# Complete positivity and variations on the Choi matrix 

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## Main Question

If $\Phi: M_{n} \rightarrow M_{m}$ is a linear map, the Choi matrix of $\Phi$ is

$$
C_{\Phi}=\sum_{i j} E_{i j} \otimes \Phi\left(E_{i j}\right)
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Topic of this talk: to what extent can $\left\{E_{i j}\right\}$ be replaced by other bases of $M_{n}$ ?

## Outline

I. Affine automorphisms and order isomorphisms (Review)

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II. Complete positivity of the map from a basis to the dual basis; variations on the Choi matrix (joint with Vern Paulsen)
III. Unique determination of states by sets of observables (joint with J. Chen, H. Dawkins, Z. Ji, N. Johnston, D. Kribs, and B. Zeng)
$H$ is a (finite or infinite dimensional) Hilbert space, and $\mathcal{B}(H)$ is the ${ }^{*}$-algebra of bounded operators on $H$.
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A state on $\mathcal{B}(H)$ is a positive linear functional $\rho$ such that $\rho(I)=1$.
If $x$ is a unit vector in $H$, then $\omega_{x}$ denotes the vector state $\omega_{x}(A)=(A x, x)$.

A state $\omega$ on $\mathcal{B}(H)$ is normal if there is a trace class operator $D$ such that $\omega(A)=\operatorname{tr}(A D)$ for $A \in \mathcal{B}(H)$.

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Normal states are the countable convex combinations of vector states: $\omega(A)=\sum_{i} \lambda_{i} \omega_{x_{i}}(A)$.
$K$ denotes the set of normal states on $\mathcal{B}(H)$. Note that $K$ is convex, and the extreme points of $K$ are the vector states.

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A map $\Phi: K \rightarrow K$ is an affine automorphism if $\Phi$ is bijective and $\Phi$ preserves convex combinations, i.e.,

$$
\Phi\left(t \rho_{1}+(1-t) \rho_{2}\right)=t \Phi\left(\rho_{1}\right)+(1-t) \Phi\left(\rho_{2}\right)
$$

for $0 \leq t \leq 1$ and all $\rho_{1}, \rho_{2}$ in $K$.

## Why we care about affine automorphisms

In the quantum mechanical formalism,

- observables are self-adjoint operators in $\mathcal{B}(H)$.
- A state represents an ensemble of physical systems each prepared in the same fashion.
- If $\rho$ is a state and $A$ is an observable, then $\rho(A)$ is the expected value of the observable $A$ in the state $\rho$.
- A convex combination of states is thought of as a statistical mixture.
- Physical symmetries (e.g., rotation) and time evolution act on states, are reversible, and preserve mixtures, hence are affine automorphisms of $K$.


## Order automorphisms

Let $\mathcal{A}=\mathcal{B}(H)_{\text {sa }}$ : the space of observables (bounded self adjoint operators on $H$ ). We order $\mathcal{A}$ in the usual way: $A \leq B$ if $B-A$ is positive semi-definite, i.e., if $\langle A \xi, \xi\rangle \leq\langle B \xi, \xi\rangle$ for all $\xi \in H$.

## Definition

Let $\mathcal{A}=\mathcal{B}(H)_{\text {sa }}$. A linear map $\Phi: \mathcal{A} \rightarrow \mathcal{A}$ is an order isomorphism if $\Phi$ is bijective and $\Phi$ and $\Phi^{-1}$ are order preserving, and is unital if $\Phi(I)=I$.

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## Example

If $C \in \mathcal{B}(H)$ is invertible, then the map $X \mapsto C^{*} X C$ is an order automorphism of $\mathcal{A}=\mathcal{B}(H)_{\text {sa }}$.

## *-automorphisms of $B(H)$

## Definition

Let $\Phi: \mathcal{B}(H) \rightarrow \mathcal{B}(H)$ be a linear map. Then $\Phi$ is a
*-automorphism

$$
\Phi\left(X^{*}\right)=\Phi(X)^{*} \text { and } \Phi(X Y)=\Phi(X) \Phi(Y)
$$

If $\Phi$ reverses products so that $\Phi(X Y)=\Phi(Y) \Phi(X)$ then $\Phi$ is said to be a *-anti-automorphism.

