Trace optimality of SIC POVMs

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Abstract

Symmetric Informationally Complete Positive Operator Valued Measures (SIC POVM) are families of $\mathtt{d}^2$ unit vectors in the complex Cartesian space $\mathbb{C}^{\mathtt{d}}$ such that the complex lines associated to them are equiangular and maximally angularly separated. We characterize SIC POVMs as minimizers for the trace of any strictly convex function of the Gram matrix associated to their orthogonal projectors. This result extends several known extremal properties of SIC POVMs and is motivated by an application in fiber optics.

1 Results

Our primary interest lies in *SIC POVMs*, which are defined as families of $\mathtt{d}^2$ unit vectors $|s_1\rangle, \ldots, |s_{\mathtt{d}^2}\rangle$ in $\mathbb{C}^{\mathtt{d}}$ satisfying

$$|\langle s_j|s_k\rangle|^2 = \frac{1}{\mathtt{d}+1} \qquad (\text{for } j \neq k). \tag{1}$$

(We assume $\mathtt{d} \geq 2$ and $\mathbb{C}^{\mathtt{d}}$ is the complex linear space of $\mathtt{d}$-tuples of complex numbers $(z_j)_{j=1}^{\mathtt{d}}$ with the standard Hermitian inner product $\langle z|z'\rangle := \sum_{j=1}^{\mathtt{d}} \overline{z}_j z'_j$.)

The acronym SIC POVMs stands for *symmetric informationally complete positive operator valued measures*, as employed in the theory of quantum measurement; see [24, 15, 3, 18] for the background and a discussion of their relevance. Existence of SIC POVMs in every dimension $\mathtt{d} \geq 2$ is a conjecture first stated in the 1999 PhD thesis of Zauner [30], corroborated by a number of exact constructions for specific $\mathtt{d}$ and extensive numerical exploration [15, 22]. From a geometrical perspective, see e.g. [14], condition (1) is asking that the vectors are equiangular with the common angle $\arccos\sqrt{1/(\mathtt{d}+1)}$, which is as close to 90° as theoretically possible.[1] In the complex projective space $\mathbb{CP}^{\mathtt{d}-1}$ — made of all unit vectors in $\mathbb{C}^{\mathtt{d}}$ up to phase — a SIC POVM corresponds to a regular $\mathtt{d}^2$-simplex of maximal size, a so called *tight simplex*. As one would expect, such highly symmetrical objects are distinguished by various *optimality properties* [21, 27, 14, 4, 10]. Our goal is to put on record the following general characterization.

Theorem 1. *Let $f : [0,\infty) \to \mathbb{R} \cup \{+\infty\}$ be any strictly convex[2] function. For any unit vectors $|s_1\rangle, \ldots, |s_{\mathtt{d}^2}\rangle$ in $\mathbb{C}^{\mathtt{d}}$, the $\mathtt{d}^2 \times \mathtt{d}^2$-matrix $\mathbf{G} = (|\langle s_j|s_k\rangle|^2)_{j,k=1}^{\mathtt{d}^2}$ satisfies*

$$\operatorname{Tr}(f(\mathbf{G})) \geq f(\mathtt{d}) + (\mathtt{d}^2-1) f\left(\frac{\mathtt{d}}{\mathtt{d}+1}\right) \tag{2}$$

and the equality holds if and only if $|s_1\rangle, \ldots, |s_{\mathtt{d}^2}\rangle$ is a SIC POVM.

The prime examples of f are the power functions $f(t) := t^p$ for $p \in (-\infty, 0) \cup (1, \infty)$ (with the proviso that $0^p = +\infty$ for $p < 0$). For $p = 2$, inequality (2) is a variant of the *frame potential bound* that is a special case of Theorem 6 in Scott's [27] — re-derived in the survey [10] — and originates from the work of Benedetto and Fickus [6] where the frame potential was first introduced. This note was spurred by the case $p = -1$ because minimization of $\operatorname{Tr}(\mathbf{G}^{-1})$ mitigates the impact of the receiver noise in a method of measurement of the mode dispersion operator for a multimode optical fiber (as explained at the end of this note). Here again [27]

[1] For the equiangular lines in $\mathbb{R}^{\mathtt{d}}$ see, e.g., [5] and [13].

[2] Mere convexity suffices for (2), and strict convexity is only needed for the SIC POVM conclusion from equality in (2).

already contains an analogous inequality but places an additional a priori constraint that the projectors associated to $|s_j\rangle$ (taken perhaps with some weights) give rise to an *operator valued measure*, which has no physical justification in the fiber optics application. Our essential contribution is then in removing this constraint, which is done by injecting an extra argument (a simple operator norm bound) and suitably adapting Scott's framework — itself grown from elements of theory of complex designs, frames, and quantum measurement. With no further claim of originality and to help the reader, we also assembled a self-contained proof that isolates the key mechanisms at play with a minimum of specialized jargon. Ultimately, the result hinges on basic Pythagorean geometry and elementary multivariable minimization. (As we proceed, we attempt to attribute the ideas. We apologize if we have missed some instances of their use.)

For a clearer perspective it is beneficial to broaden the context and recognize Theorem 1 as a specialization of the following result about families in the real linear space $\mathcal{H}$ of all $\mathtt{d} \times \mathtt{d}$ Hermitian matrices, considered as operators acting on column vectors in $\mathbb{C}^{\mathtt{d}}$ by multiplication and taken with the inner product given by the trace, $(A|A') := \operatorname{tr}(AA')$. Keep in mind that any unit $|s\rangle \in \mathbb{C}^{\mathtt{d}}$ has its associated orthogonal projector $P_s := |s\rangle\langle s| \in \mathcal{H}$ (sending $|z\rangle$ to $\langle z|s\rangle\, |s\rangle$). Such projectors are the extreme points of the convex body collecting all the non-negative trace normalized operators in $\mathcal{H}$, which play a fundamental role in quantum mechanics (see, e.g., [17, 7, 16]). The following statement is then of independent interest.

