Symmetric Informationally-Complete Quantum States as Analogues to Orthonormal Bases and Minimum-Uncertainty States

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Since Renes et al. [J. Math. Phys. \textbf{45}, 2171 (2004)], there has been much effort in the quantum information community to prove (or disprove) the existence of symmetric informationally complete (SIC) sets of quantum states in arbitrary finite dimension. This paper strengthens the urgency of this question by showing that if SIC-sets exist: 1) by a natural measure of orthonormality, they are as close to being an orthonormal basis for the space of density operators as possible, and 2) in prime dimensions, the standard construction for complete sets of mutually unbiased bases and Weyl-Heisenberg covariant SIC-sets are intimately related: The latter represent minimum uncertainty states for the former in the sense of Wootters and Sussman. Finally, we contribute to the question of existence by conjecturing a quadratic redundancy in the equations for Weyl-Heisenberg SIC-sets.

INTRODUCTION

Recently there has been significant interest in the quantum-information community to prove or disprove the general existence of so-called symmetric informationally complete (SIC) quantum measurements [1-7]. The question is simple enough: For a Hilbert space $\mathcal{H}_d$ of arbitrary dimension $d$, is there always a set of $d^2$ quantum states $|\psi_i\rangle$ such that $|\langle \psi_i | \psi_j \rangle|^2 = \text{constant}$ for all $i \neq j$? If so, then the operators $E_i = \frac{1}{d} |\psi_i\rangle \langle \psi_i|$ can be shown to form the elements of a tomographically complete positive operator-valued measure, often dubbed a SIC-POVM. Interestingly, despite the elementary feel to this question—i.e., it seems the sort of thing one might find as an exercise in a linear-algebra textbook—and the considerable efforts to solve it, the answer remains elusive. One should ask: why is there such interest in the question in the first place? Unfortunately it is hard to deny the impact that much of the motivation stems from little more than the mathematical challenge—not really a good physical reason for months of effort. In this paper, we address the issue of whether there are other, more physical motivations for seeking an answer to the existence of such states.

Indeed, there are already notable motivations from applied physics—e.g., uses of these states in quantum cryptography [8]. Here, however, we go further by deriving a few previously unobserved properties that single out SIC-sets as particularly relevant to the elementary structure of Hilbert space. These properties make no direct use of the original defining symmetry for SICs, and instead imply them. It is our hope that a better understanding of SIC-sets will lead to new and powerful tool for studying the structure of quantum mechanics [9].

Specifically, the paper is as follows. We first demonstrate a geometric sense in which SIC-sets of projectors $\Pi_i = |\psi_i\rangle \langle \psi_i|$, if they exist, are as close as possible to being an orthonormal basis on the cone of nonnegative operators. This complements the frame theoretic version of the same question proved by Scott [10]. The two results together clinch the idea that SIC-sets are uniquely singled out as a stand-in for orthonormal bases on the space of density operators, and we take the opportunity to express the structure of pure states with respect to these preferred bases. Thereafter we focus on the case of Weyl-Heisenberg (WH) covariant SIC-sets in prime dimensions. In prime dimensions, complete sets of mutually unbiased bases always exist [11] and here we demonstrate a simple expression for them in terms of the WH unitary operators. We then define a notion of minimum uncertainty state with respect to the measurement of these bases [12] and find that the Weyl-Heisenberg SIC-sets, whenever they exist, consist solely of minimum uncertainty states. This provides a strong motivation for considering WH SIC-sets as a special finite-dimensional analogue of coherent states and stresses the further interest of writing the quantum mechanical state space in terms of such operator bases. Finally, we conclude with some general remarks and conjecture a significant reduction in the defining equations for WH SIC-sets.

QUASI-ORTHONORMAL BASES AND THE SPACE OF DENSITY OPERATORS

When equipped with the usual Hilbert-Schmidt inner product $\langle A, B \rangle = \text{tr}(A^\dagger B)$, the set of operators acting on a $d$-dimensional complex vector space becomes a $d^2$-dimensional Hilbert space. Suppose we are given $d^2$ operators $A_i$ normalized so that $\text{tr}(A_i^2) = 1$. Under what conditions can the $A_i$ be orthogonal to each other? For instance, it is known that one can require the $A_i$ to be Hermitian or unitary and it is not too restrictive for orthogonality to obtain [13]. However, requiring the operators to be positive semi-definite is another matter.

