON-basis, the results obtained are mutually exclusive (for instance, $m = j$ means $m \neq j - 1, ..., -j$). For a POVM, however, this is not the case. Also, while the projectors of a PVM always commute, no such assumption is made for the elements of a general POVM - both these properties are due to the fact that the POVM elements need not necessarily be orthogonal. Another consequence of this is that the number of POVM elements need not equal the dimension even though they form a basis for the space. According to Naimark's theorem, however, any POVM is equivalent to a PVM and can hence be described in terms of a von Neumann measurement, if the latter is performed in a higher dimension.

1.2 Spaces and density matrices

The definition of a POVM given above is in terms of projection operators in the space of Hermitian matrices. This is a vector space, with the Hilbert-Schmidt product $\mathbf{V}_a \cdot \mathbf{V}_b = \mathrm{Tr}\mathbf{V}_a\mathbf{V}_b$ as inner product, and the zero matrix as origin. A projector constructed by taking the outer product of a pure state $\mid \psi\rangle\langle\psi \mid$ in a Hilbert space of dimension N with itself is an operator sitting in this N^2-dimensional space. The set $\mathscr{P}$ of positive operators, i.e. matrices with non-negative spectra, forms a convex cone in this operator space with apex at the zero matrix. $\mathscr{P}$ is defined by the property that for $P \in \mathscr{P}$, $\langle\psi \mid P \mid \psi\rangle \geq 0$ for all $\mid \psi\rangle \in \mathscr{H}$, a condition that is equivalent to P being Hermitian and having all its eigenvalues non-negative. Clearly, then, the sum of two positive operators is again positive, which justifies the claim that $\mathscr{P}$ is a convex set.

Another space that will also be of relevance to the following is what will here be called Bloch space: the $N^2 - 1$-dimensional space of Hermitian matrices with unit trace, with the maximally mixed state - $\frac{1}{N}$ times the unit matrix - as origin. This space contains the convex set $\{\rho\}$ of density matrices as those matrices in the space that have non-negative spectra. That all density matrices obey the trace one conditions follows from the quantum rule (i.e. Gleason's theorem) for calculating probabilites: given that $P_i = \mathrm{Tr}\mathbf{E}_i\rho$, the condition $\sum_i P_i = \mathbf{1}$ that the probabilities sum to unity enforces that $\mathrm{Tr}\rho = 1$.

The matrices with constant trace, of which the unit trace matrices are a special case, form parallel hyperplanes in the larger space of all Hermitian operators. In dimension two, the set of density matrices - the intersection of the cone of positive operators with the set of unit trace 2×2-matrices - is a ball known as the Bloch ball, with the sphere of pure states as its boundary. Unfortunately, as soon as N is larger than two, the situation becomes more complicated. The set of density matrices will then lie in the cross section between the positive cone and the unit trace hyperplane, but will no longer fill it completely. The reason for this dimension two anomaly can be understood by studying the symmetry group of the set of density matrices for an N-dimensional system, $SU(N)/\mathbf{Z}_N$. For all N, it is true that this is a subgroup of $SO(N^2-1)$ - for N equals two the two groups are in fact isomorphic. In general, though, a unitary transformation in Hilbert space can be interpreted as a rotation in operator space, but not conversely. In passing it can be said that the symmetry group of the set of density matrices reveals that this convex set is not a polytope - if there exists a symmetry group for a polytope, it is by necessity discrete, whereas $SU(N)/\mathbf{Z}_N$ is a continuous group of transformations.

Bloch space operators are constructed from state space vectors in the following way. Given a unit vector $\mid v\rangle$ in Hilbert space, we turn the corresponding projector $\mid v\rangle\langle v\mid$ into a vector in $\mathbf{R}^{N^2-1}$ via the formula

$$\mathbf{V} = \mid v\rangle\langle v \mid - \rho_*, \tag{1.1}$$

where ρ_* is the maximally mixed state. The trace operation then functions as inner product on this space, and a calculation shows that $\mid v\rangle$ being a unit vector leads to

$$\mathbf{V}^2 = \frac{N-1}{2N} \tag{1.2}$$

and that for unit vectors in Hilbert space

$$\langle v_i \mid v_j\rangle = 0 \quad \Leftrightarrow \quad \mathbf{V}_i \cdot \mathbf{V}_j = -\frac{1}{2N}. \tag{1.3}$$

1.3 Frames

If a set of state space vectors $\{\mid \psi_i\rangle\}$ define a POVM there always exist constants $0 < a \leq b < \infty$ such that

$$a \mid \langle v \mid v\rangle \mid^2 \quad \leq \quad \sum_k \mid \langle v \mid \psi_k\rangle \mid^2 \quad \leq \quad b \mid \langle v \mid v\rangle \mid^2 \tag{1.4}$$

for all vectors $\mid v\rangle \in \mathscr{H}$, and conversely. A set for which such constants can be found is called a frame. If $a = b$ in equation (1.4) the frame is said to be tight; any non-tight frame can be made tight by a canonical transformation.

Many other objects considered in foundational research in quantum mechanics also constitute frames. Besides the POVM, or rather certain special cases of it, a configuration here introduced as a Kochen-Specker frame will be discussed at some length in this thesis. The latter is not encountered in standard works on frame theory, and the terminology is not established. Other frames of relevance to quantum mechanics, besides the familiar ON-basis, include complete sets of MUBs and sets of coherent states.

1.4 Simplices

Another mathematical object intimately connected to the POVM is the simplex. Formally, an N-simplex in an affine space is the convex hull of a set of $N+1$ points not confined to any $N-1$ dimensional subspace, i.e. a convex polytope consisting of all points of the form

$$\mathbf{x} = \lambda_0 \mathbf{x}_0 + \lambda_1 \mathbf{x}_1 + ... + \lambda_N \mathbf{x}_N, \quad \lambda_0 + \lambda_1 + ... + \lambda_N = 1, \quad \lambda_i \geq 0, \tag{1.5}$$

with the $\mathbf{x}_i$ affinely independent. The simplex is a special case of a convex polytope, which is the convex hull of a finite number of points. The convexity property means that given two points $\mathbf{x}_1$ and $\mathbf{x}_2$ in the set, the linear combination, or mixture,

$$\mathbf{x} = \mathbf{x}_1 + (1-\lambda)\mathbf{x}_2$$

also belongs to it for all λ between zero and one.

A face F of the polytope is defined by its stability under mixing and purification, in the sense that

$$\mathbf{x} = \mathbf{x}_1 + (1-\lambda)\mathbf{x}_2, \quad 0 \leq \lambda \leq 1$$

lies in F if and only if $\mathbf{x_1}$ and $\mathbf{x_2}$ do, and that a point obtained by mixing pure points in the face cannot be obtained as a mixture of other pure points not belonging to the face.

The dimension of the faces of a convex N-polytope runs between zero and N - the single N-dimensional face is the polytope itself, whereas the zero-dimensional faces are the extremal, or pure, points of the polytope. For a simplex, the number of m-faces is equal to the mth binomial coefficient. Any point of a convex body can be expressed as a convex combination of the pure points of the body, and the rank of a point is defined as the minimal number of pure points needed in the expression. What is special about the simplex is that this expression is unique: a point in a simplex can be written as a mixture of pure points in one and only one way.

As it happens, the simplex with N^2 corners realizes a special type of POVM known as the IC-POVM, where IC stands for Informationally Complete. The meaning of this phrase is that the statistics of the POVM - now interpreted as representing a measurement - fully determines the density matrix of the system to which it is applied. Another way to state this is that the corners of the IC-POVM simplex can be used to define barycentric coordinates for any density matrix. For a quantum system of Hilbert space dimension N, the corresponding Bloch space has N^2-1 dimensions, and N^2 is just the number of measurements required to uniquely determine the state. The simplex is in this sense a minimal IC-POVM - one can of course find configurations with a larger number of elements having the same statistical properties.

Many of the configurations considered in the area of quantum foundations are geometrically simplices and as we will see below, the simplicial structure also plays a role in the search for connections between two important, but as of yet unlinked, structures: SIC-POVMs and MUBs. Polytopes of other types than simplices are also encountered, for instance in the description of quantum statistical correlations. The MUB polytope, which can be seen as a generalization of Birkhoff's four-dimensional polytope, is one example.

Chapter 2

SICs, MUBs and the search for connections

Formally, a SIC-POVM - Symmetric Informationally Complete Positive Operator Valued Measure - is a set of N^2 positive operators P_i that act on an N dimensional Hilbert space $\mathscr{H}^N$, and that satisfy

$$\frac{1}{N}\sum_{i=1}^{N^2} P_i = \mathbf{1}, \quad P_i^\dagger = P_i, \quad P_i \geq 0 \quad \text{and} \quad \text{Tr}(P_i^\dagger P_j) = \frac{1}{N+1}, \quad i \neq j. \tag{2.1}$$

Equivalently, and simpler, it is a set $| \psi_i\rangle$ of N^2 unit vectors in $\mathscr{H}^N$ that satisfy

$$|\langle\psi_i|\psi_j\rangle|^2 = \frac{1}{N+1} \qquad 1 \leq i, j \leq N \ , \quad i \neq j; \tag{2.2}$$

the first definition of the SIC-POVM (henceforth referred to as simply a SIC) is obtained from the second by from each vector $| \psi_i\rangle$ forming the operator $P_i =| \psi_i\rangle\langle\psi_i |$. The same configuration has been also studied under the name of "equiangular lines"[2], "equiangular tight frame"[3] and "maximal quantum design"[1]. Most work in recent years has focussed on the problem of proving the existence of SIC structures in arbitrary dimension. Given the relatively simple definition of the SIC one would imagine that the question in what dimensions such an object exists would be easy to answer. That this is not the case is illustrated by the fact that although they have been constructed in most (but not all) dimensions $N \leq 19$ [1, 4, 5, 6, 7] and numerical searches have been successful for all $N \leq 64$ [11, 13], a general formula has yet to emerge.

Just as IC-POVMs without the additional symmetry requirement, the SIC is important because its statistics allow us to fully determine the density matrix of the system to which it is applied. From an experimental point of view the SIC is preferrable in that it minimizes the uncertainties associated with measurement among all N^2 element IC-POVMs. Tomography of a quantum state - and this should be stressed - always makes use of a number of identical copies of the system of interest; once a measurement is performed the state of the individual system is irreversibly destroyed. In the ideal case of an infinite number of copies and measurements, the measured frequencies agree exactly with the probabilities one wishes to determine. In reality, however, the statistics are the result of a finite number of measurements, and afflicted by deviations due to this fact. The SIC is - as are the MUBs of section 2.1 - particularly insensitive to this type of uncertainty.

In the N^2-dimensional space of all Hermitian matrices, the SIC has also been shown to be as close to an orthonormal basis as is possible to find for this space given that the basis vectors are all required to lie in the cone of positive operators [12]. In contrast to a general IC-POVM the SIC elements all have the same weight, which means that the SIC (after appropriate rescaling) can be seen as sitting in Bloch space. The interpretation of the SIC as a set of points in the space of Hermitian matrices of unit trace also enables us to state the existence problem as one that concerns the shape of the convex body of density matrices mentioned in section 1.2: is it possible to inscribe a regular simplex with N^2 corners in this body? The task is not trivial; whereas the outsphere on which all pure states lie - defined to be the sphere of radius $\sqrt{\frac{N-1}{2N}}$ - has dimension N^2-2, the dimension of the set of pure states is only $2N-2$. Although a regular simplex with N^2 corners on the outsphere of the body of density matrices can be constructed, it is not clear that it can always be rotated so that its corners all coincide with pure state vectors.

2.1 Projection on the MUB planes

Besides the existence problem, another question that has received some attention in the last years is that of the connection between SICs and MUBs - Mutually Unbiased Bases. One of the motivations for investigating the relation between the two configurations also has to do with proving existence - if one could find a way of constructing a complete set of MUBs from a SIC, or vice versa, one would automatically ascertain existence of one in all dimensions where the other is known to exist. Currently, full sets of MUBs - meaning $N+1$ basis sets which are all mutually unbiased with respect to each other - are known to exist when the dimension N is a prime number, or a power of a prime - the constructive proof of existence uses the fact that $\mathbf{Z}_N$ is a field whenever N is prime. In the following, we will restrict our attention to prime dimensions larger than two.

A pair of orthogonal basis sets $\{| e_i\rangle\}$ and $\{| f_i\rangle\}$ of some N-dimensional space are said to be mutually unbiased if for all i and j it is true that

$$| \langle e_i | f_j\rangle |^2 = \text{constant} = \frac{1}{N}. \tag{2.3}$$

In Bloch space terms this is equivalent to

$$\mathbf{E}_i \cdot \mathbf{F}_j = 0, \tag{2.4}$$

again with the trace operation as scalar product. From this we see that any (Bloch space) vector in one MUB is orthogonal to any vector in any of the others. This means that the MUBs, interpreted as vectors in the $N^2 - 1$ dimensional space of Hermitian matrices with unit trace, define a set of $N + 1$ totally orthogonal hyperplanes of dimension $N - 1$ or, equivalently, a highly symmetric polytope consisting of the $N + 1$ totally orthogonal MUB-simplices. This constitutes the basis for the claim that the MUB polytope generalizes Birkhoff's polytope $\mathscr{B}_N$ for $N = 3$; the latter is the set of bistochastic 3×3 matrices, a four-dimensional convex polytope with the set of $3! = 6$ permutation matrices as its extreme points. The analogy is provided by the fact that $\mathscr{B}_3$ can be described in terms of two equilateral triangles each sitting in one of two totally orthogonal planes - as already stated, the MUB polytope then consists of four simplices in as many totally orthogonal planes, more generally of $N+1$, of them. In passing, it can also be said that the difficulties of finding a complete set of MUBs stem from the same properties of the body of density matrices as do those of proving SIC existence. Just as the task of finding a SIC is equivalent to inscribing a regular simplex in the outsphere with all corners on the submanifold of the sphere corresponding to pure states, finding a full set of MUBs means succeeding in the same maneuvre for the MUB polytope.

As it stands, the question of the connection between SICs and MUBs is not very specific, and there are of course many possible ways to go about an investigation of their relation. One well defined, and arguably relevant, question is that of the result when the SIC is projected onto the planes defined by the MUBs. To the extent that the answer is known, it indicates that looking at the projections is a fruitful way of exploring the MUB-SIC relation. If, by projecting onto the MUB planes, one would be able to substantially cut down the dimensionality of the space in which one performs the search for SIC vectors, projection would be a very valuable tool in the task of proving the existence of SICs in (possibly) all dimensions.

