A construction of general SIC-POVMs by using a complete orthogonal basis

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A general symmetric informationally complete (GSIC)-positive operator valued measure (POVM) is known to provide an optimal quantum state tomography among minimal IC-POVMs with a fixed average purity. In this paper, we provide a general construction of a GSIC-POVM by means of a complete orthogonal basis (COB), also interpreted as a normal quasiprobability representation. A spectral property of a COB is shown to play a key role for the construction of SIC-POVMs and also for the bound of the mean squared error of the state tomography. In particular, a necessary and sufficient condition to construct a SIC POVM for any $d$ are constructively given by the power of traces of a COB. We give three simple constructions of COBs from which one can systematically obtains GSIC-POVMs.

I. INTRODUCTION

An appropriate quantum state preparation rapidly increases in its importance according to the development of applications in quantum information theory such as quantum computation, quantum key distribution. Intended quantum effect can be obtained when quantum states used in such applications are not disturbed. Therefore, it is important to experimentally check whether the quantum system is appropriately prepared. Quantum state tomography provides a way to determine completely quantum states with their statistical information.

An informationally complete (IC)-positive operator valued measure (POVM) \cite{1–4} is suitable for linear quantum state tomography since any quantum state can be determined completely by its measurement statistics. Any IC-POVM for a $d$-level quantum system has at least $d^2$ POVM elements, whence an IC-POVM with $d^2$ POVM elements is called minimal. A quantum measurement represented by a symmetric informationally complete POVM (hereafter simply SIC) \cite{5} is known to be optimal for linear quantum state tomography \cite{6, 7}. However, the existence of SICs has been shown in limited dimensions \cite{8–10} and it remains an open question whether the SIC exists in all dimensions. For the most up-to-date information, see, for example, \cite{11}.

A general SIC (hereafter simply GSIC) \cite{12, 13} is a generalization of a SIC. Different from a SIC case, POVM elements in a GSIC are not necessary of rank 1, and the existence of GSICs has been shown in all dimensions \cite{12, 13}. Zhu has shown \cite{14} that a GSIC provides an optimal measurement for the linear quantum state tomography among minimal IC-POVMs with a given average purity of a POVM. Uncertainty relations of GSICs are studied in different contexts such as the entropic uncertainty relation \cite{15}, the uncertainty and complementarity relation using the generalized Wigner-Yanase-Dyson skew information \cite{16}, and the improved state-dependent entropic uncertainty relation \cite{17}. An entanglement detection by using the index of coincidence for GSICs as well as its experimental implementation have also been studied in \cite{18–22}.

In this paper, we characterize GSICs by using a complete orthogonal basis (COB) of the set of Hermitian operators. The conditions of informationally completeness, symmetric property, and completeness (normalization) of POVMs are derived directly from the properties of COBs. We observe that a spectrum property of COBs plays a key role to construct a SIC and also determines the bound of the scaled mean squared errors of the minimal IC-POVMs with a given average purity. In particular, any canonically constructed GSIC is shown to give a SIC for a qubit system, while for higher-level systems, conditions to yield SICs are given by the conditions for the power of traces of a COB. We also provide simple three constructions of COBs (and hence those of GSICs) from any sub-orthonormal operator basis and also from a complete set of mutually unbiased bases \cite{23, 24}. Incidentally, a notion of a COB can be interpreted as a normal quasiprobability representation (NQPR) studied in \cite{25}. Hence, our constructions of COBs also serve as those of NQPRs.

This paper is organized as follows. In Sec. II, we review GSICs slightly in a wider context. In Sec. III, we introduce a COB and investigate its spectral properties. In particular, we give a construction of GSICs by means of COBs. In Sec. IV, we give three constructions of COBs. We summarize this paper in Sec. V.

II. PRELIMINARIES

Throughout the paper, $\mathcal{H}$ is a finite dimensional Hilbert space with dimension $d \geq 2$ and $L(\mathcal{H})$ is the $d^2$-dimensional Hilbert space of linear operators on $\mathcal{H}$.
with respect to the Hilbert-Schmidt inner product. For both Hilbert spaces, we use the Dirac notation with a single or double bracket as follows: Inner products on $\mathcal{H}$ and $\mathcal{L}(\mathcal{H})$ are denoted by the bracket $\langle \psi | \phi \rangle$ ($\psi, \phi \in \mathcal{H}$) and the double bracket $\langle [A|B] \rangle = \text{tr} A^* B$ ($A, B \in \mathcal{L}(\mathcal{H})$), respectively. The operator $|\psi \rangle \langle \phi|$ and the super operator $|A\rangle \langle B|$ are also used in a conventional sense, e.g., $|A\rangle \langle B|C \rangle = \langle B|C\rangle A$. The set of density operators, i.e., positive operators with unit trace, is denoted by $\mathcal{S}(\mathcal{H}) := \{ \rho \in \mathcal{L}(\mathcal{H}) : \rho \geq 0, \text{tr} \rho = 1 \}$.

Let $F = (F_i)_{i=1}^n$ be a discrete POVM on $\mathcal{H}$, i.e., $F_i \geq 0$ for any $i$ and $\sum_{i=1}^n F_i = 1$ where $1$ is the identity operator. $F$ is called an informationally complete (IC)-POVM if the statistics of the measurement of $F$ determines the underlying quantum state. In other words, $F$ is an IC-POVM if for $\rho, \sigma \in \mathcal{S}(\mathcal{H})$, $\text{tr} F_i \rho = \text{tr} F_i \sigma$ ($\forall i = 1, 2, \ldots, n$) implies $\rho = \sigma$. One can show that a POVM is IC iff it spans $\mathcal{L}(\mathcal{H})$. (For the readers’ convenience, we give a simple proof for this fact in Appendix A 1.) An IC-POVM is thus called minimal if $n = d^2$.

A rank 1 POVM $F = (F_i = |\psi_i\rangle \langle \psi_i|)_{i=1}^d$ is called a symmetric informationally complete (SIC)-POVM (hereafter simply SIC) [5] if it satisfies

$$\text{tr} F_i^2 = ||\psi_i||^4 = a \quad \forall i,$$

$$\text{tr} F_i F_j = ||\psi_i \psi_j||^2 = b \quad \forall i \neq j,$$

where $a$ and $b$ are constants dependent only on the dimension $d$. Note that these constants are automatically determined as $a = \frac{1}{d^2}$ and $b = \frac{1}{d^2(d+1)}$. (These are shown by taking traces over the equations $1 = \sum_i F_i = \sum_i |\psi_i\rangle \langle \psi_i|$ and $1 = (\sum_i F_i)^2$.) Moreover, one can show a SIC spans $\mathcal{L}(\mathcal{H})$ (see the general argument below), and hence is informationally complete and minimal. However, the existence of SICs for an arbitrary dimension is a long standing open problem and has only been shown analytically (or numerically) in the limited dimensions (see, e.g., [11]).

