Optimal positive-operator-valued measures for unambiguous state discrimination

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Optimization of the mean efficiency for unambiguous (or error free) discrimination among $N$ given linearly independent nonorthogonal states should be realized in a way to keep the probabilistic quantum mechanical interpretation. This imposes a condition on a certain matrix to be positive semidefinite. We reformulated this condition in such a way that the conditioned optimization problem for the mean efficiency was reduced to finding an unconditioned maximum of a function defined on a unit $N$-sphere for equiprobable states and on an $N$-ellipsoid if the states are given with different probabilities. We established that for equiprobable states a point on the sphere with equal values of Cartesian coordinates, which we call symmetric point, plays a special role. Sufficient conditions for a vector set are formulated for which the mean efficiency for equiprobable states takes its maximal value at the symmetric point. This set, in particular, includes previously studied symmetric states. A subset of symmetric states, for which the optimal measurement corresponds to a POVM requiring a one-dimensional ancilla space is constructed. We presented our constructions of a POVM suitable for the ancilla space dimension varying from 1 till $N$ and the Neumark’s extension differing from the existing schemes by the property that it is straightforwardly applicable to the case when it is desirable to present the whole space system + ancilla as the tensor product of a two-dimensional ancilla space and the $N$-dimensional system space.

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I. INTRODUCTION

Being important for quantum communication, quantum cryptography and quantum algorithms (see e.g. [1]) the problem of finding an optimal strategy for discriminating among different non-orthogonal quantum states has gained renewed interest [2, 3, 4, 5, 6, 7, 8] (for reviews see [3, 4]). Between different strategies based on various criteria (see e.g. [4]) a special role is played by the one called unambiguous state discrimination [2, 3, 4, 5, 6, 7, 8]. It is based on pioneering works of Ivanovic, Dieks and Peres [3] who considered the problem of discriminating among two non-orthogonal states. In [6] Peres and Terno examined the case of three states. In [7] Chefles showed that non-orthogonal states may be unambiguously discriminated if and only if they are linearly independent and proved an important fact that the necessary (but not sufficient) condition for a measurement to be optimal consists in equating to unity the highest eigenvalue of a certain matrix. Chefles and Barnett [8] using this property derived an upper bound (achievable by an optimal measurement) for success probability to discriminate among $N$ so called symmetric states given with equal a priori probabilities.

Another important general result was established by Duan and Guo [9] who derived a matrix inequality for efficiencies to unambiguously discriminate among $N$ given linearly independent states. This result permitted to Sun et al [10] to reformulate the problem of finding the optimal discriminating strategy as the well-known semidefinite (conditioned) programming problem. Although this fact together with the remark that there exist softwares for numerical solution of the latter problem [10, 11] reduces any particular optimization task to a technical problem, this approach, as well as any numerical solution, usually does not bring any additional analytic insight.

In the current paper we show that the conditioned optimization problem for the mean efficiency may be reformulated as a problem of finding an unconditioned maximum of a function defined on an $N$-sphere for equiprobable states and on an $N$-ellipsoid when the states are given with different probabilities (Theorem [11] and Corollary [11]). We establish that for equiprobable states there exists a special point on the unit $N$-sphere called a symmetric point where the mean efficiency takes its maximal value for certain sets of states. In particular, this set includes all symmetric state. It happens that for $N = 2, 3$ this point is optimal only for symmetric states. Nevertheless, as we will show, starting from $N = 4$ the set of states, for which the symmetric point is optimal, is wider than the set of symmetric states. Using Theorem [11] we formulated conditions on the set of states which are sufficient for the mean efficiency to be maximal at the symmetric point (Theorem [2]). For $N = 4$ Theorem [2] is illustrated by an example of a three parameter set of states which are non-symmetric and such that one of the parameters is just the optimal mean efficiency.

We show that if one of the eigenvalues of matrix $\Psi\Psi^d$, with $\Psi$ being an $N \times N$ matrix where the given vectors are collected as columns, is $N - 1$ fold degenerate, the set is either a particular set of symmetric states or their unitary rotated form. This set may be considered as the simplest generalization of two states since the expression for the optimal mean efficiency for two states is a particular case of a more general formula obtained for the above set. Moreover, if this is the lowest eigenvalue, which is $N - 1$ fold degenerate, the ancilla space for the optimal measurement becomes one-dimensional.

For a general set of symmetric states we obtain for the optimal mean efficiency an expression alternative but
equivalent to that found by Chefles and Barnett [8].

Finally, we present our constructions of a POVM suitable for the ancilla space dimension varying from 1 till \( N \) and the Neumark’s extension differing from the existing schemes by the property that it is straightforwardly applicable to the case when it is desirable to present the whole space system + ancilla as the tensor product of a two-dimensional ancilla space and the \( N \)-dimensional system space.

II. OPTIMAL POVM

Assume that we are given a set of non-orthogonal but linearly independent and normalized to unity vectors (states) \( \psi_j, \langle \psi_j|\psi_j \rangle = 1, \ j = 1, \ldots, N \), which we collect as columns to an \( N \times N \) matrix \( \Psi = (\psi_1, \ldots, \psi_N) \). Because of the linear independence of the vectors \( \psi_j \) the matrix \( \Psi \) is non-singular, \( \det \Psi \neq 0 \), which is the property we will assume to hold throughout the paper. Below we will frequently use the following terminology.

Instead of saying the vectors (states) \( \psi_1, \ldots, \psi_N \) we will say the vectors (states) \( \Psi \). We will assume also that these vectors span an \( N \) dimensional complex Hilbert space \( \mathcal{H} \) with the usually defined inner product \( \langle \cdot | \cdot \rangle \). Evidently, they form a non-orthogonal basis in \( \mathcal{H} \). As it was previously shown [2, 3, 4, 6, 7, 8] unambiguous (or error free) strategy for discriminating among these states, is possible if and only if they are discriminated by a generalization of the POVM which is a two-dimensional ancilla space and the \( N \)-dimensional system space.

Given a two-dimensional ancilla space and the \( N \)-dimensional system space, we will say the \( N \times N \) matrix \( \Pi_x \) equivalent to that found by Chefles and Barnett [8].

By this reason without losing generality one may always assume \( \psi_k \) is captured. This confirms that we can unambiguously discriminate \( \psi_k \) from all other states \( \psi_j \), \( j \neq k \). The probability \( P_k \) for this detector to click is \( P_k = \langle \psi_k|\Pi_{L_k}|\psi_k \rangle \), which in view of \( \Pi_{L_k} \) reduces to \( P_k = x_k^2 \).

This probabilistic interpretation is valid if and only if there exists a Hermitian positive definite (or semidefinite) matrix \( \Pi_x \) such that

\[
\Pi_x + \Pi_x = I_N
\]

where \( I_N \) is the \( N \times N \) identity matrix. Relation (4) defines a (discrete in the current case) POVM which is the cornerstone of the probabilistic interpretation. From this it follows that \( \Pi_x - \Pi_x = I_N - \Xi_x \Xi_x^\dagger \) should be positive definite (or semidefinite). Note that this matrix is positive definite (semidefinite) together with \( \Psi^\dagger \Psi - X^2 \).

The last condition is just the same necessary and sufficient condition for an optimal POVM to exist first found by Duan and Guo [9]. We, thus, identify the square of our weight matrix \( X^2 \) with the efficiency matrix \( \Gamma \) used by Duan and Guo.

Note that \( \Pi_x = I_N - \Pi_x \) is positive semidefinite if the highest eigenvalue of \( \Pi_x \) is equal to 1. Thus, a POVM can always be constructed if \( X = \lambda_m^{-1}I_N \), \( \lambda_m > 0 \) where \( \lambda_m \) is the lowest eigenvalue of both the right modulus of \( \Psi \), \( \Psi^\dagger \Psi \), and its left modulus \( \Psi^\dagger \Psi \). Another important property we would like to emphasize is the following. When the mean efficiency takes its maximal value, the highest eigenvalue of \( \Pi_x \) is necessarily equal to 1 [8]. Therefore, \( \Pi_x \) is always positive semidefinite if the POVM is optimal. As we will show below in a number of cases this takes place for \( X = \lambda_m^{-1}I_N \). Moreover, rank \( \Pi_x = N - N_m := N_a \) where \( N_m = 1, \ldots, N - 1 \) is the degree of degeneracy of the highest eigenvalue of \( \Pi_x \) (for \( X = \lambda_m^{-1}I_N \) this is also the degree of degeneracy of \( \lambda_m \) so that \( N_a = 1, \ldots, N - 1 \).

If the state \( \psi_j \) can be chosen from the set \( \Psi \) with a probability \( \eta_j \), the total probability of correctly identifying any state

\[
P(x) = \sum_{j=1}^{N} \eta_j P_j = \sum_{j=1}^{N} \eta_j x_j^2
\]

is called the mean efficiency. The optimization problem becomes now a semidefinite programming problem (see [10]) consisting in finding the maximum of \( P(x) \) with respect to \( X \geq 0 \) subject to either \( \Psi^\dagger \Psi - X^2 \geq 0 \) or equivalently

\[
I_N - \Xi_x \Xi_x^\dagger = I_N - (\Psi^\dagger)^{-1}X^2\Psi^{-1} \geq 0.
\]
We shall denote this maximum by \( P_M \). In contrast to approach proposed in \cite{10} the constraint \( \Xi \), we are using, permits us to reduce the conditioned optimization problem to finding the minimal value of a function defined on an \( N \)-ellipsoid. For brevity in what follows we shall denote by \( x = (x_1, \ldots, x_N) \) Cartesian coordinates of a point from \( \mathbb{R}^N \) and by \( t = (t_1, \ldots, t_N-1) \) curvilinear coordinates on either a unit \( N \)-sphere or an \( N \)-ellipsoid with fixed axes.