Before we look at the projection properties, some mathematical preliminaries have to be put in place. More specifically, we need the definition of a certain finite group with N^2 elements: the Weyl-Heisenberg group [8]. The Weyl-Heisenberg group - also known to physicists as the generalized Pauli group and to mathematicians as the Heisenberg group - is the group generated by two elements X and Z subject to the relations

$$XZ = qXZ \ , \quad X^N = Z^N = 1 \ , \quad q \equiv e^{2\pi i/N} \ . \tag{2.5}$$

The definition of q guarantees that $q^N = 1$ but $q^r \neq 1$ for all $r \neq 0 \bmod N$. Up to unitary equivalence there is a unique unitary representation of this group such that

$$Z|a\rangle = q^a|a\rangle \qquad X|a\rangle = |a+1\rangle \ , \qquad 0 \leq a \leq N-1 \ ; \tag{2.6}$$

this is known as the clock and shift representation. The set $\{| \ a\rangle\}$ forms an orthonormal basis for Hilbert space. For prime N, the Weyl-Heisenberg group contains $N + 1$ cyclic subgroups, each with N elements, generated by X, Z, XZ, X^2Z,...,$X^{N-1}Z$.

Up to phases, which we do not have to care about, a general group element is

$$D_{ij} = X^i Z^j \ , \qquad 0 \leq i, j \leq N-1 \ . \tag{2.7}$$

The assumption here will be that the SIC that is projected is an orbit under this group, meaning that it is generated by first choosing a fiducial vector $|\psi_0\rangle$, and then acting on this vector with the N^2 elements of the (projective) Weyl-Heisenberg group. That such a group covariant SIC can be found in all dimensions (where SICs exist) is part of the content of a conjecture due to Zauner [1], likely but as of yet unproved. A further assumption that we will make is that each MUB in the complete set is the eigenbasis of a cyclic subgroup of the Weyl-Heisenberg group, which has been shown to be the case in prime dimensions. In prime power dimensions the same assumption holds if the Weyl-Heisenberg group is replaced by a related group. As we will see, the characteristics of projection of the SIC on the MUB planes are highly dependent on this assumption.
A description of the Weyl-Heisenberg group action on the MUB planes in terms of rotations is provided by the fact that the group is a subgroup of SU(N), which in turn is isomorphic to a subgroup of SO(N^2-1) - the rotation group in Bloch space. Should one be surprised by the existence of a group with the properties presented above? Basically what we ask for is rotations that, when repeated N times, take every corner of the MUB simplex back to its original position. That this works in three dimensions - when the MUB vectors form an equilateral triangle in a two-plane - is no surprise. Intuitively one realizes - and this can also be shown - that the same thing is not possible in dimension four, in which the MUB simplex is a regular tetrahedron. On the other hand, not many of us have the intuition sufficient to decide whether or not this is possible for $N = 5$, when the MUB points are the corners of a regular four-simplex with corners on the three-sphere. The Weyl-Heisenberg group does, however, accomplish this in five dimensions - in fact it does so for all prime N.

The properties of the projected SIC points differ in several ways from those of a general projection. When projecting the N^2 SIC points down on any of the MUB planes, only N distinct points are obtained. These points form a regular N-simplex inscribed in the larger N-simplex defined by the MUB vectors. The radius of the sphere on which the N points lie is independent of which MUB plane we are looking at and, as it happens, the sphere is that on which we also find the minimum uncertainty states, to be further introduced below. For $N = 3$ the projected SIC simplex is only defined up to a phase, and its orientation relative to the simplex defined by the MUB vectors spanning the plane can be chosen at will. For $N > 3$, however, the exact position of the corners of the simplex matters. In order to explain these properties, we have to look a bit further into the Weyl-Heisenberg group.

As already stated, we are assuming the MUB vectors to all be eigenvectors of some cyclic subgroup of the Weyl-Heisenberg group. This means that the corresponding plane is left invariant by action of this subgroup: for instance, the plane defined by the standard basis - which can without loss of generality always be taken to be one of the bases in a set of

MUBs - is left invariant by the cyclic subgroup generated by the element Z. The action of the Weyl-Heisenberg group on the MUB planes results in N different rotations of a given plane, meaning that several elements give the same rotation. Taken together with the assumption that a Weyl-Heisenberg covariant SIC can always be found, this implies that $|\psi_0\rangle$, $Z|\psi_0\rangle$ and $Z^2|\psi_0\rangle$,...,$Z^{N-1} \mid \psi_0\rangle$ are all elements of the SIC and hence all project to the same point on the MUB plane corresponding to the standard basis. The analogous thing goes for the other MUBs, which explains the fact that the N^2 SIC points give rise only to N points in each hyperplane when projected.

Another striking fact of the projection of the SIC is that in each MUB plane, the N projected points lie on a sphere centered at the origin, with the same radius in all of the planes. On this sphere one also finds the set of minimum uncertainty states, so called because they minimize the quadratic Rényi entropy, a relative of the possibly more reputable Shannon entropy. This functional, which as the name suggests is a measure of the randomness or level of uncertainty of a system, is defined as

$$H_R = -\log(\sum_{i=0}^{N-1} p_i^2) \tag{2.8}$$

where p_i is the probability of outcome i, which in the quantum mechanical case would correspond to the quantity $\mid \langle e_i \mid \psi\rangle \mid^2$ for some suitably chosen set of state vectors $\{\mid e_i\rangle\}$. The minimum uncertainty states minimize this quantity not for a single von Neumann measurement, but when averaged over the $N+1$ measurements corresponding to a full set of MUBs.

Letting i number the bases in a complete set of MUBs and j number the vectors in each MUB, it has been shown that for a pure state $\mid \psi\rangle$ to be a minimum uncertainty state in this sense it must hold that

$$\sum_{j=0}^{N-1} \mid \langle e_{i,j} \mid \psi\rangle \mid^2 = \frac{2}{N+1}. \tag{2.9}$$

A moderately long calculation shows that this condition is equivalent to $\mid \psi\rangle$ (or rather the operator corresponding to $\mid \psi\rangle$) making the same angle with all the MUB hyperplanes, so that the radii of the spheres on which the projections lie are the same, as already claimed - this can also be realized from the fact that the average of H_R in (2.8) over the $N+1$ MUBs is minimized by putting all the p_i equal to $\frac{1}{N}$.

The minimum uncertainty condition, as stated above, is a geometrical condition. We know in what directions from each MUB hyperplane to look for such states, and going out in any of these we sooner or later hit the outsphere of the body of density matrices. And, at the same moment, we confront the same question that has already arisen several times in this thesis: just how does the body of density matrices sit on this outsphere? It is not clear that the direction indicated by the above criterion at all corresponds to a state. Some things are, however, known. Firstly that, for prime $N > 3$, the set of SIC fiducials is discrete, and therefore smaller than the continuous set of minimum uncertainty states. A conjecture due to Wootters has it that the latter has real dimension $N - 2$, which would allow the two sets to coincide for $N = 3$ [23]. Secondly, in all odd prime dimensions the SIC vectors, if they exist, are minimum uncertainty states [12].

As has been mentioned, $N = 3$ makes for a special case in that it offers the freedom of an undetermined phase in the projected SIC simplex, so that the projection is not fixed until the exact position of the projected simplex in one of the planes is chosen. This is partly explained by the fact that the sphere - then a circle - on which the projected points lie is entirely contained in the MUB simplex, which is not the case in other dimensions. In all other cases, when the exact orientation of the simplex is important, the rotation relating the SIC simplex to that defined by the MUB vectors is apparently not of any simple form. [22]

2.2 Special configurations and elliptic curves

It is perhaps somewhat unexpected that a connection between SICs and MUBs is offered by a mathematical result dating from the 19th century, having to do with something known as the Hesse configuration. In three dimensions this construction contains the MUBs as well as the SICs. This is encouraging but maybe not as much so as one might think - from a natural generalization to higher dimensions the SICs fail to fall out, even though the MUB vectors are still there. Possible applications to the MUB-SIC problem aside, the configurations of this section are interesting in their own right, not least because they are a meeting point of mathematical disciplines such as group theory, projective geometry, combinatorics and the theory of elliptic functions.

The Hesse configuration was originally defined by Otto Hesse in 1844 [24]. While it might at first sound surprising that Hesse's construction is intimately connected to the SIC and MUB problems, closer inspection shows that the link is provided by the Weyl-Heisenberg group. We have already seen that the group plays a fundamental role in the construction of both SICs and MUBs, and it does so also for the Hessian curve. The latter results from asking for the most general homogeneous cubic polynomial in three variables left invariant by action of the Weyl-Heisenberg group. Choosing an explicit matrix representation for the group, and letting it act on a vector, its coordinates in the fixed basis transform in some way; the constraint is then that the homogeneous cubic polynomial in these three coordinates should be unaffected by this transformation. Settling for the clock and shift representation defined in (2.6) , the generators of the Weyl-Heisenberg group are

$$Z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & q & 0 \\ 0 & 0 & q^2 \end{pmatrix}$$

and

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

Choosing the basis $\{\mid a\rangle\}_{a=0}^{2}$ for our three-dimensional Hilbert space and letting x, y, z be the coordinates for a vector expressed in this basis, action by the Weyl-Heisenberg group results in these coordinates being permuted or multiplicated by a phase. For instance, application of X to the vector $x \mid 0\rangle + y \mid 1\rangle + z \mid 2\rangle$ results in the coordinate transformation $x \to y,\ y \to z,\ z \to x$. What one finds is that the most general homogeneous cubic polynomial left invariant by the Weyl-Heisenberg action is

$$f = x^3 + y^3 + z^3 + txyz, \tag{2.10}$$

for a (complex) parameter t - this is Hesse's canonical form.

Setting this polynomial equal to zero, a plane cubic curve is obtained, which assuming that $z \neq 0$, can be expressed in affine coordinates as

$$(\frac{x}{z})^3 + (\frac{y}{z})^3 + 1 + \frac{x}{z}\frac{y}{z} = 0.$$

The condition $t^3 \neq -3^3$ and $t \neq \infty$ guarantees that no points other than $(0, 0, 0)$ satisfy

$$f = 0, \quad f'_x = f'_y = f'_z = 0; \tag{2.11}$$

the curve is then said to be non-singular, implying in particular that it has no self-crossings. Here we will initially assume this assumption to hold, although we will return to the case when the curve is singular and does cross itself.

From the plane cubic curve, as from any curve, its Hessian curve can be constructed as the roots of the equation

$$h \equiv det f''_{ij} = 0; \tag{2.12}$$

this curve will again be a cubic. For the curve (2.10) it is

$$h = (6^3 + 2t)xyz - 6t^2(x^3 + y^3 + z^3) = 0. \tag{2.13}$$

As is easily seen, this is a member of the pencil of cubic curves obtained by varying the complex parameter t.

With the help of Hesse we can now proceed: one of his theorems state that each intersection of a non-singular plane cubic curve with its Hessian curve is an inflexion point of the original curve, and conversely. Given that the original curve is brought to Hesse's canonical form before constructing its Hessian, the intersection points are nine SIC-vectors. The fact that there are nine of them is a consequence of Bézout's theorem, which implies that two plane cubic curves intersect in exactly 3×3 points.

It turns out - this result is also due to Hesse[1] - that the nine SIC-points so obtained are a realization of the Hesse configuration. The latter is a set of points and lines, whose relations can be summarized as

$$(9_4, 12_3). \tag{2.14}$$

The way this is read out is that the configuration consists of 9 points, each of which lies on 4 of the 12 lines, which in turn contain 3 points each. Points and lines here refer to the objects in $\mathbf{CP}^2$ corresponding to one- and two-dimensional subspaces of $\mathbf{C}^3$, respectively. From this it is clear that a line is defined by two points, just as a two-dimensional subspace of a vector space is obtained from two one-dimensional ones.

The setup can also be inverted (using orthogonal complements in $\mathbf{C}^3$) to obtain the dual Hesse configuration,

$$(12_3, 9_4), \tag{2.15}$$

consisting of twelve points and nine lines. This maneuvre makes visible the MUB vectors, which correspond to the twelve points - i.e. twelve one-dimensional subspaces, or vectors, in $\mathbf{C}^3$. The nine lines, or two-dimensional subspaces, correspond to eigenspaces of the phase point operators originally introduced by Wootter's. We will return to these operators in a little bit, but can note here that their existence is in fact suggested already by Hesse's canonical form. One symmetry that is not required by Weyl-Heisenberg invariance but is clearly possessed by the polynomial (2.10) is given by the transformation $x \to x$, $y \leftrightarrow z$. This is exactly the action of the involution represented by a phase point operator A. The phase point operators exist in all odd prime dimensions, and the dual Hesse configuration is easily generalized to arbitrary such dimension, with its connection to MUBs and phase point operators preserved.

The Hesse configuration is, with its nine points and twelve lines, a realization of an affine plane of order three. An affine plane is defined as a set of points $\{a_\alpha\}$ and lines $\{l_\omega\}$. The lines are subsets of the set of points, each line being defined uniquely by two points, although it can of course contain a larger number. A point set constituting an affine plane satisfies the below conditions:

(1) If a_α and a_β are distinct points, there is a unique line l_ω such that $a_\alpha, a_\beta \in l_\omega$.

[1] Building on earlier work by Julius Plücker, who in addition to his work in the field in question also made many other important contributions to geometry as well as to experimental physics.

(2) If $a_\alpha \notin l_\omega$ there is a unique line l_σ such that $a_\alpha \in l_\sigma$ and $l_\omega \cap l_\sigma = \oslash$.

(3) There are at least two points on each line, and there are at least two lines.

If the point set is finite, all the lines contain the same number of points and this number, N, defines the order of the affine plane. For an affine plane of order N, it can be shown that that the total number of points must be N^2, and the number of lines $N^2 + N$. One should be aware, however, that the words 'points' and 'lines' are here in some sense arbitrary - its combinatoric properties are the real characteristics of the affine plane. As it happens, however, the points and lines as defined in the context of the Hesse configuration correspond exactly to points and lines in the abstract, combinatorial sense of the affine plane.

Hence, the characteristic intersection properties of the Hesse configuration are those of an affine plane of order three. There is, however, even more structure to the configuration than can be read directly off (2.14) or immediately derived from the affine plane axioms. Hesse provides also this information: the six inflexion points that do not lie on one particular line, lie by threes upon two other lines. This set of three lines forms a triangle in $\mathbf{CP}^2$, and the nine inflexion points all lie by threes upon the sides of any one of the four inflexion triangles. The vertices of these triangles, on the sides of which the SIC-points lie, are the twelve vectors in a complete set of MUBs. In other words, the four sets of parallell lines that can be found in the affine plane correspond to four sets of three rays arranged in a triangle in $\mathbf{CP}^2$. The intersection points of these rays - the vertices of the triangles - do not correspond to any of the points in the affine plane, but instead give the twelve MUB vectors.

This can be compared with the cases so far not considered: the choices of the parameter t for which the curve has singular points. These are the three - remember that t is complex - values that give $t^3 = -27$, and $t = \infty$. In all these four cases, the solution curve for the equation $f = 0$ collapses to three lines forming a triangle, the vertices of which are self-crossings or singular points of the curve. These vertices will again be the MUB vectors, and it turns out that the four 'forbidden' choices for t together give a full set of MUBs.

These considerations show that, in three dimensions, the SIC and the MUBs are intimately tied together by Hesse's construction in conjunction with the results stated above. This fact provides motivation for investigating generalizations of the Hesse configuration for N larger than three, in the hope of finding a corresponding link in all dimensions.