Theorem 2. *Let $f : [0, \infty) \to \mathbb{R} \cup \{+\infty\}$ be any strictly convex function. For any non-zero operators $A_1, \ldots, A_m \in \mathcal{H}$ for which*

$$\sum_{j=1}^{m} \operatorname{tr}(A_j)^2 \geq m \quad \text{and} \quad \sum_{j=1}^{m} \operatorname{tr}(A_j^2) = m \tag{3}$$

the Gram matrix $\mathbf{G} = (\operatorname{tr}(A_j A_k))_{j,k=1}^{m}$ satisfies

$$\operatorname{Tr}\left(f(\mathbf{G})\right) \geq f\left(\frac{m}{\mathtt{d}}\right) + (\mathtt{d}^2 - 1) f\left(\frac{m}{\mathtt{d}(\mathtt{d}+1)}\right). \tag{4}$$

The equality in (4) is only possible when $m \geq \mathtt{d}^2$ and $A_1, \ldots, A_m$ span $\mathcal{H}$. When $m = \mathtt{d}^2$ and $A_1, \ldots, A_m \geq 0$, the equality in (4) takes place if and only if $A_j = |s_j\rangle\langle s_j|$ for some SIC POVM $(|s_j\rangle)_{j=1}^{\mathtt{d}^2}$ in $\mathbb{C}^{\mathtt{d}}$.

Theorem 1 follows readily by applying Theorem 2 to $A_j := P_{s_j}$ (since $\operatorname{tr}(A_j A_k) = |\langle s_j|s_k\rangle|^2$). A similar looking result can be found in [4] but the functional minimized is different: it is obtained by adding the p^{th} powers of the entries of the Gram matrix $\mathbf{G}$ (for $p \geq 1$), and stronger hypotheses are imposed: $A_j \geq 0$ and $\operatorname{tr}(A_j^2) = 1$. (Theorem 6 in [27] is a further specialization to $A_j = P_{s_j}$.)

As will be clear from the proof, when restricted to the $\mathtt{d}^2 - 2$ dimensional sphere formed in $\mathcal{H}$ by the operators with unit norm and unit trace, Theorem 2 amounts to an *optimality* property of the regular $\mathtt{d}^2$-simplex among all $\mathtt{d}^2$-simplices inscribed in the sphere. For instance, taking $f(t) := -\ln t$, gives an upper bound on the volume V of the simplex spanned by the A_j in $\mathcal{H}$. (Indeed, $\mathrm{Tr}(-\ln \mathbf{G}) = -\ln\det(\mathbf{G}) = -2\ln((\mathtt{d}^2)!V)$.) The maximal volume is, predictably, that of the regular $\mathtt{d}^2$-simplex.

One can hope that the flexibility of choosing different f (as afforded by the theorem) helps in numerical searches for SIC POVMs.

2 Preliminaries

A modicum of terminology and context is needed to make the subsequent proof palatable. First, $\mathcal{H}$ has dimension $\dim_{\mathbb{R}}(\mathcal{H}) = \mathtt{d}^2$ and is often explicitly identified with the Euclidean space $\mathbb{R}^{\mathtt{d}^2}$ by associating to an operator A the real (column) vector $\vec{A} = \left(\vec{A}_0, \vec{A}_1, \ldots, \vec{A}_{\mathtt{d}^2-1}\right)$ of its coordinates with respect to some fixed orthonormal basis $\Lambda_0, \Lambda_1, \ldots, \Lambda_{\mathtt{d}^2-1}$ in $\mathcal{H}$, i.e., we have

$$A = \vec{A}_0\Lambda_0 + \vec{A}_1\Lambda_1 + \ldots + \vec{A}_{\mathtt{d}^1-1}\Lambda_{\mathtt{d}^2-1}. \tag{5}$$

One can insist that $\Lambda_1, \ldots, \Lambda_{\mathtt{d}^2-1}$ have zero trace and $\Lambda_0 := \frac{1}{\sqrt{\mathtt{d}}}I$ (where I is the identity matrix). We refer to $\mathbb{C}^{\mathtt{d}}$ as the ***Jones space***, to $\mathcal{H}$ as the ***operator space***, and to $\mathbb{R}^{\mathtt{d}^2}$ as the ***Stokes space***. The last two will be mostly treated as interchangeable because the bijection $A \leftrightarrow \vec{A}$ is an isomorphism of inner product spaces; in particular, $\mathrm{tr}(AA') = \vec{A}^{\mathtt{T}}\vec{A}'$, where the superscript $\mathtt{T}$ indicates transposition. (There are of course properties of operators $A \in \mathcal{H}$ that are not easily reflected in their Stokes vectors $\vec{A}$, most notably non-negativity $A \geq 0$.) We note that, in quantum mechanics, Stokes vectors are called *Bloch vectors* — see [17, 20, 8] and the recent discussion in [11]. The *Jones/Stokes* nomenclature originates from the theory of polarized light and is used in the context of multi-mode optical fiber [2, 19, 28, 25]. Note that we do not restrict to traceless or trace normalized operators and thus include in our Stokes vectors the 0^{th} coordinate in the direction of $\Lambda_0 = \frac{1}{\sqrt{\mathtt{d}}}I$.

