Optimal discrimination of geometrically uniform qubit and qutrit states

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We consider discrimination of geometrically uniform states, and analytically solve this problem for qubits. For qutrits, we obtain the exact solution to the optimal measurement when the defining unitary matrix for the geometrically uniform states is degenerate. We also show that if the unitary is nondegenerate then the optimal measurement for discriminating geometrically uniform qubits or qutrits can always be expressed as a rank-1 operator, which converts the original discrimination problem into an optimization of a sum of trigonometric functions with two real variables in the case of qutrits. Additionally, a geometrical interpretation of the optimal measurement for discriminating geometrically uniform qubits is given via the Bloch sphere representation.

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I. INTRODUCTION

Given an ensemble of quantum states $\{\rho_i, w_i\}$ with the prior probability distribution $\{w_i\}$, the task of discrimination is to find the optimal measurement $\{\Pi_i\}$ such that the success probability $p_s = \sum_i \mathrm{Tr}(w_i\rho_i\Pi_i)$ is maximized. This kind of problem is typical in quantum information processing [1–10], and has practical applications in quantum communications [11–16]. Investigation of quantum state discrimination was started in the 1970s, and has been a popular topic for decades; concepts such as squared-root measurements [17–22] and geometrically uniform states [18,20] are introduced and studied for a better understanding of the problem. In the theoretical aspect, the following necessary and sufficient condition for the optimal measurement is fundamental [1,2,5,23].

Theorem 1. The measurement $\{\Pi_i\}$ is optimal for discriminating the ensemble $\{\rho_i, w_i\}$ if and only if

$$\sum_i w_i\rho_i\Pi_i - w_k\rho_k \geqslant 0\,\forall k. \tag{1}$$

As a tool, Theorem 1 is indispensable in almost every derivation about quantum state discrimination. For example, condition (1) implies that $\sum w_i\rho_i\Pi_i = \sum w_i\Pi_i\rho_i$ and

$$\Big(\sum w_i\rho_i\Pi_i - w_k\rho_k\Big)\Pi_k = 0\,\forall k, \tag{2}$$

or $\Pi_k \in \mathcal{N}(\sum_i w_i\rho_i\Pi_i - w_k\rho_k)$, where $\mathcal{N}(X)$ denotes the null space of the operator X. Since $\mathrm{rank}(A+B) \leqslant \mathrm{rank}(A) + \mathrm{rank}(B)$ for any matrices A and B, we immediately conclude that the rank of Π_k cannot be larger than that of ρ_k [24], a fact that will be crucial in our later discussion.

In general, it is difficult to obtain analytical expressions for the optimal measurements. In fact, after more than 40 years of efforts, except two-state discrimination [3] and a few cases with strong symmetry properties [18–22,25–27], there exist no exact solutions. Even for the simplest case of qubits, general explicit solutions are still unknown and are expected to be of complicated form [28,29]. On the other hand, there exist numerical algorithms based on semidefinite programming [24], which solve the problem efficiently. However, numerical results provide few insights into the nature of the discrimination task, and are often insufficient to analyze its theoretical relations with other quantum mechanical problems. In fact, various links between quantum state discrimination and important concepts in quantum mechanics, such as quantum coherence [30–32], quantum discord [33,34], and complementarity [35,36], were discovered and studied recently, and hence motivate more analytical solutions to the discrimination problem which may shed light on fundamental understandings of quantum mechanics and offer quantifiers to abstract concepts with clear operational significance. For this purpose, we focus on discrimination of geometrically uniform states, which provides interesting examples of exact solutions: the problem is solved for pure states with the square-root measurement [18] and states with density matrices consisting exclusively of real numbers [25]. In this paper, we would like to further analyze the symmetry provided by geometrically uniform states, and therefore establish additional results about them. By diagonalizing the defining unitary U of the symmetry group, we provide an analytical solution to the discrimination problem of geometrically uniform qutrits whose U has a degenerate eigenvalue. On the other hand, when U is nondegenerate, we show that there exists an explicit characterization of the corresponding optimal measurement for qubits and qutrits. In particular, the optimal measurement can always be expressed as rank-1 operators. As a result, with the additional assumption that U is nondegenerate, the problem is completely solved for qubits, and an analytical expression for the optimal measurement is given, whereas for qutrits the discrimination problem is converted to an unconstrained optimization of a sum of trigonometric functions with two angle variables. In this way, the original problem is much simplified and more insights about the optimal measurement are provided.

We collect relevant results about discrimination of geometrically uniform states in Sec. II. Some notations that will be used consistently in the paper are also fixed in this section. Analyses of geometrically uniform qubits and qutrits are then carried out in Secs. III and IV, respectively, where we show the optimal measurements are always rank 1 for nondegenerate U, and provide the exact solution in the qutrit case when U is degenerate. The main result of this paper is summarized as Theorem 2 in Sec. IV. The paper is then closed with conclusions and suggestions of further works.

