Quantum measurements with prescribed symmetry

Wojciech Bruzda
Institute of Physics, Jagiellonian University, 30-348, Kraków, Poland

Dardo Goyeneche
Institute of Physics, Jagiellonian University, 30-348, Kraków, Poland
and Faculty of Applied Physics and Mathematics, Technical University of Gdańsk, 80-233 Gdańsk, Poland

Karol Życzkowski
Institute of Physics, Jagiellonian University, 30-348, Kraków, Poland
and Center for Theoretical Physics, Polish Academy of Sciences, 02-668, Warsaw, Poland
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We introduce a method to determine whether a given generalized quantum measurement is isolated or if it belongs to a family of measurements having the same prescribed symmetry. The technique proposed reduces to solving a linear system of equations in some relevant cases. As a consequence, we provide a simple derivation of the maximal family of symmetric informationally complete positive operator-valued measure SIC-POVM in dimension 3. Furthermore, we show that the following remarkable geometrical structures are isolated, so that free parameters cannot be introduced: (a) maximal sets of mutually unbiased bases in prime power dimensions from 4 to 16, (b) SIC-POVM in dimensions from 4 to 16, and (c) contextual Kochen-Specker sets in dimension 3, 4, and 6, composed of 13, 18, and 21 vectors, respectively.

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I. INTRODUCTION

Positive operator-valued measure (POVM) is the most general kind of measurement in quantum mechanics, which generalizes projective measurements. Some POVMs having a prescribed symmetry play a crucial role in quantum mechanics: symmetric informationally complete (SIC)-POVM [1,2] and mutually unbiased bases (MUBs) [3,4]. These geometrical structures have important applications in quantum theory: SIC-POVM and MUBs allow us to unambiguously reconstruct any density matrix of size d [1,3] and define entropic uncertainty relations [5,6]. Even more, MUBs are important to detect entanglement [7] and bound entanglement [8], and to lock classical information in quantum states [9].

Finitely many SIC-POVMs are known in dimension $d \leqslant 64$ [10], including a one-parameter family in dimension 3 [1]. The existence of SIC-POVM with free parameters in dimension $d > 3$ is still an open problem. Moreover, maximal sets of MUBs are known to be isolated in dimensions 2–5 [11] and finitely many nonequivalent maximal sets of MUBs are known for dimensions 3–5 [12] and N qudit systems [13]. On the other hand, families of symmetric POVMs are useful for practical applications, as the parameters can be optimized for different convenient purposes. For example, from the one-parameter family of SIC-POVM existing in dimension 3 [1] only a single member maximizes the informational power, that is, the classical capacity of a quantum-classical channel generated by the SIC-POVM [14]. Furthermore, inequivalent sets of MUBs provide different estimation of errors in quantum tomography [15].

Highly symmetric quantum measurements, like SIC-POVM or MUBs, play an important role in quantum information and foundations of quantum theory. On the one hand, it is interesting itself to design a mathematical tool that allows one to construct a family of POVMs having a prescribed symmetry from a given particular solution. On the other hand, construction of such families of solutions provides flexibility when designing experimental implementations of these measurement sets. For instance, a detailed description of a complete list of solutions of a set of k MUBs in dimension d may be helpful in tackling the problem whether an extended set of $k+1$ MUBs exists. Furthermore, it is also interesting to highlight those quantum measurements having a prescribed symmetry that do not belong to a family, which makes them special. A possible application of such isolated cases is the existence of a unique solution optimizing a given function. For instance, isolated solutions might define sets of measurement having a unique maximal violation of a Bell inequality, which is a fundamental ingredient for *self-testing* [16].

In this work, we present a method to introduce free parameters in generalized measurements having a predefined geometrical structure. The method proposed divides the entire nonlinear problem, called $\mathcal{P}_{NL}^{(1)}$, into a linear problem $\mathcal{P}_{L}^{(2)}$ and a secondary nonlinear problem $\mathcal{P}_{NL}^{(3)}$, which is simpler than $\mathcal{P}_{NL}^{(1)}$. Remarkably, in some cases the linear problem $\mathcal{P}_{L}^{(2)}$ provides a definite answer to the full problem $\mathcal{P}_{NL}$.

The paper is organized as follows: In Sec. II we establish a connection between any given POVM and certain Hermitian unitary matrices having constant diagonal.

In Sec. III we apply the notion of a defect of a unitary matrix to identify isolated cases of generalized quantum measurements having a prescribed symmetry, for which no free parameters can be introduced. Furthermore, in other cases we present a constructive method to extend known solutions to an entire family by introducing free parameters.

In Sec. IV we show that known maximal sets of MUBs in dimensions 4, 8, 9, and 16 and known SIC-POVMs in dimensions 4–16 are isolated. We also study the robustness of our results for a given accuracy in specifying the POVM, which allows us to derive conclusive results from approximate solutions. In Sec. V we find an upper bound for the maximal number of free parameters that can be introduced in sets of $2 \leqslant m \leqslant d+1$ MUBs in dimension d and in some classes of equiangular tight frames. Moreover, we show how the method works to give the known one-parameter families of SIC-POVMs in dimension 3. In Sec. VI we prove that some existing Kochen-Specker sets from quantum contextuality are isolated. In Sec. VII we summarize our results and pose open questions.