In a finite dimensional linear space, a ***frame*** is a short way to call a finite sequence of vectors spanning the space [6, 12], and the ***frame operator*** is the sum of the rank one operators (scaled orthogonal projectors) associated to the vectors. We adopt this terminology even when the spanning condition is not satisfied. Thus, for any finite sequence of operators $(A)_{j=1}^m = (A_1, \ldots, A_m)$, where $A_j \in \mathcal{H}$, we consider $\mathcal{F} : \mathcal{H} \to \mathcal{H}$ given by

$$\mathcal{F}:\ H \mapsto \sum_{j=1}^m (A_j|H)A_j = \sum_{j=1}^m \mathrm{tr}(HA_j)A_j \qquad (H \in \mathcal{H}). \tag{6}$$

Because $\mathcal{F}$ is an operator that acts on a space of operators, it could be referred to as a *frame superoperator*. It is also conveniently conflated (via the isomorphism $A \leftrightarrow \vec{A}$) with the corresponding *Stokes frame operator* — for which we use the same letter $\mathcal{F}$ — acting on $\mathbb{R}^{\mathtt{d}^2}$ as follows

$$\mathcal{F}: \ \vec{H} \mapsto \sum_{j=1}^{m} \vec{A}_j^{\mathtt{T}} \vec{H} \vec{A}_j = \left(\sum_{j=1}^{m} \vec{A}_j \vec{A}_j^{\mathtt{T}} \right) \vec{H} = \mathbf{A}^{\mathtt{T}} \mathbf{A} \vec{H}, \tag{7}$$

where the matrix $\mathbf{A} = \left(\vec{A}_1, \ldots, \vec{A}_m \right)^{\mathtt{T}}$ collects the Stokes vectors in its rows. Of course, $\mathcal{F}$ is symmetric and non-negative, if only because the same attributes apply to $\mathbf{A}^{\mathtt{T}}\mathbf{A}$, which is the matrix of $\mathcal{F}$ (in the basis $\Lambda_0, \ldots, \Lambda_{\mathtt{d}^2-1}$).

Finally, to reveal the reason for introducing $\mathcal{F}$, note how $\mathbf{G}$ — the Gram matrix of the A_j in $\mathcal{H}$ (or of the $\vec{A}_j$ in $\mathbb{R}^{\mathtt{d}^2}$) — is expressed in terms of $\mathbf{A}$:

$$\mathbf{G} = (\mathrm{tr}(A_j A_k))_{j,k=1}^m = ((A_j | A_k))_{j,k=1}^m = (\vec{A}_j^{\mathtt{T}} \vec{A}_k)_{j,k=1}^m = \mathbf{A}\mathbf{A}^{\mathtt{T}}. \tag{8}$$

One of the main ideas[3] in the proof is to get at $\mathbf{G}$ by studying $\mathcal{F}$.

Using capitalized notation "Tr" for tracing superoperators, (8) identifies the objective of our minimization as

$$\mathrm{Tr}\left(f(\mathbf{G})\right) = \sum_{i=1}^{\mathtt{d}^2} f\left(\alpha_i^2\right) \tag{9}$$

where $\alpha_1 \geq \alpha_2 \geq \ldots \geq \alpha_{\mathtt{d}^2}$ are the singular values of $\mathbf{A}$. (To be precise, $\alpha_1^2 \geq \alpha_2^2 \geq \ldots \geq \alpha_{\mathtt{d}^2}^2$ denote the eigenvalues of $\mathbf{A}^{\mathtt{T}}\mathbf{A}$ taken with multiplicity; some can be 0.)

For $f(t) = t^2$, (9) gives the *operator/Stokes frame potential*:

$$\mathrm{Tr}(\mathbf{G}^2) = \mathrm{Tr}(\mathbf{A}\mathbf{A}^{\mathtt{T}}\mathbf{A}\mathbf{A}^{\mathtt{T}}) = \mathrm{Tr}(\mathbf{A}^{\mathtt{T}}\mathbf{A}\mathbf{A}^{\mathtt{T}}\mathbf{A}) = \mathrm{Tr}(\mathcal{F}^2) = \sum_{j,k=1}^{m} \mathrm{tr}(A_j A_k)^2 = \sum_{i=1}^{\mathtt{d}^2} \alpha_i^4. \tag{10}$$

Its minimization (in conjunction with some postulated symmetries) is used in numerical searches for SIC POVMs.

3 Proof of Theorem 2

As already indicated, most of the proof combines preexisting elements found in one form or another in [27, 10, 14], about which we comment further as we proceed. One significant addition, designed to skirt the assumption that the A_j a priori

[3] an elaboration on the basic implication $\mathbf{A}\mathbf{A}^{\mathtt{T}} = I \implies \mathbf{A}^{\mathtt{T}}\mathbf{A} = I$, valid for any square $\mathbf{A}$

form an operator valued measure, comes in the form of the initial argument below, showing inequality (14) by bounding the operator norm $\|\mathcal{F}\|_{\mathrm{op}}$ of the frame superoperator. This turns out to be the right ingredient for the subsequent constrained minimization.

Unless stated otherwise, throughout this section, we assume the hypotheses of Theorem 2, i.e., $A_1, \ldots, A_m$ are non-zero operators in $\mathcal{H}$ such that

$$\sum_{j=1}^{m} \mathrm{tr}(A_j)^2 \geq m \quad \text{and} \quad \sum_{j=1}^{m} \mathrm{tr}(A_j^2) = m. \tag{11}$$

Proof of inequality (4) in Theorem 2: To avoid mathematical technicalities, let us assume that f is also differentiable. Thus we take for granted that $f'(t)$ exists and is strictly increasing in t. (It is routine to extend the argument to general convex f. In such case, $f'(t)$ may fail to exist at countably many t but one can argue by using the one-sided derivatives $f'_-(t) \leq f'_+(t)$, which exist for all t.)