II. GEOMETRICALLY UNIFORM STATES

An important family of ensembles that exhibits useful symmetry properties is the geometrically uniform (GU) states, which is defined by a generator state $\rho_0 \in \mathbb{D}(\mathbb{C}^d)$ and a cyclic symmetry group $\{U^i\}$ generated by a unitary $U \in SU(d)$ satisfying $U^n = \mathbb{1}$, where notation $\mathbb{D}(\mathbb{C}^d)$ is to denote the set of all d-dimensional density matrices and $SU(d)$ is for the Lie group of d-dimensional special unitary matrices. Throughout this paper, we will use d to denote the dimension of the generator state ρ_0, and n to denote the number of states to be discriminated. The difference between d and n is also manifested in the choice of indices: the index i is always from zero to $n-1$, while j is always from zero to $d-1$. For GU states with respect to the symmetry group $\{U^i\}$, the ensemble to be discriminated is defined as

$$\{\rho_i = U^i\rho_0 U^{-i}, 1/n\}. \tag{3}$$

It is known that for pure states [18], i.e., $\rho_0 = |\psi\rangle\langle\psi|$, the optimal measurement is the square-root measurement [17], defined generally as

$$\Pi_k = \left(\sum_i \rho_i\right)^{-1/2} \rho_k \left(\sum_i \rho_i\right)^{-1/2}. \tag{4}$$

Moreover, it is always possible to represent the optimal measurement $\{\Pi_i\}$ so that it is covariant with the symmetry group [21], i.e.,

$$\Pi_i = U^i \Pi_0 U^{-i}. \tag{5}$$

In fact, if $\{\Pi'_i\}$ is an optimal measurement for discriminating $\{U^i\rho_0U^{-i}, 1/n\}$, then for any fixed number i_0, the transformed measurement $\{U^{i_0}\Pi'_{i\ominus i_0}U^{-i_0}\}$ also gives the optimal success probability

$$p_s^{\text{opt}} = \sum_i \mathrm{Tr}(U^i\rho_0U^{-i}\Pi'_i), \tag{6}$$

where the symbol $\ominus$ denotes subtraction modulo n. Consequently, the averaged operators

$$\Pi_i = \frac{1}{n}\sum_{l=0}^{n-1} U^l \Pi'_{i\ominus l} U^{-l} \tag{7}$$

$$= \frac{1}{n}\sum_l U^{l\oplus i}\Pi'_{\ominus l}U^{-(l\oplus i)} \tag{8}$$

$$= U^i\Pi_0U^{-i} \tag{9}$$

satisfy all the requirements of being a measurement and produce the optimal success probability, so that without loss of generality, for GU ensembles, it is sufficient to consider measurements satisfying the covariance condition (5), and the discrimination problem is simplified in such a way that only the operator $\Pi_0 \geqslant 0$ satisfying

$$\sum_i U^i\Pi_0U^{-i} = \mathbb{1}, \tag{10}$$

and maximizing $\mathrm{Tr}\rho_0\Pi_0$, needs to be determined. In the following, we will restrict our attention to diagonalized $U \in SU(d)$ only, i.e.,

$$U = \sum_j |j\rangle\langle j|\lambda_j \text{ with } \lambda_j^n = 1. \tag{11}$$

In other words, the eigenbasis $\{|j\rangle\}$ of U is chosen to be the computational basis. By doing so, the conjugation $UXU^\dagger$ affects only the off-diagonal entries of any d-dimensional matrix X. In particular, this implies that for the generating operator Π_0 of any measurement $\{U^i\Pi_0U^{-i}\}$, condition (10) requires all the diagonal entries of Π_0 to be $1/n$.

In Secs. III and IV, we will apply those observations in the preceding paragraph to the special cases of discriminating GU qubits ($d = 2$) and qutrits ($d = 3$), respectively. Specifically, when $d = 2$, there is only one real parameter to be determined, which can be fixed by maximization consideration. When $d = 3$, the existence of a degenerate eigenvalue further simplifies the problem so that exact solutions can be readily constructed, while in the nondegenerate case, similarly as $d = 2$, it can be shown that the optimal measurement is rank 1, and in this way, a characterization of the optimal measurement in terms of two real phases can be established. In conclusion, by exploiting the symmetry provided by the GU states, it is possible to obtain more exact solutions to the discrimination problem.

III. GU QUBITS

In this section, we solve the discrimination problem of GU ensembles with the extra assumption of $d = 2$, i.e., $\rho_0 \in \mathbb{D}(\mathbb{C}^2)$. Without loss of generality, we may assume that $U \neq \lambda\mathbb{1}$ with any $\lambda^n = 1$ so that the Hermitian operator $\sum_i \rho_i\Pi_i$ is diagonal in the eigenbasis $\{|j\rangle\}$ of U. We would like to show that the optimal measurement is rank 1 for all interesting GU qubits, and therefore obtain an explicit expression for the generating operator Π_0. Then, by considering the Bloch sphere representation, we give a geometrical interpretation of this optimal measurement.