A natural generalization of a SIC is given by relaxing the condition for the rank: A POVM $(G_i)_{i=1}^d$ is called a special SIC-POVM (hereafter simply GSIC) [12, 13] if it satisfies

$$\text{tr} G_i^2 = a' \quad \forall i,$$

$$\text{tr} G_i G_j = b' \quad \forall i \neq j,$$

where $a'$ and $b'$ are constants dependent only on $d$. Different from a SIC, the existence and a construction of GSICs have been shown in all dimensions [12, 13].

Here we shall review some of the properties of a GSIC by further generalizing the number of POVM elements to be arbitrary $n$: $(G_i)_{i=1}^n$. Firstly, the parameters $a'$ and $b'$ are not independent and satisfy

$$a' + (n-1)b' = \frac{d}{n}. \quad (1)$$

This is seen by observing $d = \text{tr} G_i^2 = \text{tr} (\sum_i G_i) (\sum_j G_j) = \text{tr} \{\sum_i G_i^2 + \sum_{i \neq j} G_i G_j\} = na' + n(n-1)b'$. This also determines the trace of $G_i$:

$$\text{tr} G_i = \text{tr} G_i \left( \sum_j G_j \right) = a' + (n-1)b' = \frac{d}{n}. \quad (2)$$

Secondly, the parameter $a'$ satisfies

$$\frac{d}{n^2} < a' \leq \frac{d^2}{n^2}. \quad (3)$$

The first inequality follows from the Schwarz inequality: $\frac{d}{n} = \text{tr} G_i = \text{tr} G_i \leq \sqrt{\text{tr} G_i^2} \sqrt{\text{tr} G_i^2} = \sqrt{a'} \sqrt{d}$. However, the equality implies that $G_i = \frac{d}{n} I$ and is excluded in order to keep the IC condition. The second inequality is shown by the following elementary fact: For any positive operator $A \geq 0$,

$$\text{tr} A^2 \leq (\text{tr} A)^2,$$

where the equality holds iff $A$ is a rank one operator. Applying each $G_i \geq 0$ shows the second inequality and also, in the case $n = d^2$, the equality holds iff $G$ is a SIC. Finally, it holds that $G$ is IC iff $n \geq d^2$. To see this, it is enough to show that $G$ is linearly independent (hence $n \geq d^2$ iff $G$ spans $\mathcal{L}(\mathcal{H})$). Suppose that $\sum_{i=1}^n x_i G_i = 0$ for complex numbers $x_i$. By taking the trace over the equation and using Eq. (2), one has $\sum_i x_i = 0$. Next, multiplying $G_j$ to $\sum_{i=1}^n x_i G_i = 0$ and taking its trace shows $0 = \sum_i x_i \text{tr} G_i G_j = (a' - b') x_j + b' \sum_i x_i$. Combining these results, one gets $x_j = \frac{b'}{b'^2 - \sum x_i} = 0$ for all $j$. Note here that $b' \neq a'$ otherwise (1) implies $a' = \frac{d}{n}$ violating the first inequality in (3). In the following, we consider the most interesting case $n = d^2$.

In the linear quantum state tomography, Zhu [14] revealed the tomographic significance of GSICs in the following sense. For any IC POVM measurement $(\Pi_i)_{i=1}^n$, there exists a set of operators $(\Theta_i)_{i=1}^n$ with which any density operator $\rho$ can be written as $\rho = \sum_{i=1}^n p_i \Theta_i$ where $p_i = \text{tr} \Pi_i \rho$ is the probability to get the $i$th outcome of the POVM $(\Pi_i)_{i=1}^n$ under the state $\rho$. Let $f_i^{(N)}$ be the frequency to get the $i$th outcome by the individual measurement of $(\Pi_i)_{i=1}^n$ under $N$ copies of $\rho$. Then, a natural estimated state is given by $
abla (\sum_{i=1}^n f_i^{(N)} \Theta_i)$. The scaled mean squared error (MSE) $\mathcal{E}[\rho] = \mathcal{E}[\rho] = \frac{\mathcal{E}[\rho]}{\mathcal{E}[\rho] + \mathcal{E}[\rho]}$ where $||.||^2 : = \langle \rho | \cdot | \rho \rangle$ is the Hilbert-Schmidt norm. One can show that $\mathcal{E}[\rho] = \sum_{i=1}^n p_i \text{tr} \Theta_i^2 - \text{tr} \rho^2$ [6].

In [14], Zhu had shown that, among minimum IC POVMs with the fixed average purity (see below), the maximal scaled MSE $\mathcal{E}_{\text{max}}[\rho]$ over all pure states (more generally over all unitary equivalent states) is bounded from below as

$$\mathcal{E}_{\text{max}}[\rho] \geq \frac{(d^2 - 1)^2}{d^2 \rho - d + \frac{1}{d} - \text{tr} \rho^2}. \quad (4)$$

Here, $\rho$ is the average purity of an IC-POVM $(\Pi_i)_{i=1}^n$ defined by

$$\rho := \sum_i \frac{\text{tr} \Pi_i}{d}. \quad (5)$$
where \( \varphi_i := \frac{\text{tr} P_i^2}{\text{tr} P_i} \) is the purity of \( P_i \). Interestingly, Zhu had shown that the minimum of (4) is attained iff the IC-POVM is a GSIC. Therefore, one can consider a GSIC as an optimal measurement among all minimal IC-POVMs with the fixed average purity that minimize the scaled MSE for the worst case scenario of states.

### III. CHARACTERIZATION OF GSIC BY COMPLETE ORTHOGONAL BASIS

In the following, we consider the real Hilbert space of the set of all Hermitian operators \( \mathcal{K} = \{A \in \mathcal{L}(\mathcal{H}) \mid A = A^\dagger\} \). Let us start by introducing a useful operator basis for \( \mathcal{K} \).

**Definition 1** An operator basis \( (A_i)_{i=1}^d \) for \( \mathcal{K} \) is called a complete orthogonal basis (COB) if it satisfies

(i) Sub-orthonormality: \( \langle A_i | A_j \rangle = \frac{1}{d} \delta_{ij} \),

(ii) Completeness: \( \sum_i A_i = 1 \).

(See Appendix B for examples). Note that the normalization constant \( \frac{1}{d} \) in (i) is automatically determined by (ii). By completeness, one has \( \text{tr} A_i = \text{tr} A_i(\sum_j A_j) = \frac{1}{d} \). If there is a positive element \( A_i \geq 0 \) for some \( i, \frac{1}{d} = \text{tr} A_i^2 \leq (\text{tr} A_i)^2 = \frac{1}{d^2} \), contradicting \( d \geq 2 \). Therefore, any element \( A_i \) of a COB cannot be positive, and the minimum eigenvalue of each \( A_i \) is strictly negative. Here, we define an important value for a COB:

\[
\lambda^* := \frac{1}{1 + d^2 \tau},
\]

where

\[
\tau := \max_{i=1,2,\ldots,d} \{ |m_i| \mid m_i : \text{the minimum eigenvalue of } A_i \}.
\]

**Proposition 2** The value \( \lambda^* \) satisfies

\[
\lambda^* \leq \frac{1}{\sqrt{d+1}}.
\]

The upper bound is saturated iff all \( A_i \) have the same eigenvalues: \( \frac{(d-1)\sqrt{d^2+1}}{d^2} > 0 \) with multiplicity 1 and \( \frac{1-\sqrt{d^2+1}}{d} < 0 \) with multiplicity \( d-1 \).