Such a generalization is in fact provided indirectly by Wootters' phase point operator A. As has already been mentioned, this operator constitutes an important tool in the translation between the language of plane cubic curves and that of group theory, and in higher dimensions it defines an arrangement called the Segre configuration [9], a possible generalization of the Hesse configuration to all (odd) prime dimensions. Just as the phase point operator constitutes a part of the symmetry group of the plane cubic in dimension three, the group constructed by adjoining such an object to the Weyl-Heisenberg group gives the symmetry group of the corresponding elliptic curve in all these dimensions. Some further aquaintance with the operator A - or rather the N^2 operators A_{ij} obtained by acting on it with the elements of the Weyl-Heisenberg group - will now be made.

The phase point operators of Wootter's are constructed via the procedure described above for dimension three, starting from the affine plane obtained from a phase space description of an N level quantum system, namely as points (q, p), with $q, p \in \mathbf{Z}_N$. For N an odd prime, which is the case that will here be considered, $\mathbf{Z}_N$ is a field and an affine plane of order N exists. A consequence of this is that phase space can be decomposed into N parallell lines in $N + 1$ different ways - such a decomposition is called a pencil. Letting each pencil be represented by that of its lines passing through the origin and calling this line a ray, it can be shown that from these $N + 1$ rays a complete set of MUBs can be constructed, again in complete analogue with the three-dimensional case. The construction is such that each ray corresponds to a specific member of an orthogonal basis, and the other lines in the pencil are the remaining members, meaning that the rays all represent different basis sets. Choosing the projector constructed from the MUB vector corresponding to each ray to represent it, and letting the other vectors of the respective MUBs to represent the other lines in the pencils, we obtain an assignment of vectors to lines in phase space. This assignment, finally, can be used to define the phase space operator at a point (q, p) as

$$A(q, p) = \sum_{\lambda} P_{\lambda} - \mathbf{1},$$

where the projector sum runs over the $N + 1$ lines passing through the point (q, p), the projectors being constructed from the vectors associated to the lines according to the above prescription. Put in terms of the correspondence between pencil lines and MUB elements, the N^2 phase point operators are obtained by choosing one vector from each basis in a complete set of $N + 1$ MUBs.

For each of the N^2 operators $A(q, p)$ or, switching indices, A_{ij}, a projector can be defined according to

$$\Pi_{ij} = \frac{1}{2}(A_{ij} + \mathbf{1}).$$

As explained above, this will give a projection onto an n-dimensional subspace of $\mathscr{H}^N$, with $N = 2n - 1$. A pair of such subspaces will always have a common vector, but from the definition of the phase point operators follows that the subspaces obtained from the set of A_{ij} will intersect in exactly $N(N + 1)$ distinct vectors in $\mathbf{CP}^{2n-1}$, and in $\mathbf{CP}^{2n-2}$ we have the configuration

$$(N(N + 1)_N, N^2_{N+1})$$

of $N(N+1)$ points that each lie in N $(n-1)$-planes, and N^2 $(n-1)$-planes, each containing $N+1$ points. However, neither from this construction or from its dual, one directly obtains the N^2 points corresponding to a SIC.

We have already seen that the Weyl-Heisenberg group is of central importance to the construction of SICs and MUBs, as well as to the definition of Hesse's canonical form. Although not directly visible in the above account of the phase point operator construction, it lies in the background here as well: the phase point operators can in fact be seen as elements of a subgroup of all unitaries, singled out by its action on the Weyl-Heisenberg group. The Clifford group, to which the operators A_{ij} belong, is the normalizer of the Weyl-Heisenberg group in the group of all unitary matrices. This by definition means that the Clifford group is the set of unitary operators U such that sandwiching a Weyl-Heisenberg group element between U and $U^\dagger$ gives back an element of the Weyl-Heisenberg group (times an irrelevant phase). In equations:

$$UD_{ij}U^\dagger = \omega D_{i'j'}, \tag{2.16}$$

where ω is a phase factor.

The Clifford group is isomorphic to a semi-direct product between a symplectic group and the Weyl-Heisenberg group itself. In odd dimensions $N = 2n - 1$ it contains the Wootters phase point operators A_{ij} as the elements fulfilling

$$A^2 = \mathbf{1} \quad \text{and} \quad AD_{ij}A^\dagger = D_{-i-j}. \tag{2.17}$$

Each of these operators, which are both unitary and Hermitian, splits Hilbert space into two subspaces $\mathscr{H}_\pm$ with dimensions n and $n-1$, respectively. That this is so follows from the fact that they square to unity - so that their spectra consist of 1's and -1's - and that they have trace one, meaning that the number of 1's in the spectra must be exactly one more than the number of -1's. In section 2.3 some properties of these subspaces will be further investigated.

Even though the N-dimensional Segre configuration comes from (the symmetry group of) an elliptic normal curve of degree N in the complex projective space $\mathbf{CP}^{N-1}$, the connection to elliptic curves and their torsion points is not explicit in the above description. It can be made so by using the correspondence between curves and tori, making it possible to interpret the curve as a group manifold. Considering the elliptic curve as a group - there is a natural definition of group action that allows this - one can define its N-torsion points as the points, or group elements g, that satisfy $g^N = \mathbf{1}$. In this case, these points on the curve define a lattice of N^2 points on this manifold, giving the group $\mathbf{Z}_N \times \mathbf{Z}_N$ together with the point face operator involution introduced above. When lifted to the embedding space - which for a normal curve is some complex projective space - the Weyl-Heisenberg group and Wootter's phase point operators, in terms of which the problem is stated here, results. This is a generalization of what happens in $\mathbf{CP}^2$, where putting the origin at one of the nine inflexion points that an elliptic curve then has, the set of inflexion points is exactly the set of torsion points.

Another class of Clifford group elements that will be of interest in the following are those of order three, i.e. elements B satisfying

$$B^3 = \mathbf{1},$$

first studied in this context by Zauner [1]. The fiducial vector propositioned by Zauner is also conjectured to be an eigenvector of such an operator, so that it lies in one of the three subspaces corresponding to the three eigenvalues. Just as the existence of the fiducial vector, this part of Zauner's conjecture has proved to hold in all cases that have so far been checked [5]. To reconnect to the elliptic curve, it can be noted that although its torsion points do not correspond to SIC-vectors for $N > 3$, for $N = 3$ these points on the curve also lie in one of the eigenspaces of an element of order three. This opens for the possibility that it might be possible to find an alternative generalization of Hesse's configuration, for which the SICs could be obtained from order three symmetries.

2.3 The frame potential, on average

It can be shown [10] that the torsion points mentioned in the previous section lie in the $(n-1)$-dimensional subspaces defined by phase point operators in all odd prime dimensions, whereas known SIC vectors only do for $N = 3$. Given this slighty disheartening fact, we now proceed to look at these and other subspaces and their relation to SICs from a somewhat different angle.

The arguably most natural measure of how close a set of N^2 unit vectors in $\mathscr{H}^N$ is to forming a SIC is provided by the function

$$f \equiv \frac{1}{2}\sum_{i \neq j}\left(|\langle\psi_i|\psi_j\rangle|^2 - \frac{1}{N+1}\right)^2 . \tag{2.18}$$

By construction $f = 0$ if and only if the vector set is a SIC. For any frame and for any integer t one can define a frame potential according to [3, 18]

$$F_t \equiv \sum_{i,j} |\ \langle\psi_i \mid \psi_j\rangle\ |^{2t} . \tag{2.19}$$

The function f is related to the first two of these frame potentials,

$$F_t \equiv \sum_{i,j} |\langle\psi_i|\psi_j\rangle|^{2t} , \qquad t \in \{1, 2\}, \tag{2.20}$$

by

$$f = \frac{1}{2}F_2 - \frac{1}{N+1}F_1 \ . \tag{2.21}$$

Just as f does, these frame potentials assume their global minimum for a SIC. In numerical searches for SICs only F2 is usually employed, since any global minimum for the second frame potential is known to be one for F1 as well.

Computing the frame potential f for the 25 torsion points for the $N = 5$ elliptic curve, I found it to take the value 10.42, independently of how the modular parameter of the curve was varied. The question then arose if this value is to be considered high or low - in other words, can a set of N^2 vectors giving this value be said to be close to forming a SIC, or is it instead far from it?

One way to answer this question - in dimension five and other - is by considering the average of f over Hilbert space, as well as over some subspaces of possible relevance in the search for SICs. A special case of interest is when the N^2 vectors in the set form an orbit of the Weyl-Heisenberg group, in which case f is a function not of N^2 vectors but of a single fiducial i.e. a function on the projective Hilbert space $\mathbf{CP}^{N-1}$. In this case

$$|\psi_{ij}\rangle = D_{ij}|\psi_0\rangle \ , \tag{2.22}$$

for some fiducial unit vector $|\psi_0\rangle$, and the frame potential becomes

$$f_H = \frac{N^2}{2}\sum_{i,j\neq 0,0}\left(|\langle\psi_0|\psi_{ij}\rangle|^2 - \frac{1}{N+1}\right)^2 \ . \tag{2.23}$$

An explicit matrix representation of D_{ij} can be used to write [12, 14]

$$\langle\psi_0|D_{ij}|\psi_0\rangle = \bar{Z}_a q^{bj}\delta^a_{b+i}Z^b = q^{(a-b)j}\bar{Z}_a Z_{a-i} \tag{2.24}$$

and following this up by taking the Fourier transform

$$\frac{1}{N}\sum_j q^{kj}|\langle\psi_0|D_{ij}|\psi_0\rangle|^2 = \sum_a \bar{Z}_a\bar{Z}_{a+k-i}Z_{a+k}Z_{a-i} \tag{2.25}$$

we find that

$$f_H = \frac{N^3}{2}\left(\sum_{i=0}^{N-1}\sum_{k=0}^{N-1}\left|\sum_{a=0}^{N-1}\bar{Z}_a\bar{Z}_{a+k-i}Z_{a+k}Z_{a-i}\right|^2 - \frac{2}{N+1}\right) \ . \tag{2.26}$$

The results of averaging this function, as well as the unrestricted function f, over Hilbert space and four relevant subspaces are given in Article II, where arguments are also given for the results in Table 2.3 followed by a bracketed question mark, for which rigorous proofs are currently lacking. The numbers given in the table are valid for $N = 7$, in which dimension the subspaces considered are $\mathscr{H}_\pm$ - the ones singled out by the special element of order two presented in the previous section - and $\mathscr{H}_1$ and $\mathscr{H}_\alpha$, labelled by the eigenvalues of a Clifford group element of order three.

	f	f_H	$f_H(\mathcal{H}_+)$	$f_H(\mathcal{H}_-)$	$f_H(\mathcal{H}_1)$	$f_H(\mathcal{H}_\alpha)$
Minimum	0	0	12.2 (?)	4.764 (?)	0	-
Average	18.375	14.29	25.72	25.72	15.98	11.75
Maximum	900.4	128.6 (?)	128.6 (?)	42.88 (?)	-	-

Table 2.3: Averages over certain special subspaces for $N = 7$.

Chapter 3

Kochen-Specker frames

The theorem known as Kochen and Specker's theorem (KS) was formulated by Simon Kochen and Ernst Specker [28] in 1967. The effective statement of the theorem, sometimes referred to as the Bell-Kochen-Specker theorem, is that it in a Hilbert space of dimension $N \geq 3$ is impossible to assign definite values from $\{0, 1\}$ to all projection operators, i.e. vectors in such a way that each set of N orthogonal vectors contains exactly one vector with the value 1. Just as in the above, each unit vector will represent all vectors with the same direction, because only orthogonality relations are of importance. The KS result is, in effect, a corollary to Gleason's theorem [33], since it can be shown that no density matrices give such probabilities, but it was proved independently of Gleason's result (albeit 10 years later). The structure of the proof is of a somewhat different character than Gleason's - whereas the KS result is proved by using an iterated graph structure in a relatively straightforward manner, the proof of Gleason's theorem contains many subtle steps. Gleason's proof is, however, much simplified when the assumption made to prove the theorem is strengthened to include not only orthogonal bases but the full set of POVMs [17]. It can then also be shown to hold in two dimensions as well, which is not the case for Gleason's original statement. While making the assumption only for the restricted set of POVMs defined by SICs does not suffice [18], a Gleason-type theorem can very likely be proved in two dimensions [1] for all other four element POVMs [29].

The conditions, formally stated, are

$$g : \mathscr{H}^N \rightarrow \{0, 1\} \tag{3.1}$$

$$\sum_{i=1}^{N} g(P_i) = 1 \tag{3.2}$$

for all sets $\{P_i\}$ of N orthogonal vectors in $\mathscr{H}^N$.

[1]With a slight modification: continuity of the frame function is assumed instead of shown to follow from the other assumptions.

The physical implications of KS in relation to hidden variable theories have been much discussed, and the most common interpretation is that the theorem places severe restrictions on any such theory; in effect, the theorem implies that any well-defined properties possessed by particles would necessarily have to be contextual - the original authors themselves thought their result to establish the 'nonexistence of hidden variables'. However, arguments have been made for an understanding of KS rather as an epistemological statement about the limitation of the knowledge possible to obtain through measurement [30].

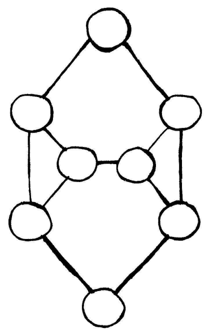

Figure 3.1: The basic building block of the graph used in the original proof of the Kochen-Specker theorem.

3.1 Kochen-Specker colourings

In proving their result, Kochen and Specker made use of a discrete subset of vectors, rather than working in continuous three-space; in fact their proof takes place in $\mathbf{R}^3$, and the result is then extended to $\mathbf{C}^N$ via $\mathbf{C}^3$. By arranging a set of 117 three-dimensional real vectors in an ingenious way they were able to prove that a non-contextuality assumption is in conflict with quantum mechanics - the impossibility of assigning truth values to all vectors in three dimensions of course follows from the impossibility of making such an assignment for a (discrete) subset, just as the KS result in all dimensions larger than two is implied by the fact that it holds in three.

For the competitionally inclined, the task of reducing the number of vectors used to prove the theorem seems a natural one to take on. Consequently, a downright contest has resulted in the record in three dimensions, due to Conway and Kochen, being pressed down to 31. This number can be further reduced in higher dimensions, and for most of them it is not known whether or not the existing record actually is a minimal set. In dimension four, however, the current record of 18 vectors [19] has been shown to be the best obtainable [20], and in three dimensions an uncolourable set must contain at least 20 vectors, even though it is not known whether or not such a minimal set exists.

The way one usually sees the problem of finding KS collections stated is in terms of colourings of vector sets. Letting the colour green represent the digit 1 (i.e. a yes-answer to some experimentally posed question) and red correspond to 0, the conditions (3.1) and (3.2) mean that only one vector in each orthogonal N-plet can be green. Non-contextuality then amounts to the assumption that each vector has one well-defined colour, no matter of what orthogonal basis it is considered a part.

