Uniqueness of Quantum States Compatible with Given Measurement Results

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We discuss the uniqueness of quantum states compatible with given results for measuring a set of observables. For a given pure state, we consider two different types of uniqueness: (1) no other pure state is compatible with the same measurement results and (2) no other state, pure or mixed, is compatible with the same measurement results. For case (1), it is known that for a d-dimensional Hilbert space, there exists a set of $4d-5$ observables that uniquely determines any pure state. We show that for case (2), $5d-7$ observables suffice to uniquely determine any pure state. Thus there is a gap between the results for (1) and (2), and we give some examples to illustrate this. The case of observables corresponding to reduced density matrices (RDMs) of a multipartite system is also discussed, where we improve known bounds on local dimensions for case (2) in which almost all pure states are uniquely determined by their RDMs. We further discuss circumstances where (1) can imply (2). We use convexity of the numerical range of operators to show that when only two observables are measured, (1) always implies (2). More generally, if there is a compact group of symmetries of the state space which has the span of the observables measured as the set of fixed points, then (1) implies (2). We analyze the possible dimensions for the span of such observables. Our results extend naturally to the case of low rank quantum states.

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I. INTRODUCTION

In a d-dimensional Hilbert space $\mathcal{H}_d$, any quantum state ρ generated by a source can be reconstructed by quantum tomography. As ρ is Hermitian and $\operatorname{tr}\rho = 1$, only d^2-1 independent measurements are needed to uniquely specify ρ. When $\rho = |\psi\rangle\langle\psi|$ is a pure state, one may not need as many measurements to uniquely determine $|\psi\rangle$. However, exactly what is meant by "uniquely" in this context needs to be specified.

Assume that a set of m linearly independent observables

$$\mathbf{A} = (A_1, A_2, \ldots, A_m) \tag{1}$$

is measured, where each A_i is Hermitian. Then for any quantum state ρ, measuring $\mathbf{A}$ (i.e., measuring every observable in $\mathbf{A}$), returns the average values

$$\mathbf{A}(\rho) := (\operatorname{tr}\rho A_1, \operatorname{tr}\rho A_2, \ldots, \operatorname{tr}\rho A_m) \in \mathbb{R}^m. \tag{2}$$

We denote the set of all vectors $\mathbf{A}(\rho)$ as follows:

$$C_m(\mathbf{A}) := \{\mathbf{A}(\rho) : \ \rho \text{ acts on } \mathcal{H}_d\}. \tag{3}$$

For a pure state $|\psi\rangle$, these values are given by

$$\mathbf{A}(|\psi\rangle) := (\langle\psi|A_1|\psi\rangle, \langle\psi|A_2|\psi\rangle, \ldots, \langle\psi|A_m|\psi\rangle). \tag{4}$$

We denote the set of all vectors $\mathbf{A}(|\psi\rangle)$ as follows, and note that this set is often called the "joint numerical range" of $\mathbf{A}$:

$$W_m(\mathbf{A}) := \{\mathbf{A}(|\psi\rangle) : \ |\psi\rangle \in \mathcal{H}_d\}. \tag{5}$$

In this work we consider two different kinds of 'unique determinedness' for $|\psi\rangle$:

1. We say $|\psi\rangle$ is *uniquely determined among pure states (UDP) by measuring* $\mathbf{A}$ if there does not exist any other pure state which has the same measurement results as those of $|\psi\rangle$ when measuring $\mathbf{A}$.

2. We say $|\psi\rangle$ is *uniquely determined among all states (UDA) by measuring* $\mathbf{A}$ if there does not exist any other state, pure or mixed, which has the same measurement results as those of $|\psi\rangle$ when measuring $\mathbf{A}$.

It is known that there exists a family of $4d-5$ observables such that any pure state is UDP, in contrast with the d^2-1 observables required in the general case of quantum tomography [1]. The physical interpretation in this case is clear: it is useful in quantum tomography to have the prior knowledge that the state to be reconstructed is pure or nearly pure. Many other techniques for pure state tomography have been developed, and experiments have been performed to demonstrate the reduction of the number of measurements needed [2–8].