II. QUANTUM MEASUREMENTS AND TIGHT FRAMES

A POVM $\{\Gamma_j\}$ is a set of N positive-semidefinite subnormalized operators defined in dimension d such that $\sum_{j=0}^{N-1}\Gamma_j = \mathbb{I}_d$, where $\mathbb{I}_d$ is the identity matrix of size d. Throughout the work, we restrict our attention to rank-1 POVMs and consider rank-1 projectors Π_j, being proportional to the elements of POVM; that is, $\Pi_j = c\Gamma_j$, where $c = N/d$. For simplicity, we refer to the set of projectors $\{\Pi_j\}$ as a POVM, understanding that they are formally proportional to the elements of a POVM. The rank-1 projectors Π_j satisfy the geometrical relation

$$\mathrm{Tr}(\Pi_i\Pi_j) = S_{ij}, \tag{1}$$

where S is a real symmetric matrix of size N. It is interesting to ask about the most general projectors having the prescribed symmetry (1) given by a real symmetric matrix S. For example, the case $S = \mathbb{I}_N + \frac{N-d}{d(N-1)}(\mathbb{J}_N - \mathbb{I}_N)$ corresponds to equiangular tight frames composed of N vectors in dimension d. Here, $\mathbb{J}_N$ denotes the matrix of size N having all entries equal to unity. We recall that a set of N vectors $\{|\phi_i\rangle\}$ defined in dimension d forms an equiangular tight frame (ETF) if $|\langle\phi_i|\phi_j\rangle|^2 = d(N-1)/(N-d)$, for every $i \neq j = 0,\ldots,d^2-1$.

A remarkably important subclass of ETF is given by the so-called SIC-POVM [1], corresponding to the case $N = d^2$. Also, two orthonormal bases $|\phi_i\rangle$ and $|\psi_j\rangle$ in dimension d define a pair of MUBs if $|\langle\phi_i|\psi_j\rangle|^2 = 1/d$, for every $i,j = 0,\ldots,d-1$. A set of m orthonormal bases is mutually unbiased if every pair of the set is mutually unbiased. Also, a set of m MUBs in dimension d has associated the symmetric matrix $S = \mathbb{I}_{dm} + \frac{1}{d}(\mathbb{J}_m - \mathbb{I}_m)\otimes\mathbb{J}_d$. For a recent review on discrete structures in Hilbert spaces, including MUBs and SIC-POVM, see Ref. [17].

Let us recall a close connection existing between POVM and *tight frames*. A set of rank-1 projectors $\{\Pi_j\}$ defines a tight frame if there exists a real number $A > 0$ such that $\sum_{j=0}^{N-1}\mathrm{Tr}(\Omega\Pi_j) = A\,\mathrm{Tr}(\Omega^2) = A$, for any rank-1 projector Ω acting on dimension d. Therefore, POVMs are tight frames for $A = c$. A crucial property for our work is the fact that the Gram matrix associated to a tight frame, or POVM, is closely related to an Hermitian unitary matrix, as we see in Proposition 1. We recall that the Gram matrix of a set of N vectors $|\phi_j\rangle$ is given by

$$G_{ij} = \langle\phi_i|\phi_j\rangle, \tag{2}$$

where $i,j = 0,\ldots,N-1$. For example, the Gram matrix of an equiangular tight frame composed of N vectors in dimension d has the form

$$G_{\mathrm{ETF}} = \begin{pmatrix} 1 & re^{i\alpha_{12}} & \cdots & re^{i\alpha_{1N}} \\ re^{-i\alpha_{12}} & 1 & \cdots & re^{i\alpha_{2N}} \\ \vdots & \vdots & \ddots & \vdots \\ re^{-i\alpha_{1N}} & re^{-i\alpha_{2N}} & \cdots & 1 \end{pmatrix}, \tag{3}$$

where $r^2 = d(N-1)/(N-d)$. Furthermore, the Gram matrix of a set of $m+1$ MUBs $\{\mathbb{I}_d, H_1, H_2, \ldots, H_m\}$ in dimension d is given by

$$G_{\mathrm{MUB}} = \begin{pmatrix} \mathbb{I}_d & H_1 & H_2 & \cdots & H_m \\ H_1^\dagger & \mathbb{I}_d & H_1^\dagger H_2 & \cdots & H_1^\dagger H_m \\ H_2^\dagger & H_2^\dagger H_1 & \mathbb{I}_d & \cdots & H_2^\dagger H_m \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ H_m^\dagger & H_m^\dagger H_1 & H_m^\dagger H_2 & \cdots & \mathbb{I}_d \end{pmatrix}, \tag{4}$$

where $H_1, H_2, \ldots, H_m$ are suitable unitary complex Hadamard matrices, so that $H_iH_i^\dagger = \mathbb{I}$ and $|(H_i)_{jk}|^2 = 1/d$ for every $j,k = 0,\ldots,N-1$ and $i = 1,\ldots,m$; see Ref. [18]. Let us establish a connection between Gram matrices of POVM and a special kind of unitary Hermitian matrices.

Proposition 1. Let Π_j be a rank-1 POVM composed of N vectors in dimension d and G be the corresponding Gram matrix. Then, the matrix $U = \mathbb{I}_N - \frac{2d}{N}G$ is unitary.

Proof. A Gram matrix G represents a POVM composed of N vectors in dimension $d \leqslant N$ if and only if $G^2 = \frac{N}{d}G$ (cf. Proposition 1 in Ref. [19]). From this property and taking into account that $\mathrm{Tr}(G) = N$, the spectrum of G satisfies

$$\lambda(G) = (\underbrace{N/d,\ldots,N/d}_{d}, \underbrace{0,\ldots,0}_{N-d}). \tag{5}$$

Therefore, $U = \mathbb{I}_N - \frac{2d}{N}G$ is a unitary matrix. ■

From Proposition 1 we realize that the existence of a POVM with a symmetry prescribed by the matrix S from Eq. (1) is equivalent to prove the existence of a unitary Hermitian matrix U having positive constant diagonal $U_{ii} = 1 - 2d/N$ and satisfying $|U_{ij}| = \frac{2d}{N}\sqrt{S_{ij}}$ for $i \neq j$. Unitary matrices $U = \mathbb{I}_N - \frac{2d}{N}G$ have been recently studied for the particular case of equiangular tight frames [20]. In the Bloch sphere associated to a one-qubit system we have some relevant geometrical structures: the orthonormal basis (line), three MUBs (three orthogonal lines), and SIC-POVM (tetrahedron). All these structures are unique, up to a global rotation. In higher dimensions, however, some geometrical structures allow one to introduce free parameters, which cannot be absorbed in a global rotation. In Sec. III we introduce the method which considerably simplifies the study of this problem.