**Theorem 1.** Let us denote
\[
P_M = \max_x \sum_{j=1}^N \eta_j x_j^2 \quad (t_N - \Xi x_2 \geq 0) \quad j = 1, \ldots, N \tag{8}
\]
and
\[
\mu_m^2 = \min_{t \in \Omega} \mu_m^2(t) \tag{9}
\]
where \( \mu_m^2(t) \) is the highest eigenvalue of the matrix \( \Xi Y^2(t) \Xi^\dagger \) with \( Y(t) \) being a diagonal matrix with the non-zero entries equal coordinates of a point lying on the positive part of an \( N \)-ellipsoid with the axes \( \eta_1^{-1/2}, \ldots, \eta_N^{-1/2} \). We denote \( \Omega \) this part of the ellipsoid, i.e.
\[
Y(t) = \text{diag} (y_1(t), \ldots, y_N(t)) , \tag{10}
\]
where
\[
y_1(t) = \eta_1^{-1/2} \sin t_1 \sin t_2 \ldots \sin t_{N-2} \sin t_{N-1} \\
y_2(t) = \eta_2^{-1/2} \sin t_1 \sin t_2 \ldots \sin t_{N-2} \cos t_{N-1} \\
y_3(t) = \eta_3^{-1/2} \sin t_1 \sin t_2 \ldots \sin t_{N-3} \cos t_{N-2} \\
\vdots \\
y_{N-1}(t) = \eta_{N-1}^{-1/2} \sin t_1 \cos t_2 \quad (\text{for } N > 2) \\
y_N(t) = \eta_N^{-1/2} \cos t_1 \\
0 < t_1, \ldots, t_N < \pi/2 . \tag{11}
\]
Then
\[
P_M = \mu_m^{-2} . \tag{13}
\]

**Proof.** First we note that \( \sum_{j=1}^N j y_j^2 = 1 \).

Let us put in \( X = rY(t) \), i.e. \( x_j = r y_j(t) \), \( j = 1, \ldots, N \). This yields \( P(x) = r^2 \) and \( \Xi X^2 \Xi^\dagger = r^2 \Xi Y^2(t) \Xi^\dagger \). Since \( r^2 \) is simply a scaling factor between eigenvalues of \( \Xi X^2 \Xi^\dagger \) and \( \Xi Y^2(t) \Xi^\dagger \) this implies
\[
\mu_m^2 = r^{-2} \bar{\mu}_m^2 = P^{-1}(x) \bar{\mu}_m^2 \tag{14}
\]
where \( \bar{\mu}_m^2 \) is the highest eigenvalue of \( \Xi X^2 \Xi^\dagger \). We note that the left hand side of Eq. \( (14) \) is a function defined on the ellipsoid, \( \mu_m = \bar{\mu}_m(t) \). Next, we shall use the property proven in \cite{2}: The necessary condition for the efficiency to be optimal is the highest eigenvalue of \( \Xi X^2 \Xi^\dagger \) being equal to 1. (Under this condition the constraint \( I_N - \Xi X \Xi^\dagger \geq 0 \) is automatically satisfied.) Let us put in \( (14) \) \( \mu_m^2 = 1 \ \forall t \in \Omega \). Under this condition Eq. \( (14) \) defines parameter \( r \) and with it the mean efficiency \( P(x) \) as functions on the ellipsoid only, i.e. \( P = P(t) = r^2(t) = \mu_m^{-2}(t) \). Thus, the maximal value of \( P(t) \) corresponds to the minimal value of \( \mu_m^2(t) \) on the part of the ellipsoid with all \( y_i(t) \geq 0 \).

For equiprobable states, when \( \eta_1 = \ldots = \eta_N = 1/N \), we find it convenient to re-scale all \( y_j(t) \) and use \( \bar{y}_j(t) = \sqrt{N} y_j(t) \) so that the point \( (\bar{y}_1(t), \ldots, \bar{y}_N(t)) \) lays on a unit \( N \)-sphere. To simplify notations below in this case we will use just the unit sphere and omit tilde over \( y_j(t) \). This leads to the following modification of Theorem 1.

**Corollary 1.** For equiprobable \( \psi_j \), i.e. for \( \eta_1 = \ldots = \eta_N = 1/N \),
\[
P_M = N^{-1} \max_{t \in \Omega} \mu_m^{-2}(t) \tag{15}
\]
where \( \Omega \) is a part of the unit \( N \)-sphere defined by \( (11) \) and \( (12) \) with \( \eta_1 = \ldots = \eta_N = 1 \), \( \mu_m^2(t) \) is the highest eigenvalue of the matrix \( \Xi Y^2(t) \Xi^\dagger \), and \( Y(t) \) is given in \( (11) \).

We would like to stress that the above condition for the highest eigenvalue of \( \Xi X^2 \Xi^\dagger \) be equal to 1 proven in \cite{2} is necessary but not sufficient for the efficiency to take the maximal value. As it is clear from the proof of Theorem 1 for \( P(t) = \mu_m^{-2}(t) \) this necessary condition is satisfied \( \forall t \in \Omega \) and, in general, \( P(t) \) is not constant for \( t \in \Omega \), which can be easily seen from the simplest \( 2 \times 2 \) example. From Eq. \( (13) \) it follows also that, in general, \( P(x) = \bar{\mu}_m^2 \mu_m^{-2} \) depends on both a point \( t \) on the ellipsoid and parameter \( r \).

On the ellipsoid there always exists a special point \( t_0 \) where \( y_1(t_0) = y_2(t_0) = \ldots = y_N(t_0) \). We will call this point the symmetric point. At this point \( Y(t) \) becomes proportional to the identity matrix and \( \Xi X^2 \Xi^\dagger \) is proportional to \( \Xi \Xi^\dagger \). By this reason the eigenvalues of \( \Xi X^2 \Xi^\dagger \) are, simply, the eigenvalues of \( \Xi \Xi^\dagger \) scaled by a factor \( r^2 \bar{y}_j^2(t_0) \). In particular,
\[
\bar{\mu}_m^2 = r^2 \bar{y}_j^2(t_0) \nu_m^2 \tag{16}
\]
where \( \nu_m^2 \) is the highest eigenvalue of \( \Xi \Xi^\dagger \) which is given through the matrix \( \Psi \) since \( \Xi = (\Psi) -1 \). If now we require for the highest eigenvalue of \( \Xi X^2 \Xi^\dagger \) to be equal to 1, \( \bar{\mu}_m^2 = 1 \), Eq. \( (16) \) defines \( r^2 \) as a function of \( t_0 \). Therefore from Eqs. \( (11) \) and \( (16) \) we obtain the mean efficiency \( P(t_0) = r^2(t_0) = \bar{y}_j^2(t_0) \nu_m^{-2} \). For equiprobable states, as we show below, in a number of cases point \( t_0 \) is just the maximal point for the mean efficiency. In particular, this point is optimal for any symmetric set of equiprobable states but not only for these states. The set of states for which the mean efficiency takes its maximal value at \( t = t_0 \) is wider than the set of symmetric states. However, as our numerical tests show, in many cases there exist points on the ellipsoid where the efficiency takes higher values. We believe that the symmetric point may be a good starting point for a numerical optimization.

Theorem 1 and Corollary 1 give a general recipe for finding the optimal weight matrix \( X(t) \) and with it the
optimal POVM defined by the set $\Xi_x = \Xi X(t)$ to unambiguously discriminate among the vectors collected to matrix $\Psi$. In general the matrix $\Psi$ is non-Hermitian and can have complex eigenvalues. Nevertheless, as we show below, for any given $\Psi$ there always exists a positive definite $\Psi_1 = \Psi_1^\dagger$ which has the same optimal weight matrix and the same optimal mean efficiency as $\Psi$.

**Corollary 2.** Both the optimal weight matrix $X = X_M$ and the optimal mean efficiency $P_M$ are invariant under a unitary rotation of the vector set $\Psi$. In particular, for any non-singular $\Psi$ given in the form

$$\Psi = U_2 E_0 U_1, \quad U_{1,1}^{-1} = U_{1,2}^\dagger$$

the optimization may be realized for $\Psi_1 = U_{1,1}^\dagger E_0 U_1$.

**Proof.** First we note that decomposition (17), (18) takes place for any non-singular matrix $\Psi$ (see e.g. 13). Denote $t = t_M$ the point on the ellipsoid where the highest eigenvalue $\mu_m^2(t)$ of the matrix $\Xi Y^2(t)\Xi^\dagger$ takes its minimal value as a function of $t$. Next, since $\Xi = (\Psi)^{-1}$, this implies $\Xi Y^2(t)\Xi^\dagger = U_2 E_0 U_1 Y^2(t) U_1^\dagger E_0 U_2$. From here it follows that the eigenvalues of matrix $\Xi Y^2(t)\Xi$ do not depend on unitary $U_2$. In particular, the eigenvalue $\mu_2^2 = \mu_2^2(t_M)$ and with it, as follows from (13), both the optimal mean efficiency $P_M$ and the weight matrix $X_M = \sqrt{P_M} Y(t_M)$ are invariant under a unitary rotation of the vectors $\Psi$. Therefore the optimization may be realized for the set $\Psi_1 = U_{1,1}^\dagger E_0 U_1$.

Note that in general properties of the vectors collected to a matrix unitarily equivalent to a given matrix change essentially. In particular, if the vectors $\Psi$ are normalized to unity, the vectors $U\Psi U^\dagger$, in general, are not normalized to unity. Nevertheless, there exist particular unitary transformations keeping unchanged both the mean efficiency and the weight matrix. These are transformations from an Abelian subgroup of the unitary group. They have the form $U = U_n = \text{diag}(e^{i\beta_1}, \ldots, e^{i\beta_k})$, $\beta_j \in \mathbb{R}$. Indeed, being multiplied from the right by $U_n$ every column vector of $\Psi$ acquires an additional essential phase factor whereas after the left multiplication the vectors $\Psi$ are simply unitary rotated. Thus, such a transformation corresponds to a re-scaling of the vector set $\Psi$ by phase factors followed by their unitary rotation. According to Corollary 2 these operations can affect neither the mean efficiency nor the weight matrix.

