A complementarity-based approach to phase in finite-dimensional quantum systems

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We develop a comprehensive theory of phase for finite-dimensional quantum systems. The only physical requirement we impose is that phase is complementary to amplitude. To implement this complementarity we use the notion of mutually unbiased bases, which exist for dimensions that are powers of a prime. For a $d$-dimensional system (qudit) we explicitly construct $d + 1$ classes of maximally commuting operators, each one consisting of $d - 1$ operators. One of this class consists of diagonal operators that represent amplitudes (or inversions). By the finite Fourier transform, it is mapped onto ladder operators that can be appropriately interpreted as phase variables. We discuss the examples of qubits and qutrits, and show how these results generalize previous approaches.

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I. INTRODUCTION

The standard formalism of quantum optics is usually presented in the context of the harmonic oscillator, where both position and momentum are represented by unbounded operators with eigenvalues in the real numbers. Systems living in a finite-dimensional Hilbert space were studied originally by Weyl [1] and also by Schwinger [2], but except for some relevant exceptions (for a complete review see [3]), they have received the attention they rightly deserve only after becoming one essential ingredient in the development of the emerging field of quantum information [4, 5]. Indeed, the promise of futuristic technologies like safe cryptography and new “super computers”, capable of handling otherwise untractable problems, relies on the ability to control the quantum states of a small number of qubits [6, 7].

In the modern parlance of quantum information the concept of phase for a $d$-dimensional system (qudit) is ubiquitous. However, in spite of being a primitive of the theory, this notion is rather imprecise and, roughly speaking, three quite distinct conceptions can be discerned.

In the first, phase is considered as a parameter and the problem is reduced to the optimal estimation of the value of the phase shift undergone by the qudit under certain operations [8]. Although very operational in style, it accommodates perfectly the practical requirements of typical applications handled in quantum information.

In the second, a semiclassical approach is adopted, and the phase is assumed to be linked to the geometry of the state space: for example, for a qubit this space is the well-known Poincaré sphere and the phase is identified with the angle that a state representative makes with the $Z$ axis [9]. This pictorial understanding of phase as an angle makes easy contact with the classical world, but once more considers the phase as a mere state parameter instead of a full quantum variable.

The third major concept emphasizes the idea that phase is a physical property and, by any orthodox picture of quantum mechanics, must be associated with a selfadjoint operator (or at least with a family of positive operator-valued measures). Within this vein, phase operators have been constructed via a polar decomposition for qubits and qutrits [10].

The main goal of this paper is to look at the fundamental problem of properly defining phase from quite a different perspective. On closer examination, one immediately discovers that the idea of complementarity is at the root of all the previous approaches: phase is complementary to some amplitude, by which we loosely mean that the precise knowledge of one implies that all possible outcomes of the other are equally probable [11]. This idea of unbiasedness leads directly to introduce mutually unbiased bases (MUBs) [12], which, for a variety of reasons, are becoming an important tool in quantum optics [13]. It is known that the maximum number of such bases cannot be greater than $d + 1$ and that this limit is certainly reached if $d$ is a power of a prime [13]. It is not known if there are nonprime-power values of $d$ for which this bound is attained. We shall be not concerned with this problem in this paper, and assume that we are always working in a prime dimension.

It is essential to recall that complementarity for the position-momentum pair is implemented by the Fourier transform, which exchanges both operators. Using the ideas introduced in Ref. [13], we construct $d + 1$ disjoint classes of maximally commuting unitary matrices (each set having $d - 1$ operators). We then note that one of these classes consists solely of diagonal operators (which
we can relate to \textit{inversions}) that can be mapped, using the finite Fourier transform, to operators acting cyclically on basis states.

This perspective leads to a natural notion of \textit{phases} as complementary to \textit{inversions}. The advantage of this approach is that it does not rely on polar decompositions or semiclassical arguments and provides a clear understanding of the behavior of such basic variables.