Note there is no notion of ${ }^{*}$-automorphism on $\mathcal{A}=\mathcal{B}(H)_{\text {sa }}$ since products of observables need not be observables.

## Examples

## Theorem

If $U$ is a unitary on $H$, then $X \mapsto U X U^{*}$ is a *-automorphism of $B(H)$ and every *-automorphism has this form.

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If $t: \mathcal{B}(H) \rightarrow \mathcal{B}(H)$ is the transpose map (with respect to an orthonormal basis), then $t$ is a *-anti-automorphism of $\mathcal{B}(H)$, and every *-anti-automorphism of $\mathcal{B}(H)$ has the form $X \mapsto U X^{t} U^{*}$ for some unitary $U$.

## Jordan automorphisms

## Definition

Let $\mathcal{A}=\mathcal{B}(H)_{\text {sa }}$. The Jordan product on $\mathcal{A}$ is given by $a \circ b=\frac{1}{2}(a b+b a)$. A Jordan automorphism $\Phi: \mathcal{A} \rightarrow \mathcal{A}$ is an linear bijection that preserves the Jordan product.

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If $\Phi: \mathcal{B}(H) \rightarrow \mathcal{B}(H)$ is a *-automorphism or *-anti-automorphism, then $\Phi$ restricted to $\mathcal{A}=\mathcal{B}(H)_{\text {sa }}$ is a Jordan automorphism.

## Physical importance of Jordan structure

The Jordan structure of a C*-algebra or von Neumann algebra was viewed as physically meaningful since it takes Hermitian operators to Hermitian operators, and is computable from the functional calculus:

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a \circ b=\frac{1}{2}(a b+b a)=\frac{1}{4}\left((a+b)^{2}-(a-b)^{2}\right) .
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Kadison called a Jordan automorphism a quantum mechanical isomorphism or a C*-isomorphism!

## Automorphisms of the space of observables

## Theorem

(Kadison) Let $\mathcal{A}=\mathcal{B}(H)_{\text {sa }}$. If $\Phi: A \rightarrow A$ is a linear map, the following are equivalent.
(i) $\Phi$ is a unital order automorphism.
(ii) $\Phi$ is an isometry on $A$. (In fact, then $\Phi$ will to an isometry on all of $B(H)$.)
(iii) $\Phi$ is a Jordan automorphism of $A$.
(iv) $\Phi$ is a ${ }^{*}$-isomorphism or a *-anti-isomorphism of $B(H)$.
(v) The map $\rho \mapsto \rho \circ \Phi$ is an affine automorphism of $K$.

## Description of order automorphisms of $B(H)_{\text {sa }}$

## Corollary

Let $\mathcal{A}=\mathcal{B}(H)_{\text {sa. }}$. If $\Phi: \mathcal{A} \rightarrow \mathcal{A}$ is an order automorphism, then there is an invertible $C$ in $B(H)$ such that either $\Phi(X)=C X C^{*}$ for all $X$ in $\mathcal{A}$, or $\Phi(X)=C X^{t} C^{*}$ for all $X$ in $\mathcal{A}$.

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## Proof.

Suppose first that $\Phi$ is unital, i.e., $\Phi(I)=I$. Then by Kadison's results above, $\Phi$ is a Jordan automorphism, hence $\Phi(X)=U X U^{*}$ for a unitary $U$ or else $\Phi(X)=U X^{t} U^{*}$.

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If $\Phi$ is not unital, then $B:=\Phi(I)^{1 / 2}$ is positive and invertible.
Then $X \mapsto B^{-1} \Phi(X) B^{-1}$ is a unital order automorphism, and now $\Phi(X)=(B U) X(B U)^{*}$ or $\Phi(X)=(B U) X^{t}(B U)^{*}$.

## Description of affine automorphisms of $K$.

## Theorem

Let $K$ be the normal state space of $B(H)$. If $\Psi: K \rightarrow K$ is an affine automorphism, then there is a unitary $U$ such that either

$$
\Psi(\rho)(X)=\rho\left(U X U^{*}\right) \text { for all } \rho \in K \text { and all } X \text { in } B(H)
$$

or such that

$$
\Psi(\rho)(X)=\rho\left(U X^{t} U^{*}\right) \text { for all } \rho \in K \text { and all } X \text { in } B(H) .
$$

These results imply that the convex structure of the normal state space $K$ (or equivalently the order structure on the space $\mathcal{A}=\mathcal{B}(H)_{\text {sa }}$ ) determine the Jordan product and the norm on $\mathcal{B}(H)$, and one of two possible associative products.