Our first step is to estimate α_1^2 from below by considering how $\mathcal{F}$ acts on the identity $I \in \mathcal{H}$. We have the following standard relationships between the operator norms:

$$\alpha_1^2 = \|\mathbf{A}\|_{\mathrm{op}}^2 = \|\mathbf{A}^{\mathtt{T}}\mathbf{A}\|_{\mathrm{op}} = \|\mathcal{F}\|_{\mathrm{op}}.$$

(Recall $\|\mathcal{F}\|_{\mathrm{op}} := \sup\{\|\mathcal{F}(H)\|/\|H\| : H \in \mathcal{H} \setminus \{0\}\}$.) Keeping in mind that $\|I\| = \sqrt{\mathrm{tr}(I^2)} = \sqrt{\mathtt{d}}$, we invoke Cauchy-Schwarz inequality (and the first part of hypothesis (11)) to write

$$\|\mathcal{F}(I)\| \geq \frac{(\mathcal{F}(I)|I)}{\|I\|} = \frac{\mathrm{tr}\left(\sum_j \mathrm{tr}(A_j)A_j\right)}{\sqrt{\mathtt{d}}} = \frac{\sum_j \mathrm{tr}(A_j)^2}{\sqrt{\mathtt{d}}} \geq \frac{m}{\sqrt{\mathtt{d}}}. \tag{12}$$

Thus

$$\|\mathcal{F}\|_{\mathrm{op}} \geq \frac{\|\mathcal{F}(I)\|}{\|I\|} \geq \frac{m/\sqrt{\mathtt{d}}}{\sqrt{\mathtt{d}}} = \frac{m}{\mathtt{d}}. \tag{13}$$

Therefore, we obtained a ***spectral radius constraint***[4]

$$\alpha_1^2 \geq \frac{m}{\mathtt{d}}. \tag{14}$$

This is accompanied by the ***trace constraint*** (from the second part of hypothesis (11) and the definition of $\mathcal{F}$):

$$\sum_{i=1}^{\mathtt{d}^2} \alpha_i^2 = \mathrm{Tr}(\mathcal{F}) = \mathrm{Tr}(\mathbf{A}^{\mathtt{T}}\mathbf{A}) = \mathrm{Tr}(\mathbf{A}\mathbf{A}^{\mathtt{T}}) = \sum_{j=1}^{m} \vec{A}_j^{\mathtt{T}}\vec{A}_j = \sum_{j=1}^{m} \mathrm{tr}(A_j^2) = m. \tag{15}$$

[4] Lemma 17 in [27] or Theorem 2.5 in [10] utilize an analogue of the equality $\alpha_1^2 = \frac{m}{\mathtt{d}}$.

We see that $\mathrm{Tr}(f(\mathbf{G}))$ is bounded below by the solution to the following minimization in a constrained variable $\vec{x} := (x_1, \ldots, x_{\mathtt{d}^2}) \in \mathbb{R}^{\mathtt{d}^2}$:

$$\mathrm{Tr}(f(\mathbf{G})) = \sum_{i=1}^{\mathtt{d}^2} f\left(\alpha_i^2\right) \geq \min\left\{\sum_{i=1}^{\mathtt{d}^2} f(x_i) :\ x_1 \geq m/\mathtt{d},\ \sum_{i=1}^{\mathtt{d}^2} x_i = m,\ x_i \geq 0\right\}. \tag{16}$$

The set Ω described by the above constraints is a convex subset — actually, a $(\mathtt{d}^2-1)$-simplex — sitting in the hyper-plane $\sum_{i=1}^{\mathtt{d}^2} x_i = m$. Note that the function $F(\vec{x}) := \sum_{i=1}^{\mathtt{d}^2} f(x_i)$ has no relative critical points in the (relative) interior of Ω. Indeed, for the gradient $\nabla F(\vec{x}) = (f'(x_i))_{i=1}^{\mathtt{d}^2}$ to be parallel to the domain's normal vector $(1,\ldots,1)$ we would have to have all $f'(x_i)$ equal, and thus $x_1 = \ldots = x_{\mathtt{d}^2}$ because f' is strictly increasing. This would give $x_1 = m/\mathtt{d}^2 < m/\mathtt{d}$, violating the first constraint. We further claim that the minimum cannot occur at a point $\vec{x}$ where $x_i = 0$ for some i but $x_1 > m/\mathtt{d}$. To fix attention, suppose $x_2 = 0$. Of course, the case when $f(0) = +\infty$ is trivially excluded (because the minimum is finite), so assume that $f(0)$ is finite. If the one sided derivative $f'(0^+)$ is also finite, then $\nabla F(\vec{x}) \cdot (-1, 1, 0, \ldots, 0) = -f'(x_1) + f'(0^+) < 0$ since $x_1 > \mathtt{d}/m > 0$ and f' is increasing. This means that $F(x_1 - \tau, \tau, x_3, \ldots, x_{\mathtt{d}^2})$ would diminish for small $\tau > 0$, a contradiction. The argument is the same when $f'(0^+) = -\infty$.

We have shown that the minimum can only occur when $x_1 = m/\mathtt{d}$. Then, however, the convexity of f, yields

$$\frac{1}{\mathtt{d}^2-1}\sum_{i=2}^{\mathtt{d}^2} f(x_i) \geq f\left(\frac{1}{\mathtt{d}^2-1}\sum_{i=2}^{\mathtt{d}^2} x_i\right) = f\left(\frac{m - m/\mathtt{d}}{\mathtt{d}^2-1}\right). \tag{17}$$

Thus

$$\sum_{i=1}^{\mathtt{d}^2} f(x_i) = f(x_1) + \sum_{i=2}^{\mathtt{d}^2} f(x_i) \geq f\left(\frac{m}{\mathtt{d}}\right) + (\mathtt{d}^2-1) f\left(\frac{m}{\mathtt{d}(\mathtt{d}+1)}\right), \tag{18}$$

which is the desired inequality (4). □

The rest of this section is devoted to elucidating what it takes for equality to hold in (4). The assertions in the second part of Theorem 2 are established via a sequence of propositions. We start with a characterization in terms of the spectrum of $\mathcal{F}$.