This is shown by the following lemma.

**Lemma 3** Let \( x_i (i = 1, 2, \ldots, d) \) be \( d \geq 2 \)-tuples of a real number in descending order with constraints

(i) \( \sum_i x_i = 1 \),

(ii) \( \sum_i x_i^2 = \frac{1}{d} \).

Then, the minimum \( x_d \) < 0 and satisfies

\[
|x_d| \geq \frac{\sqrt{d+1} - 1}{d^2}.
\]

The bound is saturated if and only if

\[
x_1 = \frac{1 + (d-1)\sqrt{d+1}}{d^2},
\]

\[
x_2, x_3, \ldots, x_d = \frac{1 - \sqrt{d+1}}{d^2}.
\]

(See Appendix A 2 for the proof.)

**Proof of Proposition 2**. Note that inequality (7) is equivalent to

\[
\tau \geq \frac{\sqrt{d+1} - 1}{d^2}.
\]

However, this is shown to hold by applying Lemma 3 to each eigenvalue of \( A_i \) (noting that \( \text{tr} A_i = \frac{1}{d} \) and \( \text{tr} A_i^2 = \frac{1}{d^2} \)). The equality condition follows from the latter statement in Lemma 3.

Now we provide a construction of a GSIC by showing the connection between a GSIC and a COB.

**Theorem 4** For any COB \( (A_i)_{i=1}^d \) and \( \lambda \in (0, \lambda^*] \),

\[
G_i = \lambda A_i + (1 - \lambda) \frac{1}{d^2}
\]

forms a GSIC. Conversely, for any GSIC \( (G_i)_{i=1}^d \) with constants \( \alpha', \beta' \), \( (A_i)_{i=1}^d \) given by (10) with \( \lambda = \sqrt{1 - \beta' d^3} = \sqrt{\frac{d^2\alpha' - 1}{d^2}} \) forms a COB.

**Proof**. Letting \( (A_i)_{i=1}^d \) be a COB and \( \lambda \in (0, \lambda^*] \), we show that \( (G_i)_{i=1}^d \) of the form (10) is a GSIC. The completeness \( \sum_i G_i = \frac{1}{d^2} \) follows from that of \( (A_i)_{i=1}^d \). Next, \( G_i \) is positive iff \( \lambda m_i + (1 - \lambda) \frac{1}{d^2} \geq 0 \) where \( m_i \) is the minimum eigenvalue of \( A_i \). Since \( m_i < 0 \) as is mentioned above, the condition is equivalent to \( \frac{1}{1 + d^2 |m_i|} \geq \lambda \). This holds since \( \lambda \in (0, \lambda^*] \), so we have \( G_i \geq 0 \). Moreover, the symmetric property of \( (G_i)_{i=1}^d \) follows as

\[
\text{tr} G_i G_j = \text{tr} \left\{ \lambda A_i + (1 - \lambda) \frac{1}{d^2} \right\} \left\{ \lambda A_j + (1 - \lambda) \frac{1}{d^2} \right\}
\]

\[
= \lambda^2 \text{tr} A_i A_j + \frac{(1 - \lambda)\lambda}{d^2} \text{tr} A_i A_j + \frac{\lambda(1 - \lambda)}{d^2} \text{tr} A_i + \frac{(1 - \lambda)^2}{d^4} \text{tr} \frac{1}{d^2}
\]

\[
= \lambda^2 \delta_{ij} + \frac{1 - \lambda^2}{d^2}.
\]

Hence, \( (G_i)_{i=1}^d \) is a GSIC with the constants

\[
\alpha' = \frac{\lambda^2}{d^2} + \frac{1 - \lambda^2}{d^2}, \quad \beta' = \frac{1 - \lambda^2}{d^3}.
\]

Conversely, letting \( (G_i)_{i=1}^d \) be a GSIC with constants \( \alpha', \beta' \), we show that \( A_i := \frac{1}{d} (G_i - \frac{1}{d^2} \mathbb{1}) \) forms a COB with \( \lambda = \sqrt{1 - \beta' d^3} = \sqrt{\frac{d^2\alpha' - 1}{d^2}} \) (reminding the relation (1) where \( n = d^2 \)) Using the symmetry \( \text{tr} G_i G_j = a' \delta_{ij} + (1 - \delta_{ij}) b' \)
and $\text{tr} G_i = \frac{1}{d^2}$, we have

$$\text{tr} A_i A_j = \frac{1}{2} \text{tr} \left( G_i - \frac{1 - \lambda}{d} \right) \left( G_j - \frac{1 - \lambda}{d} \right)$$

$$= \frac{1}{d^2} \left( (a' - b') \delta_{ij} + b' - \frac{2(1 - \lambda)}{d^3} + \frac{(1 - \lambda)^2}{d^3} \right)$$

$$= \frac{1}{d^2} \left( (a' - b') \delta_{ij} + b' - \frac{1 - \lambda^2}{d^3} \right) = \frac{1}{d} \delta_{ij}.$$  

Finally, the completeness of $(A_i)_s$ follows from that of $(G_i)_s$.  

Theorem 4 shows that any GSIC including a SIC can be constructed by a COB which is rather easy to construct (see the next section). Note that another construction of a GSIC was given in [13]. However, their construction needs two asymmetrical expressions, thereby it unnecessarily breaks a symmetry of a GSIC in appearance. In contrast, our construction (10) consists of a single expression, hence does not introduce any redundant asymmetry.

Before giving its construction, let us discuss the relation between a SIC and a COB. Although there is a freedom for the choice of $\lambda \in (0, \lambda^*]$, the extreme choice $\lambda = \lambda^*$ plays a crucial role for constructing SICs. In the following, we call such construction a canonical construction. Note that, by (11), $(G_i)_s$ is a SIC, i.e., $a' = \frac{1}{d^2}$, iff $\lambda = \frac{1}{\sqrt{d^2 + 1}}$. Therefore, Proposition 2 shows the following proposition.

**Proposition 5** A GSIC canonically constructed by a COB (i.e., $\lambda = \lambda^*$) is a SIC iff any one of the following conditions is satisfied:

(i) The upper bound of $\lambda^*$ in (7) is saturated.

(ii) $\tau = \sqrt{\frac{d^2 + 1}{d^2}}$ holds.

(iii) All $A_i$ have the same eigenvalues: $\frac{1 + (d-1)\sqrt{d^2 + 1}}{d^2} > 0$ with multiplicity 1 and $\frac{1 - \sqrt{d^2 + 1}}{d^2} < 0$ with multiplicity $d - 1$.