## II. Applications to complete positivity of certain maps

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Let $\Phi: M_{n} \rightarrow M_{m}$ be a linear map. Then $\Phi$ is positive if $a \geq 0$ implies $\Phi(a) \geq 0$.
$\Phi$ is completely positive if the map $I_{p} \otimes \Phi: M_{p} \otimes M_{n} \rightarrow M_{p} \otimes M_{n}$ is positive for all $p$.
(If we identify $M_{p} \otimes M_{n}$ with $M_{p}\left(M_{n}\right)$, this is equivalent to the entry-wise map $\left(a_{i j}\right) \rightarrow\left(\Phi\left(a_{i j}\right)\right)$ being positive.)
$M_{n}^{*}$ denotes the dual vector space of $M_{n}$.
We will be investigating complete positivity of certain maps from $M_{n}$ to $M_{n}^{*}$, so we need a definition of order on $M_{p}\left(M_{n}^{*}\right)$ for $p \geq 1$.
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## Definition

A matrix of functionals $\left(f_{i, j}\right) \in M_{p}\left(M_{n}^{*}\right)$ is positive if and only if the linear map $\Phi: M_{n} \rightarrow M_{p}$ given by $\Phi(A)=\left(f_{i, j}(A)\right)$ is completely positive.

## Definition

A linear map $\Phi$ from $M_{n}$ to $M_{n}^{*}$ is completely positive if $I \otimes \Phi: M_{p} \otimes M_{n} \rightarrow M_{p} \otimes M_{n}^{*}$ is positive, i.e. $\left(a_{i j}\right) \mapsto\left(\Phi\left(a_{i j}\right)\right)$ is a positive map.

## Definition

A linear bijection $\Phi$ from $M_{n}$ to $M_{n}$ or to $M_{n}^{*}$ is a complete order isomorphism if both $\Phi$ and $\Phi^{-1}$ are completely positive.
$\Phi$ is called a completely co-positive order isomorphism provided that its composition $\Psi \circ t$ with the transpose map $t$ on $M_{n}$ is a complete order isomorphism.

## Examples

If $\rho \in M_{n}^{*}$, then there is a unique matrix $D_{\rho} \in M_{n}$ such that $\rho(A)=\operatorname{tr}\left(A D_{\rho}\right)$. The matrix $D_{\rho}$ is called the density matrix for $\rho$.

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## Example

The map that takes $\rho \in M_{n}^{*}$ to $D_{\rho}^{*} \in M_{n}$ is a complete order isomorphism but is conjugate linear.

## Definition

Given a basis $\mathcal{B}$ of $M_{n}$, the duality $\operatorname{map} \mathcal{D}_{\mathcal{B}}: M_{n} \rightarrow M_{n}^{*}$ is the linear map that takes the basis $\mathcal{B}$ to its dual basis.

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## Theorem

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Main question: for which bases $\mathcal{B}$ is the duality map a complete order isomorphism?

## Why should one care?

1. Curiosity: what is special about the standard basis $\mathcal{E}$ of $M_{n}$ when working with complete positivity? Would other bases commonly used in applications work as well?

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3. Greater convenience when working with bases of interest in quantum information: e.g., Pauli spin matrices and their tensor products, and the Weyl basis.
4. A source of "entanglement witnesses": matrices that provide a test of entanglement.

## Definition

Let $\mathcal{B}$ be a basis of $M_{n}$ and $\mathcal{E}$ the standard basis of matrix units. Define $M_{\mathcal{B}}: M_{n} \rightarrow M_{n}$ by $M_{\mathcal{B}}=D_{\mathcal{B}}^{-1} D_{\mathcal{E}}$.

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Since $D_{\mathcal{E}}: M_{n} \rightarrow M_{n}^{*}$ is a complete order isomorphism, then $D_{\mathcal{B}}: M_{n} \rightarrow M_{n}^{*}$ will be a complete order isomorphism (resp. completely co-positive order isomorphism) iff $M_{\mathcal{B}}: M_{n} \rightarrow M_{n}$ is a complete order isomorphism (resp. completely co-positive order isomorphism.)