Proposition 1 (spectral characterization)**.** *Equality holds in (4) if and only if the eigenvalues of the frame superoperator $\mathcal{F}$ are as follows:*

$$\alpha_1^2 = \frac{m}{\mathtt{d}} \quad \textit{and} \quad \alpha_2^2 = \ldots = \alpha_{\mathtt{d}^2}^2 = \frac{m}{\mathtt{d}(\mathtt{d}+1)}. \tag{19}$$

Moreover, if equality holds in (4), then the identity operator is a (dominant) eigenvector of $\mathcal{F}$:

$$\mathcal{F}(I) = \sum_{j=1}^{m} \operatorname{tr}(A_j)A_j = \frac{m}{\mathtt{d}} I, \tag{20}$$

and we have equality in hypothesis (11):

$$\sum_{j=1}^{m} \operatorname{tr}(A_j)^2 = m. \tag{21}$$

Proof of Proposition 1: When (19) holds, equality in (4) is clear from (9). Assume now that equality holds in (4). We already know that $\alpha_1^2 = x_1 = m/\mathtt{d}$ from the previous argument. Because equality must also holds in (17), strictly convexity of f forces $x_2 = \ldots = x_{\mathtt{d}^2}$. This immediately gives (19) (via the trace constraint (15)). From $\|\mathcal{F}\|_{\mathrm{op}} = \alpha_1^2 = \frac{m}{\mathtt{d}}$, we also have all equalities in (13) and (12). In particular, we have *tightness* in the Cauchy-Schwartz inequality, forcing $\mathcal{F}(I)$ to be a multiple of I and yielding (20). Finally, (21) follows by by taking traces in (20). □

Proposition 2 (rank strain addendum)**.** *If (21) holds (alongside (11)) and $A_1, \ldots, A_m \geq 0$ then the A_j are all of rank one.*

Proof: This is a simple general observation valid for any $A_j \geq 0$. Indeed, stated in terms of the eigenvalues $\lambda_{j1}, \ldots, \lambda_{j\mathtt{d}} \geq 0$ of A_j, the conjunction of (21) and (11) reads

$$\sum_{j=1}^{m} \left(\sum_{l=1}^{\mathtt{d}} \lambda_{jl} \right)^2 = m = \sum_{j=1}^{m} \left(\sum_{l=1}^{\mathtt{d}} \lambda_{jl}^2 \right). \tag{22}$$

All terms being non-negative, each inner sum on the left has to contain only one non-zero term (or else = would become >). Thus each A_j is of rank one. □

Further characterization of the A_j at equality will use the *tightness* in the following variant of the frame bound (see e.g. Theorem 8 in [27]), which is proven by invoking Pythagorean theorem in the space of superoperators (cf. the proof of Proposition 2.4 in [14]). Note that the lemma does not require that $A_j \geq 0$. Also, inequality (24) is an instance of (4) for $f(t) = t^2$.

Lemma 1 (frame potential bound)**.** *If $A_1, \ldots, A_m \in \mathcal{H}$ are such that*

$$\frac{1}{m} \sum_{j=1}^{m} \operatorname{tr}(A_j)A_j = \frac{1}{\mathtt{d}} I \qquad \textit{and} \qquad \sum_{j=1}^{m} \operatorname{tr}(A_j^2) = m \tag{23}$$

then

$$\operatorname{Tr}(\mathcal{F}^2) \geq \frac{m^2}{\mathtt{d}^2} + \frac{m^2}{\mathtt{d}^2} \frac{(\mathtt{d}-1)}{(\mathtt{d}+1)}. \tag{24}$$

Proof of Lemma 1: The first hypothesis amounts to $\mathcal{F}(I) = \frac{m}{\mathtt{d}} I$ (as in (20)), so span(I), the linear span of I in $\mathcal{H}$, is an eigenspace of $\mathcal{F}$. We therefore focus attention on the restriction $\mathcal{F}_0 := \mathcal{F}|_{\mathcal{H}_0}$ to the $\mathtt{d}^2 - 1$-dimensional subspace $\mathcal{H}_0 := \{H \in \mathcal{H} : \mathrm{tr}(H) = 0\}$, the orthogonal complement of span(I) in $\mathcal{H}$. We consider the real linear space $\mathbb{H}_0$ of all symmetric superoperators on $\mathcal{H}_0$ with the inner product $(\mathcal{B}|\mathcal{C}) := \mathrm{Tr}(\mathcal{B}\mathcal{C})$. By the second equation in (23) (cf. (15)), we have $\mathrm{Tr}(\mathcal{F}) = m$, and so

$$\mathrm{Tr}(\mathcal{F}_0) = \mathrm{Tr}(\mathcal{F}) - \frac{m}{\mathtt{d}} = m - \frac{m}{\mathtt{d}} = m\left(1 - \frac{1}{\mathtt{d}}\right). \tag{25}$$