A. Optimal measurement

Since $\mathrm{rank}\,\Pi_0 \leqslant \mathrm{rank}\,\rho_0$, it is possible that $\mathrm{rank}\,\Pi_0 = 2$. The two conditions that $\Pi_0 \in \mathcal{N}(\sum_i \rho_i\Pi_i - \rho_0)$ and $\mathrm{rank}\,\Pi_0 = 2$ together imply that $\sum_i \rho_i\Pi_i - \rho_0 = 0$. Since $\sum_i \rho_i\Pi_i$ is diagonal, we conclude that $\rho_i = \rho_0\,\forall i$. Hence if $\mathrm{rank}\,\Pi_0 = 2$, then all measurements are equally bad, a trivial case. If otherwise

$$\rho_0 = \begin{pmatrix} \rho_{00} & \rho_{01}e^{i\phi} \\ \rho_{01}e^{-i\phi} & \rho_{11} \end{pmatrix} \text{ with } \rho_{jk} > 0 \tag{12}$$

is not diagonal, and the GU states are different so that there is a nontrivial discrimination task, we necessarily have $\mathrm{rank}\,\Pi_0 = 1$, and we claim that

$$\Pi_0 = |\mu\rangle\langle\mu|, \text{ with } |\mu\rangle = \frac{1}{\sqrt{n}}\begin{pmatrix} 1 \\ e^{-i\phi} \end{pmatrix}, \tag{13}$$

where ϕ is the off-diagonal phase in (12).

This follows immediately from Theorem 1. Explicitly, if Π_0 is defined as (13), then

$$\frac{1}{n}\sum_{i=0}^{n-1}\rho_i\Pi_i = \mathrm{diag}\,\rho_0\Pi_0 = \frac{1}{n}\begin{pmatrix}\rho_{00}+\rho_{01} & 0\\ 0 & \rho_{11}+\rho_{01}\end{pmatrix}.$$

As a result,

$$\frac{1}{n}\sum_{i=0}^{n-1}\rho_i\Pi_i - \frac{1}{n}\rho_0 = \frac{\rho_{01}}{n}\begin{pmatrix}1 & -e^{i\phi}\\ -e^{-i\phi} & 1\end{pmatrix} \geqslant 0. \tag{14}$$

Hence Theorem 1 implies that Π_0 is the optimal generator. Actually, assuming that the optimal measurement is rank 1, so that it can be expressed as

$$\Pi_0 = \frac{1}{n}\begin{pmatrix}1 & e^{i\theta}\\ e^{-i\theta} & 1\end{pmatrix}, \tag{15}$$

then

$$p_s = \mathrm{Tr}(\rho_0\Pi_0) = \frac{1}{n}[1+2\rho_{01}\cos(\theta+\phi)], \tag{16}$$

which apparently attains its maximum $(1+2\rho_{01})/n$ when $\theta+\phi=0$.

B. Bloch sphere representation

The optimal measurement generator Π_0 obtained in (13) also bears a clear geometrically meaning in terms of the Bloch sphere. Given any qubit $\rho_0 \in \mathbb{D}(\mathbb{C}^2)$, one may associate it with a point $\vec{v}_0 = (\xi,\eta,\zeta)^T \in \mathbb{R}^3$ on or inside the Bloch sphere in such a way that

$$\rho_0 = \tfrac{1}{2}(\mathbb{1}+\vec{\sigma}\cdot\vec{v}_0), \tag{17}$$

where $\vec{\sigma} = (\sigma_x,\sigma_y,\sigma_z)^T$ is formed by the three Pauli matrices and the vector $\vec{v}_0$ is called the Bloch vector. The positivity of ρ_0 requires the length of $\vec{v}_0$ to be upper bounded by 1, and this length also suggests the purity of ρ_0. Specifically, when $|\vec{v}_0| = 1$, then state ρ_0 is pure, while, on the other hand, $|\vec{v}_0| = 0$ suggests that the state is the completely mixed state $\mathbb{1}/2$. The effect of a unitary $U \in SU(2)$ on the qubit ρ_0 then corresponds to a linear transformation $R \in SO(3)$ on the three-dimensional real vector $\vec{v}_0$ such that

$$\rho_0 \to \vec{v}_0 \Longrightarrow U\rho_0U^\dagger \to R\vec{v}_0. \tag{18}$$

The correspondence (18) provides a two-to-one homomorphism between the two groups $SU(2)$ and $SO(3)$, since both U and $-U$ map to the same R. In particular, a unitary $U \in SU(2)$ satisfying $U^n = \pm\mathbb{1}$ then corresponds to $R \in SO(3)$ such that $R^n = \mathbb{1}$, or in other words, a rotation in the Bloch sphere such that rotating n times returns any vector to its original position. By Euler's rotation theorem, any $R \in SO(3)$ has an eigenvalue 1, and the corresponding eigenvector can be considered as the axis of rotation. One may always fix this axis of rotation to be the z axis, so that

$$R(\varphi) = \begin{pmatrix}\cos\varphi & -\sin\varphi & 0\\ \cos\varphi & \sin\varphi & 0\\ 0 & 0 & 1\end{pmatrix}, \tag{19}$$