\section{II. MULTICOMPLEMENTARY OPERATORS FOR FINITE-DIMENSIONAL QUANTUM SYSTEMS}

The objects we study in this paper are quantum systems described in a \(d\)-dimensional Hilbert space \(\mathcal{H}_d\). We recall \cite{12} that two different orthonormal bases \(\mathcal{A}\) and \(\mathcal{B}\) are said to be mutually unbiased if a system prepared in any element of \(\mathcal{A}\) (such as \(|a\rangle\)) has a uniform probability distribution of being found in any element of \(\mathcal{B}\)

\[ |\langle a|b\rangle|^2 = \frac{1}{d}, \quad (2.1) \]

for all \(a \in \mathcal{A}\) and all \(b \in \mathcal{B}\). As anticipated in the Introduction, we shall be concerned solely in cases where \(d\) is a prime number, as then we know that there are \(d+1\) MUBs. For dimensions which are power of a prime the argument can be easily extended with some modifications \cite{16}.

If \(|n\rangle\) \((n = 0, \ldots, d-1)\) is the standard (computational) basis in \(\mathcal{H}_d\), we introduce the generalized Pauli matrices \(X\) and \(Z\) by the following action:

\[
\begin{align*}
X|n\rangle &= |n+1\rangle, \\
Z|n\rangle &= \omega^n|n\rangle,
\end{align*}
\quad (2.2)

where

\[
\omega = \exp(2\pi i/d). \tag{2.3}
\]

Note that throughout this paper addition and multiplication must be understood mod \(d\). These operators \(X\) and \(Z\), which are generalizations of the Pauli matrices, were studied by Patera and Zassenhaus \cite{17} in a purely mathematical context, and have been used recently by many authors in a variety of applications \cite{18}. Under multiplication, they generate a finite subgroup of \(\text{SU}(d)\), known as the generalized Pauli group, and obey the finite-dimensional version of the Weyl form of the commutation relations:

\[ ZX = \omega XZ. \quad (2.4) \]

It is easily shown that the eigenvectors of \(X\) and those of \(Z\) satisfy \cite{24}.

To simplify as much as possible the following computation, we introduce the following labeling scheme: let

\[
\begin{align*}
X_0 &= Z, \\
X_k &= XZ^{k-1}, \quad k = 1, \ldots, d.
\end{align*}
\quad (2.5)
\]

Since we shall also need powers of these operators, we denote by \(\mathcal{C}_{X_k}\) the set

\[
\mathcal{C}_{X_k} = \{X_k, X_k^2, \ldots, X_k^{d-1}\}. \quad (2.6)
\]

The \(d-1\) operators in the class \(\mathcal{C}_{X_k}\) clearly commute one with another and therefore represent a maximal set of commuting operators.

Following the ideas in Ref. \cite{19}, consider now the following set (each containing \(d+1\) operators)

\[
\mathcal{S} = \{X_n, X_1, \ldots, X_d\} = \{Z, X, XZ, \ldots, XZ^{d-1}\}. \quad (2.7)
\]

By virtue of the relation \cite{24}, any two operators in this set are complementary, in the sense that their eigenvectors satisfy the unbiasedness condition \cite{24}. Furthermore, a complete MUB is obtained by constructing every eigenvector of every element in \(\mathcal{S}\), so we refer to \(\mathcal{S}\) as a maximal set of multicomplementary operators.