If we let vectors be represented by nodes and orthogonality relations by edges, our considerations here lead us into another area of combinatorics, namely that of graph colouring. The Kochen-Specker problem can be seen as a variation of the classical combinatorial problem of assigning a so-called chromatic number χ to a graph - the least number of colours needed to colour the graph in such a way that no adjacent vertices have the same colour. For instance, the complete graph with n vertices, K_n has $\chi(K_n) = n$. The definition of chromatic number can be modified for topological spaces such as the two-sphere, for which $\chi_{\mathbf{S}^2} = 4$. The latter result is due to Godsil and Zaks [31], who have also shown that the corresponding number when only rational points on the sphere are included is three. The definition of 'adjacent' is in this case orthogonal, which means that as a corollary of this result - just identify two of the three colours - a Kochen-Specker assignment of values to the rational sphere in dimension three is possible. This fact has been used to argue that the KS theorem is irrelevant from an experimental point of view [32].

Given that it is impossible to assign values from $\{0, 1\}$ according to the KS criteria to all vectors in $\mathbf{R}^3$ (and higher dimensions) in a consistent way, one might ask how close one can get to making a complete assigment. In terms of colourings: how much of $\mathbf{R}^3$ - or $\mathbf{S}^2$ because we are looking at rays rather than vectors - can be coloured, in such a way that no matter how an orthogonal triple of unit vectors is inscribed in the sphere, two of its vectors will never be red and three of its vectors will never be green at the same time. (Because of the impossibility of a complete colouring we must, however, accept that one or more of the vectors sometimes lie in an 'undefined' area.)

For a given colouring strategy, originally suggested by Appleby in dimension three, the answer is that 87% of all vectors in $\mathbf{R}^3$ can be coloured according to the criteria given above; the numbers in higher dimensions are given in Article I and can be read off the plot in Figure 3.2. That the colourable fraction does not go to zero but instead approaches 68% as N increases is perhaps somewhat unexpected, especially considering the somewhat arbitrary choice of method for colouring.
It can, however, be argued that a more physically relevant measure of colouring effectivity than the fraction of vectors (or rays) coloured is that of orthogonal bases. In this case, the result is 69% in three real dimensions and 34% in four.

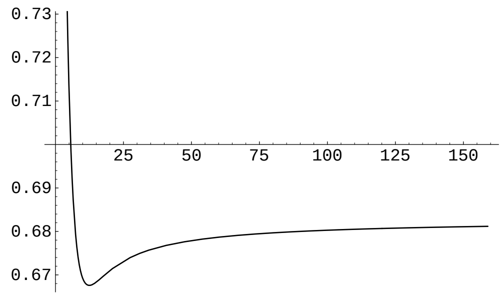

Figure 3.2: Percentage of the sphere in N dimensions that is colourable using the method suggested by Appleby, as a function of N.

3.2 A Kochen-Specker inequality

Before diving into the subject of the present section[2], we will stop to take a look at the so-called magical basis, introduced by Bennett et al in a 1996 paper [34]. This basis has the interesting and useful property that the reality of vectors expressed in it carries physical meaning.

To introduce the magical basis, we first make the trivial observation that any Hilbert space vector can be decomposed into real and imaginary parts according to

$$| \psi \rangle = \cos\sigma \mathbf{x} + \sin\sigma \mathbf{y}, \tag{3.3}$$

with $\mathbf{x}^2 = \mathbf{y}^2 = 1$ and with the trigonometric coefficients guaranteeing normalization. Further, the fact that we are looking at complex projective space - meaning that we do not differentiate between vectors that differ only by an overall multiplicative phase - gives a certain freedom, which can be used to impose the additional conditions

$$\mathbf{x} \cdot \mathbf{y} = 0, \quad 0 \leq \sigma \leq \frac{\pi}{4}. \tag{3.4}$$

This representation is useful when considering group action that preserves real and imaginary parts. This is not the situation in general: unitary transformations do not respect this decomposition. If, on the other hand, the relevant subgroup happens to be some $SO(N)$, no mixing of real and imaginary parts takes place under the group action. Examples of cases where $SO(N)$ in fact determines the orbits of interest include two entangled qubits - due to the fact that $SU(2) \times SU(2)$ is isomorphic to $SO(4)$ - as well as two entangled $j = \frac{3}{2}$ fermions, with $SU(4) \simeq SO(6)$ as the relevant subgroup. Another case - and the one that will be of interest here - is $SU(2) \simeq SO(3)$.

[2]This section is based on unpublished work together with P. Badziag, I. Bengtsson, A. Cabello and J-Å. Larsson.

For a two qubit system one can check that maximally entangled states will correspond to completely real vectors, whereas the separable states will be represented by vectors with equal real and imaginary parts, when expressed in the magical basis. For three dimensional vectors, in analogue, the (classical) spin, or $SU(2)$, coherent states have real and imaginary parts equal, while completely real corresponds to maximally non-classical states. The vectors used by Klyachko in deriving a KS-type contradiction between classical assumptions on the one hand and quantum mechanical predictions (and experimental outcomes) on the other can in this sense be viewed as maximally quantum. The advantage of choosing real vectors in the pentagram is that the resulting operator then, in addition to being Hermitian, is real and symmetrical, so that it can be diagonalized by means of rotations in $SO(2)$. As already mentioned, the transformations in this subgroup of $SU(2)$ preserve real and imaginary parts, and hence the correspondence between reality and (non-)classicality.

The configuration that will here be called a Kochen-Specker frame and that was recently discussed in relation to experimental tests of non-contextuality by Klyachko et al [27] (although, as we will see, it has implicitly appeared in other problems) is a set of vectors whose orthogonality graph forms a pentagram (or, equivalently, a pentagon); the configuration is depicted in Figure 3.2. From these vectors we can, in analogy with the Bell construction used for tests of local realism, form an operator according to

$$\Sigma = \sum_{i=0}^{4} \mid k\rangle\langle k \mid . \tag{3.5}$$

The labelling of the five vectors is chosen such that

$$\langle k \mid k+2\rangle = 0, \tag{3.6}$$

with addition modulo five understood.

As earlier mentioned, the pentagram vectors constitute a frame, and the frame bounds defined in equation (2.19) can be found for the configuration. Inspection yields that these are in fact the smallest and largest eigenvalues for the operator - hence, if the spectrum is non-degenerate, the frame will not be tight. As for the pentagram operator, it is never completely degenerate. It can, however, be partly degenerate - so that two of the eigenvalues are equal - but this is not enough to make the pentagram into a tight frame.

Also in analogy with the Bell case, we can derive an inequality from this operator that can be used to test the assumption not of local realism, but of contextuality.

Each operator in (3.5) corresponds to an observable, which is here taken to be dichotomic with values in $\{0, 1\}$. With the same reasoning used in the original KS argument, only one operator in each orthogonal triple can result in the value 1 when applied to a given state. The orthogonality relations given in (3.6) then for instance imply that given an assigment of the value 1 to the observable associated to the vector $\mid 1\rangle$, a zero must be assigned to

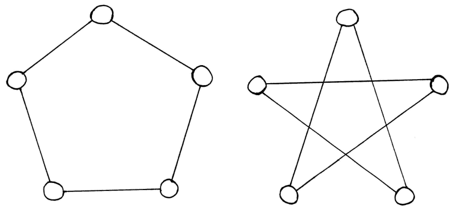

Figure 3.3: The vectors of the Kochen-Specker frame, forming a pentagram or pentagon, with orthogonality between vectors (nodes) represented by an edge between them.

both that of $\mid 3\rangle$ and that of $\mid 4\rangle$. Following this line of reasoning, one finds that at most two of the projectors in (3.5) can give the value one, so that the inequality

$$\langle \Sigma \rangle \leq 2 \tag{3.7}$$

holds. A contradiction between quantum mechanics and the classical assumptions of the above argument now arises because states can be found for which the expectation value of Σ exceeds this bound.

It is important that one understands the difference between the two types of KS configurations, with corresponding arguments, that are encountered in this thesis: the uncolourable sets and the sets giving a (probabilistic) contradiction. Although the Kochen-Specker frame figures in a fundamental way as part of the uncolourable set given by the original authors - the configuration in Figure 3.1 basically consists of a couple of pentagons with two vertices in common - the frame is itself not uncolourable. However, by assigning explicit states, fullfilling the orthogonality relations of the graph, to the nodes one is able to derive a contradiction between quantum mechanics (or experiments) and the non-contextuality assumption behind the colouring.

When a testable pentagram inequality was originally introduced by Klyachko and collaborators, it was claimed that the fact the setup is all local would make it correspond to a Bell test with the option of non-locality removed. A violation of the regular Bell inequalities - in, for example, the CHSH version - is usually taken as proof that either locality or realism must go. Meaning that, if we accept experimental violations as a fact but still want to talk about classical properties of quantum objects, we must abandon the assumption of locality. If, on the other hand, we are unwilling to negotiate with the locality principle, we must agree to question the idea that observables have well defined values before they are measured. These claims, however, are false: because the spacial distance is removed, sticking to realism does not imply having to let go of locality, because everything takes place locally. The implications of a violation of (3.7) is not that reality is a problematic assumption, either, but simply that classical properties, if they exist, have to be ascribed to full measurement situations rather than isolated objects: in short, that nature is contextual.

3.3 The Hardy paradox

As we have seen, the logical structure represented by the Kochen-Specker frame plays a central role in the proof of the original KS result, as well as in the Klyachko construction for an experimental contextuality test. A slight modification of the same structure occurs also in the formulation of another important result having to do with the non-classicality of quantum mechanics: Hardy's paradox [15, 16, 21]. In a 1993 paper, Lucien Hardy introduced a thought experiment which, without relying on inequalities, was said to demonstrate the nonlocality of almost all bipartite entangled states. (The only state for which his argument failed was, somewhat surprisingly, the maximally entangled one.) From the standpoint of actual experimental realization, the fact that it involved only two observers, each measuring two dicotomic observables, A_i and B_i, respectively, is a great advantage. On the other hand, the fact that the logical contradiction arises without any appeal to inequalities is a theoretical merit. The assumptions made are weaker than in many other Bell-type arguments, in the sense that they are not sufficient to force an assumption like that made by EPR [26] about the existence of so-called 'elements of reality', classical properties or hidden variables of the particles involved. It is, however, strong enough, to result in a contradiction according to the following.
The variables A_1, A_2, B_1 and B_2 all take values in $\{-1, 1\}$ and (adopting the notation that x stands for $X = 1$, $\bar{x}$ for $X = -1$, it is assumed that

$$P(\bar{b}_2 \mid a_1) = P(\bar{a}_2 \mid b_1) = P(b_2 \mid a_1) = 0.$$

This enforces

$$P(a_1 \mid b_1) = 0,$$

from which a contradiction is derived, because the quantum mechanical overlap between the two states giving $A_1 = 1$ and $B_1 = 1$ is non-zero.

The orthogonality graph for Hardy's paradox, which can be seen in Figure 3.4, consists of two pentagons, or Kochen-Specker frames, sharing two vectors and with two extra orthogonalities added - so far, the graph is identical to the one that occurs in the original KS argument as accounted for in the beginning of this chapter. In addition, one more vector is introduced, orthogonal to all the others in the configuration except the top one.

As noted above, the orthogonality graph of the vectors used in deriving Hardy's paradox reveals an intimate connection between the configurations used in his argument, and in the Kochen-Specker argument presented by Klyachko. One should, however, not let oneself be misled by appearances: although related the two vector sets are fundamentally different. Whereas Klyachko deals with vectors in three real dimensions, Hardy's configuration needs four dimensions to be realized and also uses vectors with complex components. Nevertheless, the similarity between the two structures suggests that the pentagram configuration - the Kochen-Specker frame - plays a central role in non-contextuality arguments. This begs

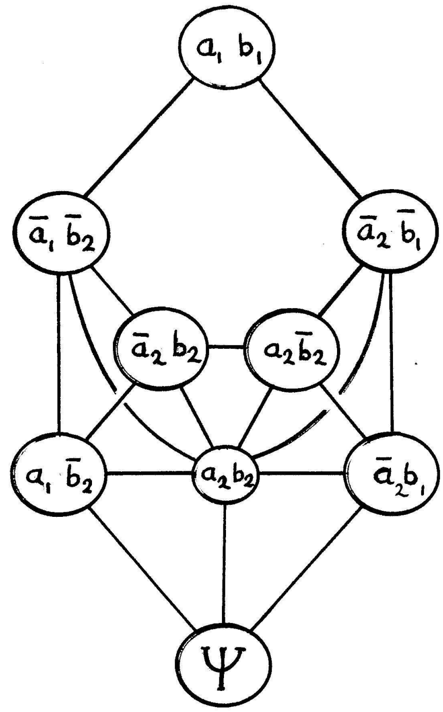

Figure 3.4: The orthogonality graph representation of the configuration used in the derivation of Hardy's paradox.

the question what relation - if any - there is between vector sets that violate the inequality (3.7) and that lead to a contradiction in the Hardy case.
A partial answer supports the strong link between the two: for Hardy's set as well as for the KS graph, the most non-classical configuration corresponds to a maximal overlap between the uppermost and lowermost vectors in Figures 3.4 and 3.1, respectively. In both cases, maximizing the non-classical probability between these two is equivalent to maximizing the violation of the pentagram inequality (3.7) when the operator Σ for the upper KS frame is applied to the bottom state.

Bibliography

[1] G. Zauner, *Quantendesigns. Grundzüge einer nichtkommutativen Designtheorie*, PhD thesis, Univ. Wien, 1999.

[2] P.W.H. Lemmens and J.J. Seidel, *Equiangular lines*, J. Algebra **24**, 494 (1973).

[3] J.J. Benedetto and M. Fickus, *Finite normalized tight frames*, Adv. Comp. Math. **18**, 357 (2003).

[4] M. Grassl, *On SIC-POVMs and MUBs in dimension 6*, in: Proc. of ERATO Conference on Quantum Information Science (2004), Tokyo 2004.

[5] D.M. Appleby, *SIC-POVMs and the extended Clifford group*, J. Math. Phys. **46**, 052107 (2005).

[6] M. Grassl, *Tomography of quantum states in small dimensions*, Electronic Notes in Discrete Math. **20**, 151 (2005).

[7] M. Grassl, *Finding equiangular lines in complex space*, talk at the Magma Workshop, 2006.

[8] H. Weyl: Theory of groups and Quantum Mechanics, Dutton, New York 1932.

[9] C. Segre, *Remarques sur les transformations uniformes des courbes elliptiques en ellesmmes*, Math. Ann. **27**, 296 (1886).

[10] K. Hulek, *Projective geometry of elliptic curves*, Asterisque **137**, 1 (1986).

[11] J.M. Renes, R. Blume-Kohout, A.J. Scott and C.M. Caves, *Symmetric informationally complete quantum measurements*, J. Math. Phys. **45**, 2171 (2004).

[12] D.M. Appleby, H.B. Dang and C.A. Fuchs, *Physical significance of symmetric informationally-complete sets of quantum states*, arXiv: 0707.2071.

[13] A. Scott, http://www.cit.gu.edu.au/∼ascott/sicpovms/

[14] M. Khatirinejad, *On Weyl-Heisenberg orbits of equiangular lines*, J. Algebr. Comb **28**, 333 (2007).