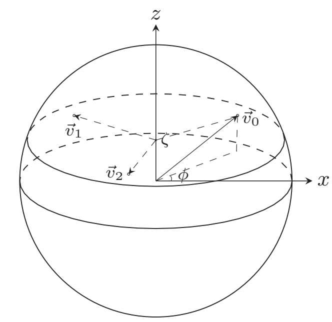

FIG. 1. The Bloch sphere representation of the generating state $\vec{v}_0$. By selecting the axis of rotation as the z axis, the three states $\vec{v}_0$, $\vec{v}_1$, and $\vec{v}_2$ all lie in the $z=\zeta$ plane, and the angle between any two adjacent vectors in the $z=\zeta$ plane is $2\pi/3$.

which corresponds to

$$U(\varphi) = \pm\begin{pmatrix}e^{i\varphi/2} & 0\\ 0 & e^{-i\varphi/2}\end{pmatrix}. \tag{20}$$

Consequently, by selecting the normalized eigenvectors $\{|0\rangle, |1\rangle\}$ of U to be the computational basis, the Bloch vectors of any GU qubit ensemble always lie in a plane parallel to the xy plane. The example of $n=3$ is shown in Fig. 1. Actually, since $\{\mathbb{1},\sigma_x,\sigma_y,\sigma_z\}$ provides an orthonormal basis for the space of 2×2 Hermitian matrices with respect to the Hilbert-Schmidt inner product, the Bloch vector representation (17) exists for any such matrices M_0 and M_1, and furthermore the inner product

$$\mathrm{Tr}(M_0^\dagger M_1) = \tfrac{1}{2}\mathrm{Tr}M_0\mathrm{Tr}M_1(\mathbb{1}+\vec{a}_0\cdot\vec{a}_1), \tag{21}$$

if $M_k = \mathrm{Tr}M_k(\mathbb{1}+\vec{\sigma}\cdot\vec{a}_k)/2$ for $k=0,1$. The positivity of M again implies that the length of the corresponding Bloch vector is less than or equal to 1. Specifically, let the optimal measurement be generated by Π_0, then the success probability

$$p_s = \mathrm{Tr}(\rho_0\Pi_0) \tag{22}$$

turns into the form

$$p_s = \tfrac{1}{2}\mathrm{Tr}\Pi_0(1+\vec{v}_0\cdot\vec{\mu}_0) \tag{23}$$

where $\vec{v}_0$ and $\vec{\mu}_0$ are the Bloch vectors for ρ_0 and Π_0, respectively. The condition

$$\sum_{i=0}^{n-1}U^i\Pi_0U^{-i} = \mathbb{1} \tag{24}$$

implies that $\mathrm{Tr}\Pi_0 = 2/n$, consequently the success probability depends completely on the inner product $\vec{v}_0\cdot\vec{\mu}_0$. Letting $\{\vec{v}_i\}$ and $\{\vec{\mu}_i\}$ be the Bloch vectors for the GU qubit states $\{\rho_i\}$ and the optimal measurement $\{\Pi_i\}$, respectively, by fixing the z axis as the axis of rotation, the z component of any vector is unchanged by the rotation, so that the condition $\sum\Pi_i = \mathbb{1}$ implies that the z component $\vec{\mu}_{i,z} = 0$ for any i. In other words, any $\vec{\mu}_i$ lies in the equator plane $z=0$. With this observation, it is obvious that the maximum inner product between $\vec{v}_i$ and $\vec{\mu}_i$ happens when $\vec{\mu}_i$ lies in the same line of the projection of $\vec{v}_i$ on the equator plane. Therefore the azimuthal angle ϕ in Fig. 1 determines the directions of the Bloch vectors $\{\vec{\mu}_i\}$ for the optimal measurement. The length of those