We would like to measure “how orthonormal” a set of positive semi-definite $A_i$ can be. A natural class of
measures for this is
\[ K_t = \sum_{i \neq j} |\langle A_i, B \rangle|^t = \sum_{i \neq j} (\text{tr}(A_i A_j))^{\frac{t}{2}}, \tag{1} \]
for any real number \( t \geq 1 \). Clearly, one will have an orthonormal basis if and only if \( K_t = 0 \) for this sum of \( N = d^2 - d^2 \) terms. But for positive semi-definite \( A_i \), as we will prove, it turns out that
\[ K_t \geq \frac{d^2(d-1)}{(d+1)^{t-1}}. \tag{2} \]
In other words, it is impossible to choose an orthonormal basis all of whose elements lie in the positive cone of operators. The natural question to ask is, is there a set of \( d^2 \) \( A_i \) for which \( K_t \) achieves the lower bound for \( t > 1 \) (for \( t = 1 \), any set of \( A_i/d \) that forms a POVM would saturate the bound for \( K_1 \))? If so, we will refer to such a set as a quasi-orthonormal basis.

Note that the linear independence of the \( A_i \) does not have to be imposed as a separate requirement. An orthonormal set of vectors is automatically linearly independent. Similarly with quasi-orthonormal sets: requiring \( K_t \) to achieve its lower bound forces linear independence. This will follow from one condition for achieving equality—that \( \{A_i, A_j\} = \text{constant} \) when \( i \neq j \) [2].

We will first prove (2) for the case \( t = 1 \), using a special instance of the Cauchy-Schwarz inequality: namely, if \( \lambda_1 \) is any set of \( n \) real numbers, \( \sum_i \lambda_i^2 \geq \frac{1}{n} (\sum_i \lambda_i)^2 \), with equality if and only if \( \lambda_1 = \cdots = \lambda_n \). Let \( G \) be a positive semi-definite operator defined by \( G = \sum_i A_i \), and note that tr\( A_i \geq 1 \) because tr\( A_i^2 = 1 \). Applying the Schwarz inequality to the eigenvalues of \( G \), we find tr\( G^2 \geq \frac{1}{n} (\text{tr} G)^2 \geq \text{tr} A_i^2 \), or equivalently, \( K_1 \geq \text{tr} A_i^2 - \text{tr} A_i \). Equality obtains if and only if \( G = d I \) and tr\( A_i = 1 \) for all \( i \), i.e., \( A_i \) are all rank-1 projectors.

Next, let \( f(x) = x^t \), then \( f(x) \) is a strictly convex function for \( t > 1 \). By writing \( K_t = \sum_{i \neq j} f(\text{tr}(A_i A_j)) \), and applying Jensen inequality, we complete the proof for (2). In Jensen inequality, the equality holds if and only if \( \text{tr}(A_i A_j) \) is a constant for all \( i \neq j \).

Putting all this together, we conclude that the necessary and sufficient conditions for the \( A_i \) to constitute a quasi-orthonormal basis are:

1. Each \( A_i \) is a rank-1 projector.
2. \( \text{tr}(A_i A_j) = \frac{1}{d^2} \) for all \( i \neq j \).

These are the same as the conditions for the operators \( A_i \) to constitute a SIC-set. In particular they imply \( \sum_i A_i = d I \) and, via [2], that the \( A_i \) must be linearly independent.

As an aside, let us point out that this derivation sheds light on the meaning of the “second frame potential” \( \Phi = \sum_{i,j} |\langle \psi_i | \psi_j \rangle|^4 \) introduced by Renes et al. [3] to aid in finding SIC-POVMs numerically. Beforehand its motivation seemed to be only the heuristic of constrained particles distancing themselves from each other because of an interaction potential—an idea that has its roots in Ref. [14]. Now, one sees that whenever \( A_i = |\psi_i \rangle \langle \psi_i | \), \( \Phi = K_2 + d^2 \)—i.e., \( \Phi \) is essentially our own orthonormality measure in this case. (2) implies that \( \Phi \geq 2d^3/(d+1) \), which was proved by different means in Ref. [3].

Returning to the general development, what we have shown is that SIC-sets \( \Pi_i = |\psi_i \rangle \langle \psi_i |, i = 1, \ldots, d^2 \), play a special role in the geometry of the cone of positive operators, and by implication, the convex set of quantum states in general—i.e., the density operators. For the purpose of foundational studies—particularly ones of the quantum Bayesian variety [9, 15]—it is worthwhile recording what this convex set looks like from this perspective.