This is to say that, in $\mathbb{H}_0$, $\mathcal{F}_0$ sits in the affine hyper-subspace $\mathbb{X} := \{\mathcal{X} : \ \mathrm{Tr}(\mathcal{X}) = m\left(1 - \frac{1}{\mathtt{d}}\right)\}$, which is clearly a translate of the null space $\mathbb{X}_0 := \{\mathcal{X} : \ \mathrm{Tr}(\mathcal{X}) = 0\}$. The identity superoperator $\mathcal{I}_0 : \mathcal{H}_0 \to \mathcal{H}_0$ is orthogonal (as an element of $\mathbb{H}_0$) to $\mathbb{X}_0$ (because $(\mathcal{X}|\mathcal{I}_0) = \mathrm{Tr}(\mathcal{X}\mathcal{I}_0) = \mathrm{Tr}(\mathcal{X}) = 0$ for $\mathcal{X} \in \mathbb{X}_0$). Therefore, $\frac{m}{\mathtt{d}(\mathtt{d}+1)}\mathcal{I}_0$ is the closest point of $\mathbb{X}$ to the origin. (It belongs to $\mathbb{X}$ because $\mathrm{Tr}(\mathcal{I}_0) = \mathtt{d}^2 - 1$.) The respective squared distances satisfy then[5]

$$\mathrm{Tr}(\mathcal{F}_0^2) \geq \mathrm{Tr}\left(\left(\frac{m}{\mathtt{d}(\mathtt{d}+1)}\mathcal{I}_0\right)^2\right) = \frac{m^2}{\mathtt{d}^2(\mathtt{d}+1)^2}(\mathtt{d}^2 - 1) = \frac{m^2}{\mathtt{d}^2}\frac{(\mathtt{d}-1)}{(\mathtt{d}+1)}. \tag{26}$$

Inequality (24) follows because $\mathrm{Tr}(\mathcal{F}^2) = \frac{m^2}{\mathtt{d}^2} + \mathrm{Tr}(\mathcal{F}_0^2)$ (with the first term contributed by the restriction $\mathcal{F}|_{\mathrm{span}(I)}$). $\square$

The rest of the argument uses ideas from theory of 2-designs [21, 30]. Specifically, it mimics the proof of Theorem 4 in [27]. In fact, had we restricted attention to A_j that are a priori non-negative and of rank one, we could have shortened the argument by invoking this theorem after first observing that equality (29) below implies that $\pi_j := \frac{1}{\mathrm{tr}(A_j)}A_j$ and $w_j := \frac{1}{\mathtt{d}^2}\mathrm{tr}(A_j)$ define a *weighted complex projective 2-design.* However, our setting is more general, so we borrow the ideas and proceed directly without the burden of additional definitions.

Proposition 3 (frame operator characterization)**.** *Equality holds in (4) if and only if the frame operator has the following form*

$$\mathcal{F}(H) = \frac{m}{\mathtt{d}(\mathtt{d}+1)}\left(\mathrm{tr}(H)I + H\right) \qquad (H \in \mathcal{H}), \tag{27}$$

which is equivalent to the matrix $\mathbf{A}^{\mathsf{T}}\mathbf{A}$ *of* $\mathcal{F}$ *being diagonal and of the form*

$$\mathbf{A}^{\mathsf{T}}\mathbf{A} = \mathrm{diag}\left(\frac{m}{\mathtt{d}}, \frac{m}{\mathtt{d}(\mathtt{d}+1)}, \ldots, \frac{m}{\mathtt{d}(\mathtt{d}+1)}\right). \tag{28}$$

[5] Those desiring algebraic verification can set $c = \frac{m}{\mathtt{d}(\mathtt{d}+1)}$ and write $0 \leq \mathrm{Tr}\left(\mathcal{F}_0 - c\mathcal{I}_0\right)^2 = \mathrm{Tr}\left(\mathcal{F}_0^2\right) - 2c\mathrm{Tr}\left(\mathcal{F}_0\right) + c^2\mathrm{Tr}\left(\mathcal{I}_0\right) = \mathrm{Tr}\left(\mathcal{F}_0^2\right) - \frac{m^2}{\mathtt{d}^2}\frac{(\mathtt{d}-1)}{(\mathtt{d}+1)}$.

Proof: First, equivalence of (27) and (28) is readily verified by using that the matrix of $\mathcal{F}$ has the jk-th entry equal to $(\mathcal{F}(\Lambda_j)|\Lambda_k)$. Also, if $\mathcal{F}$ has the stated form then its spectrum is obviously as in (19), and then equality holds in (4) by Proposition 1.

For the opposite implication, assume that equality holds in (4). From (19), we explicitly compute the Stokes frame potential by using (10):

$$\mathrm{Tr}(\mathcal{F}^2) = \sum_{i=1}^{\mathtt{d}^2} \alpha_i^4 = \frac{m^2}{\mathtt{d}^2} + (\mathtt{d}^2 - 1)\frac{m^2}{\mathtt{d}^2(\mathtt{d}+1)^2}. \tag{29}$$

This gives equality in Lemma 1; so the restriction $\mathcal{F}_0$ (in its proof) must be the closest point of $\mathbb{X}$ to the origin: $\mathcal{F}_0 = \frac{m}{\mathtt{d}(\mathtt{d}+1)}\mathcal{I}_0$. To recover the full action of the superoperator $\mathcal{F}$, we note that any $H \in \mathcal{H}$ decomposes as $H = \frac{1}{\mathtt{d}}\mathrm{tr}(H)I + H_0$ where $H_0 := H - \frac{1}{\mathtt{d}}\mathrm{tr}(H)I \in \mathcal{H}_0$. Using $\mathcal{F}(I) = \frac{m}{\mathtt{d}}I$ (per (20)) and $\mathcal{F}_0 = \frac{m}{\mathtt{d}(\mathtt{d}+1)}\mathcal{I}_0$, we write

$$\mathcal{F}(H) = \frac{m}{\mathtt{d}^2}\mathrm{tr}(H)I + \frac{m}{\mathtt{d}(\mathtt{d}+1)}\left(H - \frac{1}{\mathtt{d}}\mathrm{tr}(H)I\right) = \frac{m}{\mathtt{d}(\mathtt{d}+1)}\left(\mathrm{tr}(H)I + H\right). \tag{30}$$