The following result shows that any canonical construction in $d = 2$ gives a SIC:

**Proposition 6** For $d = 2$, a canonical construction always gives a SIC.

**Proof.** Let $(A_i)_s^{d^2}$ be a COB. The eigenvalue equation for each $A_i$ reads $0 = \det(m \mathbb{1} - A_i) = m^3 - (\text{tr} A_i) m + \frac{1}{2} ((\text{tr} A_i)^2 - d \text{tr} A_i^2)$. Therefore, $\text{tr} A_i = \text{tr} A_i^2 = \frac{1}{d}$ implies that all eigenvalues of $A_i$s are the same $m = \frac{1 + \sqrt{3}}{2}$ satisfying (iii) in Proposition 5.

Notice however that not all canonical constructions in the case $d \geq 3$ give SICs since there appear higher contributions of $\text{tr} A_i^n$ ($3 \leq n \leq d$) in the eigenvalue equations. However, we have

**Proposition 7** For any $d \geq 3$, the necessary and sufficient conditions for a canonical construction to give a SIC are systematically derived: To be specific, the conditions are $\text{tr} A_i^3 = 31/243$ for $d = 3$, and $\text{tr} A_i^4 = \frac{1}{512} (23 + 15\sqrt{5})$ and $\text{tr} A_i^4 = \frac{1}{256} (77 + 15\sqrt{5})$ for $d = 4$, etc.

**Proof.** By using Newton’s identity (see e.g., [26]), one can derive the characteristic equations for $A_i$ bearing in mind the constraints $\text{tr} A_i = \text{tr} A_i^2 = \frac{1}{d}$. For example, for $d = 3$,

$$0 = \det(m \mathbb{1} - A_i) = m^3 - \frac{1}{3} m^2 - \frac{1}{9} m - \frac{54 \text{tr} A_i^3 - 8}{162}.$$  

Therefore, by (iii) in Proposition 5 for $d = 3$, the necessary and sufficient condition for a canonical construction to give a SIC is that all $A_i$s satisfy $\text{tr} A_i^3 = 31/243$. One can obtain the conditions similarly for any $d$.  

The following proposition gives a physical meaning of the parameter $\lambda$ of a canonically constructed GSIC in the context of the quantum state tomography.

**Proposition 8** The average purity of a GSIC constructed by a COB is given by $\varphi = \frac{1}{d}((d^2 - 1)\lambda^2 + 1)$. The maximal scaled MSE for the GSIC satisfies

$$\mathcal{E}_{\max}(\rho) = \frac{d^2 - 1}{d} \frac{1}{\lambda^2} + \frac{1}{d} - \text{tr} \rho^2$$

$$\geq \frac{d^2 - 1}{d} (1 + d) + \frac{1}{d} - \text{tr} \rho^2.$$  

The inequality is saturated iff the upper bound of $\lambda^*$ in (7) is saturated which implies that the GSIC is a SIC.

**Proof.** A direct computation of (5) for a GSIC shows $\varphi = d^2 a'$ hence by (11), one obtains $\varphi = \frac{1}{d}((d^2 - 1)\lambda^2 + 1)$. The first equality is the direct application of Zhu’s result (4). The second inequality follows from (7) and $\lambda \in (0, \lambda^*]$. Finally, the last statement is shown by Proposition 5.

Hence, the larger the parameter $\lambda$, the less the maximal scaled MSE $\mathcal{E}_{\max}(\rho)$ and a SIC ($\lambda = \lambda^* = \frac{1}{\sqrt{d^2 + 1}}$) gives the minimal $\mathcal{E}_{\max}(\rho)$.

Finally, we remark that a COB $(A_i)_s$ was used by Zhu [25] as a normal quasiprobability representation (NQPR) where a quantum state $\rho$ is represented by a (possibly negative) quasiprobability $\mu_\rho(\lambda) = \text{tr} A_i \rho$. The negativity of a COB $(A_i)_s$ is naturally defined by

$$N(\{A_i\}) := \max_{\rho \in \mathcal{S}(\mathcal{H})} N(\rho)$$

where $N(\rho) := d \max\{0, -\min_{\mu_\rho(\lambda)}\}$. Theorem 1 in [25] shows a bound of the negativity where the bound is saturated iff a POVM corresponding to the NQPR is a SIC. In this context, Zhu has also observed essentially the same results as Proposition 2 and Proposition 5 because one can readily show that

$$\tau = \frac{1}{d} N(\{A_i\}).$$  

See Appendix A 3 for the proof.) Note that, combination of the relation (12) and Proposition 8 for the canonically
constructed GSIC yields the following relation between the maximal scaled MSE for the GSIC and the negativity:

\[
\epsilon_{\text{max}}(\rho) = \frac{d^2 - 1}{d} \{1 + dN(|A_j|)\}^2 + \frac{1}{d} - \text{tr} \rho^2 \\
\geq \frac{d^2 - 1}{d} (1 + d) + \frac{1}{d} - \text{tr} \rho^2.
\]

In the next section, we give several constructions of COBs for the construction of GSIC, which also serves a construction of NQPRs in Zhu’s context.

IV. CONSTRUCTIONS OF A COMPLETE ORTHOGONAL BASIS

In this section, we provide several constructions of COBs. The general ideas of Constructions 1 and 2 are explained in Appendix B in more general settings. The Construction 3 is based on the ideas developed in [27] and [28].

Construction 1. With any orthonormal basis \((T_i)_{i=0}^{d^2-1}\) for \(\mathcal{L}(\mathcal{H})\) where \(T_0 = \frac{1}{\sqrt{d}}\) (i.e., a generator of \(\text{su}(d)\)) and any orthogonal \(d^2 \times d^2\) real matrix \(O = [O_{ij}]_{i,j=0}^{d^2-1}\) satisfying

\[
O_{0j} = \frac{1}{d} \quad (j = 0,1,\ldots,d^2 - 1),
\]

\[
A_i := \frac{1}{\sqrt{d}} \sum_{j=0}^{d^2-1} O_{ij} T_j \quad (i = 0,1,\ldots,d^2 - 1)
\]  

is a COB.

Note that both \((T_i)\) and \(O\) are easily prepared, e.g., by using Gram-Schmidt orthogonalization starting from \(I\) and \((1,1,\ldots,1)^T \in \mathbb{R}^d\), respectively. Importantly, any COB can be obtained through this construction (See Appendix B for the detail in more general settings.)

The next construction only uses a generator of \(\text{su}(d)\), hence more economic and concrete than the first construction at the cost of losing the generality:

Construction 2. Let \((T_i)_{i=0}^{d^2-1}\) be an orthonormal basis for \(\mathcal{L}(\mathcal{H})\) with \(T_0 = \frac{1}{\sqrt{d}}\). Construct an orthonormal basis \((S_j)_{j=0}^{d^2-1}\) by the Gram-Schmidt orthogonalization of the set \(\{1, T_0, T_1, \ldots, T_{d^2-1}\}\) starting from the first entry. Then,

\[
A_i := \frac{1}{\sqrt{d}} \sum_{j=0}^{d^2-1} \langle S_j | T_i \rangle T_j \quad (i = 0,1,\ldots,d^2 - 1)
\]

is a COB.