Imagine introducing \( E_i = \frac{1}{d} \Pi_i \) as a canonically given quantum measurement. For a quantum state \( \rho \), the outcomes will occur with probabilities \( p(i) = \text{tr} \rho E_i \). Using the fact that \( \rho \) has a unique expansion in terms of the \( \Pi_i \), one can work out that
\[ \rho = \sum_i \left( (d+1)p(i) - \frac{1}{d} \right) \Pi_i. \tag{3} \]
On the other hand, one might imagine taking the vector of probabilities \( p(i) \) as the more basic specification, and the density operator \( \rho \) as a convenient, but derivative, specification of the quantum state. Requisite to doing this, one must have an understanding of the allowed probabilities \( p(i) \)—not every choice of probabilities in Eq. (3) will give rise to positive semi-definite \( \rho \). This can be done conveniently by taking note of the characterization of pure quantum states demonstrated in Ref. [16]. Remarkably, it is enough to specify that any Hermitian operator \( M \) satisfy only two trace conditions, tr\( M^2 = 1 \) and tr\( M^3 = 1 \), to insure that it be a rank-1 projection operator—i.e., a pure state. In terms of the \( p(i) \) these two conditions become:
\[ \sum_i p(i)^2 = \frac{2}{d(d+1)} \tag{4} \]
\[ \sum_{i,j,k} c_{ijk} p(i)p(j)p(k) = \frac{d+7}{(d+1)^3}, \tag{5} \]
where \( c_{ijk} = \text{Re} \left( \text{tr}(\Pi_i \Pi_j \Pi_k) \right) \). The full set of quantum states is thus the convex hull of the solutions to Eqs. (4) and (5). One nice thing about Eq. (5) is that it makes transparent the algebraic structure lying behind these special probability vectors: For, one can use the coefficients \( c_{ijk} \) as structure coefficients in defining the anticommutator on the space of operators.

**WEYL-HEISENBERG SIC-SETS AND MINIMUM UNCERTAINTY STATES**

A particularly important class of SIC-sets are those covariant under the action of the Weyl-Heisenberg (WH)
Finally, let us note the important case of Eqs. (8) where

\[ \sum_{r} \beta^{-1}(\alpha^2 - 2j_k^2 + \delta^2) |j_k\rangle \langle k| \quad \beta \neq 0 \]

Then it can be shown [4] that

\[ UDrU^\dagger = DF_r \]

for all \( r \). Moreover, if \( U' \) is any other unitary with this property, then \( U' = e^{i\phi}U \) for some phase \( e^{i\phi} \). In these expressions all arithmetical operations on the indices are mod \( d \). In particular \( \beta^{-1} \) is the unique positive integer less than \( d \) such that \( \beta^{-1}\beta = 1 \) mod \( d \).

If \( \beta \neq 0 \), it can be seen that \(|\langle j|U|k\rangle| = d^{-1/2} \) for all \( j, k \). So we can use symplectic transformations to generate MUBs. For definiteness take \( V, W \) to be the unitaries corresponding to \((1, 1)\) and \((0, 1)\) and define

\[ |m, j\rangle = \begin{cases} V^m|j\rangle & m = 0, 1, \ldots, d - 1 \\ W^j|j\rangle & m = \infty \end{cases} \]

This gives us a full set of \( d + 1 \) MUBs labeled by \( m \).

These bases are essentially the only ones obtainable from the standard basis by symplectic transformations. To see this let \( F \) be an arbitrary symplectic matrix with \( \beta \neq 0 \), and let \( U \) be the corresponding unitary. We have

\[ F = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \]

But, unitaries corresponding to matrices with a 0 in the top right-hand position merely permute and rephase the elements of the standard basis. So the basis \( U|0\rangle, \ldots, U|d - 1\rangle \) coincides with one of the bases \( |m, 0\rangle, \ldots, |m, (d - 1)\rangle \) up to permutation and re-phasing. We have \(|j\rangle\langle j| = (1/d) \sum_r \omega^{-jr} D_{(0,r)} \). In view of Eqs. (12) and (13) this means

\[ |m, j\rangle\langle m, j| = \begin{cases} \frac{1}{d} \sum_r \omega^{-jr} D_{(mr, r)} & m \neq \infty \\ \frac{1}{d} \sum_r \omega^{kr} |\langle j|U|k\rangle|^2 & m = \infty \end{cases} \]