In the case of the standard position-momentum complementary variables, their eigenvectors form bases related by the Fourier transform. The finite-dimensional Fourier transform can be defined as \cite{10}

\[
F = \frac{1}{\sqrt{d}} \sum_{n,n'=0}^{d-1} \omega^{nn'}|n\rangle\langle n'|, \quad (2.8)
\]

with the properties

\[
FF^\dagger = F^\dagger F = 1, \quad F^4 = 1. \quad (2.9)
\]

Using this definition one can check that \(X\) and \(Z\) are indeed Fourier pairs

\[
X = F^\dagger ZF. \quad (2.10)
\]

There exist also an operator \(V\) that transform \(X \rightarrow XZ^k\). It has a diagonal form:

\[
V = \sum_{n=0}^{d-1} \omega^{-(n^2-n)(d+1)/2} |n\rangle\langle n|, \quad (2.11)
\]

so that

\[
XZ^k = V^kXV^{-k}, \quad (2.12)
\]

where we have assumed an odd-prime dimension (the case \(d = 2\) need minor modifications, as we shall see in next Section).

In physical applications, only \(d-1\) populations can vary independently in a \(d\)-level system. In consequence, it is usual to work with \(d-1\) traceless operators \(h_j\) that measure population inversions between the corresponding levels, i.e.,

\[
h_j = S_{jj} - S_{j+1,j+1}, \quad (2.13)
\]

where

\[
S_{ij} = |i\rangle\langle j|. \quad (2.14)
\]
These \( h_j \) (usually known as the Cartan-Weyl generators) constitute a maximal Abelian subalgebra. Note that the diagonal operators in the class \( \mathcal{E}_X = \{ Z^k \} \) are linear combinations of \( h_j \), so both can be used indistinctly.

On physical grounds, we expect phases to be complementary to inversions. But inversions are invariant under phase shifts: if

\[
U(\varphi) = \exp \left( -i \sum_j \varphi_j h_j \right),
\]

where \( \varphi \) denotes \((\varphi_1, \ldots, \varphi_{d-1})\), then

\[
U(\varphi) h_k U(\varphi) = h_k.
\]

Thus, we can construct a continuous family of operators, all complementary to inversions, by conjugating any operator in the class \( \mathcal{E}_X \) by \( U(\varphi) \). In particular, the diagonal operator \( V \), which maps \( X \times Z^k \) as per Eq. (2.14) (and that is also of the form (2.15) for a definite choice of the parameters), allows us to construct any \( X_k \) starting with \( X_1 = X \). For this reason, and without any loss of generality, we shall henceforth focus on the elements of the class \( \mathcal{E}_X = \{ X, X^2, \ldots, X^{d-1} \} \) to discuss general properties of complementary phase operators. We thus define \( d - 1 \) families of operators representing the exponential of the phase by

\[
E^k(\varphi) = U^\dagger(\varphi) X^k U(\varphi), \quad k = 1, \ldots, d - 1,
\]

obtained by successive powers.

If \( |s\rangle \) is an eigenstate of \( h_j \) with eigenvalue \( h_{js} \), then the expectation value of \( E^k(\varphi) \) on an arbitrary state \( |\psi\rangle = \sum_s c_s |s\rangle \) is simply

\[
\langle E^k(\varphi) \rangle = \sum_s c_{s+k}^* c_s U^*_s(\varphi) U_s(\varphi),
\]

where

\[
U_s(\varphi) = \exp \left( -i \sum_j \varphi_j h_{js} \right).
\]

This allows us to introduce an operator kernel

\[
\Pi(\varphi) = \frac{1}{(2\pi)^{d-1}} \left[ \mathbb{1} + \sum_{k=1}^{d-1} (E^k(\varphi))^* X^k \right],
\]

which is properly normalized and generates all the moments through the relation

\[
\langle E^l(\varphi) \rangle = \frac{(2\pi)^{d-1}}{d} \text{Tr}[\Pi(\varphi) X^l],
\]

so the phase distribution is obtained as

\[
P(\varphi) = \frac{1}{(2\pi)^{d-1}} \left( 1 + \sum_{k=1}^{d-1} (E^k(\varphi))^* \langle X^k \rangle \right).
\]

We note in passing that any positive operator-valued measure of the general form

\[
\Delta(\varphi) = \frac{1}{(2\pi)^{d-1}} \left[ \mathbb{1} + \sum_{k=1}^{d-1} \gamma_k E^k(\varphi) \right],
\]

which can be associated to \( \mathcal{E}_X \), satisfies the usual requirements of real valuedness, positivity and normalization and possesses the obvious property

\[
e^{i\varphi_j h_j} \Delta(\varphi_1, \ldots, \varphi_{d-1}) e^{-i\varphi_j h_j} = \Delta(\varphi_1, \ldots, \varphi_j' + \varphi_j, \ldots, \varphi_{d-1}),
\]

which meets the usual requirements of complementarity \(^{20} \).

