Unital quantum operations on the Bloch ball and Bloch region

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Abstract

For one qubit systems, we present a short, elementary argument characterizing unital quantum operators in terms of their action on Bloch vectors. We then show how our approach generalizes to multi-qubit systems, obtaining inequalities that govern when a “diagonal” superoperator on the Bloch region is a quantum operator. These inequalities are the $n$-qubit analogue of the Algoet-Fujiwara conditions. Our work is facilitated by an analysis of operator-sum decompositions in which negative summands are allowed.

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I. INTRODUCTION

A quantum operator (or quantum superoperator) $\Phi$ on the collection $\mathcal{M}_N$ of complex $N \times N$ matrices is a completely positive, trace preserving linear map. The quantum operator $\Phi$ is unital provided that $\Phi(I) = I$, that is, provided that $\Phi$ fixes the identity matrix. A density matrix, which represents the state of a quantum system, is a positive matrix (Hermitian with nonnegative eigenvalues) having trace one. The properties of density matrices are thus preserved via the action of a quantum operation. Of course, density matrices are mapped to density matrices under any trace-preserving positive superoperator. (A positive superoperator, by definition, takes positive matrices to positive matrices.) The requirement that a quantum operation be completely positive rather than simply positive is based on the viewpoint that $\Phi$ represents the “restriction” of a positive operator on a larger system. By definition, a superoperator $\Phi$ on $\mathcal{M}_N$ is completely positive provided that $I \otimes \Phi : \mathcal{M}_m \otimes \mathcal{M}_N \rightarrow \mathcal{M}_m \otimes \mathcal{M}_N$ is positive for all positive integers $m$.

A density matrix $\rho \in \mathcal{M}_2$ represents the state of a two-level quantum system—a one qubit system. It’s not difficult to show that such matrices have the following “Bloch” representation:

$$\rho = \frac{I + \sum_{i=1}^{3} r_i \sigma_i}{2},$$

where $(r_1, r_2, r_3)$ belongs to the closed unit ball of $\mathbb{R}^3$ and where

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

are the usual Pauli matrices. The vector $\vec{r} = (r_1, r_2, r_3)$ appearing in (1) is called the Bloch vector or coherence vector of $\rho$. The correspondence between elements of the closed unit ball of $\mathbb{R}^3$ and density matrices is complete for two-level systems; that is, a trace-one matrix $\rho \in \mathcal{M}_2$ is positive if and only if it has representation (1) where $|\vec{r}| \leq 1$.

A density matrix $\rho \in \mathcal{M}_N$ has a representation analogous to (1):

$$\rho = \frac{1}{N} \left( I + \sqrt{\frac{N(N-1)}{2}} \sum_{i=1}^{N^2-1} r_i \lambda_i \right),$$

where now the Bloch vector $\vec{r}$ belongs to the closed unit ball of $\mathbb{R}^{N^2-1}$ and $\{\lambda_i\}^{N^2-1}$ consists of elements of $\mathcal{M}_N$ having the following properties:

$\lambda_i$ is self-adjoint ($\lambda_i^\dagger = \lambda_i$), $\text{tr}\lambda_i = 0$, and $\text{tr}(\lambda_i\lambda_j) = 2\delta_{ij}$. 

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One may, for example, take $\vec{\lambda}$ to consist of generators of SU($N$) (see [2, 4, 5]). In our representation (2) of density matrices, we have adopted the normalization factor $(N(N-1)/2)^{1/2}$ found in [2], which forces a pure-state density matrix to have a Bloch vector $\vec{r}$ of norm 1. Note that $\{\lambda_i\}_{i=1}^{N^2-1}$ together with the identity matrix $I$ constitutes an orthogonal basis of $\mathcal{M}_N$ relative to the Hilbert-Schmidt inner product. In contrast to the situation for two-level systems, the collection of Bloch vectors $\vec{r}$ from (2) that correspond to density matrices is a proper subset of the unit ball of $\mathbb{R}^{N^2-1}$, recently characterized in [2, 5]. We will be concerned with $n$-qubit systems, which means that in (2), $N = 2^n$ and each element of $\{\lambda_i\}_{i=1}^{N^2-1}$ may be taken to be an appropriately normalized tensor product of $n$ Pauli matrices, where $\sigma_0 := I$ is included in the “Pauli collection” but not all factors in the product can be $\sigma_0$—see Section V below for details.

Because unital quantum operators are completely positive and preserve both the trace and the identity, associated with any such operator $\Phi$ on $\mathcal{M}_N$, there is an $(N^2-1) \times (N^2-1)$ real matrix $M_\Phi$ such that

$$\Phi \left( \frac{1}{N} (I + c\vec{r} \cdot \vec{\lambda}) \right) = \frac{1}{N} \left( I + cM_\Phi \vec{r} \cdot \vec{\lambda} \right),$$

where $c = \sqrt{N(N-1)/2}$ is the normalizing constant. We call $M_\Phi$ the Bloch matrix of $\Phi$.