III. RESTRICTED DEFECT AND FREE PARAMETERS

In this section, we derive the method to introduce the maximal possible number of free parameters into a given POVM composed by N vectors in dimension d associated to a given symmetric matrix S; see Eq. (1). Using Proposition 1, this problem is equivalent to finding the most general real antisymmetric matrix R of size N such that

$$V_{ij}(t) = U_{ij}e^{itR_{ij}} \tag{6}$$

is a unitary matrix, provided that $U = \mathbb{I}_N - \frac{2d}{N}G$ is associated to a given particular POVM satisfying Eq. (1); that is, U is an Hermitian unitary matrix having constant diagonal $U_{ii} = 1 - 2d/N$ and $|U_{ij}| = \delta_{ij} - \frac{2d}{N}\sqrt{S_{ij}}$. Note that we have introduced a parameter t in Eq. (6) for convenience, which can be set to $t = 1$ after applying our method. The full problem is given as follows:

Problem $\mathcal{P}_{NL}^{(1)}$. Find the most general matrix $V_\tau(t)$ of size N of the form of Eq. (6), initially depending on τ parameters, such that

$$V_\tau(t)V_\tau(t)^\dagger = \mathbb{I}_N. \tag{7}$$

This problem implies solving a system of nonlinear coupled equations, which depends on $\tau = [N(N-1)/2 - z] - (N-1)$ nontrivial variables, where z is the number of zeros existing in the strictly upper triangular part of the matrix R. Note that τ is composed of the total number of parameters R_{ij}, i.e., $N(N-1)/2 - z$, minus the number of trivial variables $(N-1)$. These trivial parameters can be absorbed by applying the transformation $V \to EVE^\dagger$, where $E = \mathrm{Diag}(1, e^{itR_{01}}, \dots, e^{itR_{0(N-1)}})$. In order to simplify the resolution of problem $\mathcal{P}_{NL}$ we define the following linear problem:

Problem $\mathcal{P}_{L}^{(2)}$. Find the most general matrix $V_\tau(t)$ of size N, initially depending on τ parameters, such that

$$\lim_{t\to 0}\frac{d}{dt}[V_\tau(t)V_\tau(t)^\dagger] = 0. \tag{8}$$

Using Eq. (6), we can explicitly write Eq. (8) as

$$-2V_{k,k}V_{k,j}R_{j,k} + \sum_{l\neq j,k} V_{k,l}V_{l,j}(R_{k,l} - R_{j,l}) = 0, \tag{9}$$

for $1 \leqslant j < k \leqslant N$ and $1 \leqslant l \leqslant N$, which is a linear problem on variables R_{ij}. Note that $\mathcal{P}_L^{(2)} \subset \mathcal{P}_{NL}^{(1)}$, as Eq. (8) is a necessary condition to obtain Eq. (7).

The linear problem $\mathcal{P}_L^{(2)}$ allows us to simplify the full problem $\mathcal{P}_{NL}$ by determining r out of τ variables R_{ij}, where r is the number of linearly independent equations (9). After solving $\mathcal{P}_L^{(1)}$, the remaining number of free parameters R_{ij} lead us to the definition of the *restricted defect* Δ of the Hermitian unitary matrix U. It reads

$$\Delta = \tau - r, \tag{10}$$

where $\tau = (N-1)(N-2)/2 - z$ and z is the number of zeros existing in the strictly upper triangular part of the matrix U. Note that this quantity is closely related to the defect of a unitary matrix [21], adapted to the case of matrices with a special structure. The standard defect was used to define an upper bound on the number of free parameters allowed by complex Hadamard matrices [18] and forms, by construction, an upper bound for the restricted defect. In both cases, the defect equal to zero implies that a given solution is isolated, so no free parameters can be introduced.

In general, the restricted defect represents an upper bound for the maximal number of free parameters allowed by the full problem $\mathcal{P}_{NL}$. If $\Delta = 0$, then the full problem $\mathcal{P}_{NL}$ is solved by the linear problem $\mathcal{P}_L^{(1)}$. In this case, it is not possible to introduce free parameters into the matrix V. On the other hand, if $\Delta > 0$, it is necessary to solve an additional nonlinear problem in order to determine the continuous family of solutions.

Problem $\mathcal{P}_{NL}^{(3)}$. Find the most general matrix $V_\Delta(t)$ of size N, initially depending on Δ parameters, such that

$$V_\Delta(t)V_\Delta(t)^\dagger = \mathbb{I}_N. \tag{11}$$

Note that problem $\mathcal{P}_{NL}^{(2)}$ is simpler than problem $\mathcal{P}_{NL}$ as $\Delta < \tau$. This is so because $r > 0$ in Eq. (10). After solving problem $\mathcal{P}_{NL}^{(2)}$ we can assume that $t = 1$, without loss of generality. In Sec. IV we apply our results to SIC-POVM and maximal sets of MUBs.