[15] L. Hardy, *Nonlocality for Two Particles without Inequalities for Almost All Entangled States*, Phys. Rev. Lett. **71**, 1665 (1993).

[16] L. Hardy, *Ladder Proof of Nonlocality Without Inequalities: Theoretical and Experimental Results*, Phys. Rev. Lett. **79**, 2755 (1997).

[17] P. Busch, *Quantum States and Generalized Observables: A Simple Proof of Gleasons Theorem*, Phys. Rev. Lett. **91**, 120403 (2003).

[18] C.M. Caves, C.A. Fuchs, K. Manne and J.M. Renes,*Gleason-type Derivations of the Quantum Probability Rule for Generalized Measurements*, Found. Phys. **34**, 193 (2004).

[19] A. Cabello, J. M. Estebaranz, and G. García-Alcaine, *Bell-Kochen-Specker theorem: A proof with 18 vectors*, Phys. Lett. A **212**, 183 (1996).

[20] M Pavicic, J-P Merlet, B McKay, and N. D. Megill, *Kochen-Specker vectors*, J. Phys. A **38**, 1577 (2005).

[21] N. D. Mermin, *Quantum mysteries refined*, Am. J. Phys. **62**, 880 (1994).

[22] D.M. Appleby, *SIC-POVMS and MUBS: Geometrical Relationships in Prime Dimension*, in: Proc. of Foundations of probability and physics 5 (2008), Växjö (2008).

[23] D.M. Appleby, private communication.

[24] O. Hesse, *Über die Wendepuncte der Curven dritter Ordnung*, Crelle's J. **28**, 68 (1844).

[25] L. E. Dickson, *The points of inflexion of a plane cubic curve*, Ann. Math., 50 (1914).

[26] A. Einstein, B. Podolsky and N. Rosen, *Can Quantum-Mechanical Description of Physical Reality be Considered Complete?*, Phys. Rev. **47**, 777 (1935).

[27] A.A. Klyachko, M.A. Can, S. Binicioğlu and A.S. Shumovsky, *A simple test for hidden viariables in the spin-1 system*, Phys. Rev. Lett. **101**, 020403 (2008).

[28] S. Kochen and E.P. Specker, *The Problem of Hidden Variables in Quantum Mechanics*, J. Math. Mech. **17**, 59 (1967).

[29] H. Granström, *Gleason's theorem*, Master's thesis, Stockholm University, 2006.

[30] D.M. Appleby, *The Bell-Kochen-Specker theorem*, Stud. Hist. Philos. Mod. Phys. **36** (2005).

[31] C. D. Godsil and J. Zaks, *Coloring the sphere*, University of Waterloo research report CORR 88-12, 1988

[32] D. A. Meyer, *Finite precision measurement nullifies the Kochen-Specker theorem*, Phys. Rev. Lett. **83**, 3751(1999).

[33] A.M. Gleason, *Measures on the closed subspaces of a Hilbert space*, J. Math. Mech. **6**, 885 (1957).

[34] C.H. Bennett, D.P. DiVincenzo, J. Smolin and W.K. Wootters, *Mixed-state entanglement and quantum error correction*, Phys. Rev. A **54**, 3824 (1996).

Article I

Journal of Mathematical Physics, **48**, 092101 (2007)

JOURNAL OF MATHEMATICAL PHYSICS **48**, 092101 (2007)

Incomplete Kochen-Specker coloring

Helena Granström[a]
Department of Mathematics, Stockholm University, SE-10691 Stockholm, Sweden and Department of Physics, Stockholm University, SE-10691 Stockholm, Sweden

(Received 22 February 2007; accepted 13 August 2007; published online 10 September 2007)

A particular incomplete Kochen-Specker coloring, suggested by Appleby [Stud. Hist. Philos. Mod. Phys. **36**, 1 (2005)] in dimension three, is generalized to arbitrary dimension. We investigate its effectivity as a function of dimension, using two different measures. A limit is derived for the fraction of the sphere that can be colored using the generalized Appleby construction as the number of dimensions approaches infinity. The second, and physically more relevant measure of effectivity, is to look at the fraction of properly colored *ON* bases. Using this measure, we derive a "lower bound for the upper bound" in three and four real dimensions. © *2007 American Institute of Physics.* [DOI: 10.1063/1.2779764]

I. INTRODUCTION

The Kochen-Specker theorem[1] is a result that has proven to be of great conceptual interest to quantum mechanics and its interpretation. Let f be a function from the set of projection operators in some Hilbert space to the set $\{0,1\}$ such that

$$\sum_{i=1}^{N} f(P_i) = 1, \tag{1}$$

where the P_i are projection operators associated with the vectors $|e_i\rangle$, forming an *ON* basis for the Hilbert space, and N is the dimension of the space.

The statement of the Kochen-Specker theorem is that no such truth value assignments exist if the dimension of the Hilbert space is larger than 2. This result is often translated in terms of two-colorings of spheres, and the same terminology will be used here. The statement of Kochen-Specker (KS) (in N real dimensions) is in these terms that no complete coloring of the $(N-1)$-sphere obeying the KS criteria (1) is possible. The question then arises how close to complete we can possibly get. A collection of rather eccentric colorings "almost" satisfying the KS criteria has been proposed by Pitowsky,[2] Meyer,[3] Kent,[4] and Clifton and Kent.[5]

Partly in response to these constructions and the interpretations claimed for them, Appleby[6] in a 2005 paper derived an upper bound for the effectivity of a coloring that, in contrast to the colorings mentioned above, is measurable and hence arguably of greater physical interest.

Appleby considered the question of maximal effectivity in the case of three-dimensional real Hilbert space and argues that the maximal fraction of S^2 that can be satisfactorily KS colored might be as large as 99%. To provide a lower bound for the maximal effectivity in terms of area of S^2 colored, Appleby also suggested a specific incomplete coloring that covers 87% of the sphere.

Here, the Appleby construction will be generalized to an arbitrary number of real dimensions.

[a]Electronic mail: helenag@math.su.se

 © 2007 American Institute of Physics

Downloaded 30 Jul 2009 to 130.237.165.22. Redistribution subject to AIP license or copyright; see http://jmp.aip.org/jmp/copyright.jsp

For $N=4$ the coloring analogous to that proposed by Appleby in dimension three covers of 79% of S^{N-1}, 74% for $N=5$, and 71% for $N=6$. The integer giving the least percentage is $N=12$; about 66.76%.

A natural question to ask is what happens to this percentage as the number of dimensions gets very large. Does the colorable fraction, using this specific construction, go to zero? In fact, it does not, but instead tends to 68% as N approaches infinity.

A possibly more physically relevant way of phrasing the question of effectivity is in terms of the fraction of all possible *ON* bases that can be colored. In the following, we will look at the cases $N=3$ and $N=4$. The percentages turn out to be 69% and 34%, respectively. The fact that the falloff is considerably larger than was the case for vectors suggests that this fraction might go to zero with an increase in the number of dimensions.

Several questions remain unanswered, however. Perhaps most importantly, our discussion is limited to families of pure states whose components are all real in some suitable basis in complex Hilbert space, and different results might be obtained if this restriction was lifted. Secondly, one would want to evaluate the effectivity of the coloring in arbitrary dimension, using the fraction of colorable bases as a measure. One could also try to experiment with other constructions to further sharpen the lower bound for the upper bound provided by specific examples.

II. AN INCOMPLETE KOCHEN-SPECKER COLORING

Let us first consider the three-dimensional case and then go on from there to higher dimensions. We are interested in assigning the value 0 or 1 to vectors in $\mathcal{H}^3$ in such a way that no set of three mutually orthogonal vectors are all assigned the value of 0, and no pair of orthogonal vectors both have the value of 1. More precisely, we will color the one-dimensional subspaces spanned by vectors. These conditions can be expressed as

$$f{:}S^2 \rightarrow \{0,1\}, \tag{2}$$

$$f(P_1) + f(P_2) + f(P_3) = 1, \tag{3}$$

for all sets of orthogonal vectors $\{P_1, P_2, P_3\}$, S^2 being the unit two-sphere. Letting white represent the value of 0 and black the value of 1, this problem can be translated into the problem of coloring S^2, in a way that satisfies the conditions just stated. In particular, antipodal points will have the same color.

Any such assignment of truth values (probabilities from {0,1}) to all vectors in the Hilbert space of some system would correspond to (the possibility of) the system having well-defined properties, independent of measurement context. That is, for any possible observable the outcome of the corresponding measurement would be fully determined in advance. However, by the KS theorem, a complete such assigment of truth values is impossible. Hence, what we will do is to assign probabilities from {0,1} according to Eq. (3) to some of the vectors in $\mathcal{H}$—some vectors will necessarily remain uncolored, by KS.

The way to go about this suggested by Appleby is to start out by coloring the two polar caps defined by $|\tan\theta|<1$ black and the region around the equator bounded by $|\tan\theta|=\sqrt{2}$ white, where θ is the usual polar angle. This type of coloring is sketched in Fig. 1.

These limits are derived as follows. The two polar caps are made small enough so that no two vectors in an orthogonal triple can simultaneously lie in the black region, which means that they will extend down to $\theta=\pi/4$. The white section around the equator is just wide enough so that not all three vectors can lie in it at the same time.

Already in four dimensions the contribution to the total area by the black cap is close to negligible. As we will see below it reduces further with increasing dimension, which is why we will primarily be interested in the area taken up by the white section.

The fraction of the sphere in N dimensions that can be colored white with the given restriction is

Downloaded 30 Jul 2009 to 130.237.165.22. Redistribution subject to AIP license or copyright; see http://jmp.aip.org/jmp/copyright.jsp

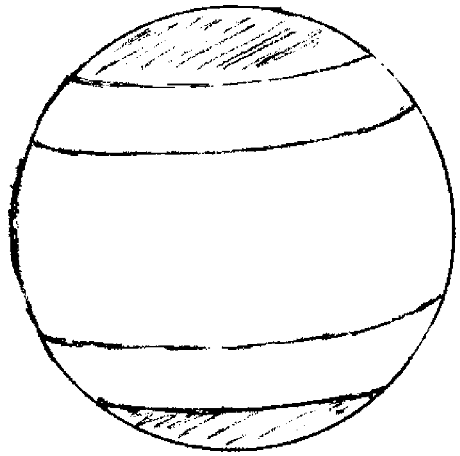

FIG. 1. A possible (incomplete) KS coloring of the unit two-sphere.

$$F = \frac{\int_{\arcsin\sqrt{(N-1)/N}}^{\pi/2} \sin^{N-2}\theta \mathrm{d}\theta}{\int_0^{\pi/2} \sin^{N-2}\theta \mathrm{d}\theta} = 2\frac{\mathrm{vol}(S^{N-2})}{\mathrm{vol}(S^{N-1})}\int_{\arcsin\sqrt{(N-1)/N}}^{\pi/2} \sin^{N-2}\theta \mathrm{d}\theta, \tag{4}$$

where $\mathrm{vol}(S^d)$ denotes the surface area of the d-dimensional sphere. The intergral limits are derived using the expression

$$R_n = \sqrt{\frac{n}{n+1}} = \sqrt{\frac{N-1}{N}} \tag{5}$$

for the radius of the circumsphere of a regular n simplex, where $n=N-1$ is the dimension of the sphere in N dimensions.

As for the black area, B_N, it will in analogy with the $N=3$ case be located around the poles of the sphere, with limiting angle $\pi/4$,

$$B_N = \mathrm{vol}(S^{N-2})\int_0^{\pi/4} \sin^{N-2}\theta \mathrm{d}\theta. \tag{6}$$

What, one may ask, is the fraction of the sphere in N dimensions that can be colored using this method in the limit $N\to\infty$? As can be seen from the expression

$$\mathrm{vol}(S^d) = \mathrm{vol}(S^{d-1})\int_0^{\pi} \sin^{d-1}\theta \mathrm{d}\theta \tag{7}$$

for high dimensions, the fraction of the area of the sphere that will lie around the poles is negligible due to the increasingly sharp peak around $\theta=\pi/2$ of the sine function power. Thus, the fraction of the surface area taken up by the black section will be very small.

To determine the fraction of the sphere taken up by the white section requires a bit more careful analysis. We will need to evaluate the expression

$$\lim_{N\to\infty} 2\frac{\mathrm{vol}(S^{N-2})}{\mathrm{vol}(S^{N-1})}\int_{\arcsin\sqrt{(N-1)/N}}^{\pi/2} \sin^{N-2}\theta \mathrm{d}\theta. \tag{8}$$

Using the known formula for $\mathrm{vol}(S^d)$ we find that

Downloaded 30 Jul 2009 to 130.237.165.22. Redistribution subject to AIP license or copyright; see http://jmp.aip.org/jmp/copyright.jsp

$$\frac{\mathrm{vol}(S^{N-2})}{\mathrm{vol}(S^{N-1})} = \frac{1}{\sqrt{\pi}}\frac{\Gamma(N/2)}{\Gamma((N-1)/2)}. \tag{9}$$

This tends to $\sqrt{N/2\pi}$ as $N\to\infty$.

Next, let us take a look at the behavior of the integral,

$$\int_{\arcsin\sqrt{(N-1)/N}}^{\pi/2} \sin^{N-2}\theta \mathrm{d}\theta = \int_0^{\arccos\sqrt{(N-1)/N}} \cos^{N-2}\theta \mathrm{d}\theta \tag{10}$$

when N grows large. The second form is convenient because all expansions can be done around zero.

In the limit of large N we can use

$$\arccos\sqrt{\frac{N-1}{N}} = \frac{1}{\sqrt{N}} + O\left(\frac{1}{N^{3/2}}\right). \tag{11}$$

Expanding $\cos t$ around $t=0$ and using the regular binomial expansion and the fact that when N is large $N-2$ can be approximated with N,

$$\lim_{N\to\infty}\cos^{N-2}\theta = \left(1-\frac{\theta^2}{2}\right)^N + h(\theta,N) = h(\theta,N) + 1 - N\frac{\theta^2}{2} + \frac{N^2}{2!}\frac{\theta^4}{4} - \frac{N^3}{3!}\frac{\theta^6}{8} + \cdots, \tag{12}$$

where $h(\theta,N)$ is a function such that

$$\lim_{N\to\infty}\sqrt{N}\int_0^{\arccos\sqrt{(N-1)/N}} h(\theta,N) = 0. \tag{13}$$

Integrating term by term and using the cosine expansion and Eq. (11) for the expansion of arccosine, we get

$$\lim_{N\to\infty}\int_0^{\arccos\sqrt{(N-1)/N}} \cos^{N-2}\theta \mathrm{d}\theta = \frac{1}{\sqrt{N}}\sum_{k=0}^{\infty}\frac{1}{2^k}\frac{1}{k!}\frac{(-1)^k}{(2k+1)} = \sqrt{\frac{\pi}{2N}}\,\mathrm{erf}\left(\frac{1}{\sqrt{2}}\right), \tag{14}$$

with erf the statistic-probabilistic error function,

$$\mathrm{erf}(z) \equiv \frac{2}{\sqrt{\pi}}\int_0^z e^{-t^2}\mathrm{d}t. \tag{15}$$

Putting all of this together, we have the result

$$\lim_{N\to\infty} 2\frac{\mathrm{vol}(S^{n-2})}{\mathrm{vol}(S^{n-1})}\int_{\arcsin\sqrt{(N-1)/N}}^{\pi/2} \sin^{N-2}\theta \mathrm{d}\theta = \mathrm{erf}\left(\frac{1}{\sqrt{2}}\right) \approx 0.68. \tag{16}$$

So, approaching the limit of an infinite number of dimensions of the Hilbert space $\mathcal{H}$ in which our projective measurements are conducted, binary probabilities (corresponding to well-defined, non-contextual properties of the system with available states in $\mathcal{H}$) can be assigned to approximately 68% of the vectors in $\mathcal{H}$.