For $N = 2$, Bloch matrices $M$ that correspond to unital quantum operators are characterized in [1] (see also [7] and [12]) in terms of signed singular values of $M$:

$$1 - d_3 \geq |d_1 - d_2| \text{ and } 1 + d_3 \geq |d_1 + d_2|,$$  (3)

where $d_1$, $d_2$, and $d_3$ may be taken to be the singular values of $M$ if det $M \geq 0$ and may be taken to be the additive inverses of the singular values of $M$ if det $M < 0$. (For information about singular values of matrices, the reader may consult [10, 11], e.g.) The inequalities (3) are the Algoet-Fujiwara conditions for a Bloch matrix corresponding to a unital quantum operator on the Bloch ball $\mathbb{B}$. In Section 4 of this paper, we present a short and completely elementary derivation of the Algoet-Fujiwara conditions, and in Section 5 we show how our methods yield a description of “diagonal” quantum operations on $n$-qubit systems, obtaining the $n$-qubit analogue of the Algoet-Fujiwara conditions (see Theorem V.1 below). C. King [6] has obtained a related description of diagonal quantum operators on three-state systems (i.e., single qutrit systems).
In the next section, we discuss operator-sum representations of superoperators that map Hermitian matrices to Hermitian matrices. As is well-known \[13\], any superoperator \( \Phi \) on \( \mathcal{M}_N \) that preserves Hermiticity must have the form

\[
\Phi(\rho) = \sum_{j=1}^k \varepsilon_j A_j \rho A_j^\dagger,
\]

where for each \( j \), \( A_j \) is an \( N \times N \) matrix and \( \varepsilon_j \in \{1, -1\} \). We show in Proposition II.1 below that if \( \Phi \) is completely positive and the operator elements \( \{A_j\} \) for \( \Phi \) are linearly independent, then \( \varepsilon_j = 1 \) for \( j = 1, 2, \ldots, k \). Proposition II.1 is the key lemma in our work of Sections 4 and 5.

Before concluding this introduction, we should add a remark about non-unital quantum operators. These superoperators correspond to affine mappings: \( (I + c\vec{r} \cdot \vec{\lambda})/N \mapsto (I + c(M\vec{r} + \vec{t}) \cdot \vec{\lambda})/N \). For \( N = 2 \), affine mappings \( \vec{r} \mapsto M\vec{r} + \vec{t} \) corresponding to quantum operators are characterized in \[12\].

II. SIGN PATTERNS IN OPERATOR-SUM DECOMPOSITIONS

Let \( \Phi \) be a superoperator on \( \mathcal{M}_N \) and suppose that for some positive integer \( k \) there exist \( N \times N \) matrices \( A_1, A_2, \ldots, A_k \) along with “signs” \( \varepsilon_j \in \{-1, 1\} \) such that

\[
\Phi(\rho) = \sum_{j=1}^k \varepsilon_j A_j \rho A_j^\dagger.
\]

The expression of the right of (4) is called an operator-sum decomposition of \( \Phi \) and \( \{A_j\}_{j=1}^k \) is corresponding set of operator elements. Operator-sum decompositions in which \( \varepsilon_j = 1 \) for every \( j \) model system-environment interactions (\[14\]; see also \[8, 11\]). For this reason, operator elements are sometimes called “interaction operators”.

Observe that if \( \Phi \) has an operator-sum decomposition (4), then \( \Phi \) preserves Hermiticity; that is, \( \Phi(\rho) \dagger = \Phi(\rho) \) whenever \( \rho \) is Hermitian. In \[13\], de Pillis shows that every superoperator on \( \mathcal{M}_N \) that preserves Hermiticity has an operator-sum decomposition. For example, by de Pillis’s result, the transpose operator \( \Phi_T \) on \( \mathcal{M}_2 \) defined by \( \Phi_T(\rho) = \rho^T \) must have an operator-sum decomposition. A simple calculation shows that one such decomposition is given by

\[
\Phi_T(\rho) = \frac{I}{\sqrt{2}} \rho \frac{I}{\sqrt{2}} + \frac{\sigma_1}{\sqrt{2}} \rho \frac{\sigma_1}{\sqrt{2}} - \frac{\sigma_2}{\sqrt{2}} \rho \frac{\sigma_2}{\sqrt{2}} + \frac{\sigma_3}{\sqrt{2}} \rho \frac{\sigma_3}{\sqrt{2}}
\]

(5)
Operator-sum representations are highly non-unique; for instance $\Phi_T$ is also given by
\[
\Phi_T(\rho) = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \rho \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \rho \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} + \frac{\sigma_1}{\sqrt{2}} \rho \sigma_1 - \frac{\sigma_2}{\sqrt{2}} \rho \sigma_2.
\]

It’s obvious that $\Phi_T$ is a positive superoperator, preserving both Hermiticity and eigenvalues. On the other hand $\Phi_T$ is the canonical example of a positive operator that is not completely positive. Can the fact that $\Phi_T$ is not completely positive be deduced from the presence of the negative sign in the operator-sum decompositions for $\Phi_T$ displayed above? Proposition 11.1 below shows that the answer to this question is yes. This is not an entirely trivial matter. For example, the identity superoperator operator $\Phi_I$, which is obviously completely positive, is given by
\[
\Phi_I(\rho) = (\sqrt{2}I)\rho(\sqrt{2}I) - I\rho I.
\]