## Definition

Let $\mathcal{B}$ be a basis of $M_{n}$ and $\mathcal{E}$ the standard basis of matrix units, with a fixed order. A change of basis map is any linear map $C_{\mathcal{B}}$ in $L\left(M_{n}\right)$ taking the set $\mathcal{E}$ to the set $\mathcal{B}$.

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## Definition

By slight abuse of notation, we write $C_{\mathcal{B}}^{T}$ for the unique linear map in $L\left(M_{n}\right)$ whose matrix in the standard basis $\mathcal{E}$ is the transpose of the matrix of $C_{\mathcal{B}}$.

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M_{\mathcal{B}}=C_{\mathcal{B}} C_{\mathcal{B}}^{T} .
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It follows that $M_{\mathcal{B}}$ depends on the basis $\mathcal{B}$, but not on the particular choice of change of basis map $C_{\mathcal{B}}$ (i.e., not on the order of the basis).

## Main theorem on complete positivity of $\mathcal{D}_{B}$.

## Theorem

Let $\mathcal{B}$ be a basis of $M_{n}$. Then $\mathcal{D}_{\mathcal{B}}: M_{n} \rightarrow M_{n}^{*}$ is a complete order isomorphism iff $C_{B} C_{B}^{T}=\operatorname{Ad}_{C}$ for some $C \in M_{n}$, and is a completely co-positive order isomorphism iff $C_{B} C_{B}^{T}=\operatorname{Ad} C \circ t$ for some $C \in M_{n}$.

## Examples: some bases closely related to the standard basis

## Theorem

Let $\left(\lambda_{i j}\right) \in M_{n}$, with all $\lambda_{i j}$ nonzero, and let $\mathcal{B}$ be the basis $\left\{\lambda_{i j} E_{i j}\right\}$. Then $\mathcal{D}_{\mathcal{B}}$ is an order isomorphism if and only if the matrix $\left(\lambda_{i j}^{2}\right)$ is positive semi-definite with rank one. In that case, $\mathcal{D}_{\mathcal{B}}$ is a complete order isomorphism.

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## Example

If $C \in M_{n}$ is invertible, for the basis $\mathcal{B}=\left\{C E_{i j} C^{*}\right\}$, the duality map $\mathcal{D}_{\mathcal{B}}$ is a complete order isomorphism. In particular, if $\mathcal{B}$ is a system of matrix units then $\mathcal{D}_{\mathcal{B}}$ is a complete order isomorphism.

## Weyl basis

## Definition

Let $e_{0}, \ldots, e_{n-1}$ be the standard basis of $\mathbb{C}^{n}$. Let $z=\exp (2 \pi i / n)$. Define $U, V \in M_{n}$ by

$$
V e_{j}=z^{j} e_{j}
$$

and

$$
U e_{j}=e_{j+1}
$$

for $j \in \mathbb{Z}_{n}$. Then $\left\{\left.\frac{1}{\sqrt{n}} U^{a} V^{b} \right\rvert\, a, b \in \mathbb{Z}_{n}\right\}$ is an orthonormal basis for $M_{n}$ which we call the Weyl basis $\mathcal{W}$.

The unitary matrices $\left\{U^{a} V^{b} \mid a, b \in \mathbb{Z}_{n}\right\}$ are usually called the discrete Weyl matrices or the generalized Pauli matrices.

## Theorem

For the Weyl basis $\mathcal{W}$, the duality map $\mathcal{D}_{\mathcal{W}}: M_{n} \rightarrow M_{n}^{*}$ is a complete order isomorphism if $n=2$, and is not an order isomorphism for $n>2$.

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## Corollary

For the basis of $M_{2}^{\otimes n}$ consisting of tensor products of the $2 \times 2$ Weyl basis, the duality map $\mathcal{D}_{\mathcal{W}}$ is a complete order isomorphism

## Testing complete positivity using non-standard bases

## Definition

If $\Phi: M_{m} \rightarrow M_{n}$ is a linear map, the Choi matrix of $\Phi$ is

$$
C_{\Phi}=\sum_{i j} E_{i j} \otimes \Phi\left(E_{i j}\right)
$$

## Theorem

(Choi) If $\Phi: M_{m} \rightarrow M_{n}$ is a linear map, then $\Phi$ is completely positive iff $C_{\Phi} \geq 0$.