Now consider an arbitrary \(|\psi\rangle\), and let \( p_{m,j} = |\langle m, j|\psi\rangle|^2 \). It follows from the above that

\[ \sum_j p_{m,j} p_{m,j+k} = \begin{cases} \frac{1}{d} \sum_r \omega^{kr} |\langle j|D_{(mr, r)}|\psi\rangle|^2 & m \neq \infty \\ \frac{1}{d} \sum_r \omega^{kr} |\langle j|D_{(r, 0)}|\psi\rangle|^2 & m = \infty \end{cases} \]

from which one sees that \(|\psi\rangle\) is fiducial if and only if

\[ \sum_j p_{m,j} p_{m,j+k} = \frac{1}{d+1}(1 + \delta_{k0}) \]
Thus, instead of imposing all of the Eqs. (8) on the components in the standard basis, we can impose just the special case Eqs. (10) for each MUB separately.

We are now ready to derive the minimum uncertainty property. Consider an arbitrary state $|\psi\rangle$ and a measurement of one of the bases $m$ in a complete set of MUBs. This will give rise to outcomes with a probability distribution $p_{m,j}$. We will quantify the uncertainty in the outcomes by the quadratic Rényi entropy [12, 19]

$$H_m = -\log_2 \left( \sum_j p_{m,j}^2 \right). \quad (18)$$

This measure and the measure related to it by deleting the logarithm seem to be playing a widening role in quantum information studies [17]. In particular, it is one of the most important measures for quantifying an eavesdropper’s information in quantum cryptography [20].

A minimum uncertainty state is one that minimizes the total uncertainty, $T = \sum_m H_m$. To see the conditions for this, we first appeal to the fact that $[17, 18]$

$$\sum_{m,j} p_{m,j}^2 = 2 \quad (19)$$

for any $|\psi\rangle$. From the convexity of the logarithm, it follows that for any sequence of positive numbers $\lambda_1, \ldots, \lambda_n$, $(1/n) \sum_j \log_2 \lambda_j \leq \log_2 \left( \sum_j \lambda_j \right)$ with equality if and only if $\lambda_1 = \cdots = \lambda_n$. Thus, in view of Eq. (19)

$$T \geq (d + 1) \log_2 \left( \frac{d + 1}{2} \right), \quad (20)$$

with equality if and only if $\sum_j p_{m,j}^2 = 2/(d + 1)$ for all $m$. Comparing this with Eq. (17), one sees that every WH fiducial vector achieves the lower bound and is therefore a minimum uncertainty state. Unfortunately, the theorem does not go the other way: it is not always the case that every minimum uncertainty state is a fiducial state.

**DISCUSSION**

We have argued that the SIC-sets in general dimensions, and more specifically the Weyl-Heisenberg covariant ones (at least in prime dimensions), are particularly interesting structures in Hilbert space geometry. Thus they call out for a better understanding, and we hope this paper is an advertisement for that cause.

There are clearly many more things that can be asked. For instance, are SIC fiducial states also minimum uncertainty states in prime-power dimensions? In non-prime-power dimensions, we face the problem that complete sets of MUBs may not even exist. In that case, can one generalize the definition of a MUB in such a way that SIC fiducial states continue to be minimum uncertainty states?

With regard to the property of quasi-orthonormality, is it possible to find non-Weyl-Heisenberg SIC-sets for which Eq. (5) takes a nicer form? Further, with regard to the property of quasi-orthonormality, is it possible to find non-Weyl-Heisenberg SIC-sets for which Eq. (5) takes a nicer form? For instance, if the $\Pi_i$ were actually orthogonal, then one would have $\text{tr} (\Pi_i \Pi_j \Pi_k) = \delta_{ij} \delta_{jk} \delta_{ki}$. How close can one come to a form like this with a SIC-set? Many questions like this loom.

But most looming is the question of whether SIC-sets exist in arbitrary dimension. In this regard, let us close with a conjecture. The necessary and sufficient conditions for $|\psi\rangle$ to be a Weyl-Heisenberg fiducial vector are captured in Eq. (8), which represents $d^2$ simultaneous equations. However, we have noted numerically (up to $d = 28$) that satisfying roughly $\frac{1}{2}d$ of these equations is enough to imply the rest. For instance, it appears to be necessary to satisfy Eq. (8) only for the cases $k = 0, 1, 2$ with $l = 0, \ldots, d/2 - 1$. Perhaps this always holds true.

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