Let us first illustrate the method in action by considering two MUBs for a single-qubit system: $|\phi_i\rangle = |i\rangle$, $i = 0,1$, and $|\psi_\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$. The Gram matrix (4) associated to this set of $m = 2$ MUBs is given by

$$G_{\mathrm{MUB}} = \frac{1}{2}\begin{pmatrix} 2 & 0 & 1 & 1 \\ 0 & 2 & 1 & -1 \\ 1 & 1 & 2 & 0 \\ 1 & -1 & 0 & 2 \end{pmatrix}. \tag{12}$$

A family of two MUBs stemming from this fixed set would have associated a Gram matrix of the form

$$G_{\mathrm{MUB}} = \frac{1}{2}\begin{pmatrix} 2 & 0 & e^{itR_{13}} & e^{itR_{14}} \\ 0 & 2 & e^{itR_{23}} & -e^{itR_{24}} \\ e^{-itR_{13}} & e^{-itR_{23}} & 2 & 0 \\ e^{-itR_{14}} & -e^{-itR_{24}} & 0 & 2 \end{pmatrix}, \tag{13}$$

and, from Proposition 1, the unitary matrix $U = \mathbb{I}_N - \frac{2d}{N}G_{\mathrm{MUB}}$. Note that the full problem $\mathcal{P}_{NL}^{(1)}$ initially depends on $\tau = 1$ nontrivial parameter, as R_{13}, R_{14}, and R_{23} can be absorbed by considering the diagonal unitary operator $E = \mathrm{diag}[1, e^{-iR_{23}}, e^{iR_{13}}, e^{iR_{14}}]$ and the redefinition $V \to EVE^\dagger$. Therefore, according to Eq. (6), and after considering the diagonal transformation E, we find that

$$V_\tau(t) = \frac{1}{2}\begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -e^{itR_{24}} \\ 1 & 1 & 0 & 0 \\ 1 & -e^{-itR_{24}} & 0 & 0 \end{pmatrix}. \tag{14}$$

Problem $\mathcal{P}_L^{(2)}$ implies the following equation:

$$R_{24} = 0, \tag{15}$$

where $r = 1$ and, therefore, $\Delta = 0$. Thus, we cannot introduce free parameters in Eq. (14), which implies that the considered pair of MUBs is isolated. Indeed, $|\phi_i\rangle = |i\rangle$, $i = 0,1$, and $|\psi_\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$ is the unique pair of MUBs existing in dimension 2, up to a global rotation [11].

IV. ISOLATED MUB AND SIC-POVM

In this section, we study the problem of introducing free parameters in MUB and SIC-POVM. Our first main result consists in proving that maximal sets of MUBs exist in low prime power dimensions.

Proposition 2. Maximal sets of $d + 1$ MUBs in dimensions $d = 4$, 8, 9, and 16 are isolated.

The results arises as follows. The upper triangular part of the Gram matrix associated to a set of m MUBs in dimension d contains $z = md(d-1)/2$ zero entries. Given that the size of the Gram matrix of the set is $N_{\rm MUB} = md$ and $m = d + 1$ we have $z = d(d^2 - 1)/2$. Therefore, the matrix G contains $\tau = (N_{\rm MUB} - 1)(N_{\rm MUB} - 2)/2 - z$ parameters. The next step consists in determining how many of these parameters are remaining after solving the linear problem $\mathcal{P}_L^{(1)}$. To this end, we calculated the number of linearly independent equations of the linear system defined in Eq. (9) for the cases $d = 4, 8, 9$, and 16, finding $r_4 = 141$, $r_8 = 2233$, $r_9 = 3556$, and $r_{16} = 34545$, respectively. By using these results and Eq. (10) we find that the restricted defect Δ vanished in all these cases. We based our calculation of the restricted defect Δ on the maximal sets of MUBs provided in Refs. [4,12]. In dimension $d = 9$, we considered Ref. [22] to obtain simpler expressions of results presented in Ref. [4].

Let us now consider the case of SIC-POVM. It is well known that SIC-POVM for a qubit system is essentially unique, as it represents the regular tetrahedron inscribed into the Bloch sphere, up to a global rotation. Furthermore, single-parameter families of SIC-POVM for a qutrit system exist [1], which represents the most general solution [23]. For higher dimensions, the problem of introducing free parameters in SIC-POVM is still open. As a preliminary result, exhaustive numerical simulations indicate that free parameters cannot be introduced in SIC-POVM, at least in low dimensions higher than three. For this problem, we have solved the linear problem $\mathcal{P}_L^{(1)}$ in dimensions $d = 4, \ldots, 16$, obtaining the following results.

Proposition 3. SIC-POVMs in dimensions $d = 4, \ldots, 16$ are isolated.

This result also includes the *Hoggar lines* [24], a special class of SIC-POVM defined in dimension $d = 8$. We considered the total number of parameters $\tau = (N_{\rm SIC} - 1)(N_{\rm SIC} - 2)/2$, as there is no pair of orthogonal vectors in SIC-POVM ($z = 0$), and $N_{\rm SIC} = d^2$. In order to prove Proposition 3 we solved the linear problem $\mathcal{P}_L^{(1)}$ for both analytical [24–28] and highly accurate numerical SIC-POVMs [10]. In all the cases we have found $\Delta = 0$, which implies that free parameters cannot be introduced. Calculations of the restricted defect have been done in MATLAB.

Let us now study the robustness of the restricted defect Δ under the presence of inaccuracies in describing the POVM. Given the set of vectors $\{\phi_j\}$ defined in Eq. (2) we quantify the inaccuracy in approximate vectors $\{\phi'_j\} \approx \{\phi_j\}$ by introducing the inaccuracy factor:

$$s = \frac{1}{\sqrt{d}} \max_j \|\phi'_j - \phi_j\|. \tag{16}$$

The factor s_μ quantifies the maximal allowed inaccuracy in entries of vectors ϕ_j. For example, in the case of approximate solutions $\{\phi'_j\}$ having k digits of precision we have $s \approx 10^{-k}$. In our study of robustness of the defect Δ, we simulate the introduction of inaccuracies by considering

$$(\phi'_j)_i = (\phi_j)_i + s\xi_i, \tag{17}$$

where $(x)_i$ denotes the ith entry of the vector x and ξ_i are random numbers uniformly distributed in the interval $[-1,1]$.