As we discussed in the Introduction, quantum operations are completely positive. Observe that since Hermitian matrices are differences of positive matrices (immediate from the spectral decomposition), positive (and hence completely positive) superoperators must preserve Hermiticity. Thus any quantum operator $\Phi$ has an operator-sum decomposition (4). In Theorem 1 of [3], Choi shows that a completely positive operator $\Phi$ has an operator-sum decomposition (4) in which each sign is positive ($\varepsilon_j = 1$ for every $j$). Of course this doesn’t mean that every operator-sum decomposition of a completely positive map must feature only positive signs, as (6) shows. Choi does not prove his Theorem 1 as a corollary of de Pillis’s theorem for Hermiticity-preserving superoperators. Rather, he gives an elegant independent proof that also yields de Pillis’s characterization (as Choi points out [3, p. 277]). More important for our purposes is that Choi investigates the relationship between different operator-sum representations of the same superoperator, proving [3, Remark 4] that if $\{A_j\}_{j=1}^k$ and $\{E_j\}_{j=1}^m$ are collections of operator elements for the same superoperator on $\mathcal{M}_N$ and if $\{A_j\}_{j=1}^k$ is linearly independent in $\mathcal{M}_N$, then there is an isometric $m \times k$ matrix $[\alpha_{jn}]$ such that for each $j \in \{1,2,\ldots,m\}$
\[
E_j = \sum_{n=1}^k \alpha_{jn} A_n.
\]

Note that because $[\alpha_{jn}]$ is an isometry, we must have $m \geq k$; if both $\{A_j\}_{j=1}^k$ and $\{E_j\}_{j=1}^m$ are linearly independent collections of operator elements for the same superoperator, then Choi shows $m = k$ and the matrix of scalars $[\alpha_{jn}]$ relating them by (7) is unitary.
**Proposition II.1** Suppose that $\Phi : \mathcal{M}_N \to \mathcal{M}_N$ is given by

$$\Phi(\rho) = \sum_{j=1}^{k} \varepsilon_j A_j \rho A_j^\dagger$$

where $\{A_j\}_{j=1}^{k}$ is linearly independent in $\mathcal{M}_N$ and $\varepsilon_j \in \{-1,1\}$ for $j = 1, 2, \ldots, k$. Then $\Phi$ is completely positive if and only if $\varepsilon_j = 1$ for each $j \in \{1, 2, \ldots, k\}$.

*Proof.* If each sign “$\varepsilon_j$” is positive, then $\Phi$ is easily seen to be completely positive (and the independence of $\{A_j\}$ is irrelevant).

Conversely, suppose that $\Phi$ is completely positive and has the form displayed in the statement of the proposition with $\{A_j\}_{j=1}^{k}$ independent. We assume, in order to obtain a contradiction, that some of the signs $\varepsilon_j$ are $-1$. Without loss of generality, we take $\varepsilon_j = -1$ for $j = 1$ to $p$ for some $p \in \{1, 2, \ldots, k - 1\}$. (Clearly, not all of the signs can be negative: the linear independence of the set of operator elements means that no element $A_j$ is the zero matrix so that if all signs were negative, $\Phi$ would map positive matrices to negative ones and hence couldn’t be completely positive).

Because $\Phi$ is completely positive, Choi’s work shows that there exists an operator-sum decomposition for $\Phi$ with all signs positive:

$$\Phi(\rho) = \sum_{j=1}^{m} E_j \rho E_j^\dagger.$$ 

We have for every $N \times N$ matrix $\rho$,

$$\sum_{j=1}^{k} \varepsilon_j A_j \rho A_j^\dagger = \sum_{j=1}^{m} E_j \rho E_j^\dagger,$$

or

$$\sum_{j=p+1}^{k} A_j \rho A_j^\dagger = \sum_{j=1}^{m} E_j \rho E_j^\dagger + \sum_{j=1}^{p} A_j \rho A_j^\dagger,$$

so that we have two different operator-sum representations for the same superoperator $\rho \mapsto \sum_{j=p+1}^{k} A_j \rho A_j^\dagger$. Thus, in particular, there are scalars $(\alpha_n)$ (forming one row of the isometric matrix relating the operator elements on the left of (8) to those on the right) such that

$$A_1 = \sum_{n=p+1}^{k} \alpha_n A_n,$$

contradicting the linear independence of $\{A_j\}_{j=1}^{k}$. QED

In the sequel, we will use the following quick corollary of the preceding proposition.
Corollary II.2 Suppose that $\Phi$ is a completely positive superoperator on $\mathcal{M}_N$ having the representation

$$\Phi(\rho) = \sum_{j=1}^{k} \beta_j A_j \rho A_j^\dagger,$$

where $\{A_j\}_{j=1}^{k}$ is linearly independent in $\mathcal{M}_N$ and $\beta_j$ is real for $j = 1, 2, \ldots, k$. Then $\beta_j \geq 0$ for $j \in \{1, 2, \ldots, k\}$.

Because the Pauli matrices $\sigma_1$, $\sigma_2$, and $\sigma_3$ together with the $2 \times 2$ identity matrix $\sigma_0$ form a linearly independent set in $\mathcal{M}_2$, the preceding corollary shows that the superoperator $\Phi$ defined on $\mathcal{M}_2$ by

$$\Phi(\rho) = \beta_0 \sigma_0 \rho \sigma_0 + \beta_1 \sigma_1 \rho \sigma_1 + \beta_2 \sigma_2 \rho \sigma_2 + \beta_3 \sigma_3 \rho \sigma_3$$

(9)

is completely positive only when $\beta_j \geq 0$ for $j = 0, 1, 2, 3$. It’s not difficult to obtain a characterization of positivity for the superoperator $\Phi$ defined by (9). The characterization, presented in the next proposition, shows that if $\Phi$ is positive but not completely positive and $\Phi$ is written in the form of (9) above, then exactly one of the scalars $\beta_j$ will be negative, as illustrated in equation (5).