Note that we can obtain the explicit formula for this construction as follows:

\[
A_0 = \frac{1}{d\sqrt{d}} \left( T_0 - \sum_{j=1}^{d^2-1} f(j) T_j \right),
\]

\[
A_i = \frac{1}{d\sqrt{d}} \left( T_0 - \sum_{j=1}^{i-1} f(j) T_j + (d^2 - i) f(i) T_i \right) \\
\quad (i = 1,2,\ldots,D - 1),
\]

where \(f(j) = \frac{d}{\sqrt{(d^2 - j)(d^2 - (j - 1))}}\).

The canonical construction (10) for \(d = 2\) using the standard Pauli matrices reads the following SIC:

\[
G_0 := \frac{1}{12} \begin{pmatrix} -\sqrt{6} + 3 & -1 + \sqrt{2}i \\ -1 - 2\sqrt{2}i & \sqrt{6} + 3 \end{pmatrix},
\]

\[
G_1 := \frac{1}{4} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix},
\]

\[
G_2 := \frac{1}{12} \begin{pmatrix} 3 & -1 - 2\sqrt{2}i \\ -1 + 2\sqrt{2}i & 3 \end{pmatrix},
\]

\[
G_3 := \frac{1}{12} \begin{pmatrix} \sqrt{6} + 3 & -1 + \sqrt{2}i \\ -1 - 2\sqrt{2}i & \sqrt{6} + 3 \end{pmatrix}.
\]

For a general \(d \geq 3\), we can also compute the COB using the generalized Gell-Mann matrices:

\[
T_{nm} := \begin{cases} \frac{1}{\sqrt{d}} |n\rangle \langle m| + |m\rangle \langle n| & (n < m), \\
\frac{\sqrt{d} - 1}{\sqrt{d}} |n\rangle \langle m| - |m\rangle \langle n| & (n > m), \\
\frac{1}{n\sqrt{n + 1}} \sum_{k=1}^{n} \langle k | \langle n| - n |n + 1\rangle \langle n + 1| \\
& (n = 1,2,\ldots,d - 1),
\end{cases}
\]

and \(T_{dd} := \frac{1}{d}\). We have numerically computed \(\tau\) of the COB and plotted \(\lambda^*\) in Fig. 1. Except for \(d = 2\), \(\lambda^*\) is less than the maximum value \(\frac{\sqrt{d}}{d+1}\), so the corresponding GSICs are not SICs.

The third construction is based on the complete sets of mutually unbiased bases (MUBs) and mutually unbiased straitions (MUSs) [23, 24]. Let us first give a short review for those concepts.

Two orthonormal bases (ONBs) \(|\psi_i\rangle_{i=1}^{d^2}\) and \(|\phi_i\rangle_{i=1}^{d^2}\) for \(\mathcal{H}\) are called mutually unbiased if \(|\langle \psi_i | \phi_j \rangle|^2 = \frac{1}{d}\) for all \(i,j\). The set of ONBs \(|J,i\rangle_{i=1}^{d^2}\) \((J = 1,2,\ldots,m)\) is called mutually unbiased if any pair of the bases are mutually unbiased:

\[
|\langle J,i | J',i' \rangle|^2 = \delta_{JJ'}\delta_{ii'} + \frac{1}{d}(1 - \delta_{JJ'}).
\]

The maximum number of MUBs is known to be \(d + 1\) and the set of MUBs with \(d + 1\) elements is called complete. Similar to the problem of SICs, the existence of the complete set of MUB for all \(d\) is still open.

Next, let \(M\) denotes a set with the cardinality \(\#(M) = d^2\), which we label as \(M = \{1,2,\ldots,d^2\}\). A subset of \(M\)
is a COB as is shown below.

Following [28], we introduce a vector $|\Phi_{j,k\ell}\rangle := |J,i\rangle \otimes |J,\bar{i}\rangle$ on $\mathcal{H} \otimes \mathcal{H}$ where $|\psi\rangle := \sum_{i} |i\rangle |\psi_i\rangle$ denotes the complex conjugate vector with respect to a (fixed) ONB $|i\rangle$ for all $i \neq j$. Let $|\Psi\rangle := \frac{1}{\sqrt{d}} \sum_{i=1}^{d} |i\rangle \otimes |i\rangle$ be a maximally entangled state. Then, it is easy to see $|\Psi\rangle = \frac{1}{\sqrt{d}} \sum_{i=1}^{d} |J,i\rangle \otimes |J,i\rangle$ for any $J$. Let

$$|\hat{k}\rangle := \frac{1}{\sqrt{d}^{d+1}} \sum_{j=1}^{d+1} |\Phi_{j,k(s(k,j))}\rangle - |\Psi\rangle \quad (k = 1, 2, \ldots, d^2).$$

Then, one can show that $|\hat{k}\rangle$ is a unit vector and $\langle \Phi_{j,k}\rangle |\hat{k}\rangle = \frac{1}{\sqrt{d}} \delta_{s(k,j)}$. Moreover, one can show $\sum_{i} |\hat{k}\rangle |\hat{k}\rangle = I$ by the completeness conditions for MUBs and MUSs, hence $\{|\hat{k}\rangle\}_{k=1}^{d}$ forms an ONB for $\mathcal{H} \otimes \mathcal{H}$ (see [28] for the detail).

Now consider an isomorphism $A \in \mathcal{L}(\mathcal{H}) \to \mathcal{I}(A) := \{ (\otimes \otimes) \Psi \} \in \mathcal{H} \otimes \mathcal{H}$ between an operator and a vector. As $(|i\rangle)$ forms a basis for $\mathcal{H}$, it is easy to see that $\mathcal{I}$ is a linear bijection between $\mathcal{L}(\mathcal{H})$ and $\mathcal{H} \otimes \mathcal{H}$, and $\langle A | B \rangle = d \mathcal{I}(A) \mathcal{I}(B)$ for any $A, B \in \mathcal{L}(\mathcal{H})$. We define $A_k \in \mathcal{L}(\mathcal{H}) (k = 1, 2, \ldots, d^2)$ by

$$\mathcal{I}(A_k) = \frac{1}{d} |\hat{k}\rangle$$

Then, the normalization condition holds:

$$\langle A_k | A_{k'} \rangle = d \mathcal{I}(A_k) \mathcal{I}(A_{k'}) = \frac{\langle \hat{k} | \hat{k} \rangle}{d} = \delta_{kk'}.$$ 

Noting that $|\Phi_{j,k}\rangle = \sqrt{d} \mathcal{I}(|J,i\rangle \langle J,i|)$, we have $\langle A_k | J,i \rangle \langle J,i| A_{k'} \rangle = d \mathcal{I}(A_k) \mathcal{I}(A_{k'}) = \frac{1}{d} \langle k | \Phi_{j,k}\rangle = \frac{\langle \hat{k} | \hat{k} \rangle}{d} = \delta_{kk'}$. So, we observe $|J,i\rangle \langle J,i| = d \sum_{k=1}^{d^2} \langle A_k | J,i \rangle \langle J,i| A_k \rangle = \sum_{k \in L_i^{(J)}} A_k$. Then,

$$1 = \sum_{i} \sum_{k \in L_i^{(J)}} |J,i\rangle \langle J,i| A_k = \sum_{k=1}^{d^2} A_k.$$

Hence, the set $(A_k)_k$ is a COB.