Choi's characterization of complete positivity doesn't necessarily hold for other bases of $M_{m}$ in place of $\left\{E_{i j}\right\}$. The following is a consequence of the preceding results.

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## Corollary

Let $\mathcal{B}=\left\{B_{j}: 1 \leq j \leq n^{2}\right\}$ be a basis for $M_{n}$, and let $\psi: M_{n} \rightarrow M_{p}$ be a linear map.
(1) If the duality map $\mathcal{D}_{\mathcal{B}}$ is a complete order isomorphism, then $\Psi$ is completely positive if and only if $\sum_{j=1}^{n^{2}} \Psi\left(B_{j}\right) \otimes B_{j} \in\left(M_{p} \otimes M_{n}\right)^{+}$.

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(2) If the duality map $\mathcal{D}_{\mathcal{B}}$ is a completely co-positive order isomorphism, then $\Psi$ is completely positive if and only if $\sum_{j=1}^{n^{2}} \Psi\left(B_{j}\right) \otimes B_{j}^{t} \in\left(M_{p} \otimes M_{n}\right)^{+}$.

## Entanglement witnesses

## Definition

A state $\rho$ on $M_{n} \otimes M_{n}$ is entangled if it is not a convex combination of product states.

It is not easy to tell if a state is entangled. One way is by finding an entanglement witness.

## Definition

If $W=W^{*} \in M_{n} \otimes M_{n}$, then $W$ is an entanglement witness if $W$ is positive on product states but $\rho(W)<0$ for some state $\rho$. (This implies $\rho$ is entangled, and we say $W$ witnesses the entanglement of $\rho$.)

## Corollary

Let $\mathcal{B}$ be a basis of $M_{n}$ such that the duality map $\mathcal{D}_{\mathcal{B}}$ is a complete order isomorphism. If $\Psi: M_{n} \rightarrow M_{n}$ is any map that is positive but not completely positive, then $\sum_{B_{i} \in \mathcal{B}} B_{i} \otimes \Psi\left(B_{i}\right)$ is an entanglement witness.

## A basis-free description of the Choi matrix

Recall the Choi matrix for $\Phi: M_{n} \rightarrow M_{n}$ is defined by $C_{\Phi}=\sum_{i} E_{i j} \otimes \Phi\left(E_{i j}\right)$. Here the basis $\left\{E_{i j}\right\}$ can't be replaced by an arbitrary orthonormal basis. The following result provides an alternate description of the Choi matrix that does have this independence property. Given a matrix $B=\left(b_{i, j}\right)$ we set $\bar{B}=\left(\overline{b_{i, j}}\right)$.

## A basis-free description of the Choi matrix

Recall the Choi matrix for $\Phi: M_{n} \rightarrow M_{n}$ is defined by
$C_{\Phi}=\sum_{i} E_{i j} \otimes \Phi\left(E_{i j}\right)$. Here the basis $\left\{E_{i j}\right\}$ can't be replaced by an arbitrary orthonormal basis. The following result provides an alternate description of the Choi matrix that does have this independence property. Given a matrix $B=\left(b_{i, j}\right)$ we set $\bar{B}=\left(\overline{b_{i, j}}\right)$.

## Theorem

Let $\left\{B_{l}\right\}_{l=1}^{n^{2}}$ be an orthonormal basis for $M_{n}$, and $\Phi: M_{n} \rightarrow M_{p}$ linear. Then Choi's matrix is given by

$$
\begin{equation*}
C_{\Phi}=\sum_{l=1}^{n^{2}} \overline{B_{l}} \otimes \Phi\left(B_{l}\right) \tag{1}
\end{equation*}
$$

This expression shows that the Choi matrix is the partial transpose of a matrix defined by Jamiołkowski

$$
\begin{equation*}
\mathcal{J}(\Phi)=\sum_{i j} E_{i j}^{*} \otimes \Phi\left(E_{i j}\right) . \tag{2}
\end{equation*}
$$

Jamiołkowski defined this correspondence as a tool in studying linear maps from $M_{n}$ into $M_{p}$. Here $E_{i j}$ could be replaced by any orthonormal basis, but positivity of $\mathcal{J}(\Phi)$ is not equivalent to complete positivity of $\Phi$.

## Reference

V. Paulsen and F. Shultz., Complete positivity of the map from a basis to its dual basis, Journal of Mathematical Physics 54 (2013) 072201.