Proposition II.3 The superoperator $\Phi : \mathcal{M}_2 \rightarrow \mathcal{M}_2$ defined by (9) is positive if and only if every pair from $\{\beta_j\}_{j=0}^{3}$ sums to a nonnegative number:

$$\beta_0 + \beta_1 \geq 0, \beta_0 + \beta_2 \geq 0, \beta_0 + \beta_3 \geq 0, \beta_1 + \beta_2 \geq 0, \beta_1 + \beta_3 \geq 0, \beta_2 + \beta_3 \geq 0.$$  

(10)

Proof. The following observation will facilitate some calculations in the proof; it will also play in a crucial role in the final two sections of this paper.

$$\sigma_i \sigma_j \sigma_i = \pm \sigma_j, \ i, j \in \{0, 1, 2, 3\},$$  

(11)

where the sign is positive when $i = 0$, $j = 0$, or $i = j$, and negative otherwise.

We assume that $\Phi$, defined by (9), is positive and obtain the inequalities stated in the proposition. Suppose $\rho$ is a positive matrix. Without loss of generality we will assume that $\rho$ has trace 1 and hence has the form $(I + r_1 \sigma_1 + r_2 \sigma_2 + r_3 \sigma_3)/2$, where $\vec{r} = (r_1, r_2, r_3)$ lies in the unit ball of $\mathbb{R}^3$. A simple calculation shows

$$\Phi(\rho) = \frac{s_0 I + r_1 s_1 \sigma_1 + r_2 s_2 \sigma_2 + r_3 s_3 \sigma_3}{2},$$  

(12)
where \( s_0 = \beta_0 + \beta_1 + \beta_2 + \beta_3, \) \( s_1 = \beta_0 + \beta_1 - \beta_2 - \beta_3, \) \( s_2 = \beta_0 - \beta_1 + \beta_2 - \beta_3, \) and \( s_3 = \beta_0 - \beta_1 - \beta_2 + \beta_3. \) Because \( \Phi(\rho) \) is positive, its trace is nonnegative; thus,

\[
\text{tr}(\Phi(\rho)) = s_0 \geq 0.
\]

If \( s_0 = 0, \) then the positive matrix \( \Phi(\rho) \) is the zero matrix (independent of \( \rho \)), which, in view of (12), forces \( s_1, s_2, \) and \( s_3 \) to be zero as well. It follows that \( \beta_j = 0 \) for each \( j, \) and the inequalities (10) hold for this case.

Suppose \( \text{tr}(\Phi(\rho)) > 0. \) Then we may rewrite the right-hand side of (12) as follows:

\[
s_0 \left( I + \frac{r_1 s_1}{s_0} \sigma_1 + \frac{r_2 s_2}{s_0} + \frac{r_3 s_3}{s_0} \sigma_3 \right),
\]

which represents a positive matrix if and only if

\[
\left( \frac{r_1 s_1}{s_0} \right)^2 + \left( \frac{r_2 s_2}{s_0} \right)^2 + \left( \frac{r_3 s_3}{s_0} \right)^2 \leq 1.
\]

Substituting, respectively, \( \vec{r'} = (1, 0, 0), (0, 1, 0), \) and \( (0, 0, 1) \) into (14) yields the following three inequalities

\[
|s_1| \leq s_0, |s_2| \leq s_0, |s_3| \leq s_0,
\]

which, in turn, yield the desired inequalities (10).

For the proof of the converse, suppose that \( \Phi \) acts on the positive matrix \( (I + \vec{r'} \cdot \vec{\sigma})/2) \) and that the inequalities (10) hold. Adding the first and last inequalities of (10), we must have \( \beta_0 + \beta_1 + \beta_2 + \beta_3 \geq 0. \) If \( \beta_0 + \beta_1 + \beta_2 + \beta_3 = 0, \) then by grouping summands appropriately, one obtains that each of the inequalities of (10) must be an equality and it follows from (12) that \( \Phi \) is the zero operator. On the other hand, if \( \beta_0 + \beta_1 + \beta_2 + \beta_3 > 0, \) then it’s easy to see that the quotients multiplying \( r_1, r_2, \) and \( r_3 \) in (13) must each have absolute value less than or equal to 1 and this shows that the quantity on the left of (14) is \( \leq r_1^2 + r_2^2 + r_3^2, \) which is \( \leq 1 \) since \( \rho \) is positive. Thus \( \Phi(\rho) \) is positive, as desired. QED

III. UNITARY SUPEROPERATORS AND ROTATIONS OF THE BLOCH REGION

In this section, we summarize known information about quantum operators having an operator-sum decomposition with single unitary operator element.
Suppose that $\Phi : M_N \to M_N$ is unitary in the sense that it has an operator-sum representation of the form

$$\Phi(\rho) = U\rho U^\dagger,$$

where $U$ is a unitary $N \times N$ matrix. Clearly such unitary $\Phi$’s are unital quantum operators.