The next theorem establishes sufficient conditions for the symmetric point on the $N$-sphere to be a point of the maximal mean efficiency for equiprobable states. To prove this result, according to Corollary 1 one has to find the minimum of the highest eigenvalue of the matrix $\Xi Y^2(t)\Xi$ for $t$ on the unit $N$-sphere.

**Theorem 2.** Let $\Psi$ be Hermitian, positive definite and the states $\Psi$ are equiprobable. If there exists an eigenvector $\varphi_m^0 = (\varphi_{m,1}^0, \ldots, \varphi_{m,N}^0)^\dagger$, $\varphi_{m}^0 | \varphi_{m}^0 = 1$, of $\Psi$ corresponding to its lowest eigenvalue $\lambda_m$, i.e. $\Psi \varphi_m^0 = \lambda_m \varphi_m^0$, $\lambda_m = \min_j \lambda_j$, such that $|\varphi_{m,1}^0| = |\varphi_{m,2}^0| = \ldots = |\varphi_{m,N}^0| = N^{-1/2}$, then $P_M = \lambda_m^2$.

**Proof.** First we note that because of Hermiticity of $\Psi$, matrices $\Psi, \Psi^\dagger = \Psi^\dagger \Psi = \Psi^\dagger, \Xi = \Psi^{-1}$ and $\Xi \Xi = \Xi^\dagger \Xi = 1$ may have the same set of eigenvectors. In particular, $\Xi \varphi_m^0 = \lambda_m \varphi_m^0$ and $\Xi \Xi \varphi_m^0 = \lambda_m^2 \varphi_m^0$ so that $\lambda_m^2$ is the highest eigenvalue of $\Xi \Xi$.

Let us denote $H(t) = \Xi Y^2(t)\Xi^\dagger$ where $Y(t)$ is given in (10) with $y_j(t)$ being given in (11) and (12) with $y_1(t) = \ldots = y_N(t) = 1$. Let also $\mu_m^2(t)$ be the highest eigenvalue of $H(t)$ and $\varphi_m(t)$ be one of the eigenvectors with eigenvalue $\mu_m^2(t)$, i.e.

$$H(t) \varphi_m(t) = \mu_m^2(t) \varphi_m(t).$$

Since $\mu_m^2(t)$ is the highest eigenvalue then according to the variational principle the following inequality holds true $\forall \varphi \in \mathcal{H}$. In particular, for any $t$ we have

$$\mu_m^2(t) \geq \langle \varphi_m^0 | H(t) | \varphi_m^0 \rangle = \langle \varphi_m^0 | \Xi Y^2(t) \Xi \varphi_m^0 \rangle \geq \lambda_m^2 \sum_{i=1}^N \varphi_m | y_i^2 = N^{-1} \lambda_m^2.$$  

Let $t_0$ be a point on the unit sphere where $y_j(t_0) = \ldots = y_N(t_0) = N^{-1/2}$ and, hence, $Y(t) = N^{-1/2} I_N$. This implies that $\varphi_m(t_0) = \varphi_m^0$ and $\mu_m^2(t_0) = \langle \varphi_m^0 | H(t_0) | \varphi_m^0 \rangle = N^{-1} \lambda_m^2 \Xi | \varphi_m^0 = N^{-1} \lambda_m^2$. Comparing this result with (20) we conclude that $\mu_m^2(t_0) \geq \mu_m^2(t)$ for any $t$ and, hence, according to Corollary 1 $P_M = [\lambda_m^2(t_0)]^{-1} = \lambda_m^2$.

This theorem has an interesting implication which we formulate as the next theorem.

**Theorem 3.** Let matrix $\Psi$ be such that matrix $\Psi^\dagger$ has only two distinct eigenvalues $\lambda_1^2$ and $\lambda_N^2$ and one of them is $N-1$ fold degenerate, then for equiprobable states $P_M = \min(\lambda_1^2, \lambda_N^2)$.

We would like to remind that the positive square roots $\lambda_j$ of the eigenvalues of the left modulus of $\Psi$, i.e. of the eigenvalues $\lambda_j^2$ of $\Psi^\dagger$, are called singular numbers of $\Psi$ (13). Thus, by the theorem assumption one of these numbers is $N-1$ fold degenerate.

**Proof.** Let for definiteness $\lambda_2^2 = N-1$ fold degenerate. Using Corollary 2 without losing generality one may assume $\Psi$ to be Hermitian and positive definite, $\Psi = U^\dagger E_0 U$, $U^\dagger = U^{-1} = (u_{k,j})$, $E_0 = \text{diag}(E_{0,j})$, $E_{0,j} = \lambda_1 > 0$, $j = 1, \ldots, N-1$, $E_{0,N} = \lambda_N > 0$, so that matrix $\Psi^\dagger \Psi = \Psi^\dagger \Psi$ has eigenvectors $U$. Thus the first $N-1$ vectors $u_k = (u_{k,1}, \ldots, u_{N,k})^\dagger$, $k = 1, \ldots, N-1$ collected as columns to $U^\dagger$ correspond to the eigenvalue $\lambda_1$ of $\Psi$ and the last column of $U^\dagger$, $u_N = (u_{1,N}, \ldots, u_{N,N})^\dagger$, corresponds to $E_{0,N} = \lambda_N$. Moreover, since any unitary transformation $\Psi \rightarrow U\Psi$, $U^{-1} = U^\dagger$ does not affect the norms of the vectors,
diagonal entries of $\Psi^2 = \Psi^\dagger \Psi$ remain equal to 1 after any unitary rotation. (Note nevertheless that the whole overlap matrix $\Psi^\dagger \Psi = \Psi^2$ remain unchanged after such a transformation.) Below we prove that under these conditions the eigenvector $u_N$ of $\Psi^2$ corresponding to $\lambda_N^2$ has coordinates with equal absolute values. Moreover, in the eigensubspace of $\Psi^2$ corresponding to eigenvalue $\lambda_1^2$ there always exists an eigenvector $u_{N-1} = (u_{1,N-1}, \ldots, u_{N,N-1})^\dagger$, $\langle u_{N-1}|u_{N-1}\rangle = 1$, $\Psi^2 u_{N-1} = \lambda_1 u_{N-1}$, such that $|u_{1,N-1}| = |u_{2,N-1}| = \ldots = |u_{N,N-1}| = N^{-1/2}$. Then the statement will follow from Theorem 2.

Condition $(\Psi^2)_{k,k} = 1$ or explicitly

$$\lambda_1^2 \sum_{j=1}^{N-1} |u_{k,j}|^2 + |u_{k,N}|^2 \lambda_N^2 = 1, \quad k = 1, \ldots, N \quad \text{(21)}$$

and unitarity of $U$, $\sum_{j=1}^{N-1} |u_{k,j}|^2 + |u_{k,N}|^2 = 1$, imply

$$|u_{k,N}|^2 = \frac{1 - \lambda_1^2}{\lambda_N^2 - \lambda_1^2}, \quad k = 1, \ldots, N. \quad \text{(22)}$$

Using this result and unitarity of $U$ once again one gets

$$u_{k,N} = \frac{1}{\sqrt{N}} e^{i\alpha_{k,N}}, \quad k = 1, \ldots, N, \quad \text{(23)}$$

where real phases $\alpha_{k,N}$ are defined by a concrete choice of $\Psi$.

From (22) and (23) we find a link between eigenvalues $\lambda_1^2$ and $\lambda_N^2$:

$$\lambda_N^2 + (N-1)\lambda_1^2 = N, \quad \text{(24)}$$

which results in a restriction for the lowest eigenvalue $0 < \min(\lambda_1^2, \lambda_N^2) < 1$.

Since by assumption the first $N-1$ vectors collected to $U^\dagger$ correspond to the same eigenvalue of $\Psi$ there is a freedom to choose in the eigensubspace spanned by these vectors any orthonormal basis. For our purpose it is sufficient to show that there exist real phases $\alpha_{k,N-1}$, $k = 1, \ldots, N$ such that a vector $u_{N-1} = (u_{1,N-1}, \ldots, u_{N,N-1})^\dagger$,

$$u_{k,N-1} = \frac{1}{\sqrt{N}} e^{i\alpha_{k,N-1}}, \quad k = 1, \ldots, N \quad \text{(25)}$$

is orthogonal to the vector $u_{k,N}$ (23). Indeed, from (23) and (25) one obtains

$$\sum_{k=1}^{N} e^{i(\alpha_{k,N} - \alpha_{k,N-1})} = 0. \quad \text{(26)}$$

This equation means that $\alpha_{k,N} - \alpha_{k,N-1}, k = 1, \ldots, N$ is $(k-1)$th root of unity, i.e. $\alpha_{k,N} - \alpha_{k,N-1} = \frac{2\pi}{N}(k-1)$ so that

$$\alpha_{k,N-1} = \alpha_{k,N} - \frac{2\pi}{N}(k-1), \quad k = 1, \ldots, N. \quad \text{(27)}$$

We, thus, explicitly constructed the vector $u_{N-1}$ from the eigensubspace corresponding to the eigenvalue $\lambda_1$ having the necessary form.