III. APPLICATION: QUANTUM PHASE FOR FINITE-DIMENSIONAL SYSTEMS

A. The case of qubits

To fully appreciate the details of the method, we shall work out some relevant examples. First, we focus on the simplest case of a two-dimensional Hilbert space \( \mathcal{H}_2 \), and a state space that coincides with the sphere \( S_2 \).

The basic operators are the standard Pauli matrices

\[
X = 2\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Z = 2\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},
\]

such that

\[
\sigma_x \sigma_z = -\sigma_z \sigma_x.
\]

The transformation \( \sigma_z \to \sigma_x \) is accomplished by the finite Fourier transform

\[
F = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.
\]

However, it is impossible to find a unitary transformation \( V \) such that \( \sigma_x \to \sigma_z \sigma_x \). For this reason, instead of \( \sigma_x, \sigma_z \) the matrix \( \sigma_y = i\sigma_x \sigma_z \) is used, so that \( \sigma_y = V^\dagger \sigma_z V \), where \( V \) is the unitary operator

\[
V = \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix}.
\]

If \( \vartheta_A \) describes a point in the Bloch sphere \( S_2 \) in an arbitrary direction parametrized by \( \mathbf{n} = (\cos \vartheta_A \sin \varphi_A, \sin \vartheta_A \sin \varphi_A, \cos \vartheta_A) \), let \( A \) be

\[
A = \mathbf{n}_A \cdot \sigma = R(\vartheta_A, \varphi_A) \sigma_z R^{-1}(\vartheta_A, \varphi_A),
\]

where

\[
R(\vartheta, \varphi) = \exp \left[ \frac{\vartheta}{2} \left( \cos \varphi \sigma_x - \sin \varphi \sigma_y \right) \right].
\]
The condition of complementarity between $A$ and a generic operator $B$ [expressed also as in Eq. (3.5)] can be written as \[ n_A \cdot n_B = 0; \] (3.7)
that is, the subspace spanned in $S_2$ by $n_A$ is orthogonal to that by $n_B$. We have then a one-parameter set of complementary operators of the general form \[ B = n_B \cdot \sigma, \] (3.8)
where the unit vector $n_B$ satisfies (3.7), which is equivalent to \[ \cot \vartheta_B = -\tan \vartheta_A \cos(\varphi_B - \varphi_A). \] (3.9)
In particular, the complementary set to the inversion $\sigma_z$ consists in the one-parameter family \[ E(\varphi) = \cos \varphi \sigma_x - \sin \varphi \sigma_y = \begin{pmatrix} 0 & e^{i\varphi} \\ e^{-i\varphi} & 0 \end{pmatrix}, \] (3.10)
where $\varphi$ represents a reference phase. This in fact agrees with the exponential of the phase operator obtained via a polar decomposition \[ 10].\]

According to the approach developed in this paper, we have now one family of phase operators that can be constructed as \[ E(\varphi) = \exp(i\varphi \sigma_z/2) \sigma_x \exp(-i\varphi \sigma_z/2). \] (3.11)
This coincides also with (3.10), and can be recast in the suggestive form \[ E(\varphi) = \xi(\varphi)^t F \xi, \] (3.12)
where $t$ denotes the transpose and \[ \xi(\varphi) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\varphi} \\ e^{i\varphi} \end{pmatrix}, \quad \sigma = \begin{pmatrix} \sigma_x \\ \sigma_x \sigma_z \end{pmatrix}. \] (3.13)