The behavior of the percentage as a function of dimension is given in Fig. 2. The results are $1-1/\sqrt{2}+1/\sqrt{3}=87\%$ of all vectors for $N=3$, 79% for $N=4$, 74% for $N=5$, and 71% for $N=6$. The integer giving the least percentage is $N=12$, about 66.76%.

What has been derived above is a lower bound for the area of the sphere that is KS colorable in arbitrary dimension. The possibility remains, however, that a maximally effective coloring could cover a much larger area—possibly, in fact, as much as 99% of the sphere in $\mathbb{R}^3$, see Ref. 6.

Downloaded 30 Jul 2009 to 130.237.165.22. Redistribution subject to AIP license or copyright; see http://jmp.aip.org/jmp/copyright.jsp

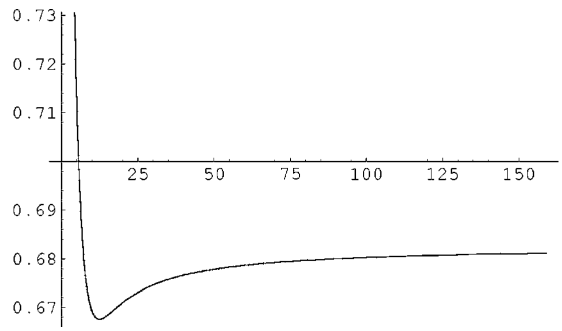

FIG. 2. Percentage of the sphere in N dimensions that is colorable using the above method, as a function of N.

III. A SECOND EFFECTIVITY MEASURE

The physically relevant question is, arguably, not how large a fraction of all states can be assigned probabilities 1 or 0, but rather what percentage of all complete orthogonal bases (measurements) can have all their basis vectors assigned binary probabilities in a consistent way. We will answer this question specifically for the Appleby coloring in three and four dimensions.

Let us first consider the coloring of the two-sphere proposed above—a black cap and a white equatorial belt covering in total 87% of the sphere—and make use of the regular measure on $\mathbb{R}^3$ to compare the number of properly colored bases consisting of vectors from these sections with the total number of ordered orthonormal triples in $\mathbb{R}^3$.

In a properly colored base exactly one vector is black, so one of the three vectors in an orthogonal triple has to be chosen to lie on one of the black caps. The remaining two orthogonal vectors can then be chosen from a great circle orthogonal to the first vector—the question is how large a fraction of this great circle will lie within the white section and also how the second vector (which determines the third basis vector up to a sign) can be chosen so that the third vector will also be contained within the white section.

Figure 3 depicts the plane of the great circle orthogonal to the first (black) vector on which the remaining two vectors in the orthogonal triple will have to lie. The circle segment bounding the shaded area is the cut between the white belt and the orthogonal great circle. For any choice of second vector from this section, the third vector will be fully determined (up to a sign). Hence, we cannot choose our second vector in a properly colored triple from any part of the circle-belt overlap in Fig. 3, but only from the sectors that will result in the third vector lying in the white belt as well. Given a second vector, the third is obtained by rotation in the great circle plane by an

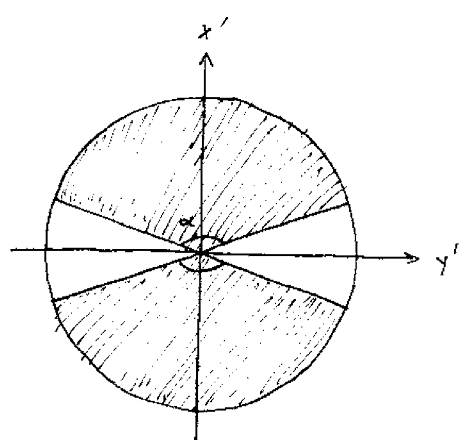

FIG. 3. A cut through the plane of the great circle orthogonal to the vector chosen to lie on the black cap. The intersection with the white area is shaded.

Downloaded 30 Jul 2009 to 130.237.165.22. Redistribution subject to AIP license or copyright; see http://jmp.aip.org/jmp/copyright.jsp

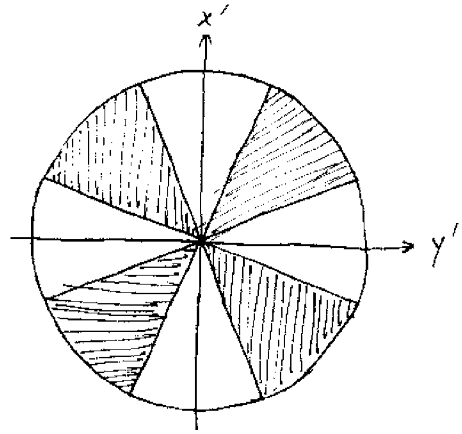

FIG. 4. The overlap between the white section of the great circle and its rotation by $\pi/2$ is the shaded section.

angle of $\pi/2$. The allowed choices for second vector are then the points such that the points corresponding to a $\pi/2$ rotation of these points are also white. This set of points is just the overlap between the white (shaded) sector in Fig. 3 and the same sector rotated by $\pi/2$, as illustrated in Fig. 4, an overlap that can be shown to always be nonempty. Hence, what we will need to find is the total angle taken up by the shaded section in Fig. 4—this will be denoted by β. It is clear that this β can be expressed in terms of the α of Fig. 3 as

$$\beta = 4\alpha - 2\pi. \tag{17}$$

The angle α, in turn, can be expressed in terms of the regular polar angle θ that specifies our choice of black vector using the following procedure.

First, consider the plane spanned by the vector chosen to lie in the black section, call it z', and a vector y' in the plane orthogonal to z'; $\{x,y,z\}$ is a reference coordinate system as shown. The vector x' orthogonal to y' and z' is chosen so that its z component equals zero. From Fig. 5 it is clear that

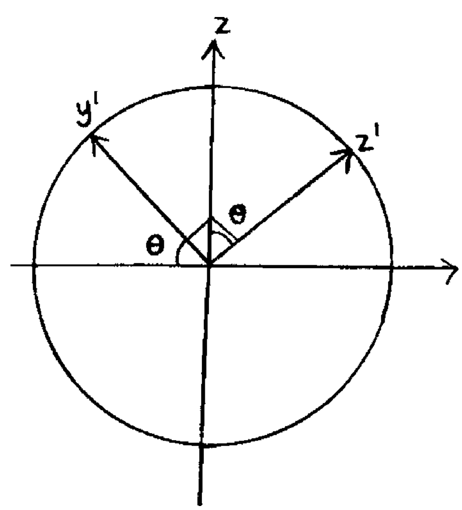

FIG. 5. The vector y' will make an angle π-θ with the z axis.

Downloaded 30 Jul 2009 to 130.237.165.22. Redistribution subject to AIP license or copyright; see http://jmp.aip.org/jmp/copyright.jsp

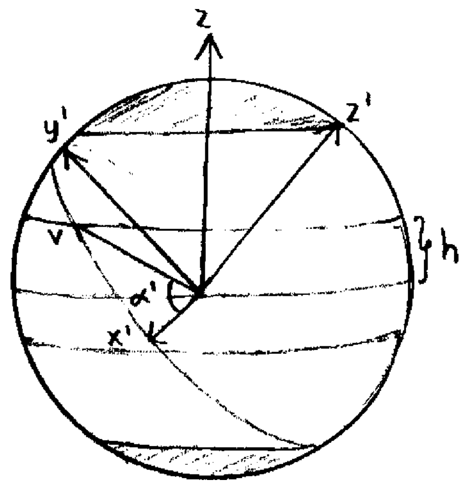

FIG. 6. Coordinates x' and y' are introduced in the plane of the great circle orthogonal to the vector z'.

$$z = 0x' + \sin\theta y' + \cos\theta z'. \tag{18}$$

Meanwhile, as can be seen from Fig. 6, a vector v lying just on the boundary of the white belt can be expressed in terms of y' and x' as

$$v = \cos\alpha' x' + \sin\alpha' y', \tag{19}$$

with $\alpha' = \alpha/2$, its z component being equal to zero. We also know that the z component of our vector v is just h, with $h = 1/\sqrt{3}$ according to our earlier deliberations. Taken together, this gives

$$v \cdot z = h = (\cos\alpha' x' + \sin\alpha' y') \cdot z = \sin\alpha' y' \cdot z = \sin\alpha' \sin\theta, \tag{20}$$

so that

$$\alpha = 2 \arcsin\frac{h}{\sin\theta} \tag{21}$$

and

$$\beta = 8 \arcsin\frac{h}{\sin\theta} - 2\pi. \tag{22}$$

When $\theta < \arcsin 1/\sqrt{3}$ expression [Eq. (21)] for α is not defined, for those angles all of the vectors orthogonal to the black section vector defined by the angle θ lie within the white section.

This enables us to express the fraction of the orthogonal great circle corresponding to every choice of vector z' in terms of the angle θ, making possible integration over all values of θ and thereby the comparison we have in mind.

So, the integrals we want to evaluate are

$$I = 2\pi \int_0^{\arcsin 1/\sqrt{3}} \sin\theta \mathrm{d}\theta + \int_{\arcsin 1/\sqrt{3}}^{\pi/4} \left(8 \arcsin\frac{h}{\sin\theta} - 2\pi\right) \sin\theta \mathrm{d}\theta. \tag{23}$$

This sum turns out to equal 1.4572.

This, multiplied by a combinatorial factor of 3 because what we considered the first vector could as well have been the second or third, should be compared to the value of the integral

Downloaded 30 Jul 2009 to 130.237.165.22. Redistribution subject to AIP license or copyright; see http://jmp.aip.org/jmp/copyright.jsp

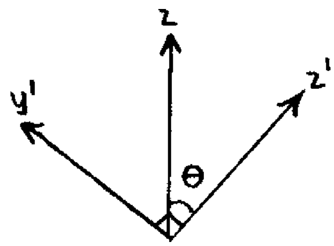

FIG. 7. y' lies on the two-sphere orthogonal to the vector z'.

$$2\pi\int_0^{\pi/2} \sin\,\theta \mathrm{d}\theta = 2\pi. \tag{24}$$

The result is that approximately 69% of all ordered bases in $\mathbb{R}^3$ can be KS colored using the given construction.

The above considerations for the three-dimensional case can, with some modification, be applied also in four dimensions. Introducing spherical coordinates $\{\phi,\theta_1,\theta_2\}$ on the three sphere, we will start out by finding the intersectional area of the orthgonal two-sphere and the white "belt." Let z' denote the black vector, let z be a reference coordinate, and let y' be a vector on the orthogonal two-sphere, as in Fig. 7.

The white section is the set of vectors,

$$\{u: |u\cdot z| \leq A\}, \quad A = \tfrac{1}{2}. \tag{25}$$

For any vector u in this set we have that

$$u\cdot z' = 0. \tag{26}$$

Now, let us make the ansatz,

$$y' = az + bz'. \tag{27}$$

Normalization together with condition (26) then gives

$$a = \frac{1}{\sin\,\theta_2}, \quad b = -\frac{\cos\,\theta_2}{\sin\,\theta_2}. \tag{28}$$

Also,

$$u\cdot z' = 0 \Rightarrow u\cdot y' = u\cdot(az+bz') = au\cdot z. \tag{29}$$

So, using Eq. (25), the belt on the orthogonal two-sphere will be the set of vectors,

$$\{v: |v| \leq B\}, \quad B = aA = \frac{1}{2\,\sin\,\theta_2}. \tag{30}$$

For $0 \leq \theta_2 \leq \arcsin 1/2$ the orthogonal two-sphere will lie entirely within the white section.

This intersection between the orthogonal two-sphere and the white section on the three sphere can now be treated in analogy with the previous case. Given a black first vector, when placing the second vector in the white section, the segment of the great circle orthogonal to this second vector on which we can choose the third in order for the fourth to lie in the white section is given by

Downloaded 30 Jul 2009 to 130.237.165.22. Redistribution subject to AIP license or copyright; see http://jmp.aip.org/jmp/copyright.jsp

$$\gamma = 8 \arcsin \frac{B}{\sin \theta_1} - 2\pi. \tag{31}$$

Also in analogy with the previous case, all of the orthogonal great circle will be white for $\arccos B \leqslant \theta_1 \leqslant \arcsin B$. To summarize, we have integration over the angle θ_2 which runs between 0 and $\pi/2$, covering the black cap; and the possibilities available for choosing the remaining three vectors are governed by a function of θ_2, obtained from an integration over the angle θ_1 between $\arccos B$ and $\pi/2$, that is, over the white section of the two-sphere orthogonal to the first vector specified by θ_2, B being a function of θ_2.

To make all of this explicit, we have the following integrals

$$I = 2\pi \int_{\arccos B}^{\arcsin B} \sin \theta_1 \mathrm{d}\theta_1 + \int_{\arcsin B}^{\pi/2} \left(8 \arcsin \frac{B}{\sin \theta_1} - 2\pi\right) \sin \theta_1 \mathrm{d}\theta_1 \tag{32}$$

and, finally,

$$4\pi \int_0^{\arcsin 1/2} \sin^2 \theta_2 \mathrm{d}\theta_2 + \int_{\arcsin 1/2}^{\pi/4} I \sin^2 \theta_2 \mathrm{d}\theta_2. \tag{33}$$

The result when comparing this, multiplied by an overall combinatorial factor of 4, to the value of the expression

$$4\pi \int_0^{\pi/2} \sin^2 \theta \mathrm{d}\theta \tag{34}$$

is that 34% of the ordered orthogonal triples in $\mathbb{R}^4$ are properly colored using the chosen method.

IV. CONCLUSIONS

Generalizing a method of coloring proposed by Appleby in three real dimensions, we have found a lower bound on the area of the n sphere that can be KS colored, but we are still ignorant as to a sharp upper bound. In three and four dimensions, we have calculated how large a fraction of all bases the colored area corresponds to, and the behavior of the percentage (69% in three dimensions and 34% in four dimensions) suggests that the asymptotic value for a large number of dimensions might well be zero. These results are restricted to families of pure states that span a real subspace of complex Hilbert space, and clearly it would be interesting to see this restriction lifted. It should also be noted that the main advantage of the Appleby coloring is that it is easily generalized to higher dimensions, but that there is no reason to believe that it is particularly effective. It is also not obvious that the same method of coloring would be maximal in different dimensions, and our lower bound for the upper bound might be considerably sharpened by experimenting with other constructions.

ACKNOWLEDGMENTS

Thanks are due to Hans Rullgård for support in numerical computations.