When the state is UDP, one needs to make sure that the state is indeed pure in order for the tomography to be meaningful. This is not practical in general, but one can readily generalize the previously-mentioned UDP results to low rank states, where the physical constraints (e.g., low temperature or locality of interaction) may ensure that the actual physical state (which ideally is supposed to be pure) indeed has low rank. If the state is UDA, however, one does not need to bother with these physical assumptions, because there is only one state compatible with the measurement results, which must necessarily be pure (or of low rank).

There is also another clear physical meaning for the states that are UDA by measuring $\mathbf{A}$. Consider a Hamiltonian of the form

$$H_{\mathbf{A}} = \sum_{i=1}^{m} \alpha_i A_i. \quad (6)$$

Then any unique ground state $|\psi\rangle$ of $H_{\mathbf{A}}$ is UDA by measuring $\mathbf{A}$. This is easy to verify: if there were any other state ρ that gave the same measurement results, then ρ would have the same energy as that of $|\psi\rangle$, which is the ground state energy. Therefore, any pure state in the range of ρ must also be a ground state, which contradicts the fact that $|\psi\rangle$ is the unique ground state. In other words, UDA is a necessary condition for $|\psi\rangle$ to be a unique ground state of $H_{\mathbf{A}}$. It is in general not sufficient, but the exceptions are likely rare [9, 10].

The uniqueness properties for pure states, for both UDP and UDA, have also been studied extensively in the case of multipartite quantum systems, where the observables correspond to reduced density matrices (RDMs). That is, the observables are chosen to act nontrivially on only some subsystems. For an n-particle system and a constant $k < n$, there are a total of $\binom{n}{k}$ k-RDMs, and the corresponding measurements $\mathbf{A}$ are those $\leq k$-body operators. For example, for a three-qubit system and $k = 2$, one can choose $\mathbf{A}$ as a tuple of all one and two-particle Pauli operators. Of course, one can also choose to look at just some of the $\binom{n}{k}$-RDMs, rather than all of them. For instance, for a three-particle system, one can look at the 2-RDMs of particle pairs $\{1, 2\}$ and $\{1, 3\}$.

It is known that almost all three-qubit pure states are UDA by their 2-RDMs [11]. These authors also show that UDP implies UDA for 2-RDMs of three-qubit pure states. This result can be further improved to 2-RDMs of particle pairs $\{1, 2\}$ and $\{2, 3\}$ [9]. More generally one can consider a three-particle system of particles $1, 2, 3$ with Hilbert spaces whose dimensions are d_1, d_2, d_3, respectively. If $d_1 \geq d_2 + d_3 - 1$, then almost all pure states are UDA by their 2-RDMs of particle pairs $\{1, 2\}$ and $\{1, 3\}$ [12]. However, a much stronger result is known when considering UDP instead of UDA: it was shown by Diosi [13] that if $d_1 \geq 2$ then almost all pure states are UDP by their 2-RDMs of particle pairs $\{1, 2\}$ and $\{1, 3\}$.

For n-particle quantum systems with subsystems of equal dimension, almost all pure states are UDA by their k-RDMs of just over half of the parties (i.e., $k \sim n/2$). Furthermore, $\sim n/2$ properly chosen RDMs among all of the $\binom{n}{k}$ k-RDMs suffice [14]. W-type states are UDA by their 2-RDMs, and $n-1$ of those 2-RDMs are enough [15]. General symmetric Dicke states are UDA by their 2-RDMs [16]. It has been shown that the only n-particle pure states that cannot be UDP by their $(n-1)$-RDMs are the GHZ-type states, and this result has been further improved to the case of UDA [17]. Their results also show that UDP implies UDA for $(n-1)$-RDMs of n-qubit pure states.