It’s well known (see, e.g., [11, Exercise 8.13]) that if $\Phi$ is unitary and acts on $M_2$ (the one qubit situation), then its Bloch matrix $M_\Phi$ is a rotation matrix on $\mathbb{R}^3$, that is, $M_\Phi^TM_\Phi = I$ and $\det(M_\Phi) = 1$. Furthermore, it’s not difficult to show that the correspondence between rotation matrices on $\mathbb{R}^3$ and unitary superoperators is complete in the $N = 2$ setting; that is, given any rotation matrix $A$ there is a unitary $2 \times 2$ matrix $U$ such that

$$U \left( \frac{I + \vec{r} \cdot \vec{\sigma}}{2} \right) U^\dagger = \left( \frac{I + A\vec{r} \cdot \vec{\sigma}}{2} \right).$$

Now suppose $N > 2$ and $\Phi : M_N \to M_N$ is a unitary quantum operator. As one would expect, once again $\Phi$ has a Bloch matrix $M_\Phi$ that is a “rotation”, where by rotation we mean $M_\Phi$ is orthogonal ($M_\Phi^TM_\Phi = I$) and orientation preserving ($\det(M_\Phi) = 1$). It’s very easy to see that $M_\Phi$ must be orthogonal: let $\Phi(\rho) = U\rho U^\dagger$ and $\rho = (I + c\vec{r} \cdot \vec{\lambda})/N$ and note

$$\frac{1}{N} + (1 - \frac{1}{N})|\vec{r}|^2 = \text{tr}(\rho^2) = \text{tr}(U\rho U^\dagger U\rho U^\dagger) = \text{tr} \left( \frac{I + cM_\Phi\vec{r} \cdot \vec{\lambda}}{N} \right)^2 = \frac{1}{N} + (1 - \frac{1}{N})|\vec{M_\Phi\vec{r}}|^2$$

(15)

so that $|M_\Phi\vec{r}| = |\vec{r}|$. Thus $M_\Phi$ is an isometry and since it has real entries, $M_\Phi$ is orthogonal. The proof that $\det(M_\Phi) = 1$, which we will also present, requires a bit more effort. Because $U$ is unitary, there is an orthonormal basis $|v_j\rangle \in \mathbb{C}^N$ consisting of eigenvectors of $U$ with corresponding eigenvalues $e^{ia_j}\in\mathbb{C}$, where the $a_j$’s are real. For $s \in [0, 1]$, define

$$U_s = \sum_j e^{i(1-s)a_j}|v_j\rangle\langle v_j|,$$

so that $U_0 = U$ and $U_1 = I$. Let $\Phi_s : M_N \to M_N$ be given by $\Phi_s(\rho) = U_s\rho U_s^\dagger$ and let $M_{\Phi_s}$ be the corresponding Bloch matrix. We have already shown that $M_{\Phi_s}$ is orthogonal for each $s$ in $[0, 1]$. Hence $\det(M_{\Phi_s}) = \pm 1$ for each such $s$. Since $\det(M_{\Phi_s})$ varies continuously with $s$ and since $\det(M_{\Phi_1}) = \det I = 1$, we see $\det(M_{\Phi}) = \det(M_{\Phi_0}) = 1$, as desired.

When $N > 2$, the correspondence between rotations and unitary quantum operators is complicated; for example, the angle $\theta$ between pure-state Bloch vectors $\vec{r}_1$ and $\vec{r}_2$ must satisfy $\cos(\theta) \geq -1/(N - 1)$, or, equivalently, $\vec{r}_1 \cdot \vec{r}_2 \geq -1/(N - 1)$ [4].
Returning to the one-qubit situation, suppose that $M$ is an arbitrary $3 \times 3$ real matrix and the linear superoperator $\Phi_M: M_2 \rightarrow M_2$ is defined by

$$\Phi_M \left( \frac{I + \vec{r} \cdot \vec{\sigma}}{2} \right) = \frac{I + M\vec{r} \cdot \vec{\sigma}}{2}. \tag{16}$$

An interesting problem is to determine when $\Phi_M$ is a quantum operation. An obvious necessary condition is $\|M\| \leq 1$, where $\|M\| = \max\{|M\vec{r}| : |\vec{r}| = 1\}$. A complete description of those $M$ such that $\Phi_M$ is a quantum operator may be found in [1] (see also [7] and [12]). This description is based on the singular-value decomposition of $M$, which, in turn, easily yields the following.

**Proposition III.1** Suppose $M$ is a $3 \times 3$ matrix with real entries. Then there exist $3 \times 3$ rotation matrices $A$ and $B$ as well as a $3 \times 3$ diagonal matrix $D$ with real entries such that

$$M = BDA.$$

Moreover, if $\det M \geq 0$, then the diagonal entries of $D$ may be chosen to be the singular values of $M$ listed in decreasing order; otherwise, the diagonal entries of $D$ may be chosen to be the negatives of the singular values of $M$ listed in increasing order.

Let $\Phi_M$ be the unital superoperator [16] on $M_2$ induced by the real $3 \times 3$ matrix $M$. Let $M = BDA$ be the factorization of $M$ promised by Proposition III.1 and let let $U_A$ and $U_B$ be the unitary $2 \times 2$ matrices such that

$$U_A \left( \frac{I + \vec{r} \cdot \vec{\sigma}}{2} \right) U_A^\dagger = \frac{I + A\vec{r} \cdot \vec{\sigma}}{2} \quad \text{and} \quad U_B \left( \frac{I + \vec{r} \cdot \vec{\sigma}}{2} \right) U_B^\dagger = \frac{I + B\vec{r} \cdot \vec{\sigma}}{2}. \tag{17}$$