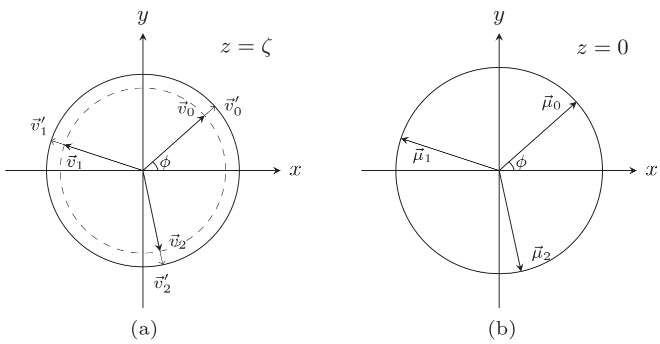

FIG. 2. (a) The projection of the Bloch vectors $\vec{v}_0$, $\vec{v}_1$, and $\vec{v}_2$ of the qubit states on $z = \zeta$. Since the states are not required to be pure, their Bloch vectors may not touch the border circle $x^2 + y^2 = 1 - \zeta^2$. The angle between any two adjacent vectors is $2\pi/3$, and their position is completely determined by the length of the generating state $\vec{v}_0$ and the azimuthal angle ϕ. Only when the states are pure, i.e., the vector $\vec{v}_i$ reaches the border circle, the optimal measurement is the square-root measurement. In general, the optimal measurement for discriminating $\{\vec{v}_0, \vec{v}_1, \vec{v}_2\}$ is the square-root measurement obtained for $\{\vec{v}'_0, \vec{v}'_1, \vec{v}'_2\}$. (b) The optimal measurement on the equator plane. The representing vectors $\vec{\mu}_0$, $\vec{\mu}_1$, and $\vec{\mu}_2$ are all of unit length, and the measurement is completely determined by the azimuthal angle ϕ. The Bloch vectors $\{\vec{v}_0, \vec{v}_1, \vec{v}_2\}$ and $\{\vec{v}'_0, \vec{v}'_1, \vec{v}'_2\}$ both correspond to the optimal measurement represented by the vectors $\{\vec{\mu}_0, \vec{\mu}_1, \vec{\mu}_2\}$.

vectors is determined by $\sum \Pi_i = \mathbb{1}$, or equivalently $\mathrm{Tr}\Pi_i = 2/n$ for any i, which puts no restriction on the vectors $\vec{\mu}_i$. This suggests that one can always make them as large as possible, which corresponds to pure states whose Bloch vectors are unit length. In conclusion, the geometrical consideration from the Bloch sphere solves the problem of discriminating GU qubits completely. By expressing the generator state ρ_0 in the eigenbasis of U, the Bloch vector $\vec{\mu}_0$ for the generating operator Π_0 lies in the equator plane with unit length and has the same azimuthal angle ϕ as the Bloch vector $\vec{v}_0$ for ρ_0. The case of $n = 3$ is shown in Fig. 2.

Fixing the axis of rotation as the z axis, the phase ϕ of the off-diagonal entries of $\rho_0 \in \mathbb{D}(\mathbb{C}^2)$ can be removed by rotating the corresponding Bloch vector to make it lie in the xz plane. For general d-dimensional states $\rho \in \mathbb{D}(\mathbb{C}^d)$, there are totally $d(d-1)/2$ independent phases for the off-diagonal entries, and therefore cannot by completely removed by the rotational symmetry alone. Hence the off-diagonal phases start to play a role in the discrimination problem of GU ensembles when $d \geqslant 3$. As a result, except a few special cases, the problem necessarily involves analysis of the phases, and is hence much more complicated.

IV. GU QUTRITS

In this section, we consider the three-dimensional generator state

$$\rho_0 = \begin{pmatrix} \rho_{00} & \rho_{01}e^{i\phi_{01}} & \rho_{02}e^{i\phi_{02}} \\ \rho_{01}e^{-i\phi_{01}} & \rho_{11} & \rho_{12}e^{i\phi_{12}} \\ \rho_{02}e^{-i\phi_{02}} & \rho_{12}e^{-i\phi_{12}} & \rho_{22} \end{pmatrix}, \quad \rho_{jk} \geqslant 0, \quad (25)$$

which is nondiagonal in the eigenbasis $\{|j\rangle\}$ of U and hence gives a nontrivial discrimination problem. The optimal measurement $\{U^i\Pi_0U^{-i}\}$ for discriminating the GU ensemble $\{U^i\rho_0U^{-i}, 1/n\}$ depends on the unitary U. Specifically, we will give an explicit solution to the generator Π_0 when U has a degenerate eigenvalue and show that it is rank 1 otherwise.

A. Degenerate U

If the defining unitary U has a degenerate eigenvalue, then the optimal measurement $\{U^i\Pi_0U^{-i}\}$ for discriminating the GU ensemble $\{U^i\rho_0U^{-i}, 1/n\}$, which is generated by an arbitrary qutrit $\rho_0 \in \mathbb{D}(\mathbb{C}^3)$, can be analytically solved. Explicitly, without loss of generality, we may assume that

$$U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{pmatrix} \text{ with } \lambda \neq 1 \text{ and } \lambda^n = 1. \quad (26)$$

As discussed in Sec. II, condition $\sum_i U^i\Pi_0U^{-i} = \mathbb{1}$ requires all diagonal entries of Π_0 to equal $1/n$, and the degeneracy of λ further implies that

$$\Pi_0 = \frac{1}{n}\begin{pmatrix} 1 & x & y \\ x^* & 1 & 0 \\ y^* & 0 & 1 \end{pmatrix} \text{ with } x, y \in \mathbb{C}, \quad (27)$$

for any covariant measurement generator Π_0 satisfying (10). Then the optimal value of x and y can be determined by considering the maximization of $p_s = \mathrm{Tr}(\rho_0\Pi_0)$. Explicitly,