This result confirms in this simple case the complementary character of $E(\varphi)$ obtained via Fourier transform. For a pure state such as \[ \vert \psi \rangle = \begin{pmatrix} \cos(\vartheta/2) \\ \sin(\vartheta/2) e^{i\chi} \end{pmatrix}, \] (3.14)
with $0 \leq \vartheta \leq \pi$, $0 \leq \chi \leq 2\pi$, the average value of $E(\varphi)$ is \[ \langle E(\varphi) \rangle = \sin \vartheta \cos(\chi + \varphi). \] (3.15)
The main features of this description are obviously independent of the reference phase $\varphi$.

**B. The case of qutrits**

For a three-dimensional Hilbert space $\mathcal{H}_3$ the basic operators are \[ X = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega^2 \end{pmatrix}, \] (3.16)
and $\omega = \exp(2\pi i/3)$. We have four classes of disjoint traceless operators, each containing two commuting operators \[ \mathcal{C}_x = \{Z, Z^2\}, \quad \mathcal{C}_x = \{X, X^2\}, \] (3.17)
\[ \mathcal{C}_x = \{XZ, (XZ)^2\}, \quad \mathcal{C}_x = \{XZ^2, (XZ^2)^2\}. \]
The discrete Fourier transform is \[ F = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \omega^2 \end{pmatrix}, \] (3.18)
and $V$ is the diagonal unitary matrix \[ V = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \] (3.19)
In this case we have two Cartan operators associated with the two independent inversions \[ h_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad h_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \] (3.20)
which can be easily expressed as linear combinations of $Z$ and $Z^2$. Note that $X$ and $X^2$ correspond to two different physical situations: in the computational basis $X$ acts as $X \vert n \rangle = \vert n + 1 \rangle$, while $X^2 \vert n \rangle = \vert n + 2 \rangle$.

Thus, we have two families of commuting phase operators:
\[ E(\varphi_1, \varphi_2) = e^{i(\varphi_1 h_1 + \varphi_2 h_2)} X e^{-i(\varphi_1 h_1 + \varphi_2 h_2)} \] (3.21)
\[ E^2(\varphi_1, \varphi_2) = e^{i(\varphi_1 h_1 + \varphi_2 h_2)} X^2 e^{-i(\varphi_1 h_1 + \varphi_2 h_2)}. \]
In this particular case, they essentially coincide because $E^2(\varphi_1, \varphi_2) = E(\varphi_1, \varphi_2)$. The phase operator $E(\varphi_1, \varphi_2)$ can be represented in a form similar to (3.12), namely \[ E(\varphi_1, \varphi_2) = \xi(\varphi_1, \varphi_2)^t F \xi, \] (3.22)
with
\[ \xi(\varphi_1, \varphi_2) = \frac{1}{\sqrt{3}} \begin{pmatrix} e^{i(\varphi_2 - 2\varphi_1)} \\ e^{i(\varphi_1 + \varphi_2)} \\ e^{i(\varphi_1 - 2\varphi_2)} \end{pmatrix}, \quad \xi = \begin{pmatrix} X \\ XZ \\ XZ^2 \end{pmatrix}. \] (3.23)
Its explicit form is
\[ E(\varphi_1, \varphi_2) = \begin{pmatrix} e^{-i(\varphi_1 - \varphi_2)} & 0 & e^{i(\varphi_1 + \varphi_2)} \\ 0 & e^{i(\varphi_1 - 2\varphi_2)} & 0 \\ 0 & 0 & e^{i(\varphi_1 + 2\varphi_2)} \end{pmatrix}, \] (3.24)
where again $\varphi_1$ and $\varphi_2$ are reference phases. The average value of $E(\varphi_1, \varphi_2)$ in an arbitrary pure state such as \[ \vert \psi \rangle = \begin{pmatrix} \cos(\vartheta/2) \\ \sin(\vartheta/2) \cos(\xi/2) e^{i\chi_1} \\ \sin(\vartheta/2) \sin(\xi/2) e^{i\chi_2} \end{pmatrix}, \] (3.25)
We can observe that when only two levels are involved, $\xi = 0$, 
\[
\langle E(\varphi_1, \varphi_2) \rangle = \frac{1}{2} \sin^2(\varphi/2) \sin \theta e^{i(\lambda_1 - \lambda_2 + (\varphi - 2\varphi_1))} 
+ \frac{1}{2} \sin \theta \{\sin(\xi/2) e^{i(\lambda_1 + (\varphi_1 + \varphi_2))} 
+ \cos(\xi/2) e^{-i(\lambda_1 + (2\varphi_1 - \varphi_2))}\}. 
\] 
(3.26)