Let us assume that $\mathcal{R}$ is the real matrix associated to the linear system of equations (9). Note that the number of linearly independent equations of such a system is given by $\text{rank}(\mathcal{R}) = r$. When considering inaccuracies in the POVM the rank of the perturbed matrix $\mathcal{R}'$ and $\mathcal{R}$ may differ. Therefore, we need to study how much the singular values of $\mathcal{R}'$ are affected under the presence of inaccuracies. In particular, we are interested in the perturbation of the two smallest singular values $\sigma_0 = 0$ and $\sigma_1 > 0$, which are responsible for the variation of the rank. In order to obtain a confidence region for the restricted defect (10) we need to consider the following two bounds: (i) an upper bound for the maximal perturbation of σ_0 and (ii) a lower bound for the maximal perturbation of σ_1. In Appendix we show that

$$|\sigma'_i - \sigma_i| \leqslant f(d,N)\,s \tag{18}$$

for $i = 0,1$, where s is the inaccuracy quantifier defined in Eq. (16) and

$$f(d,N) = \frac{2^6 d^2}{N}\left(1 - \frac{2d}{N}\right)^2 \sqrt{\frac{N-d}{N(N-1)}} \tag{19}$$

for $N > 2d$. Let us now find the smallest possible value of s such that the critical condition $\sigma'_0 = \sigma'_1$ holds, which imposes an upper bound for the confidence region of the restricted defect Δ. By considering Eq. (18) we find that Δ does not change its value for $0 \leqslant s \leqslant s_{\max}$, where $s_{\max} = \sigma_1(2f(d,N))^{-1}$. Note that σ_1 depends on the exact solution, which is not known if the exact solution is not available. By using Eq. (18) we find that $\sigma_1 \leqslant \sigma'_1 + f(d,N)\,s$, which implies

$$s_{\max} \leqslant \frac{\sigma'_1 + f(d,N)\,s}{2f(d,N)}. \tag{20}$$

Note that this inequality provides a confidence region only if $f(d,N)\,s \ll 1$.

Confidence regions for SIC-POVM and maximal sets of MUBs for two and three qubits are depicted in Figs. 1 and 2, respectively. For the case of four-qubit systems we

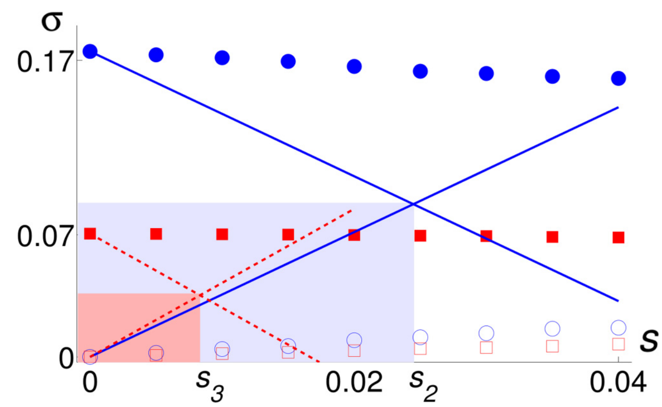

FIG. 1. Smallest singular values σ_0 and σ_1 of $\mathcal{R}$ as a function of the inaccuracy factor s for SIC-POVM. Open and solid symbols represent σ_0 and σ_1, respectively, for two- (○) and three-qubit (□) systems. Each case is averaged over eight samples randomly chosen and generated from the approximate SIC-POVM provided in Ref. [10], which has accuracy $s = 1 \times 10^{-32}$. The confidence regions (blue and red rectangles) are given by values of s existing between zero and the value determined by the intersection of the lower and upper bounds. Here, s_2 and s_3 stand for two- and three-qubits systems, respectively. Outside the confidence regions it is not possible to discriminate between singular values σ_0 and σ_1.

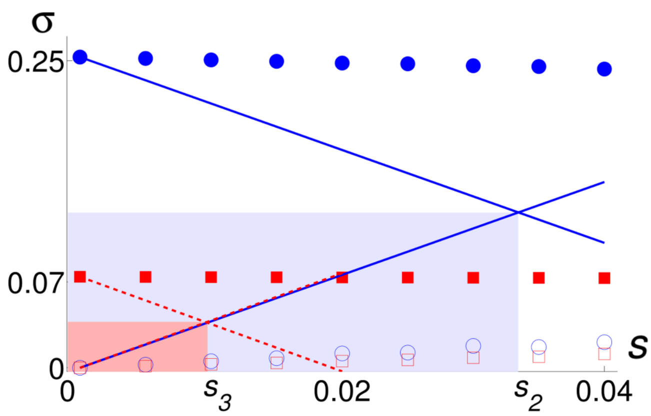

FIG. 2. Smallest singular values σ_0 and σ_1 of $\mathcal{R}$ as a function of the inaccuracy factor s for maximal sets of MUBs. Open and solid symbols represent σ_0 and σ_1, respectively, for two- (○) and three-qubit (□) systems. Each case is averaged over eight samples randomly chosen and generated from analytic solutions.

have solutions with precision $s = 1\times10^{-32}$, whereas the upper bound for the confidence region is $s_4 \approx 4\times10^{-3}$. For MUBs, we calculated the restricted defect Δ by considering analytic solutions in all the cases [4,12,22].