## UDA and UDP

I'm going to discuss a result from the paper
J. Chen, H. Dawkins, Z. Ji, N. Johnston, D. Kribs, F. Shultz, and
B. Zeng, Uniqueness of quantum states compatible with given measurement results, Physical Review A 88 (2013) 012109.
and its connection with the results on affine automorphisms above.

One goal of quantum tomography is to make measurements to determine a state.

## Definition

A set of observables $\mathcal{A}$ in $M_{n}$ is informationally complete if $\operatorname{tr} A \rho_{1}=\operatorname{tr} A \rho_{2}$ for all $A \in \mathcal{A}$ implies $\rho_{1}=\rho_{2}$.

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Clearly there are informationally complete sets of $n^{2}-1$ observables whose span (with the identity) is all of $M_{n}$, hence $n^{2}-1$ observables suffice, and one can show no smaller number of observables suffices.

Suppose one has additional information, for example, that the states to be distinguished are all pure states. Then Heinosaari, Mazzarella, Wolf showed that $4 n-5$ observables suffice.

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## Definition

Let $\rho$ be a pure state on $H$ and $\mathbf{A}$ a finite set of observables. We say $(\rho, \mathbf{A})$ has the UDA property if $\sigma(A)=\rho(A)$ for a state $\sigma$ and for all $A \in \mathbf{A}$ implies $\sigma=\rho$. If this holds when $\sigma$ is restricted to being a pure state, we say $(\rho, \mathbf{A})$ has the UDP property. (The acronym "UDA" stands for "uniquely determined for all".)

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Chen, Dawkins, Ji, Johnston, Kribs, S., and Zeng construct a set of observables with $|\mathcal{A}|=\mathbf{5 n}-\mathbf{7}$ possessing the UDA property.

## Another UDP/UDA result

## Lemma

Let $G$ be a compact group of unitaries on a real or complex finite dimensional Hilbert space $H$, and let $L$ be the set of fixed points of $G$. Let $\mu$ be Haar measure on $G$, and define $P: H \rightarrow H$ to be the linear map satisfying

$$
\begin{equation*}
\langle P \xi, \eta\rangle=\int_{G}\langle g \xi, \eta\rangle d \mu(g) \tag{3}
\end{equation*}
$$

for $\xi, \eta \in H$. Then $P$ is the orthogonal projection onto $L$, $P g=g P=P$ for all $g \in G$, and $P$ is in the convex hull of $G$.

Let $K_{n}$ be the state space of $M_{n}$. Recall that symmetries of $K_{n}$ are given by conjugation by unitaries or by the transpose map or by composition of these two types of symmetries.

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If we view $L\left(M_{n}\right)_{s a}$ as a real Hilbert space (with the usual inner product $\langle X, Y\rangle=\operatorname{tr}(X Y)$ ), then conjugation by unitaries in $M_{n}$ and the transpose map on $M_{n}$ both preserve this inner product, so these symmetries are unitaries on the Hilbert space $L\left(M_{n}\right)_{s a}$. Thus we can apply the lemma above.

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In the following theorem we are identifying states with the associated density matrices: $\rho(A)=\operatorname{tr}(A D)$ and conversely observables with members of the linear span of $K_{n}$.

## Theorem

Let $A$ be a finite set of observables on $H_{n}$ with real linear span $L$. Assume there exists a compact group $G$ of affine automorphisms of $K_{n}$ whose fixed point set is $L \cap K_{n}$. Then each pure state which is UDP for measuring $A$ is also UDA.

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## Corollary

For $n=2$, for all pure states and all sets $\mathbf{A}$ of observables, UDP implies UDA.

## Corollary

Let $\mathbf{A}=\left\{A_{1}, \ldots, A_{p}\right\}$ be observables in $M_{n}$. If the (complex) linear span of $\mathbf{A}$ is a ${ }^{*}$-subalgebra $\mathbf{A}$ of $M_{n}$, then UDP $=$ UDA for pure states measured by these observables.

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## Example

Let $\mathbf{A}=\left\{E_{11}, \ldots, E_{n n}\right\}$. Then the complex linear span of $\mathbf{A}$ consists of the diagonal matrices. From the corollary it follows that for each pure state $\rho$ on $M_{n}$, UDP for $\mathbf{A}$ implies UDA.