From the proof of this theorem one can extract a particular representation of a vector set $\Psi$ when $\Psi$ is Hermitian, positive definite and has only two distinct eigenvalues. First we note that using proper rescaling and unitary rotation one can always guarantee equal values of all coordinates of the vector $u_N$, i.e. $u_N = (1, \ldots, 1)/\sqrt{N}$. By this reason the vectors $u_j = (\exp(ia_{1,j}), \ldots, \exp(ia_{N,j}))/\sqrt{N}, j = 1, \ldots, N-1$ with $\alpha_{k,j-1} = \alpha_{k,j} - 2\pi(k-1)/N, k = 1, \ldots, N, j = N, N-1, \ldots, 2$ are orthogonal to $u_N$ since they differ from each other only by permutations of coordinates. Moreover, it is straightforward to check that together with $u_N$ they form an orthonormal set in $\mathcal{H}_N$. (They correspond to all $N$ roots of unity.) Using property (26) of roots of unity one can find the entries $\psi_{j,k}$ of $\Psi = U^\dagger E_0 U$

$$\psi_{j,k} = (\lambda_N - \lambda_1)/N, \quad j \neq k, \quad \text{(28)}$$

$$\psi_{j,k} = (\lambda_N + (N-1)\lambda_1)/N, \quad j, k = 1, \ldots, N \quad \text{(29)}$$

where $\lambda_1$ and $\lambda_N$ should satisfy Eq. (24).

Note that the inner products of the vectors $\Psi$ (28), (29) are equal to the same value $\langle \psi_i | \psi_j \rangle = s = (\lambda_N - \lambda_1)/N$, $i \neq j, |s| < 1$. Using Eq. (24) one can express eigenvalues of $\Psi^2$ in terms of $s$ as $\lambda_1^2 = 1 - s, \lambda_N^2 = 1 + N s$. In turn, the optimal mean efficiency in terms of $s$ reads

$$P_M = 1 - s + N (s - |s|)/2. \quad \text{(30)}$$

Our last comment here is that $N_0 = \text{rank} \mathcal{P}_x = 1$ for $s > 0$ and $N_0 = N-1$ for $s < 0$.

## III. PARTICULAR CASES

In this section we show that for $N = 2$ and $N = 3$ the maximal mean efficiency obtained from Theorem 2 corresponds to a set of symmetric equiprobable states and this theorem may lead to a wider set of equiprobable states starting from $N = 4$. In Section III A we illustrate our theorems for the case of two non-orthogonal states. In particular, if the states are given with different prior probabilities we specify a domain in the parameter space when Theorem 2 results in a von Neumann measurement. In the sections III B, III C and III D we consider equiprobable states only. In Section III B we construct a four-parameter set of three vectors normalized to unity and described by a Hermitian positive definite $3 \times 3$ matrix and present an example of states for which the symmetric point is not optimal. In Section III C we construct a three parameter set of four normalized to unity vectors described by a $4 \times 4$ Hermitian matrix with the optimal point being the symmetric point. In Section III D we show that for any set of $N$ symmetric states the symmetric point is the maximal point for the mean efficiency and re-derive the result obtained by Chefles and Barnett [8] for the value of the maximal mean efficiency. We obtain also an alternative formula for the maximal mean efficiency which may be useful when the states are given in a form different from that used by Chefles and Barnett [8].
A. \( N = 2 \)

Although the case of two states is well studied (see e.g. \cite{2, 5, 10}) we find it useful for illustrating our theorems above.

The most general Hermitian \( 2 \times 2 \) matrix \( \Psi \) composed of the vectors normalized to unity has the form

\[
\Psi = \begin{pmatrix} \sqrt{1-r^2} & e^{-i\alpha}r \\ e^{i\alpha}r & \sqrt{1-r^2} \end{pmatrix}, \quad 0 < r < 1, \quad \frac{1}{\sqrt{2}}. \tag{31}
\]

The inequality in (31) guarantees the positivity of eigenvalues of \( \Psi \), \( \lambda_{1,2} = \sqrt{1-r^2} \mp r \).

First we note that using a matrix \( U_a = \text{diag}(1, \exp(-i\beta)) \) for rescaling and unitarily rotating the set (31), i.e. \( \Psi \rightarrow U_a\Psi U_a^\dagger \), we can eliminate the inessential phase factors in the off-diagonal entries of \( \Psi \). Therefore in (31) we can put \( \alpha = 0 \). Now we see that if for matrix (31) with \( \alpha = 0 \) we displace the first coordinate of the vector \( \psi_1 \) to the next position and put its last (second in the current case) coordinate at the first place, we obtain \( \psi_2 \). The same transformation applied to \( \psi_2 \) gives \( \psi_1 \). Since this transformation is unitary, the states (31) are symmetric (see [8] for a definition).

For equiprobable states using \( Y(t) = \text{diag}(\sin t, \cos t) \) we obtain the highest eigenvalue of \( \Xi Y^2(t)\Xi = \Psi^{-1} Y^2(t)\Psi^{-1} \)

\[
\mu_m^2(t) = \frac{2 - \sqrt{2} \left[ 1 + 4 r^2 - 4 r^4 + (1 - 2 r^2)^2 \cos(4t) \right]^{1/2}}{4(1 - 2 r^2)^2}, \tag{32}
\]

which has a minimum (\( \mu_m^{-2}(t) \) has a maximum) at \( t = \pi/4 \). Note that this is just the symmetric point on the unit circle and, hence, for \( N = 2 \) the mean efficiency acquires the maximal value at the symmetric point. Thus, using Corollary 1 one obtains the optimal mean efficiency \( P_M = 1 - 2r\sqrt{1-r^2} = 1 - |\langle \psi_1 | \psi_2 \rangle| \).

The coordinates of eigenvectors of \( \Psi \), \( u_{1,2} = (\mp 1 + e^{i\alpha})/\sqrt{2} \) have equal absolute values. Therefore according to Theorem 2, \( P_M = \min(\lambda_1^2, \lambda_2^2) = (\sqrt{1-r^2}-r)^2 \) which is just the same as above.

For \( N = 2 \) the degree of degeneracy of the lowest eigenvalue assumed in Theorem 3 is \( N - 1 = 1 \). Thus using Eq. (30) for \( N = 2 \) one obtains the same value once again \( P_M = 1 - |\psi| = 1 - |\langle \psi_1 | \psi_2 \rangle| \), the result previously reported by numerous authors [2, 5, 8, 10]. This means that Eq. (30) presents the simplest generalization from \( N = 2 \) to an arbitrary \( N \).

For states given with different probabilities \( \eta_1 \) and \( \eta_2 = 1 - \eta_1 \), \( \eta_1 \neq \frac{1}{2} \) it is instructive to illustrate the case when Theorem 1 leads to a projective (i.e. von Neumann) measurement.

First we note that without losing generality one may assume \( 1/2 < \eta_1 < 1 \). Then choosing \( Y(t) = \text{diag}(\eta_1^{-1/2} \sin t, \eta_2^{-1/2} \cos t) \) we find the highest eigenvalue of \( \Xi Y^2(t)\Xi \)

\[
\mu_m^2(t) = \frac{\cos(2t)(2\eta_1 - 1) - 2G(t)}{4\eta_1 \eta_2(1 - 2 r^2)^2}, \tag{33}
\]

where

\[
G(t) = \left[ \frac{1}{2} + (\eta_1 - \frac{1}{2}) \cos(2t) \right]^2 - \eta_1 \eta_2 (2r^2 - 1)^2 \sin^2(2t). \tag{34}
\]

Function (33) may have minima only at points where \( d\mu_m^2(t)/dt = 0 \), i.e. at points satisfying the equation

\[
\sin(2t)G_1(t) = 0 \tag{35}
\]

In particular this may happen at \( t = 0 \) and \( t = \pi/2 \) where the function \( \mu_m^2(t) \) takes the values

\[
\mu_m^2(0) = (1 - 2 r^2)^{-2} \eta_2^{-1}, \quad \mu_m^2(\frac{\pi}{2}) = (1 - 2 r^2)^{-2} \eta_1^{-1} < \mu_m^2(0). \tag{37}
\]

Note that at these points either \( x_1 = 0 \) or \( x_2 = 0 \) meaning that either detection operator \( \Pi_{x1} \) or \( \Pi_{x2} \) does not participate at the optimal measurement and can be omitted from POVM so that the resolution of the identity \( \Xi \) contains in this case two terms only. For one-dimensional operators and \( N = 2 \) this necessarily leads to orthoprojectors as detection operators and, hence, to a von Neumann measurement.

According to (33) and (34) we have \( \mu_m^2(t) = \mu_m^2(\pi - t) \) and therefore \( t = \frac{\pi}{2} \) cannot be an inflexion point for this function. Moreover there exists no more than one point \( t \in (0, \pi/2) \) where \( d\mu_m^2(t)/dt := (d\mu_m^2(t)/dt)|_{t = \frac{\pi}{2}} = 0 \). This follows from the fact that this point should be found from the equation \( G_1(t) = 0 \) with \( G_1(t) \) given in (36) where, according to (33), \( G(t) \) is a second order polynomial on \( \cos(2t) \). By this reason to specify a domain in the space of parameters \((r, \eta_1)\) where the optimal measurement is a von Neumann measurement it is sufficient to find the values of \((r, \eta_1)\) such that \( t = \frac{\pi}{2} \) is just the point of a minimum for \( \mu_m^2(t) \), i.e. the point where \( d^2\mu_m^2(\pi/2)/dt^2 > 0 \). Thus from Eqs. (32) and (33) we find the condition

\[
2 + 2(4r^4 - 4r^2 - 1)\eta_1 > 0 \tag{38}
\]

or equivalently

\[
\frac{1}{1 + 4r^2 - 4r^2} < \eta_1 < 1. \tag{39}
\]

From Eq. (37) we find the optimal mean efficiency for this measurement \( P_M = \eta_1 \left( 1 - 2 r^2 \right)^2 = \eta_1 \left( 1 - \langle \psi_1 | \psi_2 \rangle^2 \right) \) which is just the “von Neumann value” \( \eta_1 \cos^2(\frac{\pi}{2} - \theta) = \eta_1 \sin^2 \theta \) where \( \theta \) is the angle between the vectors \( \psi_1 \) and \( \psi_2 \).