V. FREE PARAMETERS IN MUB AND SIC-POVM

In Sec. IV we prove that some maximal sets of MUBs and SIC-POVMs are isolated in low dimensions. In this section, we first calculate the restricted defect for sets of $m = 2,\dots,d+1$ MUBs in dimensions $d = 2,\dots,8$ (see Table I). Interestingly, the restricted defect for a pair of MUBs B_1 and B_2 coincides with the standard defect of the complex Hadamard matrix $H = B_1^\dagger B_2$. Indeed, the maximal number of free parameters that can be introduces in the Gram matrix

$$G_{\rm MUB} = \begin{pmatrix} \mathbb{I}_d & H \\ H^\dagger & \mathbb{I}_d \end{pmatrix} \tag{21}$$

coincides with the maximal number of parameters that can be introduced in H. Let us explain some details concerning Table I. First, note that $\Delta = 0$ for every subset of $2 \leqslant m \leqslant d+1$ MUBs in prime dimensions $d = 2,3,5,7$. This is so because every complex Hadamard matrix involved in the set is equivalent to the Fourier matrix, which is isolated in prime dimensions [18]. For triplets in dimension 4, we have $\Delta = 3$, which coincides with the maximal number of free parameters that can be introduced [11]. The number of generic restricted defects for a pair of MUBs in dimension 6 is four, coinciding with the generic defects of complex Hadamard matrices of size 6 [21]. However, note that there is an exceptional pair of MUBs for which $\Delta = 0$, as an isolated complex Hadamard matrix of size 6 exists [29]. Generic defects for triplets of MUBs are not well understood (⋄); see Table I and Ref. [30].

In dimensions 8 and 9 we restricted our attention to subsets of MUBs arising from the maximal sets defined in Refs. [4,12]. Note that subsets of $m \geqslant 6$ MUBs are isolated in dimension 8, whereas several families of $m = 5$ MUBs exist [31]. Another observation is that the restricted defect Δ for maximal sets of $d+1$ MUBs in dimension d coincides with the defect for d MUBs. This is so because the $(d+1)$th MUB is univocally determined by the first d MUBs. For subsets of $m < d$, the restricted defect for m MUBs may depend on the subset chosen. However, results presented in Table I are consistent for every subset of MUB.

We also studied the restricted defect for equiangular tight frames composed of $N = k^2$ vectors in dimension $d = k(k-1)/2$, typically denoted as ETF(d,N) [32]. These ETFs have associated the following Hermitian unitary matrices [20]:

$$U_{i_1+ki_2+1,\,j_1+kj_2+1} = \omega^{i_1 j_2 - j_1 i_2}, \tag{22}$$

where $i_1,i_2,j_1,j_2 \in \{0,\dots,k-1\}$ and $\omega = e^{2\pi i/k}$. Matrix (22) is equivalent to the tensor product of Fourier matrices, $F_k \otimes F_k$, where $(F_k)_{st} = \omega^{st}$. Table II summarizes the restricted defect for matrix U in low dimensions. Results are shown in Table II. For prime values of k, the formula

$$\Delta = \tfrac{1}{2}(k+1)(k-1)(k-2) \tag{23}$$

matches all solutions presented in Table II, so we are tempted to believe that it holds for any prime k.

Let us now study the SIC-POVM problem in dimension $d = 3$. By considering the fiducial state $|\phi_{00}\rangle = (1,-1,0)/\sqrt{2}$ a

TABLE I. Upper bound on the maximal number of free parameters Δ allowed by subsets of m MUBs in dimension d. The results do not depend on selecting m subsets of MUBs out of the full set of $d+1$ MUBs. As a remarkable observation, maximal sets of MUBs are isolated. Also, subsets of $m \geqslant 6$ in dimension 8 and $m \geqslant 5$ MUBs in dimension 9 are isolated in all the cases. Question marks denote our lack of knowledge about given number of MUB, while ⋄ indicates the case of three MUBs in dimension 6, which is still considered unresolved.

$m \setminus d$	2	3	4	5	6	7	8	9
2	0	0	3	0	4	0	21	16
3	0	0	3	0	⋄	0	27	20
4		0	0	0	?	0	19	32
5			0	0	?	0	7	0
6				0	?	0	0	0
7					?	0	0	0
8						0	0	0
9							0	0
10								0

TABLE II. Maximal number of free parameters that can be introduced in ETF composed by $N = k^2$ vectors in dimension $d = k(k-1)/2$. The case $k = 2$ corresponds to an ETF(3,4) which is isolated (regular simplex in dimension 3). Also, $k = 3$ has associated a SIC-POVM in dimension 3, where $\Delta = 4$ but only two-parameter families exist [1]. For the case $k = 4$ there exists several six-parameter families of ETF(6,16) [20].

k	Δ	k	Δ	k	Δ
2	0	7	120	12	1237
3	4	8	273	13	924
4	21	9	352	14	1632
5	36	10	576		
6	112	11	540		

SIC-POVM is given by [25]

$$|\phi_{st}\rangle = X^s Z^t |\phi_{00}\rangle, \tag{24}$$

where $X|j\rangle = |[j \oplus 1]\rangle$, $Z|j\rangle = \omega^j |j\rangle$, $\omega = e^{2\pi i/3}$, and $\oplus$ means addition modulo 3. The 9×9 Gram matrix G_{SIC} of the SIC-POVM and its associated unitary matrix $U = \mathbb{I}_N - \frac{2d}{N} G_{\mathrm{SIC}}$ depends on $\tau = 36 - 8 = 28$ parameters, where the $N - 1 = 8$ trivial parameters $R_{1,j}$ for $j = 2,\dots,9$ have been set as zero. The linear system of equations (8) associated with problem $\mathcal{P}_L^{(1)}$ has $r = 24$ linearly independent equations, which provides a four-dimensional complex set of solutions R_{ij}, depending on four parameters: R_{23}, R_{26}, R_{48}, and R_{89}. The additional restriction to have real parameters implies