Finally, the explicit form of $A_k$ is shown as follows. We have $\mathcal{I}(|\phi\rangle \langle \phi|) = \frac{1}{\sqrt{d}} |\delta \rangle \otimes |\delta\rangle$ for any $|\phi\rangle$ and $\mathcal{I}(I) = |\Psi\rangle$. By using these properties, as well as (18), and (19), one arrives at the expression (17).

Let us construct a SIC for $d = 2$ using Construction 3.

We employ the sets $L_1^{(1)} := \{ 1, 2 \}, L_2^{(1)} := \{ 3, 4 \}, L_1^{(2)} := \{ 1, 3 \}, L_2^{(2)} := \{ 2, 4 \}, L_1^{(3)} := \{ 1, 4 \}, L_2^{(3)} := \{ 2, 3 \}$ as a complete set of MUBs and the set of bases $(1, 1) := \frac{1}{\sqrt{2}} (1, 1)^T, (1, 2) := \frac{1}{\sqrt{2}} (1, -1)^T, (2, 1) := \frac{1}{\sqrt{2}} (1, i)^T, (2, 2) := \frac{1}{\sqrt{2}} (1, -i)^T, (3, 1) := (1, 0)^T, (3, 2) := (0, 1)^T$ as a complete set of MUBs. According to the direct computation using (17), a
canonical construction (10) gives the following SIC:

\[
\begin{align*}
G_1 & = \frac{1}{4\sqrt{3}} \begin{pmatrix} 1 + \sqrt{3} & 1 - i \\ 1 + i & -1 + \sqrt{3} \end{pmatrix}, \\
G_2 & = \frac{1}{4\sqrt{3}} \begin{pmatrix} -1 + \sqrt{3} & 1 + i \\ 1 - i & 1 + \sqrt{3} \end{pmatrix}, \\
G_3 & = \frac{1}{4\sqrt{3}} \begin{pmatrix} -1 + \sqrt{3} & -1 - i \\ 1 + i & 1 + \sqrt{3} \end{pmatrix}, \\
G_4 & = \frac{1}{4\sqrt{3}} \begin{pmatrix} 1 + \sqrt{3} & -1 + i \\ -1 - i & -1 + \sqrt{3} \end{pmatrix}.
\end{align*}
\]

V. CONCLUSIONS AND DISCUSSIONS

In this paper, we gave the construction of GSICs by means of COBs and investigated the condition to give a SIC by the spectrum property of a COB (Theorem 4). In particular, for \( d = 2 \), any canonically constructed GSIC is a SIC (Proposition 6), while for \( d \geq 3 \), conditions for the power of traces of a COB were given to yield SICs (Proposition 7). A characteristic value \( \lambda \) of a COB gives the bound of the scaled MSE for the linear quantization of NQPRs. The constructions provided three different constructions of COBs, one of which shows a relation with MUBs. The constructions serve as not only for those of GSICs, but also for those of NQPRs.

Finally, we remark another idea of constructions of COBs, and hence of GSICs, based on Zauner’s conjecture for a SIC [5, 29]: Let \( (D_{jk})_{j,k=0}^{d-1} \) be the tuple of unitary operators defined by

\[
D_{jk} = \omega^{\frac{j}{2}} \sum_{m=0}^{d-1} \omega^{jm} |k+m\rangle \langle m|
\]

where \( \omega = \exp\left(\frac{2\pi i}{d}\right) \), \(|k\rangle \) is an ONB for \( \mathcal{H} \), and \( \oplus \) denotes the addition modulo \( d \). Then, it is believed that there is a normalized fiducial vector \( |\phi\rangle \in \mathcal{H} \) with which \( (|\psi_{jk}\rangle \langle \psi_{jk}|)_{j,k=0}^{d-1} = (D_{jk} |\phi\rangle \langle \phi| D_{jk}^\dagger) \) is a SIC. Note that \( (D_{jk})_{j,k} \) is a faithful projective unitary representation of a group \( G = Z_d \times Z_d \). More generally, for a group \( G \) with the identity \( e \) and the order \( \#(G) = d^2 \), let \( (U_g)_{g \in G} \) be a faithful projective unitary representation:

\[
U_g U_{g'} = c(g,g') U_{gg'} \quad (g,g' \in G) \quad (\text{20})
\]

with \( |c(g,g')| = 1 \) which is orthogonal

\[
\langle U_g | U_{g'} \rangle = d \delta_{gg'} \quad (\text{21})
\]

These bases are sometimes called nice error bases [30, 31]. Note that the faithfulness is required to guarantee \( \#(U_g) = d^2 \). By the properties (20) and \( |c(g,g')| = 1 \), it is easy to see that if a fiducial vector satisfies

\[
|\langle \phi | U_g \phi \rangle|^2 = \frac{1}{d + 1} \quad \forall g \neq e, \quad (\text{22})
\]

\( \frac{1}{d} |\langle U_g \phi | U_g \phi \rangle|_{g \in G} \) forms a SIC. Note that [32] the orthogonality condition (21) is equivalent to the relation

\[
\sum_g U_g U_g^\dagger = d (\text{tr} \mathbb{1}) \quad \forall C \in \mathcal{L}(\mathcal{H}), \quad (\text{23})
\]

hence the completeness of the POVM follows automatically.

Let \( (U_g)_{g \in G} \) be a faithful projective unitary representation of a group \( G \) with \( \#(G) = d^2 \). Let \( A \) be an Hermitian operator with \( \text{tr} A^2 = \frac{1}{d} \). Moreover, let \( A \) satisfies the condition

\[
\text{tr} A U_g U_g^\dagger = 0 \quad \forall g \neq e.
\]

Then, it is easy to see that \( (A_g := U_g A U_g^\dagger)_{g \in G} \) is a COB: The orthogonality and the completeness conditions follow from (22) and (23), respectively. Note also that \( \text{tr} A_g = \frac{1}{d} \) follows automatically. Such an operator \( A \) might be called a fiducial operator. Hence, a construction for both SICs and GSICs reduces to be a problem to find a fiducial operator. We think the problem interesting even for GSICs.

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Appendix A: Proofs of some propositions

In this appendix, we shall give proofs of some propositions and lemmas.

1. Spanning property of IC-POVM

First, the following is a well-known fact for IC POVM (see e.g. [4]), but here we provide its simple proof:

**Proposition 9** A POVM \( F = (F_i)_{i=1}^n \) is informationally complete if and only if \( F \) spans \( \mathcal{L}(\mathcal{H}) \).