Below we will consider equiprobable states only.
B. \(N = 3\)

The most general Hermitian \(3 \times 3\) matrix \(\Psi = (\psi_1, \psi_2, \psi_3)\), contains three real and three complex parameters. Since the vectors \(\psi_j\) are assumed to be normalized to unity, the diagonal entries of \(\Psi\) can always be expressed in terms of off-diagonal elements. Moreover, one can always re-scale the vectors \(\psi_2\) and \(\psi_3\) such that their first components become real. After re-scaling the Hermiticity of \(\Psi\) can be restored by a proper unitary rotation of the vectors \(\Psi\). Thus, in the current case without losing generality matrices \(\Psi\) may be assumed to form a four-parameter family with a real parametrization. In general, eigenvalues of such a matrix should be found from a third order algebraic equation. Although any third order algebraic equation can be solved analytically, solutions, in general, are rather complicated and difficult for analyzing. Therefore below we show that there exists a parametrization where both the eigenvalues and eigenvectors of \(\Psi\) have a rather simple form but first we find convenient to illustrate our Theorem 2.

Let \(u_j = (u_{1j}, u_{2j}, u_{3j})^T\), and \(\lambda_j > 0, j = 1, 2, 3\) be eigenvectors and eigenvalues of \(\Psi\) respectively so that \(\Psi = U_j U_j^T\), where \(U_j = (u_1, u_2, u_3)\) and \(E_0 = \text{diag}(\lambda_1, \lambda_2, \lambda_3)\). According to Theorem 2 the components of (for instance) vector \(u_3\) should have equal absolute values. First we note that since the state vectors are defined up to phase factors one can always choose \(u_{3,3} = 1/\sqrt{3}\). Then using a similar re-scaling and unitary rotation of the vectors \(\Psi\) as discussed above, i.e. \(\Psi \rightarrow U_a \Psi U_a^T = U_a U_2 U_3 U_0 E_0 U_a U_2 U_3 U_0^T\) with \(U_a = \text{diag}(\exp(i \beta_3))\), \(j = 1, 2, 3\), one can always guarantee the choice \(u_{1,3} = u_{2,3} > 0\). Since this transformation does not affect \(u_{3,3}\), from here it follows that \(u_{1,3} = u_{2,3} = u_{3,3} = 1/\sqrt{3}\). Since \(\Psi\) is Hermitian, its eigenvectors \(u_j\) are orthogonal to each other. Therefore the vectors \(u_1\) and \(u_2\) can be obtained by applying a general transformation (rotation) from the group \(SU_2\) to arbitrary two orthonormal vectors chosen to be orthogonal to the vector \(u_3 = (1, 1, 1)/\sqrt{3}\). In particular, one can choose \(u_1 = (−2, 1, 1)/\sqrt{6}\) and \(u_2 = (0, 1, −1)/\sqrt{2}\). In this way we obtain the following unitary matrix

\[
U_3^T = \left(\begin{array}{ccc}
-\sqrt{\frac{1}{3}} K_{za} & -i \sqrt{\frac{2}{3}} K_{xy} & \frac{1}{\sqrt{3}} \\
\frac{1}{\sqrt{6}} K_{za} + \frac{1}{\sqrt{2}} K_{xy} & \frac{1}{\sqrt{6}} K_{za} - \frac{i}{\sqrt{2}} K_{xy} & \frac{i}{\sqrt{3}} \\
\frac{1}{\sqrt{6}} K_{za} - \frac{i}{\sqrt{2}} K_{xy} & \frac{1}{\sqrt{6}} K_{za} + \frac{i}{\sqrt{2}} K_{xy} & \frac{1}{\sqrt{3}}
\end{array}\right)
\]  

(40)

where \(K_{za} = \cos \frac{\theta}{2} + i K_z \sin \frac{\theta}{2}\), \(K_{xy} = (K_x + i K_y) \sin \frac{\theta}{2}\) and we have used the usual parametrization for the \(SU_2\) group [14] with \(0 \leq \alpha \leq 2\pi\) and \(K_x, K_y, K_z\) being the coordinates of a real unit 3-dimensional vector, \(K_x^2 + K_y^2 + K_z^2 = 1\), \(K_{xy,z} \in \mathbb{R}\). Below we find more convenient to use two complex parameters \(K_{xy}\) and \(K_{za}\) subject to the normalization condition

\[
|K_{xy}|^2 + |K_{za}|^2 = 1.
\]  

(41)

The normalization condition for the vectors \(\Psi\), \((\Psi^2)_{ij} = 1\), or explicitly

\[
\sum_{j=1}^{N} \lambda_j^2 |u_{k,j}|^2 = 1, \quad k = 1, 2, \ldots, N, \quad N = 3, \quad \lambda_j^2 = \frac{3 - \lambda_j^2}{2|K_{xy}|^2 + 2|K_{za}|^2} = \frac{3 - \lambda_j^2}{2}.
\]  

(42)

may be considered as a system of linear inhomogeneous equations with respect to eigenvalues \(\lambda_j^2\). Note that because of the unitarity of \(U_3\) this system always has a solution \(\lambda_1^2 = \lambda_2^2 = \lambda_3^2 = 1\). This trivial solution is not suitable for our purposes and we need another one. This means that system (42) should be linearly dependent with a vanishing main determinant, \(\det(|u_{k,j}|^2) = 0\). In this case one of the eigenvalues, say \(\lambda_k^2\), is arbitrary while two others are linear functions of \(\lambda_k^2\). It is straightforward to check that for \(u_{k,j}\) given in (10) the determinant vanishes and from the system (42) we find

\[
\lambda_2^2 = \frac{3 - \lambda_3^2}{2}.
\]  

(43)

Since we assume \(\Psi\) to be positive definite, this means that \(\lambda_1 = \lambda_2\) and the unitary rotation of the vectors \(u_1\) and \(u_2\) considered above does not affect \(\Psi\). Thus the vectors \(\Psi\) are parameterized by one parameter \((\lambda_3)\) only,

\[
\Psi = \left(\begin{array}{ccc}
A_0 & A_1 & A_1 \\
A_1 & A_0 & A_1 \\
A_1 & A_1 & A_0
\end{array}\right),
\]  

(44)

where

\[
A_0 = \frac{1}{3}(\lambda_1 + \lambda_2 + \lambda_3), \quad A_1 = \frac{1}{3}(\lambda_3 - \lambda_2).
\]  

(45)

From here we see that similarly to the previous section the coordinates of the vector \(\psi_3\) are obtained from the coordinates of the vector \(\psi_1\) by a simple permutation (denote it \(P\)) and the coordinates of the vector \(\psi_3\) are obtained from the coordinates of the vector \(\psi_2\) by the same permutation \(P\). Applying \(P\) to the vector \(\psi_3\) one obtains \(\psi_1\). This means that \(P^3 = I_3\) (identity). Since such a permutation of coordinates is a unitary transformation, the set (44) is a particular case of symmetric states (for a definition see e.g. [8]). From theorems 2 and 3 for the states (44) we find the optimal mean efficiency \(P_M = \lambda_3^2\) for \(0 < \lambda_3 < 1\) and \(P_M = \frac{3 - \lambda_j^2}{2}\) for \(1 < \lambda_3 < \sqrt{3}\). Note that the vectors (44) have equal inner products \(s = \langle \psi_j | \psi_k \rangle = \frac{1}{3}(\lambda_j^2 - \lambda_k^2), j \neq k, -1/2 < s < 1\) and the optimal mean efficiency is obtained from Eq. (60) at \(N = 3\).

The condition \(\lambda_1^2 \neq \lambda_2^2\) is incompatible with the system (42) when it is considered as a system of linear equations with respect to \(\lambda_j^2\). Nevertheless, for \(\lambda_1^2 \neq \lambda_2^2\) this system has a solution with respect to \(SU_2\) group parameters. In particular, after simple calculations one finds

\[
|K_{za}|^2 = \frac{1}{2}, \quad K_{xy} = \pm K_{za}
\]  

(46)
For this parameter set matrix $\Psi$ assumes the form

$$
\Psi = \begin{pmatrix}
A_0 & A_2 & A_4 \\
A_2^* & A_0 & A_2 \\
A_4^* & A_2 & A_0
\end{pmatrix}
$$

(47)

where $A_0$ is given in (46) and

$$
A_2 = \frac{1}{3}(\lambda_3 - e^{i\theta_2}\lambda_2 - e^{-i\theta_2}\lambda_1)
$$

(48)

for the upper sign in (46). It follows from (47) that the vectors $\Psi$ have the same permutation symmetry as in the previous case. Hence, this is a set of symmetric states also. The same conclusion takes place for the lower sign in (46). Note that $A_2$ defined by (48) cannot be real. Therefore the vectors (44) are not a particular case of the previous case. Hence, this is a set of symmetric states vectors $\Psi$ have the same permutation symmetry as in the previous case. It follows from (47) that the main determinant is replaced by its transposed form, i.e. $u_k \rightarrow u_j$. Since such a replacement does not affect the main determinant, the system remains to be overfull and one can express, for instance, $\lambda_1^2$ and $\lambda_2^2$ in terms of $\lambda_3^2$

$$
\lambda_1^2 = \frac{1 - 3|u_{2,2}|^2 + \lambda_2^2(|u_{2,2}|^2 - |u_{3,2}|^2)}{|u_{1,2}|^2 - |u_{2,2}|^2}
$$

(49)

and

$$
\lambda_2^2 = 3 - \lambda_1^2 - \lambda_3^2.
$$

(50)

Thus, we have obtained a four-parameter set of matrices $\Psi$ where three parameters come from $SU_2$ group and one parameter is $\lambda_3 > 0$.