$$\begin{aligned} \mathrm{Tr}(\rho_0\Pi_0) &= \frac{1}{n} + \frac{2}{n}\mathrm{Re}(x\rho_{01}e^{-i\phi_{01}} + y\rho_{02}e^{-i\phi_{02}}) \\ &\geqslant \frac{1}{n} + \frac{2}{n}(|x|\rho_{01} + |y|\rho_{02}) \quad (28) \\ &\geqslant \frac{1}{n} + \frac{2}{n}\big[(|x|^2 + |y|^2)(\rho_{01}^2 + \rho_{02}^2)\big]^{1/2}, \quad (29) \end{aligned}$$

where the equality in (28) is attained with

$$\arg x = \phi_{01}, \quad \arg y = \phi_{02} \quad (30)$$

and the equality in (29) is attained with

$$|x| : |y| = \rho_{01} : \rho_{02}. \quad (31)$$

Together with the positivity requirement

$$\Pi_0 \geqslant 0 \Rightarrow |x|^2 + |y|^2 \leqslant 1, \quad (32)$$

Eqs. (30) and (31) determine the optimal measurement operator Π_0 in (27) completely:

$$x = \frac{1}{\sqrt{\rho_{01}^2 + \rho_{02}^2}}\rho_{01}e^{i\phi_{01}}, \quad (33)$$

$$y = \frac{1}{\sqrt{\rho_{01}^2 + \rho_{02}^2}}\rho_{02}e^{i\phi_{02}}, \quad (34)$$

and the corresponding success probability

$$p_s^{\mathrm{opt}} = \frac{1}{n} + \frac{2}{n}\sqrt{\rho_{01}^2 + \rho_{02}^2}. \quad (35)$$

For a consistency check, let $\lambda = -1$ for the unitary U defined in (26), then the Helstrom bound [3] gives

$$p_s^{\mathrm{Hel}} = \frac{1}{2} + \frac{1}{4}\mathrm{Tr}|\rho_0 - U\rho_0U^\dagger|, \quad (36)$$

with ρ_0 defined in (25) and

$$U\rho_0 U^\dagger = \begin{pmatrix} \rho_{00} & -\rho_{01}e^{i\phi_{01}} & -\rho_{02}e^{i\phi_{02}} \\ -\rho_{01}e^{-i\phi_{01}} & \rho_{11} & \rho_{12}e^{i\phi_{12}} \\ -\rho_{02}e^{-i\phi_{02}} & \rho_{12}e^{-i\phi_{12}} & \rho_{22} \end{pmatrix}, \tag{37}$$

so that the eigenvalues of the operator $\rho_0 - U\rho_0 U^\dagger$ are $\{0, \pm 2\sqrt{\rho_{01}^2 + \rho_{02}^2}\}$, and the Helstrom bound (36) is the same as (35), as it should be.

B. Nondegenerate U

If the eigenspace of U is nondegenerate, i.e.,

$$U = \sum_j |j\rangle\langle j|\lambda_j \tag{38}$$

with $\lambda_j^n = 1$ and $\lambda_j \neq \lambda_k$ for any unequal pair (j,k), then for any d-dimensional matrix X, the condition $[U, X] = 0$ is sufficient to ensure that X is diagonal. In particular, since the two operators $\sum_i \rho_i \Pi_i$ and $\sum_i \Pi_i$ both commute with U, we have

$$\sum_i \rho_i \Pi_i = \sum_i U^i \rho_0 \Pi_0 U^{-i} = n\mathrm{diag}\, \rho_0 \Pi_0, \tag{39}$$

$$\sum_i \Pi_i = \sum_i U^i \Pi_0 U^{-i} = n\mathrm{diag}\, \Pi_0. \tag{40}$$

Therefore if U is nondegenerate, any positive operator whose diagonal entries all equal $1/n$ is guaranteed to generate a measurement. In particular, we may focus on rank-1 measurements whose generator is of the following form:

$$\Pi_0 = |\mu\rangle\langle\mu| \text{ with } \mu = \frac{1}{\sqrt{n}}\sum_j |j\rangle e^{i\theta_j}, \tag{41}$$

where all matrix elements of Π_0 have the same absolute value $1/n$. Note that such kind of operators fail to generate a measurement when U is degenerate. In the remainder of this section, we will show that the optimal measurement for discriminating any GU ensemble that is defined by a nondegenerate unitary U and an arbitrary qutrit $\rho_0 \in \mathbb{D}(\mathbb{C}^3)$ is rank 1, so that only the phases $\{\theta_j\}$ in (41) need to be determined.

Similarly as in Sec. III, the rank of the operator

$$\Delta_0 = \sum_i \rho_i \Pi_i - \rho_0 \tag{42}$$

can be either 1 or 2, which implies that the rank of Π_0 can be either 2 or 1. Define

$$\Phi = \phi_{01} + \phi_{12} - \phi_{02}. \tag{43}$$

Since

$$\tilde{\rho}_0 = D\rho_0 D^\dagger = \begin{pmatrix} \rho_{00} & \rho_{01} & \rho_{02} \\ \rho_{01} & \rho_{11} & \rho_{12}e^{i\Phi} \\ \rho_{02} & \rho_{12}e^{-i\Phi} & \rho_{22} \end{pmatrix} \tag{44}$$

with the transformation matrix

$$D = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i\phi_{01}} & 0 \\ 0 & 0 & e^{i\phi_{02}} \end{pmatrix}, \tag{45}$$

discriminating the GU ensemble $\{\rho_i, 1/n\}$ is equivalent to discriminating $\{\tilde{\rho}_i = U^i \tilde{\rho}_0 U^{-i}, 1/n\}$, but this time with only one off-diagonal phase Φ. We next consider the two cases $\Phi = 0$ and $\Phi \neq 0$ separately.