**Proof.** Note first that \( F \) is informationally complete iff for any \( C, D \in \mathcal{L}(\mathcal{H}) \) and any \( i \), \( \text{tr} F_i C = \text{tr} F_i D \Rightarrow C = D \) by noting that any linear operator can be expressed as a linear combination of density operators.

Let \( F = (F_i)_{i=1}^n \) be an informationally complete POVM. Assume contrary that \( F \) does not span \( \mathcal{L}(\mathcal{H}) \). Then, \( (\text{span} F)^\perp \neq \{0\} \). Namely, there is non-zero \( X \in \mathcal{L}(\mathcal{H}) \) such that for any \( i \), \( \langle F_i | X \rangle = \text{tr} F_i X = 0 = \text{tr} F_i 0 \). However, IC then implies \( X = 0 \), which is a contradiction. The converse is trivial. \( \blacksquare \)
2. Proof of Lemma 3

Proof of Lemma 3. Conditions (i) and (ii) imply that $x_1 > 0$ and $x_d < 0$. To see this, assume contrary that $x_d \geq 0$, so that all $x_i \geq 0$. Then, $(\sum_i x_i)^2 - (\sum_i x_i^2) = \sum_{i \neq j} x_i x_j \geq 0$. On the other hand, by (i) and (ii), $(\sum_i x_i)^2 - (\sum_i x_i^2) = (\frac{1}{d} - \frac{1}{d}) = \frac{1}{d} > 0$. Thus we have a contradiction. Similar argument (by flipping the sign) shows $x_1 > 0$.

Let $a_i := \frac{\sqrt{n}}{\sqrt{d(d-1)}}(d^2 x_i - 1)$. It follows from (i) and (ii) that

\[(i)' \sum_i a_i = 0, \quad (ii)' \sum_i a_i^2 = 2.
\]

Similar to the above argument, $a_d < 0$ and one sees $|a_d| = \frac{\sqrt{n}}{\sqrt{d(d-1)}}(d^2 |x_d| + 1)$ (note that $x_d < 0$ implies $1 - d^2 x_d = d^2 |x_d| + 1$). Proposition 1-[I] in [33] shows

\[
|a_d| \geq \frac{2}{d(d-1)}. \tag{A1}
\]

Therefore, we have

\[
\frac{\sqrt{n}}{\sqrt{d(d-1)}}(d^2 |x_d| + 1) \geq \frac{2}{d(d-1)},
\]

from which we obtain (3). By Proposition 1-[III] in [33], (A1) is saturated, which implies (3) is saturated, iff

\[a_1 = \sqrt{\frac{2}{d-1}},
\]

\[a_2, a_3, \ldots, a_d = -\sqrt{\frac{2}{d(d-1)}},
\]

which imply that (8) and (9) hold.

3. Proof of (12)

Proof of (12). We denote by $m_i$ the minimum eigenvalue of $A_i$, which is strictly negative as is shown in the main text. Clearly, $-|m_k| = m_k \leq \tau \rho A_k$ for any $\rho \in S(\rho)$. Hence, we have $\tau = \max_i \{|m_i|\} \geq -\tau \rho A_k$ and thus $\tau = \max_i \{|m_i|\} \geq -\min_i \tau \rho A_k$. Since the positivity of $\tau$ trivially holds, this shows

\[
\frac{1}{d} N(\{A_i\}) \leq \tau.
\]

To prove the converse inequality, let $\rho_k = |\phi_k\rangle \langle \phi_k| \in S(H)$ where $|\phi_k\rangle$ is the unit eigenvector of $A_k$ corresponding to the minimum eigenvalue $m_k$. We have, for any $k$,

\[\min_i \text{tr } A_i \rho_k = \min_i \langle \phi_k | A_i | \phi_k \rangle \leq \langle \phi_k | A_k | \phi_k \rangle = m_k.
\]

Therefore, $\frac{1}{d} N(\{A_i\}) \geq \max \{0, -\min_i \text{tr } A_i \rho_k\} \geq -\min_i \text{tr } A_i \rho_k \geq -m_k = |m_k|$. Since this holds for any $k$, we have

\[
\frac{1}{d} N(\{A_i\}) \geq \tau.
\]

Appendix B: Orthogonal basis with a fixed sum

Let $\mathcal{K}$ be a $D$-dimensional real inner product space. In this appendix, we provide two constructions of an orthogonal basis $\{|\phi_i\rangle\}_{i=0}^{D-1}$ with constant norms, i.e., $\langle \phi_i | \phi_j \rangle = d \delta_{ij}$ ($c > 0$), as well as the fixed sum $\sum_{i=0}^{D-1} |\phi_i\rangle = |i\rangle$. Note that automatically $c = \frac{|||\rangle||^2}{D}$ since $||| \rangle \rangle^2 = \sum_i \langle \phi_i | \phi_j \rangle = \sum_{i,j} c \delta_{ij} = CD$. For our purpose to construct a COB, just apply $|i\rangle \mapsto |i\rangle$ where $\mathcal{K}$ is the real Hilbert space of Hermitian operators, noting that $||| \rangle \rangle = \sqrt{\bar{D}}$ and $D = d^2$.

Construction 1. With a given $|i\rangle$, prepare an orthonormal basis $\{|t_i\rangle\}_{i=0}^{D-1}$ where $|t_0\rangle = \frac{|i\rangle}{||| \rangle \rangle}$. Prepare also an orthogonal $D \times D$ real matrix $O = |O_{ij}|_{i,j=0}^{D-1}$ (i.e., $OO^T = O^T O = I$) such that

\[
O_{0i} = \frac{1}{\sqrt{D}} \quad (\forall i = 0, 1, \ldots, D - 1), \tag{B1}
\]

where $I$ is the $D \times D$ identity matrix. Then,

\[
|\phi_i\rangle := \frac{||| \rangle \rangle}{\sqrt{D}} \sum_{j=0}^{D-1} O_{ij} |t_j\rangle \quad (i = 0, 1, \ldots, D - 1) \tag{B2}
\]

gives the desired basis.

Indeed, since $O$ is an orthogonal matrix, one has $|t_i\rangle = \frac{||| \rangle \rangle}{\sqrt{D}} \sum_j O_{ij} |\phi_j\rangle$ so that the condition (B1) implies

\[
||| \rangle \rangle = ||| |t_0\rangle\rangle = \sum_j \sqrt{D} O_{0j} |\phi_j\rangle = \sum_j |\phi_j\rangle.
\]

The orthogonality of $|\phi_i\rangle$ is also satisfied by the orthogonality of $O$.

Note here that both $\{|t_i\rangle\}$, and $O$ can be easily constructed by using the Gram-Schmidt orthogonalization starting from $|i\rangle$ and $(1, 1, \ldots, 1)^T \in \mathbb{R}^D$, respectively.