In particular, the choice $K_{xy} = 0$ and $K_{zo} = \exp(i\pi/4)$ selects from this set a one parameter ($\lambda_3$) subset

$$
\Psi = \frac{1}{6} \begin{pmatrix}
6 + \lambda_+ & -i\sqrt{3}\lambda_- & (1 - i)\lambda_+ \\
i\sqrt{3}\lambda_- & 3(2 + \lambda_+) & (1 + i)\sqrt{3}\lambda_- \\
(1 + i)\lambda_+ & (1 - i)\sqrt{3}\lambda_- & 2(3 + \lambda_+)
\end{pmatrix}
$$

(51)

where we have abbreviated $\lambda_+ = \lambda_2 + \lambda_3 - 2$, $\lambda_- = \lambda_2 - \lambda_3$. The eigenvalues of $\Psi$ are $\lambda_1 = 1$, $\lambda_2 = \sqrt{2 - \lambda_3}$ and $\lambda_3$.

As a numerical example we choose $\lambda_3^2 = 3/2$. The optimal point on the sphere is found using Corollary (42) $(t_1, t_2) = (0.919, 0.992)$, which corresponds to the weights $(x_1, x_2, x_3) = (0.67, 0.43, 0.99)$ and the optimal mean efficiency $P_M = 0.535$. The mean efficiency at the symmetric point $t_0 = (\arccos\frac{1}{\sqrt{3}}$, $\pi/4)$, $P(t_0) = \lambda_2^2 = 1/2 < P_M$, is not optimal.

C. $N = 4$

We start with an orthonormal set of 4-vectors where one of the vectors has equal coordinates

$$
U_4 = \frac{1}{2} \begin{pmatrix}
0 & -1 & -\sqrt{2} & 1 \\
-\sqrt{2} & 1 & 0 & 1 \\
0 & -1 & \sqrt{2} & 1 \\
\sqrt{2} & 1 & 0 & 1
\end{pmatrix}.
$$

(52)

In general one can apply a 8-parameter transformation from the group $SU_3$ to the vectors $(u_1, u_2, u_3)$ to get a general orthonormal set having a vector with equal coordinates. For the sake of simplicity we will use $SU_2$ group once again and apply it to the vectors $u_1$ and $u_2$ in a similar way as it was described in the previous section. In such a way one obtains the following elements of matrix $4\Psi$:

$$
\psi_{1,1} = 2\lambda_3 + \lambda_4 + \lambda_1|K_{xy}|^2 + \lambda_2|K_{zo}|^2,
\psi_{1,2} = \lambda_4 + \lambda_2|\sqrt{2}K_{xy} + K_{zo}|^2 + \lambda_1|K_{xy} - \sqrt{2}K_{zo}|^2,
\psi_{3,3} = \psi_{1,1},
\psi_{3,4} = \psi_{1,4}, 4(\lambda_3 + \lambda_4) - 2\psi_{1,1} - \psi_{1,2},
\psi_{2,3} = \psi_{1,2},
\psi_{2,4} = \psi_{1,1} - \psi_{1,2} + \psi_{1,3} + \psi_{1,4} - \psi_{1,2},
\psi_{3,4} = \psi_{1,4}.
$$

(53)

One can easily check that after this transformation system (52) at $N = 4$ is overfull and has a solution $\lambda_1^2 = \lambda_2^2 = \lambda_3^2 = \lambda_4^2 = \frac{1}{4}(4 - \lambda_3^2)$ useless for our purposes since it corresponds to symmetric states. To get another solution we will assume $\lambda_3^2 \neq \lambda_4^2$ for $i \neq j$ and solve the system (42) with respect to $SU_2$ group parameters thus obtaining

$$
|K_{xy}|^2 = \frac{\lambda_1^2 - \lambda_3^2}{\lambda_2^2 - \lambda_3^2},
|K_{zo}|^2 = \frac{\lambda_2^2 - \lambda_3^2}{\lambda_1^2 - \lambda_3^2}.
$$

(54)

$$
K_{xy} = \pm \sqrt{\frac{\lambda_1^2 - \lambda_3^2}{\lambda_2^2 - \lambda_3^2}}K_{zo},
$$

(55)

With this set of parameters the vectors $\Psi = \Psi$ have unit norm for arbitrary $\lambda_j$ provided $\sum_{j=1}^4 \lambda_j^2 = 4$. For the upper sign in (55) the basic elements of the matrix $4\Psi$ given in (53) read

$$
\psi_{1,1} = \lambda_1 + \lambda_4 + 2\lambda_3 + \lambda_2^2 - \lambda_3^2,
\psi_{2,2} = \psi_{1,1} + \frac{2(\lambda_1 - \lambda_2)(\lambda_2 - \lambda_3)}{\lambda_1 + \lambda_2},
\psi_{4,4} = \psi_{2,2},
\psi_{1,2} = 2(\lambda_3 + \lambda_4) - \psi_{1,1} + \frac{2\lambda_4}{\lambda_1 + \lambda_2}.
$$

(56)
where
\[ B_1 = \sqrt{\frac{(\lambda_2^2 - \lambda_3^2)(\lambda_3^2 - \lambda_4^2)}{\sqrt{2}}} \]  

(57)

Thus we have obtained a 3-parameter \((\lambda_2, \lambda_3, \lambda_4)\) set of the vectors \(\Psi\).

Note that Eq. (54) imposes restrictions on possible values of \(\lambda_i^2\). In particular, the following inequalities:
\[ \lambda_1^2 < \lambda_2^2 < \lambda_3^2 < \lambda_4^2 \]  

(58)

should hold. Here we imposed the condition that \(\lambda_1^2\) is the lowest eigenvalue of \(\Psi^2\). Since under the last restriction the eigenvector of \(\Psi^2\) corresponding to the lowest eigenvalue has equal coordinates, we can apply Theorem 2. According to this theorem the optimal mean efficiency coincides with \(\lambda_1^2\), \(P_M = \lambda_1^2\), provided the parameters are ordered according to (58) and \(\lambda_1^2 + \lambda_2^2 + \lambda_3^2 < 4\).

Finally, to show that the vectors from this set are neither symmetric states nor their unitary rotated form we give matrix \(\Psi^2\)

\[ \Psi^2 = \begin{pmatrix} 1 & B_1^* & B_2 & B_3 & B_4 \\ B_1 & 1 & B_2 & B_3 + iB_1 & B_4 \\ B_2 & B_1 & 1 & B_2 & B_3 \\ B_3 & B_2 & B_1 & 1 & B_2 \\ B_4 & B_3 & B_2 & B_1 & 1 \end{pmatrix} \]  

(59)

where \(B_1\) in given in (57), \(B_2 = \frac{1}{2}(2 - \lambda_2^2 - \lambda_3^2 - iB_1)\) and \(B_3 = 1 - \lambda_3^2\). In the next section we will show that a matrix \(\Psi^2\) of the form (69) cannot correspond to symmetric states.

D. Symmetric states

In this section we prove that the mean efficiency for the equiprobable so called symmetric states (see e.g. [8] for some discussion and literature overview) is maximal at the symmetric point on the unit sphere.

As shown in [8] symmetric states \(\psi_k\) may be defined in terms of any orthonormal basis \(\{\epsilon_k\}\), \(k = 0, \ldots, N - 1\), \(\langle \epsilon_k | \epsilon_j \rangle = \delta_{kj}\) in \(\mathcal{H}\) as follows

\[ \psi_k = \sum_{j=0}^{N-1} c_j e^{2\pi ijk/N} \epsilon_j, \quad k = 0, \ldots, N - 1, \]  

(60)

where coefficients \(c_k\) may be arbitrary complex numbers provided

\[ \sum_{k=0}^{N-1} |c_k|^2 = 1. \]  

(61)

In what follows we choose a representation where \((\epsilon_0, \ldots, \epsilon_{N-1}) = I_N\). Then using the fact that the additional phase factors in (60) are either \(N\)th roots of unity or their integer powers and therefore they satisfy the following identity

\[ \sum_{k=0}^{N-1} e^{2\pi i(j-j')k/N} = N\delta_{jj'}, \quad j, j' = 0, 1, \ldots \]  

(62)

one easily sees that

\[ \Phi \Phi^\dagger = N\text{diag}(|c_0|^2, \ldots, |c_{N-1}|^2) \]  

(63)

where as above \(\Phi = (\psi_0, \ldots, \psi_{N-1})\). By the same reason and in view of condition (61) matrix \(\Phi^\dagger \Phi\) has the form

\[ \Phi^\dagger \Phi \equiv A = \begin{pmatrix} A_0 & A_{N-1} & A_{N-2} & \cdots & A_1 \\ A_1 & A_0 & A_{N-1} & \cdots & A_2 \\ A_2 & A_1 & A_0 & \cdots & A_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A_{N-1} & A_{N-2} & A_{N-3} & \cdots & A_0 \end{pmatrix} \]  

(64)

where \(A_0 = 1\) and

\[ A_k = \sum_{j=0}^{N-1} |c_j|^2 e^{2\pi ijk/N}, \quad k = 1, \ldots, N - 1. \]  

(65)

A matrix of the form (64) is called circulant [15]. For any complex \(A_k\) it has eigenvalues \(F(\varepsilon^{k+1})\), \(k = 0, \ldots, N - 1\) where

\[ F(x) = \sum_{k=0}^{N-1} A_k x^k, \quad x = e^{2\pi i/N} \]  

(66)

and eigenvectors

\[ v_{k-1} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \varepsilon^{(N-k)j} v_{j-1}, \quad k = 1, \ldots, N, \]  