$$R_{23} - 3R_{89} = R_{23} - 3R_{26} = R_{89} - R_{26} = 0,$$

which is equivalent to $R_{26} = R_{89} = R_{23}/3$. After setting $t = 1$, we obtain three solutions to problem $\mathcal{P}_L^{(1)}$: $V_\Delta(R_{23},R_{48})$, $V_\Delta(R_{26},R_{48})$, and $V_\Delta(R_{89},R_{48})$. Now, we are in position to solve the nonlinear problem $\mathcal{P}_{NL}^{(2)}$, which is much simpler than the full nonlinear problem $\mathcal{P}_{NL}$. Indeed, $\mathcal{P}_{NL}^{(2)}$ implies solving trivial trigonometric equations, which give us the solutions $R_{26} \in \{0,\pi\}$, $R_{89} \in \{0,\pi\}$, and $R_{23} \in \{0,\pi\}$, respectively. Therefore, we generate six one-parameter families of SIC-POVM in dimension 3:

$$\begin{aligned} &\mathcal{S}_1 : V_\Delta(R_{23} = 0, R_{48}), \quad \mathcal{S}_2 : V_\Delta(R_{23} = \pi, R_{48}), \\ &\mathcal{S}_3 : V_\Delta(R_{26} = 0, R_{48}), \quad \mathcal{S}_4 : V_\Delta(R_{26} = \pi, R_{48}), \\ &\mathcal{S}_5 : V_\Delta(R_{89} = 0, R_{48}), \quad \mathcal{S}_6 : V_\Delta(R_{23} = \pi, R_{48}). \end{aligned} \tag{25}$$

Here we note that $\Delta = 4$ and six one-parameter real solutions exist. These six solutions belong to the four-dimensional tangent plane defined by Eq. (8) and do not fit into a lower-dimensional tangent space, which explains why Δ cannot take a lower value. Furthermore, solutions (25) are equivalent, in the sense that we can transform one into the other by applying a permutation of rows or columns and multiplication of diagonal unitary operations to the Gram matrix, which is equivalent to relabeling and applying global phases to vectors. Solution (25) represents the most general SIC-POVM existing in dimension 3 [23], up to equivalence. We remark that the generic Hermitian defect for a SIC-POVM in dimension 3 is $\Delta = 2$, with the only exception of the particular vector $|\phi_{00}\rangle$, where $\Delta = 4$; however, from this fact we cannot define a larger family.

VI. ISOLATED KOCHEN-SPECKER SETS

In this section, we apply our method presented in Sec. III to show that some sets of vectors used in a proof of the Kochen-Specker contextually theorem [33], typically called KS sets, are isolated.

KS sets are collections of N vectors in dimension d, which contain m subsets of d vectors forming orthonormal basis. Some of these orthonormal bases have common vectors, so that $N < md$. These intersections are crucial to prove that a deterministic local hidden variable theory is not possible [33]. That is, for a system prepared in a quantum state ρ and a set of KS vectors $\{\phi_0,\dots,\phi_{N-1}\}$ it is not possible to end up with N deterministic probabilities $P_k = \mathrm{Tr}(\rho|\phi_k\rangle\langle\phi_k|) \in \{0,1\}$, for $k = 0,\dots,N-1$. Therefore, the assumption of hidden determinism in quantum mechanics implies that predefined values of observables depend on the context in which measurements were implemented. The original proof given by Kochen and Specker involves $N = 117$ vectors in dimension $d = 3$ [33]. Subsequently, examples exhibiting a lower number of vectors were found. Some remarkable examples are KS sets composed of $N = 13$ vectors in dimension $d = 3$ [34], $N = 18$ vectors in dimension $d = 4$ [35], and $N = 21$ vectors in dimension $d = 6$ [36].

TABLE III. Isolated KS sets composed of 13 vectors in dimension 3, 18 vectors in dimension 4, and 21 vectors in dimension 6. The number of zeros (z) appearing into the upper triangular part of the Gram matrix of the KS set, total number of parameters (τ), rank of the linear system defined in Eq. 8 (r), and restricted defect ($\Delta = \tau - r$) are defined in Sec. III. For these three KS sets the free parameters produced by a positive restricted defect Δ can be absorbed as global phases of the vectors.

N	d	z	τ	r	Δ	No. free parameters
13	3	24	78	66	12	0
18	4	63	90	83	7	0
21	6	105	105	103	2	0

Let us now apply our method to prove that these three inequivalent KS sets are isolated. The first important observation is that the three KS sets form three POVMs. This means that Proposition 1 holds for these sets and, therefore, the method to introduce free parameters presented in Sec. III can be applied. In order to do so we have to calculate the restricted defect Δ defined in Eq. (10), which is a function of the total number of parameters τ and the number of linearly independent equations associated to problem $\mathcal{P}_{\mathbf{L}}^{(\mathbf{2})}$ (see Sec. III). The geometrical structure is determined by the orthogonality restrictions imposed by the KS sets. For the above-mentioned three KS sets we have shown that they are isolated. The way to proceed is similar to the proof that maximal sets of MUBs or SIC-POVMs are isolated (see Proposition 2). However, there is a minor additional remark: the sets are isolated despite that the restricted defect Δ of the sets is nonzero. This is so because the apparently remaining Δ free parameters can be absorbed by considering a sequence of nontrivial emphasing in the Gram matrices, which means that the free parameters can be absorbed as global phases of the KS vectors. Table III resumes the details of our calculations.

VII. CONCLUSION

We studied the problem to introduce free parameters in a given POVM having prescribed symmetry, where mutually unbiased bases (MUBs) and symmetric informationally complete-positive operator-valued measurement (SIC-POVM) are relevant examples (see Sec. II). In particular, our method allows us to determine whether a given quantum t design having prescribed symmetry [25] forms an isolated structure. We introduced a powerful method that divides this fully nonlinear problem into a linear problem and a simpler nonlinear problem (see Sec. III).