We established (27), and thus also (28). □

Proposition 4 (SIC POVM characterization)**.** *Suppose equality holds in (4). Then* $m \geq \mathtt{d}^2$ *and* $A_1, \ldots, A_m$ *span all of* $\mathcal{H}$*. If additionally* $m = \mathtt{d}^2$ *and* $A_1, \ldots, A_{\mathtt{d}^2} \geq 0$*, then* $A_1, \ldots, A_{\mathtt{d}^2}$ *are the projectors associated to a SIC-POVM.*

Proof: Solving (27) for H expresses it as a linear combination of the A_j:

$$H = \frac{\mathtt{d}(\mathtt{d}+1)}{m}\mathcal{F}(H) - \mathrm{tr}(H)I = \sum_j \frac{\mathtt{d}(\mathtt{d}+1)}{m}\mathrm{tr}(HA_j)A_j - \frac{\mathtt{d}}{m}\mathrm{tr}(H)\mathrm{tr}(A_j)A_j, \tag{31}$$

where we used the definition of $\mathcal{F}$ and $\sum_j \mathrm{tr}(A_j)A_j = \mathcal{F}(I) = \frac{m}{\mathtt{d}}I$ (per (20)) to express I in terms of the A_j. By arbitrariness of $H \in \mathcal{H}$, $A_1, \ldots, A_m$ span all of $\mathcal{H}$ and $m \geq \mathtt{d}^2 = \dim(\mathcal{H})$.

Under the additional assumption that $m = \mathtt{d}^2$, the A_j must also be linearly independent and we can draw stronger conclusions. Indeed, setting $H := A_k$ in (31) gives

$$A_k = \sum_j \left(\frac{\mathtt{d}+1}{\mathtt{d}}\mathrm{tr}(A_kA_j) - \frac{1}{\mathtt{d}}\mathrm{tr}(A_k)\mathrm{tr}(A_j)\right)A_j. \tag{32}$$

Matching the coefficients in front of the A_j on both sides gives (for all $j \neq k$)

$$\frac{\mathtt{d}+1}{\mathtt{d}}\mathrm{tr}(A_k^2) - \frac{1}{\mathtt{d}}\mathrm{tr}(A_k)^2 = 1 \quad \text{and} \quad \frac{\mathtt{d}+1}{\mathtt{d}}\mathrm{tr}(A_kA_j) = \frac{1}{\mathtt{d}}\mathrm{tr}(A_k)\mathrm{tr}(A_j). \tag{33}$$

So far we have not used the hypothesis that $A_1, \ldots, A_m \geq 0$. Assuming it now, each A_k is also of rank one by Proposition 2 (because (21) holds by Proposition 1). The first equation in (33) implies then that A_k is a projector onto the direction of some unit vector $|s_k\rangle \in \mathbb{C}^{\mathtt{d}}$. (Indeed, the sole eigenvalue $\lambda_k \geq 0$ of A_k satisfies $\frac{\mathtt{d}+1}{\mathtt{d}}\lambda_k^2 - \frac{1}{\mathtt{d}}\lambda_k^2 = 1$, which gives $\lambda_k = 1$.) In view of $\mathrm{tr}(A_l) = \langle s_l|s_l\rangle = 1$ (for all l), the second equation in (33) gives the SIC-POVM condition

$$|\langle s_j|s_k\rangle|^2 = \mathrm{tr}(A_jA_k) = \frac{1}{\mathtt{d}+1}\mathrm{tr}(A_j)\mathrm{tr}(A_k) = \frac{1}{\mathtt{d}+1} \qquad (j \neq k). \tag{34}$$

We have shown that $A_1, \ldots, A_{\mathtt{d}^2}$ are the projectors associated to a SIC-POVM. □

Finally, we note that, when A_j do come from a SIC POVM, equality (4) is attained. Indeed, (1) reveals the Gram matrix as

$$\mathbf{G} = \frac{\mathtt{d}}{\mathtt{d}+1}I + \frac{1}{\mathtt{d}+1}E \tag{35}$$

where E is the $\mathtt{d}^2 \times \mathtt{d}^2$ matrix with all entries 1. The eigenvalues α_i^2 of such $\mathbf{G}$ are easily computed to be as in (19). Combined with Proposition 4, this concludes the characterization of equality in (4) as asserted in Theorem 2, thus ending the proof of the theorem.

We finish with a comment highlighting the geometry underlying the proof.

Remark 1. *Assuming* $\mathrm{tr}(A_j) = 1$ *and* $m = \mathtt{d}^2$*, equality in (4) takes place exactly when the vectors* $\vec{A}_1, \ldots, \vec{A}_{\mathtt{d}^2}$ *in the Stokes space* $\mathbb{R}^{\mathtt{d}^2}$ *form a regular simplex of maximum side-length in the* $\mathtt{d}^2 - 2$*-dimensional sphere corresponding to the operators of unit trace and unit norm. Such* $\vec{A}_1, \ldots, \vec{A}_{\mathtt{d}^2}$ *are unique up to an orthogonal transformation of* $\mathbb{R}^{\mathtt{d}^2}$*. SIC POVMs arise from such simplices with the additional property that all vertices* $\vec{A}_j$ *come from non-negative operators (*$A_j \geq 0$*).*