Finally, let $\Phi_D$ be the unital superoperator defined by

$$\Phi_D \left( \frac{I + \vec{r} \cdot \vec{\sigma}}{2} \right) = \frac{I + D\vec{r} \cdot \vec{\sigma}}{2}.$$

Note that

$$\Phi_M(\rho) = (\Psi \circ \Phi_D \circ \Omega)(\rho), \tag{18}$$

where $\Psi(\rho) = U_B\rho U_B^\dagger$ and $\Omega(\rho) = U_A\rho U_A^\dagger$. Because $\Psi$ and $\Omega$ and their inverses are quantum operations and compositions of quantum operations are quantum operations [18] shows that $\Phi_M$ is a quantum operation if and only if $\Phi_D$ is a quantum operation. Thus, to characterize unital quantum operators on the Bloch ball, one need only understand which diagonal matrices $M$ are such that $\Phi_M$ is a quantum operator. Necessary and sufficient conditions on
the diagonal entries of $M$ (which are given by (3) in the Introduction) that ensure $M$ induces a quantum operation are obtained in [1] as well as [12] and [7]. The method employed in [1] and [12] to obtain the conditions is based on the proof of Theorem 1 of [3]: one analyzes the positivity of

$$(I \otimes \Phi_M)(E)$$

where $I$ is the identity on $\mathcal{M}_2$ and where $E$ is the $4 \times 4$ matrix composed of elementary $2 \times 2$ blocks:

$$E = \begin{bmatrix}
1 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1
\end{bmatrix}.$$ 

The method employed in [7] involves starting with an operator-sum decomposition of the unital quantum operator in question and expressing its operator elements as linear combinations of the Pauli matrices.

In the next section, we take a new approach to characterizing the diagonal matrices corresponding to quantum operators on the Bloch ball. Our approach is based on our work with sign patterns in operator-sum decompositions in Section II and allows convenient generalization to the $n$-qubit situation.

IV. DIAGONAL QUANTUM OPERATORS ON THE BLOCH BALL

Suppose that

$$D = \begin{bmatrix}
d_{11} & 0 & 0 \\
0 & d_{22} & 0 \\
0 & 0 & d_{33}
\end{bmatrix}$$

and $\Phi_D$ is the linear superoperator on $\mathcal{M}_2$ defined by

$$\Phi_D \left( \frac{I + \vec{r} \cdot \vec{\sigma}}{2} \right) = \frac{I + D\vec{r} \cdot \vec{\sigma}}{2}. \quad (19)$$

Letting $\vec{r} = 0$, shows $\Phi_D(I) = I$. Even if one assumes that (19) holds only when $(I + \vec{r} \cdot \vec{\sigma})/2$ is positive (that is when $|\vec{r}| \leq 1$), then (19), combined with the linearity of $\Phi_D$, completely determines $\Phi_D$. Letting $\vec{r} = (1, 0, 0)$, we obtain $\Phi_D((I + \sigma_1)/2) = (I + d_{11}\sigma_1)/2$. Hence, by
linearity,
\[ \Phi_D(\sigma_1) = 2\Phi_D \left( \frac{I + \sigma_1}{2} - \frac{I}{2} \right) = 2\Phi_D \left( \frac{I + \sigma_1}{2} \right) - 2\Phi_D \left( \frac{I}{2} \right) = d_{11}\sigma_1 \]
Similarly, \( \Phi_D(\sigma_2) = d_{22}\sigma_2 \) and \( \Phi_D(\sigma_3) = d_{33}\sigma_3 \). Thus \( \Phi_D \) is a diagonal operator on \( \mathcal{M}_2 \) with respect to the basis \((\sigma_0, \sigma_1, \sigma_2, \sigma_3)\). Of course, \( \Phi_D \) is completely determined by its action on this basis.

Because
\[ \sigma_i\sigma_j\sigma_i = \pm\sigma_j, \]
the superoperator \( \Psi \) on \( \mathcal{M}_2 \), defined by
\[ \Psi(\rho) = \sum_{i=0}^{3} \beta_i \sigma_i \rho \sigma_i, \]  
for some real constants \( \{\beta_j\}_{j=0}^{3} \), will have \( I, \sigma_1, \sigma_2, \) and \( \sigma_3 \) as eigenvectors. Thus \( \Psi \) will equal \( \Phi_D \) if we can arrange to have \( \Psi \) yield the appropriate corresponding eigenvalues: 1, \( d_{11}, d_{22}, \) and \( d_{33} \). This is a simple matter of solving the following linear system, the \( j \)-th equation of which is obtained by substituting \( \rho = \sigma_j \) into (20):
\[
\begin{align*}
1 &= \beta_0 + \beta_1 + \beta_2 + \beta_3 \\
1 + d_{11} &= \beta_0 - \beta_1 - \beta_2 - \beta_3 \\
1 + d_{22} &= \beta_0 - \beta_1 + \beta_2 - \beta_3 \\
1 + d_{33} &= \beta_0 - \beta_1 - \beta_2 + \beta_3.
\end{align*}
\]
Let \( C \) denote the \( 4 \times 4 \) matrix of coefficients of the preceding system and observe that \( C \) is a symmetric matrix such that \( C^2 = 4I \). This observation permits quick solution of the system:
\[
\begin{align*}
\beta_0 &= \frac{1 + d_{11} + d_{22} + d_{33}}{4}, \quad \beta_1 = \frac{1 + d_{11} - d_{22} - d_{33}}{4}, \\
\beta_2 &= \frac{1 - d_{11} + d_{22} - d_{33}}{4}, \quad \beta_3 = \frac{1 - d_{11} - d_{22} + d_{33}}{4}.
\end{align*}
\]
Hence we see that the superoperator \( \Phi_D \) has operator-sum decomposition given by
\[ \Phi_D(\rho) = \sum_{i=0}^{3} \beta_i \sigma_i \rho \sigma_i, \]
with the constants \( \beta_j \) given by (22). By Corollary [11.2], \( \Phi_D \) is completely positive if and only if \( \beta_j \geq 0 \) for \( j = 0, 1, 2, \) and 3. Thus we have arrived at our desired characterization
of diagonal quantum superoperators on \( M_2 \). Observe that the nonnegativity of the \( \beta_j \)'s is equivalent to the Algoet-Fujiwara conditions (3).