Despite these many results, there is no systematic study of these two different types of uniqueness for pure states. This will be the focus of the present paper, where we are interested in knowing, for given measurements $\mathbf{A}$, whether UDP and UDA are the same or different. We will give a general argument that there is a gap between the number of observables needed for the two different cases, however the gap seems to be surprisingly small. Moreover, in many interesting circumstances, UDP and UDA can coincide. Our discussions extend naturally to the case of low rank quantum states instead of just pure states. Here one can also look at two kinds of uniqueness when measuring given observables $\mathbf{A}$: one is uniqueness among all low rank states, the other is among all states of any rank.

We organize the paper as follows. In Sec. II, we first show that there is a set of $5d - 7$ observables that insures every pure state is UDA; this should be compared to $4d - 5$ result in the UDP case. Thus in general there is a gap between the best known results for the UDP and UDA cases, and we illustrate this with some examples. Sec. III discusses the case of observables corresponding to RDMs of a multipartite quantum state, where for the three particle case, we show that if $d_1 \geq \min(d_2, d_3)$, then almost all pure states are UDA by their 2-RDMs of particle pairs $\{1, 2\}$ and $\{1, 3\}$, improving the bounds given in [12]. However, this still leaves a gap with the Diosi result for the case of UDP in [13]. We further discuss circumstances where UDP can imply UDA for all pure states. In Sec. IV, we use convexity of the numerical range of operators to show that UDP always implies UDA when there are only two independent measurements performed. In a more general case, if there is a compact group of symmetries of the state space which has the span of the measurement operators as its set of fixed points, then UDP implies UDA for all pure states. We analyze the possible dimensions for those fixed point sets. A summary and some discussion is included in Sec. VI.

II. THE NUMBER OF OBSERVABLES FOR UDA

In this section, we discuss the minimum number of observables needed to have all pure states be UDA. We start by choosing a Hermitian basis $\{\lambda_i\}_{i=0}^{d^2-1}$ for the operators on $\mathcal{H}_d$. Without loss of generality we choose $\lambda_0 = I$, the identity operator on $\mathcal{H}_d$, which has trace d. We further require that the λ_i's are orthogonal, in the sense that for $i, j \geq 0$,

$$\operatorname{tr} \lambda_i \lambda_j = d(d-1)\delta_{ij}. \quad (7)$$

The $d \times d$ Hermitian matrices are a real inner product space for $\langle A, B\rangle = \operatorname{tr}(AB)$, so such a basis $\{\lambda_i\}_{i=0}^{d^2-1}$ exists for any dimension d. For instance, for the qubit case ($d = 2$), we can choose the Pauli basis

$$\begin{aligned} \lambda_1 &= X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\ \lambda_2 &= Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \\ \lambda_3 &= Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned} \quad (8)$$

For the qutrit case ($d = 3$), one can choose $\lambda_i = \sqrt{3}M_i$ for $i > 0$, where the M_is are the Gell-Mann matrices given by

$$\begin{aligned} M_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad M_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\ M_3 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad M_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \\ M_5 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad M_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \\ M_7 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad M_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}. \end{aligned} \tag{9}$$

For general d, one can choose $\lambda_i = \sqrt{\frac{d(d-1)}{2}} M_i$ for $i > 0$, where the M_is are the generalized Gell-Mann matrices.

We can now write any density operator ρ as

$$\rho = \frac{1}{d}(I + \vec{r} \cdot \vec{\lambda}), \tag{10}$$

where $\vec{\lambda} = (\lambda_1, \lambda_2, \ldots, \lambda_{d^2-1})$, and $\vec{r} = (r_1, r_2, \ldots, r_{d^2-1})$ has real entries.

Because $\operatorname{tr} \rho^2 \leq 1$, we have $\vec{r} \cdot \vec{r} \leq 1$ and equality holds if ρ is a pure state. However, not every state satisfying $\vec{r} \cdot \vec{r} = 1$ is a pure state. Indeed, ρ is a pure state if and only if $\rho^2 = \rho$, which gives a family of equations that $\vec{r}$ needs to satisfy.