(67)

\[ Av_k = F(\varepsilon^{k+1})v_k, \quad k = 0, \ldots, N - 1. \]  

(68)

From (67) it follows that if \(v_{k,j}\) are the coordinates of the vectors \(v_k\) then \(|v_{k,j}| = N^{-1/2}\) for \(k, j = 0, \ldots, N - 1\). Using Theorem 2 the fact that matrices \(\Phi\Phi^\dagger\) and \(\Phi^\dagger \Phi\) have the same set of eigenvalues and formula (63) we obtain for \(P_M\) just the value reported by Chefles and Barnett [8]

\[ P_M = N \times \min(|c_0|^2, \ldots, |c_{N-1}|^2). \]  

(69)

Note that the entries of matrix (64) are inner products of the vectors \(\psi_j\), i.e. \(A = (\langle \psi_i | \psi_j \rangle)\). Therefore they are independent on a unitary rotation of the set \(\Psi\). By this reason, for any set of symmetric states \(\Psi\), matrix of their inner products has always form (64). The opposite statement, evidently, is also true. If for a set of states \(\Psi\)
the matrix $\Psi^\dagger \Psi$ has the form (64), then the states are either symmetric states or their unitary rotated form. This follows from the fact that one of the square roots of matrix (64) is a Hermitian matrix of symmetric states. If for a Hermitian matrix $B^2 = (B^2)^\dagger$ a Hermitian matrix $B = B^1$ is given, then any other Hermitian square root of $B^2$, $B = B^1, B^2 = B^2$, is defined up to a unitary matrix $V = (V^\dagger)^{-1}, V^\dagger V$ such that $V B = B V^\dagger$.

The entries of a matrix given in (23) and (29) correspond to a set of symmetric states. This means that any set of states satisfying Theorem $\Psi$ i.e. a set, for which one of the eigenvalues of the matrix $\Psi^\dagger \Psi$ is $N - 1$ fold degenerate, is either a set of symmetric states or its unitary rotated form. From this viewpoint Theorem 2 gives another recipe how one can identify such a set when it is presented by a non-Hermitian matrix. From the other hand matrix (59) does not have this form meaning that the states $\Psi$ obtained in Section III C are not symmetric.

Another remarkable property of matrix (64) we would like to emphasize is the following. Assume we are given vectors collected as the columns to matrix (64), i.e. we put $\Psi = (\psi_1, \ldots, \psi_N) = A$. In this case, evidently, $\psi_j + 1 = P \psi_j, j = 1, \ldots, N - 1, \psi_1 = P \psi_N$ where $P$ displaces every coordinate of a vector to the next position and places the last coordinate in place of the first one. Such an operator is unitary and, hence, according to a definition of symmetric states (see e.g. [8]) the states (64) are symmetric. Using Theorem 2 we can obtain another (but equivalent to (69)) expression for the optimal mean efficiency for symmetric states. It may be useful when symmetric states are given in a form different from that used by Chefles and Barnett [8].

This possibility is based on the property of matrix (64) to be normal, i.e. $AA^\dagger = A^\dagger A$ which can be checked by a direct calculation. Therefore matrices $A, A^\dagger$ and $A^\dagger A$ may have the same set of eigenvectors given in (67). Absolute values of coordinates of any eigenvector coincide and we can apply Theorem 2 to find the optimal mean efficiency. According to Corollary 2 for the optimization procedure we can replace $\Psi$ by positive definite Hermitian matrix $\Psi = \epsilon^\dagger E_0 U$ where diagonal matrix $E_0$ contains absolute values of matrix $A$ eigenvalues as non-zero entries, $E_{0,k} = |F(\epsilon^k)|, k = 0, 1, \ldots, N - 1$ where $F(x)$ and $\epsilon$ are given in (69). To apply Theorem 2 the vectors $\Psi = A$ should have unit norm. This condition is satisfied if $\sum_{j=1}^{N-1} |A_j|^2 = 1$. Now using Corollary 1 we conclude that $P_M = \min(|E_{0,0}|^2, \ldots, |E_{0,N-1}|^2)^2$. Parameters $A_k$ should be chosen such that $E_{0,k} \neq 0, k = 0, \ldots, N - 1$. Otherwise the set $\Psi$ becomes linearly dependent.

IV. POVM AND NEUMARK’S EXTENSION

In the previous section we formulated conditions to be imposed on the set of the vectors $\Psi$ when, from the one hand, the mean efficiency takes its maximal value at the symmetric point and from the other hand there exists a Hermitian positive semidefinite matrix $\Pi_x$ satisfying (5). Another important property we established is that although $\Pi_x$ is an $N \times N$ matrix its rank may vary from 1 till $N - 1$ so that if we associate a set of the vectors with the columns of this matrix, this set is necessarily linearly dependent with a linearly independent subset spanning the space of dimension $N_x$ varying from 1 till $N - 1$.

Below we will discuss the so called Neumark’s extension which, in particular, consists in considering an additional space called ancilla space related just with the set of the vectors collected to $\Pi_x$. In particular, the dimension of the ancilla space is $N_x = \text{rank} \Pi_x$.

The notion of an ancilla first introduced in quantum information theory [10] permits one to reduce generalized measurements to conventional von Neumann measurements in a higher dimensional space [12]. Usually this extended space is considered as the direct product of spaces of the system to be measured with another (auxiliary) known system called the ancilla (see e.g. [11]). But as is stressed in [18] it may have a wider sense as any extra degrees of freedom related with the Neumark’s extension theorem. Since there are two ways to extend the initial Hilbert space, there are two different realizations of the extended Hilbert space: (i) the extended space is the tensor product of the initial (i.e. system) space and the ancilla space (TPE) and (ii) the extended space is the direct sum of the initial space and the ancilla space (DSE) [18]. As is stressed in [18] DSE is much more economical from the experimental viewpoint since in this case the dimension of the extended space is much less than the corresponding dimension for TPE. In particular, the authors [18] claim that to unambiguously discriminate among $N$ given linearly independent non-orthogonal states by DSE an $(N - 1)$-dimensional ancilla space is sufficient whereas for TPE $N^2$ additional dimensions are necessary, where $N$ is just the space dimension of the main system, i.e. the number of the given linearly independent vectors collected to $\Psi$. From the other hand, as it is pointed out by Preskill [12], the tensor product extension is much more transparent from physical viewpoint since additional dimensions can always be interpreted as extra degrees of freedom of the extended system (e.g. internal degrees of freedom like spin or external degrees of freedom corresponding to an interaction of the system with a reservoir).

As is stressed in Section II $(N - 1)$-dimensional ancilla space is the maximal space appearing as result of the optimization procedure and the actual ancilla space dimension varies from 1 till $N - 1$. Thus for $N > 2$ we give a stronger limit to the minimal ancilla space dimension for the DSE-case than the one found in [18]. To the best of the author’s knowledge in the current literature there are no explicit constructions of POVMs accepting ancilla spaces of such low dimension as 1 for $N > 2$ [22]. The next section is just devoted to fill in this gap. We will present a general construction of a simple form for a POVM with the ancilla space dimension in the range between 1 and $N$.

Another point we would like to emphasize is the following. According to the necessary condition [8] for the
optimization of the mean efficiency the highest singular number of matrix $\Xi_x$ should be equal to 1. Just this property leads to a linear dependence between the vectors $\tilde{\Pi}_x$. If after the optimization one can sacrifice the very optimal POVM in favor of a bit less optimal POVM where all the vectors collected to matrix $\Xi_x$ are scaled by a factor a bit less than 1 (real scaling factor should be chosen in agreement with how much from the optimal efficiency one is able to sacrifice), then the rank of $\tilde{\Pi}_x$ becomes equal to $N$ and the ancilla space acquires the same dimension as the system space ($N_a = N$). In such a case, as we show below by an explicit construction of the corresponding Neumark’s extension, one may enjoy an advantage of the direct sum extension of two copies of the same $N$-dimensional space being presented in the form of the tensor product of the two-dimensional ancilla space and $N$-dimensional system space with a clear physical meaning of the ancilla space as an additional (e.g. internal) degree of freedom of an extended system. Thus, similar to DSE-case, we indicate on a stronger limit (e.g. internal) degree of freedom of an extended system.

Below we will consider only the vectors $\Xi_x$ and to simplify notations will omit subscript $x$.

A. POVM

Let the vectors $\xi_i \in \mathcal{H}$, $i = 1, \ldots, N$, collected to the matrix $\Xi$, be given. Denote as $\Xi$ matrix with unknown linearly independent vectors $\tilde{\xi}_j \in \mathcal{H}$, $j = 1, \ldots, N_a \leq N$ such that the identity decomposition

$$\Xi\Xi^\dagger + \Xi\Xi^\dagger = I_N$$

holds. Since by assumption the vectors $\Xi$ are linearly independent $\text{rank} \Xi = N$ but $\text{rank} \Xi = N_a \leq N$ and $\Xi\Xi^\dagger$ is positive definite while $\Xi\Xi^\dagger$ may be positive both definite and semidefinite. In both cases matrix $(I_N - \Xi\Xi^\dagger)^{1/2}$ is well defined and Hermitian. Therefore from (70) it follows

$$\Xi = (I_N - \Xi\Xi^\dagger)^{1/2} \tilde{V}, \quad \tilde{V}^{-1} = \tilde{V}^\dagger$$

where $\tilde{V}$ is an $N \times N$ arbitrary unitary matrix. In particular, for $N_a = N$ one may choose $\tilde{V} = (\Xi\Xi^\dagger)^{-1/2}$ leading to

$$\Xi = (I_N - \Xi\Xi^\dagger)^{1/2}(\Xi\Xi^\dagger)^{-1/2} = [(\Xi\Xi^\dagger)^{-1} - I_N]^{1/2}\Xi.$$  

(72)

Note that the $N \times N$ matrix $\Xi$ (72) contains $N$ linearly independent vectors as columns only if $N_a = N$. If $N_a < N$ among $N$ columns of this matrix only $N_a$ columns are linearly independent. Since we want this matrix to contain only linearly independent columns it should be rectangular of dimension $N \times N_a$ in this case. Moreover, there is no need to rotate all $N$ vectors by transformation $\tilde{V}$. It is sufficient to use an arbitrary $N_a \times N_a$ unitary rotation instead of $\tilde{V}$. Below we explicitly construct a matrix $\Xi$ having this property.