[1] S. Kochen and E. P. Specker, J. Math. Mech. **17**, 59 (1967).
[2] I. Pitowsky, Philos. Sci. **52**, 154 (1985).
[3] D. A. Meyer, Phys. Rev. Lett. **83**, 3751 (1999).
[4] A. Kent, Phys. Rev. Lett. **83**, 3755 (1999).
[5] R. Clifton and A. Kent, Proc. R. Soc. London, Ser. A **456**, 2101 (2000).
[6] D. M. Appleby, Stud. Hist. Philos. Mod. Phys. **36**, 1 (2005).

Downloaded 30 Jul 2009 to 130.237.165.22. Redistribution subject to AIP license or copyright; see http://jmp.aip.org/jmp/copyright.jsp

Article II

Accepted for publication in Open Systems and Information Dynamics

arXiv:0808.2947v2 [quant-ph] 24 Oct 2008

Stockholm
August 2008
Revised October 2008

THE FRAME POTENTIAL, ON AVERAGE

Ingemar Bengtsson[1]

Stockholm University, AlbaNova
Fysikum
S-106 91 Stockholm, Sweden

Helena Granström[2]

Stockholm University
Institutionen för matematik
S-106 91 Stockholm, Sweden

Abstract

A SIC consists of N^2 equiangular unit vectors in an N dimensional Hilbert space. The frame potential is a function of N^2 unit vectors. It has a unique global minimum if the vectors form a SIC, and this property has been made use of in numerical searches for SICs. When the vectors form an orbit of the Heisenberg group the frame potential becomes a function of a single fiducial vector. We analytically compute the average of this function over Hilbert space. We also compute averages when the fiducial vector is placed in certain special subspaces defined by the Clifford group.

[1]Email address: ingemar@physto.se. Supported by VR.
[2]Email address: helenag@math.su.se.

1. Introduction

Symmetric Informationally Complete Positive Operator Valued Measures, or SICs, is the unwieldy name for a simple idea [1, 2]: a set of N^2 unit vectors in an N dimensional Hilbert space, equiangular in the sense that

$$|\langle\psi_I|\psi_J\rangle|^2 = \frac{1}{N+1} \ , \qquad 1 \leq I, J \leq N \ , \quad I \neq J \ . \tag{1}$$

If the vectors are reinterpreted as projectors, that is as points in the set of Hermitian matrices of unit trace (the space where the density matrices live), they form a regular simplex in an $N^2 - 1$ dimensional Euclidean space. This also explains why we want their number to be N^2. The corners of such a simplex can be used to define barycentric coordinates for any density matrix, which is what "informationally complete" stands for. In quantum information theory SICs have attracted attention because they—if they exist—are useful for quantum state tomography [2, 3]. In quantum foundations they have attracted attention as a preferred kind of measurement [4]—and they have been studied in many other branches of science under names such as "equiangular lines" [5], "equiangular tight frames" [6], and "maximal quantum designs" [1]. Strohmer and Heath provide a mathematical survey [7].

The question whether SICs exist for all N has turned out to be extraordinarily difficult to answer. They have been constructed in most (but not all) dimensions $N \leq 19$ [1, 8, 9, 10, 11]. Numerical searches have been successful for all $N \leq 45$ [2], but no general formula has emerged. This is a bit surprising, given that we are really asking a very simple question about the shape of the convex body of density matrices: is it possible to inscribe a regular simplex in this body, with N^2 corners on its outsphere? The available evidence does however suggest that the answer is "yes" for all N, and moreover one can always find a SIC covariant under the Heisenberg-Weyl group, meaning that it can be constructed by first choosing a fiducial vector $|\psi_0\rangle$, and then acting on this vector with the N^2 elements of the (projective) Heisenberg-Weyl group.

A natural measure of how close a given set of N^2 unit vectors $|\psi_I\rangle$ is to forming a SIC is given by the function

$$f \equiv \frac{1}{2}\sum_{I\neq J}\left(|\langle\psi_I|\psi_J\rangle|^2 - \frac{1}{N+1}\right)^2 \ . \tag{2}$$

By construction $f = 0$ if and only if the vectors form a SIC. The function f is related to the frame potentials

$$F_t \equiv \sum_{I,J} |\langle \psi_I | \psi_J \rangle|^{2t} \ , \qquad t \in \{1, 2\} \tag{3}$$

by

$$f = \frac{1}{2} F_2 - \frac{1}{N+1} F_1 \ . \tag{4}$$

These frame potentials also assume their global minimum for a SIC, and in fact it is enough if F_2 assumes its minimum, since F_1 is known to follow suit. Therefore numerical searches for SICs have focused on minimizing F_2. Actually a frame potential is defined for any integer t [2, 6], but this does not concern us here.

We will have nothing to say about the existence problem here, rather we will compute averages of the function f, with and without the assumption of group covariance. We use the Fubini-Study measure on complex projective space to perform the averaging. We also compute averages when the fiducial vector is restricted to lie in certain subspaces defined by the Heisenberg group and its normalizer (the so-called Clifford group). These calculations were made for a reason: in the course of an investigation of certain configurations of N^2 vectors that occur in a related problem (to be precise but perhaps not informative, the torsion points of an elliptic curve defined by a complete set of mutually unbiased bases) we computed the values of f for these configurations. And the question then arose whether the values we obtained were high or low. To answer questions like this—and there are many such questions—one needs to know these averages.

Our final results have a certain elegance. Our paper is organized as follows: in section 2 we state some definitions, and in section 3 we describe the special subspaces we are interested in. In section 4 we give details concerning our calculations, which were carried out by brute force. Readers who are familiar with the SIC problem, and who do not want the details of an involved calculation, are advised to go directly to section 5, where we state our results and make some comments.[3]

[3]The first version of this paper contained a mistake, in eq. (34). A counterintuitive and exciting result ensued. The mistake was spotted by Christopher Fuchs and by an anonymous referee; it is better to be right than to be exciting, and we thank them for this.

2. Definitions

The Heisenberg-Weyl group [12] is the group generated by two elements τ and σ subject to the relations

$$\sigma\tau = q\tau\sigma \ , \qquad \tau^N = \sigma^N = 1 \ , \qquad q \equiv e^{2\pi i/N} \ . \tag{5}$$

Up to unitary equivalence there is a unique unitary representation of this group such that

$$\sigma|a\rangle = q^a|a\rangle \qquad \tau|a\rangle = |a+1\rangle \ , \qquad 0 \leq a \leq N-1 \ . \tag{6}$$

This is how we fix coordinates in Hilbert space; vectors can then be defined by their components

$$|\psi\rangle = \sum_{a=0}^{N-1} Z^a|a\rangle \ . \tag{7}$$

Up to phases, a general group element is

$$D_{ij} = \tau^i\sigma^j \ , \qquad 0 \leq i,j \leq N-1 \ . \tag{8}$$

The phases do not matter to us.

Now consider N^2 unit vectors forming an orbit under the Heisenberg group,

$$|\psi_{ij}\rangle = D_{ij}|\psi_0\rangle \ , \tag{9}$$

where $|\psi_0\rangle$ is some fiducial unit vector. The frame potential evaluated on such an orbit becomes a function on the projective Hilbert space $\mathbf{CP}^{N-1}$. This is the case we are most interested in, so we define

$$f_H = \frac{N^2}{2} \sum_{i,j \neq 0,0} \left(|\langle\psi_0|\psi_{ij}\rangle|^2 - \frac{1}{N+1} \right)^2 \ . \tag{10}$$

Because of group covariance there are only $N^2 - 1$ terms in the sum.

The definition of f_H can be manipulated further [4, 13]. Following Appleby, Dang and Fuchs we use an explicit matrix representation of D_{ij} to write

$$\langle\psi_0|D_{ij}|\psi_0\rangle = \bar{Z}_a q^{bj}\delta^a_{b+i}Z^b = q^{(a-b)j}\bar{Z}_a Z_{a-i} \ . \tag{11}$$

Then we take the Fourier transform

$$\frac{1}{N}\sum_j q^{kj}|\langle\psi_0|D_{ij}|\psi_0\rangle|^2 = \sum_a \bar{Z}_a\bar{Z}_{a+k-i}Z_{a+k}Z_{a-i} \ . \tag{12}$$

From this it is easy to show that the first frame potential $F_1 = N^3$ (this is true for all SIC-POVMs), and moreover that

$$f_H = \frac{N^3}{2}\left(\sum_{i=0}^{N-1}\sum_{k=0}^{N-1}\left|\sum_{a=0}^{N-1}\bar{Z}_a\bar{Z}_{a+k-i}Z_{a+k}Z_{a-i}\right|^2 - \frac{2}{N+1}\right) \ . \tag{13}$$

This is the expression we will work with in the sequel.

We will be interested in averages of f and f_H. To compute these averages we use the Fubini-Study measure $\mathrm{d}\mu_{\mathrm{FS}}$ on projective Hilbert space [14]; this is the natural definition of an average in the absence of any special information. What we wish to compute is

$$\langle f\rangle \equiv \frac{1}{\mathrm{vol}[\mathbf{CP}^{N-1}]}\int \mathrm{d}\mu_{\mathrm{FS}} \ f \ , \tag{14}$$

and similarly for f_H. Computing $\langle f\rangle$ is straightforward: using first the linearity of the expectation value and then the unitary invariance of the measure we obtain

$$\langle f\rangle = \frac{N^2(N^2-1)}{2}\left\langle\left(|\langle\psi_0|\psi\rangle|^2 - \frac{1}{N+1}\right)^2\right\rangle \ . \tag{15}$$

Here $|\psi_0\rangle$ is any fixed vector. To compute $\langle f_H\rangle$ requires more work—we will fall back on the explicit expression (13), and then collect terms.

We have now defined the functions we wish to average, and we have defined "average". It remains to define the special subspaces of Hilbert space that we are about to consider.

3. Special subspaces

We will compute averages of f_H also when the fiducial vector is confined to lie in certain interesting subspaces of the Hilbert space, picked out by the Clifford group. By definition the latter is the normalizer of the Heisenberg-Weyl group in the group of all unitaries. Thus the Clifford group is the group of all unitaries U such that

$$UD_{ij}U^{\dagger} = \omega D_{i'j'} \ , \tag{16}$$

where ω is a phase factor. We are interested in representations up to a phase, and it can be shown that the Clifford group with the phases ignored is isomorphic to a semi-direct product of a symplectic group with the Heisenberg group itself. The importance of this automorphism group was stressed by Zauner [1] and Grassl [8]; for a self-contained account see Appleby [9].

When the dimension is odd the Clifford group contains elements of order 2. They play a major role in the definition of discrete Wigner functions for the odd dimensional case [15, 16], and for the special case when the dimension is an odd prime number they are also known as Wootters' phase point operators [17]. They are symmetries of an elliptic curve associated to a complete set of mutually unbiased bases [18]. An elliptic curve can be defined as an embedding of a torus into complex projective space. The Heisenberg group acts on this torus, and gives rise to N^2 torsion points on the curve, roughly analogous to the Nth roots of unity on a circle. Hughston [19] has made the interesting comment that, in the special case $N = 3$, these torsion points define a SIC. In general it is known that the torsion points lie in the N^2 subspaces defined by elements of the Clifford group of order 2. In particular there is such an element A obeying

$$AD_{ij}A = D_{-i,-j} \ . \tag{17}$$

Because $A^2 = 1$, the operator A is both unitary and Hermitean. It splits Hilbert space into two subspaces $\mathcal{H}^{\pm}$ of dimensions n and $n-1$, respectively, where $N = 2n - 1$. Explicitly these subspaces are defined by

$$\mathcal{H}^+ : \quad \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2}x_0 \\ x_1 \\ \vdots \\ x_{n-1} \\ x_{n-1} \\ \vdots \\ x_1 \end{pmatrix} \qquad \mathcal{H}^- : \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ x_1 \\ \vdots \\ x_{n-1} \\ -x_{n-1} \\ \vdots \\ -x_1 \end{pmatrix} . \tag{18}$$

Unfortunately the fiducial vectors of the SICs do not lie in these subspaces when $N > 3$. However, we believe that f_H averaged using the Fubini-Study measure in such subspaces gives some feeling for the systematics of the SIC problem, and we will compute this average.

For any N the Clifford group contains elements of order 3. Zauner [1] conjectured that there always exists a SIC such that the fiducial vector is an eigenvector of a symplectic transformation of order 3, and his conjecture has been verified by Appleby [9] in all available cases [2]. We would therefore like to know the average of f_H over such subspaces. Unfortunately it is not so easy to describe these subspaces for arbitrary N, and we therefore confined ourselves to the special case $N = 7$. Then there exists an element of order 3 acting like a permutation matrix, and the subspaces are explicitly

$$\mathcal{H}_1 : \quad \frac{1}{\sqrt{3}} \begin{pmatrix} \sqrt{3}x_0 \\ x_1 \\ x_1 \\ x_2 \\ x_1 \\ x_2 \\ x_2 \end{pmatrix} \qquad \mathcal{H}_\alpha : \quad \frac{1}{\sqrt{3}} \begin{pmatrix} 0 \\ x_1 \\ \alpha^2 x_1 \\ x_2 \\ \alpha x_1 \\ \alpha x_2 \\ \alpha^2 x_2 \end{pmatrix} \tag{19}$$

where α, the eigenvalue, is a primitive third root of unity. The dimension of the subspace $\mathcal{H}_1$ is 3, and the dimensions of the two orthogonal subspaces are 2. There is a fiducial vector for a SIC in $\mathcal{H}_1$ [9]. It seemed reasonable to expect that the average f_H over this subspace would be quite low, but this expectation was not borne out.

4. Calculations

In order to average the frame potential (13) over the entire Hilbert space, we observe—see eq. (25) below—that the angular integrals will make all non-real terms of the sum disappear. We also note that a term of the form $|Z_1|^4|Z_2|^4$ gives the exact same contribution to the average as one of, say, the form $|Z_3|^4|Z_5|^4$, and all one needs to keep track of is the number of different $|Z_i|$ in a term, as well as the exponents present. Consequently, we look at the sum (13), and ask in how many ways we can get a term of the type $|Z_1|^8$, in how many ways one of the type $|Z_1|^6|Z_2|^2$, and so on. The problem has then been reduced to elementary equation solving.