Combining our work on diagonal superoperators with the factorization (18), we find an operator-sum decomposition of the unital superoperator \( \Phi_M \) defined by (16):

\[
\Phi_M(\rho) = \sum_{i=0}^{3} \beta_i(U_B \sigma_i U_A) \rho (U_B \sigma_i U_A)^\dagger
\]  

(23)

where \( M = BDA \) is the factorization of Proposition III.1, where \( U_A \) and \( U_B \) are the unitary matrices given by (17), and where the scalars \( \beta_i \) are defined by (22). As discussed above the superoperator \( \Phi_M \) will be completely positive if and only if the scalars \( \beta_i \) leading each summand are nonnegative. In [9, Theorem 1(1)], Landau and Streater show that every unital quantum superoperator on \( M_2 \) is a convex combination of unitary maps. Observe that (23) recaptures the Landau-Streater result, and says a bit more: every unital superoperator \( \Phi \) on \( M_2 \) that preserves both Hermiticity and trace is a linear combination of unitary superoperators: \( \Phi(\rho) = \sum_{i=0}^{3} \beta_i U_i \rho U_i^\dagger \) where \( \sum_{i=0}^{3} \beta_i = 1 \) for real, but not necessarily positive, scalars \( \beta_i \).

V. DIAGONAL QUANTUM OPERATORS ON THE BLOCH REGION

Let \( S = \{0,1,2,3\} \) be the index set for the Pauli matrices (including \( \sigma_0 = I \)) and let \( S^n_0 = S^n \setminus \{(0,0,\ldots,0)\} \) be the Cartesian product of \( n \) copies of \( S \) with the zero \( n \)-tuple removed. We represent the state \( \rho \) of an \( n \)-qubit system in Bloch form

\[
\frac{1}{2^n} \left( I + \sqrt{2^{n-1}(2^n - 1)} \sum_{i=1}^{2^{n-1}} r_i \lambda_i \right),
\]

where \( \{\lambda_i\}_{i=1}^{2^{n-1}} \) consists of all (appropriately normalized) \( n \)-factor tensor products of the Pauli matrices, excluding \( I = \sigma_0 \otimes \cdots \otimes \sigma_0 \):

\[
\{\lambda_i\}_{i=1}^{2^{n-1}} = \left\{ \frac{1}{\sqrt{2^{n-1}}} \sigma_{j_1} \otimes \sigma_{j_2} \otimes \cdots \otimes \sigma_{j_n} : (j_1,j_2,\ldots,j_n) \in S^n_0 \right\}.
\]

Observe that \( \{\lambda_i\}_{i=1}^{2^{n-1}} \) together with \( \lambda_0 := I/\sqrt{2^{n-1}} \) constitutes an orthogonal basis for \( M_2^n \) such that \( \langle \lambda_i|\lambda_j \rangle = 2\delta_{ij} \), where \( \langle \cdot | \cdot \rangle \) is the Hilbert-Schmidt inner product: \( \langle A|B \rangle = \text{tr}(A^\dagger B) \).
A basis should be ordered and we will use the “dictionary” ordering:

\[
\begin{align*}
\lambda_0 &= \frac{1}{\sqrt{2^{n-1}}} \sigma_0 \otimes \sigma_0 \otimes \cdots \otimes \sigma_0 \otimes \sigma_0, \\
\lambda_1 &= \frac{1}{\sqrt{2^{n-1}}} \sigma_0 \otimes \sigma_0 \otimes \cdots \otimes \sigma_0 \otimes \sigma_1, \\
\lambda_2 &= \frac{1}{\sqrt{2^{n-1}}} \sigma_0 \otimes \sigma_0 \otimes \cdots \otimes \sigma_0 \otimes \sigma_2, \\
\lambda_3 &= \frac{1}{\sqrt{2^{n-1}}} \sigma_0 \otimes \sigma_0 \otimes \cdots \otimes \sigma_0 \otimes \sigma_3, \\
\lambda_4 &= \frac{1}{\sqrt{2^{n-1}}} \sigma_0 \otimes \cdots \otimes \sigma_0 \otimes \sigma_1 \otimes \sigma_0, \ldots, \\
\lambda_{2^{2n-1}-1} &= \frac{1}{\sqrt{2^{n-1}}} \sigma_3 \otimes \cdots \otimes \sigma_3 \otimes \sigma_3 \otimes \sigma_3.
\end{align*}
\]

Note that the dictionary ordering is equivalent to that produced by ordering according to the size of the index sequence \(i_1 i_2 \ldots i_n\) associated with \(\sigma_{i_1} \otimes \cdots \otimes \sigma_{i_n}\), where \(i_1 i_2 \ldots i_n\) is interpreted as the base 4 representation of a number.