For $N_a < N$ denote as $U$ unitary matrix bringing $\Xi\Xi^\dagger$ to a diagonal form

$$\Xi\Xi^\dagger U = US_d$$

(73)

where $S_d$ is a diagonal matrix, in which the highest $(N - N_a)$ fold degenerate eigenvalue, which is equal to 1, occupies the last $(N - N_a)$ positions. Then from (70) one finds

$$\Xi\Xi^\dagger = U(I_N - S_d)U^\dagger.$$  

(74)

It is clear that by construction only the first $N_a$ columns of matrix $U(I_N - S_d)^{1/2}$ are nonzero. Therefore, the solution we need is obtained if $\Xi$ is composed of all nonzero columns of $U(I_N - S_d)^{1/2}$, which we denote $\Xi_1$, times an arbitrary unitary $N_a \times N_a$ matrix $V$, i.e.

$$\Xi = \Xi_1 V, \quad V^{-1} = V^\dagger.$$  

(75)

Note that all $N_a$ columns of $N \times N_a$ matrix $\Xi$ (75) are linearly independent by construction.

B. Neumark’s extension

Neumark [10] proved a very general statement concerning a representation of an additive operator-valued function in a unitary space in terms of orthogonal spectral functions in higher spaces. In the context of our problem it, in particular, means that any non-orthogonal identity decomposition in the space $\mathcal{H}_N$ may be presented as a projection from a space of a higher dimension of an orthogonal identity decomposition (see e.g. [12]). Although there exists a number of constructions extending a given non-orthogonal identity decomposition to an orthogonal one in a higher dimensional space (see e.g. [12, 18, 20]) they are based on either the tensor product extension [12] or are not suitable for establishing an isomorphism between Hilbert spaces $\mathcal{H}_N \oplus \mathcal{H}_N$ and $\mathcal{H}_2 \otimes \mathcal{H}_N$. Therefore in this section we give an explicit realization of the Neumark’s theorem suitable for this purpose.

Let us consider $(N + N_a) \times (N + N_a)$ matrix $(N_a \leq N)$

$$U = \begin{pmatrix} \Xi & \tilde{\Xi} \\ Z & Y \end{pmatrix}.$$  

(76)

As it is noted by Preskill [12] the rows $(z_{k,1}, \ldots, z_{k,N}, y_{1,1}, \ldots, y_{N_a,1})$, $k = N + 1, \ldots, N + N_a$ of matrix (76) should be orthogonal to all its rows $(\xi_{j,1}, \ldots, \xi_{j,N}, \tilde{\xi}_{j,1}, \ldots, \tilde{\xi}_{j,N_a})$, $j = 1, \ldots, N$ where $z_{k,j}$, $y_{k,j}$, $\xi_{k,j}$ and $\tilde{\xi}_{k,j}$ are entries of blocks $Z$, $Y$, $\Xi$ and $\tilde{\Xi}$ of $U$ respectively. Below we find explicit expressions for
Z and Y in terms of the given Ξ and \( \tilde{Ξ} \) such that \( \mathcal{U} \) is unitary

\[
\mathcal{U}^\dagger \mathcal{U} = I_{N+N_a},
\]

(or equivalently \( \mathcal{U} \mathcal{U}^\dagger = I_{N+N_a} \)).

Condition (77) is equivalent to the following set of equations for Z and Y

\[
\begin{align*}
\Xi \dagger \Xi + Z \dagger Z &= I_N, \\
\tilde{Ξ} \dagger \tilde{Ξ} + Y \dagger Y &= I_{N_a}, \\
\Xi \dagger \Xi + Z \dagger Z &= 0.
\end{align*}
\]

(78)\hspace{1cm}(79)\hspace{1cm}(80)

Now we note that the condition \( \mathcal{U} \mathcal{U}^\dagger = I_{N+N_a} \) is an implication of (77). This, in particular, means that the POVM condition (70) follows from (78)-(80). Therefore we can replace Eq. (79) by Eq. (70). From (78) we find matrix Z. For that we multiply (70) from the left by unitary matrix \( \Phi \) and from the right by \( \Phi \) where \( \Phi = (\Xi \Xi) \dagger^{-1/2} \Xi \) which gives \( \Xi \dagger \Xi + \Phi \Xi \Xi \dagger \Phi = I_N \). Comparing this equation with (78) we conclude that \( Z \dagger Z = \Phi \Xi \Xi \dagger \Phi \) and, hence,

\[
Z = V \tilde{Ξ} \dagger \Phi = V \tilde{Ξ} \dagger (\Xi \Xi) \dagger^{-1/2} \Xi, \quad V^{-1} = V \dagger (81)
\]

where \( V \) is an arbitrary unitary matrix. Note that \( ZZ \dagger = V \tilde{Ξ} \dagger \tilde{Ξ} V \dagger \) is \( N_a \times N_a \) overlap matrix of the unitary rotated linearly independent by construction vectors \( \xi_i \), \( i = 1, \ldots, N_a \) collected as columns to \( \tilde{Ξ} \) and, therefore, \( ZZ \dagger \) is non-singular. Using this fact we find from (80)

\[
Y = -V (\tilde{Ξ} \dagger \tilde{Ξ})^{-1} \tilde{Ξ} (\Xi \Xi) \dagger^{1/2} \Xi. \quad (82)
\]

Note that for \( Y \) given in (82) condition (70) is automatically satisfied which may be checked by a direct calculation.

It is important to note that if a non-singular \( \tilde{Ξ} \) given in (72) is used in (70), in which case \( N_a = N \), Eqs. (81) and (82) assume simpler form

\[
\begin{align*}
Z &= V \Phi \dagger \tilde{Ξ}, \\
Y &= -V \Phi \dagger \Xi.
\end{align*}
\]

(83)\hspace{1cm}(84)

These equations suggest the choice \( V = \Phi \) leading to the simplest expressions for \( Z \) and \( Y \)

\[
Z = \tilde{Ξ}, \quad Y = -\Xi, \quad (85)
\]

and the following expression for \( \mathcal{U} \) [23]

\[
\mathcal{U} = \sigma_z \otimes \Xi + \sigma_+ \otimes \tilde{Ξ},
\]

(86)

where \( \sigma_x, \sigma_z \) are the usual Pauli matrices. Since all Hilbert spaces of the same dimension are isomorphic to each other, \( 2N \)-dimensional Hilbert space, which is the direct sum of two \( N \)-dimensional spaces, \( \mathcal{H}_N \oplus \mathcal{H}_N \), is isomorphic to \( \mathcal{H}_2 \otimes \mathcal{H}_N \). Relation (86) may be used to map the operator \( \mathcal{U} \) presented by matrix (70) in the space \( \mathcal{H}_N \oplus \mathcal{H}_N \) to the space \( \mathcal{H}_2 \otimes \mathcal{H}_N \).

V. CONCLUSION

The main feature of our approach to optimization of the mean efficiency for discriminating among \( N \) given linearly independent non-orthogonal states from methods usually used by previous authors consists in choosing a different form for the constraint to be imposed on optimization parameters to assure the existence of a POVM and, hence, the necessary probabilistic interpretation. The form of the constraint, we have used, permitted us to reduce the conditioned optimization problem for the mean efficiency to a problem of finding an unconditioned maximum of a function defined on an \( N \)-ellipsoid [Theorem 1] for the states given with different probabilities and on a unit \( N \)-sphere for equiprobable states (Corollary 1). Using Theorem 1 we established the invariance of both the weight matrix and the optimal mean efficiency with respect to unitary rotations of the vector set. Therefore for any vector set \( \Psi \) the optimization procedure may be realized for its equivalent Hermitian form, \( \Psi = \Psi^\dagger \) with \( \Psi \) being a positive definite matrix. Using this fact for equiprobable states we succeeded to formulate a criterion when the optimal point is the symmetric point on the \( N \)-sphere. This selects a set of matrices for which a numerical optimization becomes unnecessary. By the symmetric point on the sphere we mean a point with equal values of Cartesian coordinates when the sphere is centered at the origin. We have shown that for \( N = 2, 3 \) only symmetric states satisfy this criterion but starting from \( N = 4 \) the indicated set becomes wider than the set of symmetric states. The whole family of states satisfying this criterion is still unspecified.

We have also found a subset of \( N \) symmetric states which may be considered as the simplest generalization of two states since the expression for the optimal mean efficiency for two states is a particular case of a more general formula valid for the subset. The vectors from this subset are characterized by the following property. If \( \Psi \) is a matrix where the state vectors are collected as columns then \( \Psi^\dagger \Psi \) has only two distinct eigenvalues one of which is \( N - 1 \) fold degenerate.

Our approach is illustrated by examples with \( N = 2, 3, 4 \) nonorthogonal states.

Finally we presented our constructions of POVM and Neumark’s extension. We indicated on an explicit procedure how to construct a POVM for the case when the dimension of the ancilla space varies from 1 till \( N \). As to Neumark’s extension we presented a formula for the unitary matrix realizing the corresponding orthogonal identity decomposition suitable for its use both in the Hilbert space \( \mathcal{H}_N \oplus \mathcal{H}_N \) and \( \mathcal{H}_2 \otimes \mathcal{H}_N \).

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