Using our method, we proved that known maximal sets of MUBs in dimensions 4, 8, 9, and 16 and known SIC-POVM in dimensions 4–16 are isolated. In particular, a special class of SIC-POVM existing for three-qubit systems, called Hoggar lines, is isolated (see Sec. IV). Moreover, we calculated an upper bound for the maximal number of free parameters that can be introduced in subsets of $2 \leqslant m \leqslant d+1$ MUBs in dimensions $d = 2$–9 (see Sec. V). The same study has been done for equiangular tight frames in low dimensions, which define equiangular POVM (see Table II).

As a further result, we studied the robustness of our method under the presence of inaccuracies in defining the generalized measurement, which allowed us to establish a confidence region for the maximal possible number of free parameters that can be introduced (see Sec. IV). The importance of robustness relies on the fact that some geometrical structures, like SIC-POVM, are established analytically in low dimension only, whereas accurate numerical solutions exist in every dimension $d \leqslant 121$ and also in $d = 124$, 143, 147, 168, 172, 195, 199, 228, 259, and 323 [10,37].

Additionally, we proved that three Kochen-Specker contextuality sets are isolated (see Sec. VI). Namely, 13 vectors in dimension 3 [34], 18 vectors in dimension 4 [35], and 21 vectors in dimension 6 [36].

Finally, we pose some intriguing open questions: (i) Are maximal sets of MUBs isolated in every prime power dimension? (ii) Are SIC-POVMs isolated in every dimension $d > 3$? Furthermore, it would be welcome to develop a more efficient software to solve the linear problem $\mathcal{P}_L^{(1)}$ for POVMs having $N > 300$ elements, e.g., maximal sets of MUBs or SIC-POVM in dimension $d > 16$.

A MATLAB source code to support calculation of the restricted defect and additional features is available on the GitHub platform: https://github.com/matrix-toolbox/defect.

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APPENDIX: ROBUSTNESS OF RESTRICTED DEFECT

In this Appendix we derive the function $f(d,N)$ which appears in Eq. (18) and allows us to show that the restricted defect of a unitary matrix associated to a given generalized measurement is stable with respect to small perturbations. Consider a set of vectors ϕ_j and the approximate vectors $\phi'_j = \phi_j + \delta\phi_j$. The perturbed Gram matrix is given by

$$\begin{aligned}(G+\delta G)_{ij} &= \langle \phi_i + \delta\phi_i | \phi_j + \delta\phi_j \rangle \\ &\approx \langle \phi_i|\phi_j\rangle + \langle \delta\phi_i|\phi_j\rangle + \langle \phi_i|\delta\phi_j\rangle,\end{aligned}$$

which implies that

$$|\delta G_{ij}| \leqslant \|\phi_i\|\|\delta\phi_i\| + \|\phi_j\|\|\delta\phi_j\| \leqslant 2\sqrt{d}\, s. \tag{A1}$$

Here, we used Eq. (16). Also, from $U = \mathbb{I} - \frac{2d}{N} G$ we have $|\delta U_{ii}| = 0$ and $|\delta U_{ij}| \leqslant 4d^{3/2}\, s/N$ for $i \neq j$. Let us now calculate the perturbations on entries of the matrix $\mathcal{R}$, which defines the system of equations (9). It is simple to show that if $N > 2d$ the maximal perturbations are produced by the entries of $\mathcal{R}_{jk} = -2U_{kk}U_{kj}$, associated to the left-hand term of Eq. (9). Therefore,

$$\begin{aligned}|\delta\mathcal{R}_{ij}| &= 2|U_{kk}||\delta U_{ij}| \leqslant 2\left(1 - \frac{2d}{N}\right)\frac{4d^{3/2}}{N}\, s \\ &\leqslant \frac{8\, d^{3/2}}{N}\left(1 - \frac{2d}{N}\right) s.\end{aligned} \tag{A2}$$

Using this result, we have

$$\begin{aligned}|\delta(\mathcal{R}^\dagger\mathcal{R})_{ij}| &= |\delta(\mathcal{R}^\dagger)_{ij}\mathcal{R}_{ij} + (\mathcal{R}^\dagger)_{ij}\delta(\mathcal{R})_{ij}| \\ &\leqslant 2 \max_{\mathcal{R}_{ij}} |\delta(\mathcal{R}^\dagger)_{ij}\mathcal{R}_{ij}| \\ &\leqslant 2 \max_{\mathcal{R}_{ij}} |\delta(\mathcal{R}^\dagger)_{ij}| \max_{\mathcal{R}_{ij}} |\mathcal{R}_{ij}| \\ &\leqslant \frac{2^6 d^{5/2}}{N^2}\left(1 - \frac{2d}{N}\right)^2 \sqrt{\frac{N-d}{d(N-1)}}\, s.\end{aligned} \tag{A3}$$

Now we are in position to estimate the maximal perturbation on the eigenvalues of $\mathcal{R}^\dagger\mathcal{R}$:

$$\lambda' = \lambda_k + \delta\lambda_k \approx \lambda_k + \langle \delta(\mathcal{R}^\dagger\mathcal{R})\rangle. \tag{A4}$$

From the Gerschgorin circle theorem [38] we have

$$|\langle \delta(\mathcal{R}^\dagger\mathcal{R})\rangle| \leqslant \sum_{ij} |\delta(\mathcal{R}^\dagger\mathcal{R})_{ij}|. \tag{A5}$$

From combining Eqs. (A3), (A4), and (A5) we find that $|\lambda'_i - \lambda_i| \leqslant f(d,N)\, s$, where

$$f(d,N) = \frac{2^6 d^{5/2}}{N^2}\left(1 - \frac{2d}{N}\right)^2 \sqrt{\frac{N-d}{d(N-1)}}\, s.$$

Given that $\mathcal{R}^\dagger\mathcal{R}$ is a positive operator, its eigenvalues λ_i coincide with its singular values σ_i. Therefore, $|\sigma'_i - \sigma_i| \leqslant f(d,N)\, s$, which proves Eq. (18).

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