If one of the observables is a multiple of the identity, then we can drop it from the list of observables without affecting UDA and UDP. If two states agree on an observable A_i, then they agree on $A_i + tA_i$ for any real scalar t, so we can adjust each of the observables $\mathbf{A} = (A_1, \ldots, A_m)$ to have trace zero without affecting UDA or UDP. We thus assume that all A_i are traceless from here on.

We can expand any observable A_i in terms of $\{\lambda_i\}$ as

$$A_i = \sum_{j=1}^{d^2-1} \alpha_{ij} \lambda_j. \tag{11}$$

Then the average value of A_i is given by

$$\operatorname{tr}(A_i \rho) = \frac{1}{d}(d + \sum_j r_j \alpha_{ij} d(d-1)) = 1 + (d-1)\vec{r} \cdot \vec{\alpha_i}, \tag{12}$$

where $\vec{\alpha_i} = \{\alpha_{i1}, \alpha_{i2}, \ldots, \alpha_{i(d^2-1)}\}$.

To discuss the problem for any pure state to be UDA, the constant 1 and constant factor $d - 1$ can be ignored, as these constants are the same for all states. Therefore we have

$$\operatorname{tr}(A_i \rho) \sim \vec{r} \cdot \vec{\alpha_i}, \tag{13}$$

where $\sim$ means that the average value of A_i for the state ρ is geometrically equivalent to the projection of $\vec{r}$ onto $\vec{\alpha_i}$.

Alternatively, define $T : \mathbb{R}^{d^2-1} \to \mathbb{R}^m$ by $T(\vec{r}) = (\vec{r} \cdot \alpha_1, \ldots, \vec{r} \cdot \vec{\alpha}_m)$. Let L be the linear subspace of $\mathbb{R}^{d^2-1}$ spanned by $\vec{\alpha}_1, \ldots, \vec{\alpha}_m$, and let π be the orthogonal projection from $\mathbb{R}^{d^2-1}$ onto L. Then π and T have the same kernel, namely $L^\perp$. Thus for states ρ_1, ρ_2, we have $T(\rho_1) = T(\rho_2)$ if and only if $\pi(\rho_1) = \pi(\rho_2)$, so in considering UDA and UDP we can treat T as being the orthogonal projection onto L.

If we subtract the density matrix I/d from all states, then the translated set of states sits in the real $d^2 - 1$ dimensional subspace of trace zero Hermitian matrices. In this sense, we are actually working with real geometry in $\mathbb{R}^{d^2-1}$. All quantum states then sit inside the $(d^2 - 1)$-dimensional unit ball, with pure states corresponding to unit vectors, but not every vector on the unit $(d^2 - 2)$-dimensional sphere corresponding to a pure state. The observables span an m-dimensional subspace that all the quantum states will be projected onto. We will simply say the subspace is spanned by $\mathbf{A}$ when no confusion arises, and we will no longer distinguish an operator A_i from the corresponding vector $\vec{\alpha_i}$. Indeed we only consider the real span of $\mathbf{A}$, and we denote it by $\mathcal{S}(\mathbf{A})$. For each $\mathcal{S}(\mathbf{A})$, there is an orthogonal subspace in $\mathbb{R}^{d^2-1}$ of dimension $d^2 - 1 - m$, which we denote by $\mathcal{S}(\mathbf{A})^\perp$. Here we are taking the orthogonal complement in the space of traceless Hermitian matrices, so that every $V \in \mathcal{S}(\mathbf{A})^\perp$ is traceless.

We now are ready to state our first theorem.

Theorem 1. *For a d-dimensional system ($d > 2$), there exists a set of $5d - 7$ observables for which every pure state is UDA.*

To see why this is the case, note that in the above-mentioned geometrical picture, it is clear that a pure state $|\psi\rangle\langle\psi|$ is UDA by measuring $\mathbf{A}$ if there does not exist any operator $V \in \mathcal{S}(\mathbf{A})^\perp$ such that $|\psi\rangle\langle\psi| + V$ is positive. It thus suffices to find $\mathcal{S}(\mathbf{A})^\perp$ such that any operator $V \in \mathcal{S}(\mathbf{A})^\perp$ has at least two positive and two negative eigenvalues.