Notice also that, conversely, any orthogonal basis $\{|\phi_i\rangle\}_{i=0}^{D-1}$ with a fixed sum $|i\rangle$ can be constructed in this way (with two alternatives (i) and (ii) below):

(i) Given arbitrary orthonormal basis $\{|t_i\rangle\}$ with $|t_0\rangle = \frac{|i\rangle}{||| \rangle \rangle}$, there exists an orthogonal matrix $O$ satisfying (B1) such that any orthogonal basis $\{|\phi_i\rangle\}_{i=0}^{D-1}$ with a fixed sum $|i\rangle$ is constructed by (B2) 1.

1 As $\{|t_i\rangle\}$, and $\{|\phi_i\rangle\}$ are both orthogonal basis, there exists an orthogonal matrix $O = |O_{ij}|$ which connects them: $|t_i\rangle = \frac{1}{\sqrt{D}} \sum_j O_{ij} |\phi_j\rangle$. Since $\frac{1}{\sqrt{D}} \sum_j |\phi_j\rangle = |t_0\rangle = \frac{1}{\sqrt{D}} \sum_j O_{0j} |\phi_j\rangle$, one has $O_{0j} = \frac{1}{\sqrt{D}}$ for all $j$. 

(ii) Given arbitrary orthogonal matrix $O$ satisfying (B1), there exists $\{ |t_i \rangle \}$, with $|t_0 \rangle = |o \rangle$, such that any orthogonal basis $\{ |\phi_i \rangle \}^{D-1}_{i=0}$ with a fixed sum $|i\rangle$ is constructed by (B2) \footnote{Let $O = [O_{ij}]$ be an orthogonal matrix satisfying (B1). Then it is straightforward to see $|t_i \rangle = \frac{\sqrt{D}}{D-1} \sum_j O_{ij} |\phi_j \rangle$ is the desired basis.}

The next construction is not general but uses only one orthonormal basis and is more concrete.

**Construction 2.** Prepare an orthonormal basis $\{ |t_i \rangle \}^{D-1}_{i=0}$ where $|t_0 \rangle = |o \rangle$. Construct an orthonormal basis $\{ |s_i \rangle \}^{D-1}_{i=0}$ by the Gram-Schmidt orthogonalization of the set $S = \{ |s\rangle, |t_1\rangle, \ldots, |t_{D-1}\rangle \}$ where $|s\rangle := \sum_j |t_j\rangle$ starting from $|s\rangle$.

Then, using the unitary operator $U = \sum_j |t_j\rangle \langle s_j |$, it is easy to see that

$$|\phi_i \rangle := \frac{\|t\|}{\sqrt{D}} U |t_i \rangle$$

(B3) gives a desired orthogonal basis. In particular, $\sum_i |\phi_i \rangle = \frac{\|t\|}{\sqrt{D}} U |s\rangle = \sum_i |t_i \rangle$ since $|s\rangle_0 = |\phi \rangle = \frac{1}{\sqrt{D}} \sum_i |t_i \rangle$.

Note that the linearly independence of the set $S$ is easily shown. The choice of the latter $D-1$ vectors in $S$ can be arbitrary from $\{ |t_i \rangle \}^{D-1}_{i=0}$. However, by the symmetric argument, one can show that the obtained orthonormal basis $\{ |s_i \rangle \}^{D-1}_{i=0}$ is independent on the choice.

One can continue this construction more concretely as follows. First, the direct computation of the Gram-Schmidt orthogonalization gives $|s_0 \rangle = \frac{1}{\sqrt{D}} \sum_j |t_j \rangle$ and

$$|s_i \rangle = \frac{(D-i)|t_i \rangle - \sum_{k \neq i} |t_k \rangle}{\sqrt{(D-i)(D-i-1)}} (1 \leq i \leq D-1).$$

Plugging this into (B3), one arrives at the COB given by

$$|\phi_0 \rangle = \frac{\|t\|}{D} \left( |t_0 \rangle - \sum_{j=1}^{D-1} f(j) |t_j \rangle \right)$$

$$|\phi_i \rangle = \frac{\|t\|}{D} \left( |t_0 \rangle - \sum_{j=1}^{i-1} f(j) |t_j \rangle + (D-i) f(i) |t_i \rangle \right) (i = 1, 2, \ldots, D-1)$$

where $f(j) = \sqrt{\frac{D}{(D-j)(D-j-1)}}$.

Finally, here are some examples of COBs. In $d = 2$, Construction 1 using $T_0 = 1/\sqrt{2} \mathbb{I}, T_1 = 1/\sqrt{2} \sigma_y, T_2 = 1/\sqrt{2} \sigma_y, T_3 = 1/\sqrt{2} \sigma_z$, and $O = \frac{\sqrt{D}}{D-1} \sum_j O_{ij} |\phi_j \rangle$ is the desired basis.

Thus, we have the following COB:

$$A_1 = \left( \frac{1}{\sqrt{2}}, \frac{1-i}{\sqrt{2}} \right) \cdot \left( \frac{1}{\sqrt{2}}, \frac{-1-i}{\sqrt{2}} \right), \quad A_2 = \left( 0, \frac{-1-i}{\sqrt{2}} \right),$$

$$A_3 = \left( \frac{1}{\sqrt{2}}, \frac{1+i}{\sqrt{2}} \right) \cdot \left( \frac{1}{\sqrt{2}}, \frac{-1+i}{\sqrt{2}} \right).$$

(B5)

Construction 2 using the above $\{T_i\}^3_{i=0}$ gives the following COB:

$$A_1 = \left( \frac{1}{\sqrt{2}}, \frac{1-i}{\sqrt{2}} \right) \cdot \left( \frac{1}{\sqrt{2}}, \frac{-1-i}{\sqrt{2}} \right),$$

$$A_2 = \left( \frac{1}{\sqrt{2}}, \frac{1+i}{\sqrt{2}} \right) \cdot \left( \frac{1}{\sqrt{2}}, \frac{-1+i}{\sqrt{2}} \right),$$

$$A_3 = \left( \frac{1}{\sqrt{2}}, \frac{1-i}{\sqrt{2}} \right) \cdot \left( \frac{1}{\sqrt{2}}, \frac{-1+i}{\sqrt{2}} \right).$$

(B5)

Construction 3 using $L_1^{(1)} = \{1, 2\}, L_2^{(1)} = \{3, 4\}, L_1^{(2)} = \{1, 3\}, L_2^{(2)} = \{2, 4\}, L_1^{(3)} = \{1, 4\}, L_2^{(3)} = \{2, 3\}$ and a complete set of MUBs which consists of the normalized eigenvectors of the Pauli matrices gives the same COB as (B5).

In $d = 2$, as mentioned in the proof of Proposition 6, all eigenvalues of $A_i \phi$ are the same $\frac{1+i\sqrt{3}}{\sqrt{3}}$. Therefore, we observe $\lambda^* = \frac{1}{\sqrt{2}} \mathbb{I}$ which saturates the upper bound.

In three or more dimensions, the matrix forms of COBs are more complex. For example, Construction 2 for $d = 3$ using the generalized Gell-Mann matrices (16) gives the following COB:
We numerically observed $\tau = 0.291347$ and $\lambda^* = 0.276081$ which cannot saturate the upper bound 0.5.

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