Our goal is to characterize those \((2^{2n-1}) \times (2^{2n-1})\) diagonal matrices \(D\), with real entries \(d_{jj}\), along the diagonal, such that \(\Phi_D : M_{2^n} \rightarrow M_{2^n}\) defined by

\[
\Phi_D \left( \frac{1}{2^n} \left( I + c\vec{r} \cdot \vec{\lambda} \right) \right) = \frac{1}{2^n} \left( I + cD\vec{r} \cdot \vec{\lambda} \right)
\]

is a quantum operator. Just as in the single-qubit setting, (24) together with the linearity of \(\Phi_D\) yields

\[
\Phi_D(I) = I \quad \text{and} \quad \Phi_D(\lambda_j) = d_{jj} \lambda_j \quad \text{for} \quad j = 1, \ldots, 2^{2n} - 1.
\]

Because \(\Phi_D\) preserves Hermiticity, we know that it has an operator-sum decomposition; moreover, we know that \(\Phi_D\) has \(\{\lambda_j\}_{j=0}^{2^{2n}-1}\) as eigenvectors. The one-qubit situation, analyzed in the preceding section, suggests that \(\Phi_D\) has the form

\[
\Phi_D(\rho) = \sum_{i=0}^{2^{2n}-1} \beta_i \lambda_i \rho \lambda_i
\]

for some real constants \(\{\beta_j\}_{j=1}^{2^{2n}-1}\).

Using (11), it is easy to check that

\[
\lambda_i \lambda_j \lambda_i = \pm \frac{1}{2^{n-1}} \lambda_j \quad \text{for} \quad i, j \in \{0, 1, 2, \ldots, 2^{2n} - 1\}
\]

so that \(\Phi_D\), given by (25), will have the right eigenvectors. We need only arrange for \(\Phi_D\) to have the correct eigenvalues (namely, 1, \(d_{1,1}\), \(d_{2,2}\), \ldots, \(d_{2^{2n-1},2^{2n-1}}\)).

We need a way to keep track of the signs that appear on the right of (26). Let \(C\) be the \(4 \times 4\) matrix of 1’s and -1’s defined by

\[
\sigma_i \sigma_j \sigma_i = c_{ij} \sigma_j
\]
so that $C$ is the matrix of coefficients of the system (21) of the preceding section. Note that $C$ has 1’s along its main diagonal and $C/2$ is a symmetric, orthogonal matrix. Moreover the “one-qubit” Algoet-Fujiwara conditions—$\beta_j \geq 0$ for $j = 0, 1, 2, 3$ where the $\beta_j$’s are given by (22)—are equivalent to the requirement that the column vector

$$\begin{bmatrix}
1 \\
d_{11} \\
d_{22} \\
d_{33}
\end{bmatrix}$$

have nonnegative components.

Now let $F$ be the $16 \times 16$ “sign” matrix corresponding to (26) in the $n = 2$ qubit situation: $\lambda_i \lambda_j \lambda_0 = f_{ij} \lambda_j/2$. It’s not difficult to see that $F = C \otimes C$; for example, to find the “upper-left” $4 \times 4$ block of $F$, one calculates

$$(\sigma_0 \otimes \sigma_j)(\sigma_0 \otimes \sigma_k)(\sigma_0 \otimes \sigma_j) = (\sigma_0 \sigma_0 \sigma_0) \otimes (\sigma_j \sigma_k \sigma_j) = c_{00}c_{jk}\sigma_0 \otimes \sigma_k$$

so that $c_{00}C$ is the upper-left block of $F$, which is the appropriate submatrix in the Kronecker product. Thus when $n = 2$, the matrix of coefficients of the $\beta_i$’s in the $16 \times 16$ system that results when $\lambda_0$ through $\lambda_{15}$ are subsituted into (25) is $\frac{1}{2}C \otimes C$, and thus, because the inverse of $\frac{1}{2}C \otimes C$ is $\frac{1}{8}C \otimes C$, the necessary and sufficient conditions for $\Phi_D$ to be completely positive is that

$$\begin{bmatrix}
1 \\
d_{1,1} \\
\vdots \\
d_{15,15}
\end{bmatrix}$$

have nonnegative components. Moreover, these components are precisely the $\beta_i$’s in (25) that lead to an operator-sum decomposition of $\Phi_D$.

In complete generality, we have the following.

**Theorem V.1 (Algoet-Fujiwara Conditions for $n$-qubits)** The diagonal linear superoperator $\Phi_D : M_{2^n} \rightarrow M_{2^n}$ defined by (24) is completely positive if and only if the column
vector

\[
\begin{bmatrix}
1 & 1 & 1 \\
1 & 1 & -1 \\
1 & -1 & 1 \\
1 & -1 & -1
\end{bmatrix}^{\otimes n}
\begin{bmatrix}
1 \\
d_{1,1} \\
\vdots \\
d_{2^n-1,2^n-1}
\end{bmatrix}
\]

has nonnegative components. Moreover, if \(\beta_{j-1}\) denotes \(j\)-th component of this column vector (for \(j = 1, \ldots, 2^n\)), then \(\Phi_D\) has operator-sum decomposition

\[
\Phi_D(\rho) = \sum_{j=0}^{2^n-1} \beta_j \lambda_j \rho \lambda_j.
\]

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