In order to construct $\mathcal{S}(\mathbf{A})^\perp$, we explicitly construct a set of $m = d^2 - 5d + 6$ linearly independent Hermitian matrices $H_1, H_2, \ldots, H_m \in M_d(\mathbb{C})$ such that the Hermitian matrix

$$\sum_{j=1}^{m} r_j H_j$$

has at least two positive eigenvalues for any nonzero real vector $r = (r_j) \in \mathbb{R}^m$.

Our construction is motivated by, and similar to, the diagonal filling technique used in Ref. [18], but along the other direction of the diagonals.

This then means that measuring $d^2 - 1 - (d^2 - 5d + 6) = 5d - 7$ observables is enough for any pure state to be UDA, which proves the theorem. There are indeed technical details to be clarified that we leave to Appendix A.

If we compare our results with those given in [1], which shows that measuring $4d - 5$ observables are enough for any pure state to be UDP, there exists an obvious gap. We claim that this gap cannot be closed in general. To see this, let us look at the simplest case of $d = 3$, where the results just compared state that 7 observables are enough for any pure state to be UDP but 8 observables are enough for any pure state to be UDA.

If one could measure a particular set $\mathbf{A}$ with 7 observables and have all pure states be UDA, then in fact every state must be UDP by measuring $\mathbf{A}$. According to [1], this only happens if $\mathcal{S}(\mathbf{A})^\perp$ contains a single invertible traceless operator V, which implies that V is rank 3. Without loss of generality we can assume the largest eigenvalue V is positive with an eigenstate $|\psi\rangle$. Then $|\psi\rangle$ is not UDA by measuring $\mathbf{A}$ since as observed in [1] there exists a mixed state which also has the same average values as those of $|\psi\rangle$. Therefore, one cannot measure only 7 observables for all pure states to be UDA.

For general d, our construction needs $5d-7$ observables. We do not know whether this is the optimal construction, but it is very unlikely one can get this down to $4d-5$. In other words, in general UDA and UDP for pure states should be indeed two different concepts and there should always be gaps between the number of observables needed to be measured for each case to uniquely determine any pure quantum state. There is one exception though, which is for the qubit case (i.e., $d=2$) where it is shown in [1] that for all pure states to be UDP, one needs to measure $3=2^2-1$ variables, which then uniquely determine any quantum state among all states.

Finally, we remark that our results in Theorem 1 naturally extend to the case of low rank states. That is, for a rank $q < d/2$ quantum state ρ, we can similarly consider two different cases: (1) ρ is uniquely determined among all rank $\leq q$ states by measuring $\mathbf{A}$ (which was considered in [1]), and (2) ρ is uniquely determined among all quantum states of any rank by measuring $\mathbf{A}$.

Theorem 2. *For a d-dimensional system ($d>2$), measuring $(4q+1)d-(4q^2+2q+1)$ observables is enough for a rank $\leq q$ state to be uniquely determined among all states.*

Compared to the results in [1], where $4q(d-q)-1$ observables are needed to uniquely determine any rank $\leq q$ states among all rank $\leq q$ states, when d is large the difference in the leading term has a gap of size d. The proof idea is similar to that of Theorem 1, so we leave the details to Appendix A.

III. THE CASE OF REDUCED DENSITY MATRICES

In this section we discuss the case where the Hilbert space $\mathcal{H}_d$ is a multipartite quantum system, where the observables correspond to reduced density matrices (RDMs). That is, the observables are chosen to be acting nontrivially only on a subset of the subsystems. For instance, for a three-qubit system, the observables corresponding to the 2-RDM of the first two particles can be chosen as

$$\begin{aligned}\mathbf{A} = \quad & (X_1, X_2, Y_1, Y_2, Z_1, Z_2 \\ & X_1X_2, X_1Y_2, X_1Z_2, Y_1X_2, Y_1Y_2, \\ & Y_1Z_2, Z_1X_2, Z_1Y_2, Z_1Z_2),\end{aligned} \tag{14}$$

where X_i, Y_i, Z_i are Pauli X, Y, Z operators acting on the ith qubit.