If $\Phi = 0$, then we claim that the optimal measurement is generated by

$$\tilde{\Pi}_0 = |\tilde{\mu}\rangle\langle\tilde{\mu}|, \text{ with } |\tilde{\mu}\rangle = \frac{1}{\sqrt{n}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \tag{46}$$

so that the optimal measurement for discriminating the original ensemble is generated by

$$\Pi_0 = D^\dagger \tilde{\Pi}_0 D. \tag{47}$$

This is again a direct application of Theorem 1, since

$$\tilde{\Delta}_0 = \sum_i \tilde{\rho}_i \tilde{\Pi}_i - \tilde{\rho}_0 = n\mathrm{diag}\, \tilde{\rho}_0 \tilde{\Pi}_0 - \tilde{\rho}_0$$
$$= \begin{pmatrix} \rho_{01} + \rho_{02} & -\rho_{01} & -\rho_{02} \\ -\rho_{01} & \rho_{01} + \rho_{12} & -\rho_{12} \\ -\rho_{02} & -\rho_{12} & \rho_{02} + \rho_{12} \end{pmatrix} \geqslant 0.$$

Similar consideration can be generalized to qudit

$$\rho_0 = \sum_j |j\rangle\langle j|\rho_{jj} + \sum_{k\neq j} |j\rangle\langle k|\rho_{jk}e^{i\phi_{jk}} \in \mathbb{D}(\mathbb{C}^d), \tag{48}$$

and we therefore establish the following fact: if there are d phases $\{\theta_j\}$ so that the $d(d-1)/2$ independent off-diagonal phases $\{\phi_{jk}\}$ in (48) can be expressed as $\phi_{jk} = \theta_j - \theta_k$, then the optimal measurement is rank 1 and generated by $|\mu\rangle = \sum_j |j\rangle e^{i\theta_j}/\sqrt{n}$. This generalizes the main result in [25].

Otherwise, if $\Phi \neq 0$, then we claim that $\tilde{\Delta}_0$ cannot be rank 1, and therefore $\tilde{\Pi}_0$ and Π_0 are rank 1. Indeed, assuming that

$$\tilde{\Delta}_0 = |\nu\rangle\langle\nu| \text{ with } |\nu\rangle = \begin{pmatrix} \nu_0 \\ \nu_1 e^{-i\alpha_1} \\ \nu_2 e^{-i\alpha_2} \end{pmatrix} \tag{49}$$

since $\sum \tilde{\rho}_i \tilde{\Pi}_i$ is diagonal, the off-diagonal entries of $\tilde{\Delta}_0$ coincide with that of $-\tilde{\rho}_0$. Then by comparing the off-diagonal phases, we obtain that

$$\alpha_1 = \alpha_2 = 0 \text{ but } \alpha_1 - \alpha_2 = \Phi \neq 0, \tag{50}$$

which is a contradiction. In conclusion, regardless of the value of Φ, we always have rank $\Pi_0 = 1$.

We summarize the results about discrimination of GU qubits and qutrits as the following theorem.

Theorem 2. The optimal measurement for discrimination of the n equiprobable GU states $\{\rho_i = U^i \rho_0 U^{-i}\}_{i=0}^{n-1}$ generated by a qubit or qutrit state

$$\rho_0 = \sum_{j,k=0}^{d-1} |j\rangle\langle k|\rho_{jk}e^{i\phi_{jk}} \text{ with } \rho_{jk} \geqslant 0, d = 2 \text{ or } 3,$$

and a nondegenerate diagonal unitary matrix

$$U = \sum_{j=0}^{d-1} |j\rangle\langle j|\lambda_j \text{ with } \lambda_j \neq \lambda_k\, \forall\, j \neq k, \tag{51}$$

which satisfies $U^n = \mathbb{1}$, is the rank-1 measurement $\{\Pi_i = U^i|\mu\rangle\langle\mu|U^{-i}\}_{i=0}^{n-1}$, with the generator

$$|\mu\rangle = \frac{1}{\sqrt{n}}\sum_{j=0}^{d-1}|j\rangle e^{i\theta_j}. \tag{52}$$

The phases $\{\theta_j\}$ are determined by maximizing the following expression:

$$\sum_j \sum_{k\neq j} |\rho_{jk}|\cos(\theta_k - \theta_j + \phi_{jk}). \tag{53}$$