We can observe that when only two levels are involved, $\xi = 0$, 
\[
\langle E(\varphi_1, \varphi_2) \rangle = \frac{1}{2} \sin \theta e^{i(\lambda_1 + (2\varphi_1 - \varphi_2))}, 
\] 
(3.27)

which measure the relative phase between the states 1 and 2, and depends only on a single effective phase $2\varphi_1 - \varphi_2$. Since $E^2(\varphi_1, \varphi_2) = E'(\varphi_1, \varphi_2)$, which includes all the possible moments, the phase distribution remains constant at the direction $2\varphi_1 - \varphi_2 = \text{constant}$.

It is instructive to compare our construction of phase operators with the more common algorithm, based on the polar decomposition of $S_{12}$, $S_{23}$, and $S_{13}$, defined in Eq. (2.11). The polar decomposition of $S_{ij}$ implicitly focuses of the $i \rightarrow j$ transition, without analyzing the role of the third “spectator” state of the system. This observation can be used to explain the lack of uniqueness in the polar decomposition of singular operators like $S_{12}$, for instance. This approach produces a phase operator $E_{12}$ of the form

\[
E_{12} = \begin{pmatrix} 0 & 1 & 0 \\ x & 0 & y \\ y^* & 0 & -x^* \end{pmatrix}, \quad |x|^2 + |y|^2 = 1, 
\] 
(3.28)

where $S_{12} = E_{12} R_{12}$ and $R_{12} = \sqrt{S_{12} S_{21}}$ is the “modulus”. The only constraints on $E_{12}$ are imposed by the requirement of unitarity.

A particular solution to Eq. (3.28) is obtained by “isolating” the third state from the first two by choosing $y = 0$ and thus $x = e^{i\varphi_{12}}$. Since $(S_{12}, S_{21}, h_1)$ span a $su(2)$ subalgebra, this choice amounts to limiting the action of the phase operator $E_{12}$ to a specified $su(2)$ subspace. A similar argument holds for $E_{23}$, with $(S_{23}, S_{32}, h_2)$ spanning another $su(2)$ subalgebra.

This perspective in terms of polar decomposition and transitions leads to phase operators that fulfill the requirements of complementarity only between pairs of states involved in each transition. The corresponding positive operator-valued measure obtained in this construction is still of the general form found in Eq. (2.22). However, this restricted point of view is to be contrasted with the approach of this paper, where complementarity is imposed for the three-level system as a whole.

**IV. CONCLUDING REMARKS**

Mutually unbiased bases are a primitive of quantum theory, as they embody the importance of the superposition principle. In this paper we have used them to develop a comprehensive quantum theory of the phases as complementary to inversions in finite-dimensional systems.

The construction presented in this paper is devoid of any ambiguity associated with the non-uniqueness of polar decomposition of ladder operators. In prime dimensions, phase operators and inversions are elegantly related by a finite Fourier transform, much like positions and momenta are related by an ordinary Fourier transform in infinite-dimensional systems, and provides an appealing way of treating a concept as central as the phases of a system.

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