Computing the average of f_H as given in (13), amounts to computing the average

$$\langle \Sigma \rangle = \left\langle \sum_{i=0}^{N-1} \sum_{k=0}^{N-1} \left| \sum_{a=0}^{N-1} \bar{Z}_a \bar{Z}_{a+k-i} Z_{a+k} Z_{a-i} \right|^2 \right\rangle . \tag{20}$$

For calculational convenience, the sum can be split into two parts: the $i = 0$ part where all terms are real and we have to keep track of cross terms, and the remaining $i \neq 0$ part, where cross terms contribute only in special cases:

$$\langle \Sigma \rangle = \sum_{k=0}^{N-1} \left(\sum_{a=0}^{N-1} |Z_a|^2 |Z_{a+k}|^2 \right)^2 + \sum_{i=1}^{N-1} \sum_{k=0}^{N-1} \left| \sum_{a=0}^{N-1} \bar{Z}_a \bar{Z}_{a+k-i} Z_{a+k} Z_{a-i} \right|^2 . \tag{21}$$

Let us first consider the $i = 0$ term, which can be rewritten as

$$\sum_{k=0}^{N-1} \sum_{a=0}^{N-1} \sum_{b=0}^{N-1} |Z_a|^2 |Z_{a+k}|^2 |Z_b|^2 |Z_{b+k}|^2 .$$

We will divide our analysis into two cases, the case $a = b$ and the case $a \neq b$. When $a = b$ the terms we get will be either of the type $|Z_1|^8$—this will occur for $k = 0$—or of the type $|Z_1|^4|Z_2|^4$, which will be the case for all remaining values of k, no matter what is the value of a and b. The total contribution, modulo integration, from the $i = 0$ term will for $a = b$ then be

$$N|Z_1|^8 + N(N-1)|Z_1|^4|Z_2|^4 , \tag{22}$$

where the factor N in front of the first term comes from the number of possible choices of $a = b$, and the second term is multiplied by the factor $N(N-1)$ for N different choices of $a = b$ and $N - 1$ choices of $k \neq 0$.

We now turn to the sum for different values of a and b. In this case, we will have four different types of $|Z_i|$, each to the power of two, in each term, except in the three special cases where the values of two or more of the indices coincide, namely when $a = b + k$, $b = a + k$ and $k = 0$. In the first two cases we get terms of the $|Z_1|^4|Z_2|^2|Z_3|^2$ type, in the last we get a $|Z_1|^4|Z_2|^4$ type term. The remaining choices of k, a and b—there are $N(N-1)(N-3)$ of them—give terms with all indices different, i.e. terms of the type $|Z_1|^2|Z_2|^2|Z_3|^2|Z_4|^2$. The total contribution from the $i = 0$ term is given in table 1.

Moving on to the $i \neq 0$ case, we can forget about cross terms except when $k = 0$. Consequently, when $k \neq 0$ we can consider the sum

$$\sum_{i=1}^{N-1} \sum_{k=1}^{N-1} \sum_{a=0}^{N-1} |Z_a|^2 |Z_{a+k-i}|^2 |Z_{a+k}|^2 |Z_{a-i}|^2,$$

while when $k = 0$ we still have to work with the expression from equation (21). As in the previous case, we ask what special cases occur, i.e. when two or more indices take on equal values. These cases turn out to be $k = i$, $k = -i$ and $k = 0$. The respective contributions to the average are given in the table, as is the contribution for all other choices of indices.

	Z_1^8	$Z_1^6 Z_2^2$	$Z_1^4 Z_2^4$	$Z_1^4 Z_2^2 Z_3^2$	$Z_1^2 Z_2^2 Z_3^2 Z_4^2$
$i = 0, a = b$	N	—	$N(N-1)$	—	—
$i = 0, a \neq b, k = 0$	—	—	$N(N-1)$	—	—
$i = 0, a \neq b, k = a - b$	—	—	—	$N(N-1)$	—
$i = 0, a \neq b, k = b - a$	—	—	—	$N(N-1)$	—
$i = 0$, others	—	—	—	—	$N(N-1)(N-3)$
$i \neq 0, k = 0$	—	—	$N(N-1)$	$2N(N-1)$	$N(N-1)(N-3)$
$i \neq 0, k = i$	—	—	—	$N(N-1)$	—
$i \neq 0, k = -i$	—	—	—	$N(N-1)$	—
$i \neq 0$, others	—	—	—	—	$N(N-1)(N-3)$
total	N	—	$3N(N-1)$	$6N(N-1)$	$3N(N-1)(N-3)$

Table 1: Number of different type terms in the average for odd N.

Subtracting the constant term and multiplying by the initial factor of (13) yields an expression which can be integrated over all of Hilbert space in order to obtain the SIC-function average. To perform the integrals we parametrize the unit vectors as

$$Z^a = (\sqrt{p_0}, \sqrt{p_k}e^{i\nu_k}) \ , \tag{23}$$

where the ranges of the parameters are

$$p_0 + p_1 + \ldots + p_{N-1} = 1 \ , \quad p_0 \geq 0 \ , \quad p_k \geq 0 \ , \qquad 0 \leq \nu_k < 2\pi \ . \tag{24}$$

We solve for p_0, and obtain the explicit expression [14]

$$\langle f \rangle = \frac{(N-1)!}{(2\pi)^{N-1}} \int_0^1 \mathrm{d}p_1 \ldots \int_0^{1-p_1-\ldots-p_{N-2}} \mathrm{dp}_{N-1} \int_0^{2\pi} \mathrm{d}\nu_1 \ldots \int_0^{2\pi} \mathrm{d}\nu_{N-1} \ f \ . \tag{25}$$

In calculating the averages a number of standard integrals will be used, namely

$$\left\langle |Z_1 Z_2 Z_3 Z_4|^2 \right\rangle = \frac{(N-1)!}{(N+3)!} \tag{26}$$

$$\left\langle |Z_1|^4 |Z_2 Z_3|^2 \right\rangle = 2\frac{(N-1)!}{(N+3)!} \tag{27}$$

$$\left\langle |Z_1 Z_2|^4 \right\rangle = 2^2 \frac{(N-1)!}{(N+3)!} \tag{28}$$

$$\left\langle |Z_1|^6 |Z_2|^2 \right\rangle = 3! \frac{(N-1)!}{(N+3)!} \tag{29}$$

$$\left\langle |Z_1|^8 \right\rangle = 4! \frac{(N-1)!}{(N+3)!} \ . \tag{30}$$

The computations for odd values of N are straightforward, with few complications. Even N are, however, a somewhat different story. To begin with, cross terms play in also for non-zero values of i and k, and in a somewhat different manner than in the odd N case. Whereas we get cross term contributions for odd N only when all terms are real in a sum—as for $k = 0$, for instance—we here find pairwise equal terms inside the modulus sign of the $i \neq 0$ term of equation (21), so that care has to be exercised when squaring. Using the same strategy as for odd N—dividing the sum into $i = 0$ and $i \neq 0$ parts and asking when two or more indices are equal—we find a number of index choices for which terms of order higher than two occur, some of which coincide with the ones for odd N. As opposed to in the odd N case, though, the number of possible choices for the summation indices depend on the parity of i, as well as on the modulo four value of N, so that the calculational details differ beteween, for instance, $N = 6$ and $N = 8$. This is because the restrictions one gets when solving the equal-indices-equations, are sometimes equivalent for, say, $i = 3$ and $N = 0$ mod 4 and independent for $N = 2$ mod 4 for the same i, giving a different number of combinatorial possibilities. The final results for the frame potential average taken over Hilbert space, on the other hand, turns out to be identical for the two cases; this average is given in section 5.

Also when considering the sum average over $\mathcal{H}^+$ and $\mathcal{H}^-$, the calculations get more involved than in the non-restricted odd N case. As for even N, we get cross term contributions to the integral, and further technical complications are due to the fact that the respective subspace conditions,

$$Z_i = Z_{-i} \tag{31}$$

and

$$Z_i = -Z_{-i} \ , \tag{32}$$

make the number of equations to solve when asking what possibilities there are for the power of any Z_i to be higher than two in a term larger. In other words, the calculations have to be divided into a greater number of different cases, but the logic is much the same as in the calculations for all of Hilbert space sketched above. In using equations (26 - 30), one should keep in mind that the dimension of the space over which the average is taken is no longer equal to N.

5. Results

Our results are easy to state. The function f attains its global minimum at a SIC, and its global maximum if all the N^2 unit vectors coincide. Thus

$$0 \leq f \leq \frac{N^4}{2}\frac{N-1}{N+1} \ . \tag{33}$$

Its Fubini-Study average value is

$$\langle f \rangle_{\rm FS} = \frac{N^2}{2}\frac{N-1}{N+1} \ . \tag{34}$$

When the dimension is large, the scalar product between randomly choosen vectors is close to zero, and this is reflected by the average.

If we specialize to N^2 unit vectors forming an orbit under the Weyl-Heisenberg group we believe that the global maximum occurs if the fiducial vector is an eigenvector of some element in the group, in which case the orbit collapses to an eigenbasis. Thus

$$0 \leq f_H \leq \frac{N^3}{2}\frac{N-1}{N+1} \ .$$

(Unfortunately we were unable to prove that the eigenbasis represents the global maximum. It seems obvious that this is so, and we did check that it is a local extremum. For safety, we do not number this equation.) The average value depends on whether the Hilbert space dimension is odd or even:

$$N = 2n-1 \ : \qquad \langle f_H \rangle_{\rm FS} = \frac{N^2}{2}\frac{N(N-1)}{(N+2)(N+1)} \tag{35}$$

$$N = 2n \ : \qquad \langle f_H \rangle_{\rm FS} = \frac{N^2}{2}\frac{N^2}{(N+3)(N+1)} \ . \tag{36}$$

Asymptotically there is no difference. It is perhaps somewhat unexpected that the average of f_H has the same asymptotic behaviour as the average of f.

We also computed the average when the fiducial vector is restricted to lie in certain interesting subspaces defined by elements of the Clifford group (the normalizer of the Weyl-Heisenberg group). Elements of order 2 occur in odd dimensions $N = 2n-1$. Their eigenspaces have dimension $\dim[\mathcal{H}^-] = n-1$ and $\dim[\mathcal{H}^+] = n$. As observed by Hughston [19], when $N = 3$ $\mathcal{H}^-$ contains only one vector, and it is a fiducial vector for a SIC. However, 3 is a very special dimension. The complementary subspace $\mathcal{H}^+$ contains a SIC fiducial vector too, as well as four vectors from a complete set of four mutually unbiased bases, for which f_H attains its (conjectured) maximum. The average over $\mathcal{H}^+$ is $\langle f_H \rangle = 81/40$. For $N > 3$ the situation is quite different. We find

$$N = 2n - 1 > 3 \ : \qquad \langle f_H \rangle_{\mathcal{H}^-} = \langle f_H \rangle_{\mathcal{H}^+} = N^2 \frac{N(N-1)}{(N+3)(N+1)} \ . \tag{37}$$

Asymptotically this is twice the average over the full Hilbert space. It is a bit striking that the averages are equal.

It is harder to deal with the subspaces defined by elements of order 3. At the same time they are more interesting, because Zauner's conjecture [1, 9, 20] says that the fiducial vector can always be choosen to lie in the subspace with eigenvalue 1. We did compute averages for $N = 7$. There are three subspaces $\mathcal{H}_1$, $\mathcal{H}_\alpha$, $\mathcal{H}_{\alpha^2}$, labelled by the eigenvalues of the element that cubes to one ($\alpha = e^{2\pi i/3}$). Their dimensions are respectively 3, 2, and 2. The average values of f_H in the three subspaces are

$$\langle f_H \rangle_{\mathcal{H}_1} = \frac{151 \cdot 7^3}{5 \cdot 3^4 \cdot 2^3} \approx 15.985 \tag{38}$$

$$\langle f_H \rangle_{\mathcal{H}_\alpha} = \langle f_H \rangle_{\mathcal{H}_{\alpha^2}} = \frac{37 \cdot 7^3}{5 \cdot 3^3 \cdot 2^3} \approx 11.751 \ . \tag{39}$$

The average over the subspace that contains the SIC fiducial vector is above the average $\langle f_H \rangle$ over the full Hilbert space. This surprised us.

The values of f_H vary widely, also within the special subspaces (except that f_H is actually constant on $\mathcal{H}^-$ when $N = 5$). We describe the situation for $N = 7$ in the following table:

	f	f_H	$f_H(\mathcal{H}^+)$	$f_H(\mathcal{H}^-)$	$f_H(\mathcal{H}_1)$	$f_H(\mathcal{H}_\alpha)$
Minimum	0	0	12.2 (?)	4.764 (?)	0	?
Average	18.375	14.29	25.72	25.72	15.98	11.75
Maximum	900.4	128.6 (?)	128.6 (?)	42.88 (?)	?	?

Some entries were left uncomputed, and some without proofs—we marked the latter with a question mark within bracket, even though we are sure they are correct.

Unfortunately we are unable to see how to compute the asymptotic behaviour of $\langle f_H \rangle$ for a fiducial vector in subspaces of the kind considered by Zauner. We expect them to depend on number theoretical details of the dimension. It would be interesting to see numerical studies of such averages however.

References

[1] G. Zauner: *Quantendesigns. Grundzüge einer nichtkommutativen Designtheorie*, PhD thesis, Univ. Wien 1999.

[2] J. M. Renes, R. Blume-Kohout, A. J. Scott, and C. M. Caves, *Symmetric informationally complete quantum measurements*, J. Math. Phys. **45** (2004) 2171.

[3] A. J. Scott, *Tight informationally complete quantum measurements*, J. Phys. **A39** (2006) 13507.

[4] D. M. Appleby, H. B. Dang, and C. A. Fuchs, *Physical significance of symmetric informationally-complete sets of quantum states*, arXiv:0806.1339.

[5] P. W. H. Lemmens and J. J. Seidel, *Equiangular lines*, J. Algebra **24** (1973) 494.

[6] J. J. Benedetto and M. Fickus, *Finite normalized tight frames*, Adv. Comp. Math. **18** (2003) 357.

[7] T. Strohmer and R. W. Heath Jr., *Grassmannian frames with applications to coding and communication*, Appl. Comput. Harmon. Anal. **14** (2003) 257.

[8] M. Grassl, *On SIC-POVMs and MUBs in dimension 6*, in Proc. of ERATO conference on Quantum Information Science (2004), Tokyo 2004.

[9] D. M. Appleby, *SIC-POVMs and the extended Clifford group*, J. Math. Phys. **46**, 052107 (2005).

[10] M. Grassl, *Tomography of quantum states in small dimensions*, Electronic Notes in Discrete Math. **20** (2005) 151.

[11] M. Grassl, *Finding equiangular lines in complex space*, talk at the Magma workshop, 2006.

[12] H. Weyl: *Theory of Groups and Quantum Mechanics*, Dutton, New York 1932.

[13] M. Khatirinejad, *On Weyl-Heisenberg orbits of equiangular lines*, J. Algebr. Comb., published online 6 November 2007.

[14] I. Bengtsson and K. Życzkowski: *Geometry of Quantum States*, Cambridge UP 2006.

[15] S. Chaturvedi, E. Ercolessi, G. Marmo, G. Morandi, N. Mukunda and R. Simon, *Wigner distributions for finite dimensional quantum systems: An algebraic approach*, Pramana J. Phys. **65** (2005) 981.

[16] D. Gross, *Hudson's theorem for finite-dimensional quantum systems*, J. Math. Phys. **47** (2006) 122107.

[17] W. K. Wootters, *A Wigner-function formulation of finite-state quantum mechanics*, Ann. Phys. **176** (1987) 1.

[18] K. Hulek, *Projective geometry of elliptic curves*, Asterisque **137** (1986) 1.

[19] L. P. Hughston, unpublished.

[20] S. T. Flammia, *On SIC-POVMs in prime dimensions*, J. Phys. **A39** (2006) 13483.