Note that the success probability corresponding to the measurement $\{\Pi_i\}$ is

$$\begin{aligned} p_s^{\{\Pi_i\}}(\rho_0) &= \langle\mu|\rho_0|\mu\rangle = \frac{1}{n}\sum_{j,k}|\rho_{jk}|\cos(\theta_k - \theta_j + \phi_{jk}) \\ &= \frac{1}{n} + \frac{1}{n}\sum_j\sum_{k\neq j}|\rho_{jk}|\cos(\theta_k - \theta_j + \phi_{jk}), \end{aligned} \tag{54}$$

so that the optimal condition (53) is well posed. Actually, the variables can be reduced by setting $\theta_0 = 0$, since an overall phase factor makes no difference. It is also clear from (53) that the diagonal entries play no role in such discrimination, which is as expected. The choice of the computational basis ensures that the unitary transformation does not change the diagonal entries, and the difference between the discriminated states $\{\rho_i\}$ lies completely in the off-diagonal entries. It is tempting to conjecture that similar results holds in every finite dimension. Unfortunately, even in dimension 4, there are GU ensembles, with nondegenerate defining unitary U, whose optimal discrimination measurement cannot be expressed as rank-1 operators [37].

By transformation (44), the optimal choice of the phases $\{\theta_1, \theta_2\}$ can be determined by solving the system of trigonometric equations:

$$\rho_{01}\sin\tilde{\theta}_1 + \rho_{02}\sin\tilde{\theta}_2 = 0, \tag{55}$$

$$-\rho_{01}\sin\tilde{\theta}_1 + \rho_{12}\sin(\tilde{\theta}_2 - \tilde{\theta}_1 + \Phi) = 0, \tag{56}$$

where Φ is defined as in (43), and then performing the transformation

$$\theta_1 = \tilde{\theta}_1 - \phi_{01}, \quad \theta_2 = \tilde{\theta}_2 - \phi_{02}. \tag{57}$$

If the off-diagonal entries of ρ_0 have the same absolute value, i.e.,

$$\rho_0 = \begin{pmatrix} \rho_{00} & ae^{i\phi_{01}} & ae^{i\phi_{02}} \\ ae^{-i\phi_{01}} & \rho_{11} & ae^{i\phi_{12}} \\ ae^{-i\phi_{02}} & ae^{-i\phi_{12}} & \rho_{22} \end{pmatrix} \text{ with } a > 0, \tag{58}$$

then (55) and (56) admit simple analytical solutions. This time, these equations become

$$\sin\tilde{\theta}_1 + \sin\tilde{\theta}_2 = 0, \tag{59}$$

$$-\sin\tilde{\theta}_1 + \sin(\tilde{\theta}_2 - \tilde{\theta}_1 + \Phi) = 0, \tag{60}$$

and the solution for the optimal $(\tilde{\theta}_1, \tilde{\theta}_2)$ is

$$\tilde{\theta}_1 = -\tilde{\theta}_2 = \Phi'/3, \tag{61}$$

where $\Phi' = \Phi + 2k\pi$ for some $k \in \mathbb{Z}$ so that $\Phi' \in [-\pi, \pi]$. The optimal success probability is then

$$p_s^{\text{opt}} = \frac{1}{n} + \frac{6a}{n}\cos(\Phi'/3). \tag{62}$$

V. CONCLUSION

We have derived the exact solution to discriminating three-dimensional GU states whose defining unitary U has a degenerate eigenvalue, and shown that if the unitary U is nondegenerate, then the optimal measurement for discriminating GU qubits or qutrits satisfies Theorem 2. In particular, this solves the problem of discriminating GU qubits completely, and simplifies that for GU qutrits. Although Theorem 2 cannot be generalized to arbitrary dimensions, some of the observations will be helpful in further studies of discriminating GU states. For example, by setting the basis such that the unitary U is diagonalized, all the information useful for discrimination is gathered into the off-diagonal entries; additionally, only the degeneracy of the unitary U plays a role in determination of the optimal measurement, the actual eigenvalues and the number of discriminated states are immaterial for the problem, and hence without loss of generality one may focus on discriminating δ GU qudit states, where $\delta \leqslant d$ is the number of different eigenvalues of U. It is also an interesting problem to find extra conditions which will make Theorem 2 valid in higher dimensions.

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[37] For example, numerically, the best success probability of discriminating the GU ensemble defined by

$$\rho_0 = \frac{1}{20}\begin{pmatrix} 4 & 1 & 2 & 2 \\ 1 & 2 & e^{i\frac{\pi}{3}} & e^{-i\frac{\pi}{3}} \\ 2 & e^{-i\frac{\pi}{3}} & 10 & 4e^{i\frac{2\pi}{3}} \\ 2 & e^{i\frac{\pi}{3}} & 4e^{-i\frac{2\pi}{3}} & 4 \end{pmatrix}, U = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \mathrm{i} & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -\mathrm{i} \end{pmatrix}$$

with rank-1 measurement is $p_s^{r=1} \approx 0.4198$, while the actual optimal success probability is $p_s^{\rm opt} \approx 0.4213$.