Proof: Under the extra hypotheses, equations (33) that characterize equality in (4) read

$$\mathbf{G}_{kk} = \mathrm{tr}(A_k^2) = 1 \qquad \text{and} \qquad \mathbf{G}_{jk} = \mathrm{tr}(A_jA_k) = \frac{1}{d+1}, \tag{36}$$

which is equivalent to (35). Now, for the $\mathtt{d}^2 \times \mathtt{d}^2$ matrix $\mathbf{A}$, perform the polar decomposition: $\mathbf{A} = SQ$ where $S = S^{\mathtt{T}} \geq 0$ and Q is orthogonal. Because $S^2 = \mathbf{A}\mathbf{A}^{\mathtt{T}} = \mathbf{G}$, the matrix S is uniquely determined as the square root of the right side of (35). Therefore $\mathbf{A}$ is unique up to a composition with an orthogonal matrix (on the right). This means that $\vec{A}_1, \ldots, \vec{A}_{\mathtt{d}^2}$ are unique up to an orthogonal transformation of $\mathbb{R}^{\mathtt{d}}$. We leave it to the reader to see that the Gram matrix of the form (36) corresponds to a regular $\mathtt{d}^2$-simplex. That the side length is the maximal possible follows from inequality (4). The assertion about SIC POVMs follows by combining (36) and Proposition 2. □

4 Application

Let us briefly indicate how Theorem 1 for $f(t) := t^{-1}$ is motivated by a problem in measurement of multimode optical fiber [23, 29, 26]. An unknown operator $T \in \mathcal{H}$ has to be recovered from $\mathtt{d}^2$ measurements of the scalars

$$a_j := \operatorname{tr}(A_j T) = \vec{A}_j^{\mathtt{T}} \vec{T} \qquad (j = 1, \ldots, \mathtt{d}^2). \tag{37}$$

This is to say that the vector $\vec{a} = (a_1, \ldots, a_{\mathtt{d}^2})$ satisfies the system $\vec{a} = \mathbf{A}\vec{T}$, so $\vec{T}$ can be found by linear inversion

$$\vec{T} = \mathbf{A}^{-1}\vec{a}, \tag{38}$$

which then gives $T = \sum_j \vec{T}_j \Lambda_j$ (per (5)). Note that this formulation is nearly identical to the basic problem of quantum tomography (see e.g. [1, 9]), the key difference being that there is no requirement that $T \geq 0$.

In a practical engineering setting, the measurements of individual a_j are subject to noise-induced perturbations δa_j. This creates *noise* $\delta\vec{T} = \mathbf{A}^{-1}\delta\vec{a}$ in the measured $\vec{T}$, where $\vec{\delta a} := (\delta a_1, \ldots, \delta a_{\mathtt{d}^2})$. Assume that the noise covariance matrix $E\left[\vec{\delta a}\vec{\delta a}^{\mathtt{T}}\right]$ is of the form $\sigma^2 I$, which is the case when, e.g., the δa_j are independent identically distributed with variance $\sigma^2 > 0$. Then the variance of the magnitude $\|\delta\vec{T}\|$ of $\delta\vec{T}$ is given by the expected value

$$E\left[\delta\vec{T}^{\mathtt{T}}\delta\vec{T}\right] = E\left[\operatorname{Tr}\left(\mathbf{A}^{-1}\vec{\delta a}\vec{\delta a}^{\mathtt{T}}\left(\mathbf{A}^{-1}\right)^{\mathtt{T}}\right)\right] = \sigma^2 \operatorname{Tr}\left(\left(\mathbf{A}\mathbf{A}^{\mathtt{T}}\right)^{-1}\right) = \sigma^2 \operatorname{Tr}(\mathbf{G}^{-1}). \tag{39}$$

Thus $\operatorname{Tr}(\mathbf{G}^{-1})$ is the *noise magnification factor*, and Theorem 1 shows that the projectors associated with a SIC POVM should be used as the A_j in order to minimize this factor.

Before we go, let us mention that, when A_j do come from a SIC POVM, equation (38) takes a simple form that does not require numerical matrix inversion. Indeed, (28) yields

$$\left(\mathbf{A}^{\mathtt{T}}\mathbf{A}\right)^{-1} = \operatorname{diag}\left(\frac{1}{\mathtt{d}}, \frac{\mathtt{d}+1}{\mathtt{d}}, \frac{\mathtt{d}+1}{\mathtt{d}}, \ldots, \frac{\mathtt{d}+1}{\mathtt{d}}\right). \tag{40}$$

Therefore, using $\mathbf{A}^{-1} = \left(\mathbf{A}^{\mathtt{T}}\mathbf{A}\right)^{-1}\mathbf{A}^{\mathtt{T}}$ gives

$$\mathbf{A}^{-1} = \left[\frac{1}{\mathtt{d}}\vec{A}_0, \frac{\mathtt{d}+1}{\mathtt{d}}\vec{A}_1, \ldots, \frac{\mathtt{d}+1}{\mathtt{d}}\vec{A}_{\mathtt{d}^2-1}\right]. \tag{41}$$

The explicit formula for recovering $\vec{T}$ from $\vec{a}$ reads then

$$\vec{T} = \mathbf{A}^{-1}\vec{a} = \frac{1}{\mathtt{d}}a_0\vec{A}_0 + \frac{\mathtt{d}+1}{\mathtt{d}}a_1\vec{A}_1 + \ldots + \frac{\mathtt{d}+1}{\mathtt{d}}a_{\mathtt{d}^2-1}\vec{A}_{\mathtt{d}^2-1}. \tag{42}$$

This is a version of formula (53) in [27].

A full explanation of the application, including the engineering aspects, will be given elsewhere.

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