For simplicity, in this section we only consider 3-particle systems, labelled by $1,2,3$, with Hilbert space dimensions d_1, d_2, d_3, respectively. That is, $\mathcal{H}_d = \mathcal{H}_{d_1}\otimes\mathcal{H}_{d_2}\otimes\mathcal{H}_{d_3}$ and $d=d_1d_2d_3$. Nevertheless, our method naturally extends to systems of more than 3 particles.

Recall that for a three particle system, it is known that almost all three-qubit pure states are UDA by their 2-RDMs [11]. This result can be further improved to 2-RDMs of particle pairs $\{1,2\}$ and $\{2,3\}$ [9]. More generally, if $d_1 \geq d_2+d_3-1$, then almost all pure states are UDA by their 2-RDMs of particle pairs $\{1,2\}$ and $\{1,3\}$ [12]. Similarly, if $d_1 \geq 2$, then almost every pure state is UDP by its 2-RDMs of particle pairs $\{1,2\}$ and $\{1,3\}$ [13].

We notice that, in contrast with the discussion of Sec. II, one no longer considers uniqueness for all pure states, but 'almost all' of them. This means there exists a measure zero set of pure states which are not uniquely determined. For instance, for the three qubit case, any state which is local unitarily equivalent to the GHZ-type state

$$|GHZ\rangle_{type} = a|000\rangle + b|111\rangle \tag{15}$$

cannot be UDP, as any state of the form $a|000\rangle + be^{i\theta}|111\rangle$ has the same 2-RDMs as those of $|GHZ\rangle_{type}$. This means that, for a three qubit pure state $|\psi\rangle$, it is either UDA or not UDP. In other words, if any three qubit pure state $|\psi\rangle$ is UDP, then it is UDA by its 2-RDMs of particle pairs $\{1,2\}$ and $\{1,3\}$. In this sense, we say in this case UDP implies UDA for all three-qubit pure states.

However, for the general case of a three particle system, there is a gap between known results of UDA and UDP. Our following result improves the bound for the UDA case.

Theorem 3. *If $d_1 \geq \min(d_2,d_3)$, then almost every tripartite quantum state $|\phi\rangle \in \mathcal{H}_{d_1}\otimes\mathcal{H}_{d_2}\otimes\mathcal{H}_{d_3}$ is UDA by its 2-RDMs of particle pairs $\{1,2\}$ and $\{1,3\}$.*

To see why this is the case, an arbitrary pure state $|\phi_{123}\rangle$ of this system can be written as

$$|\phi_{123}\rangle = \sum_{i_1=1}^{d_1}\sum_{i_2=1}^{d_2}\sum_{i_3=1}^{d_3} c_{i_1i_2i_3}|i_1\rangle|i_2\rangle|i_3\rangle. \tag{16}$$

If there is another state ρ which agrees with $|\phi\rangle$ in its subsystems $\{1,2\}$ and $\{1,3\}$, then we can find a pure state $|\psi_{1234}\rangle \in \mathcal{H}_{d_1}\otimes\mathcal{H}_{d_2}\otimes\mathcal{H}_{d_3}\otimes\mathcal{H}_{d_4}$ which agrees with ρ on the subsystem $\{1,2,3\}$ and also agrees with $|\phi_{123}\rangle$ on subsystems $\{1,2\}$ and $\{1,3\}$.

Without loss of generality, we assume $d_2 \geq d_3$. Since the rank of the 2-RDM of the subsystem $\{1,2\}$ is at most d_3, the pure state $|\psi_{1234}\rangle$ can be written as

$$|\psi_{1234}\rangle = \sum_{i_1=1}^{d_1}\sum_{i_2=1}^{d_2}\sum_{i_3=1}^{d_3} c_{i_1i_2i_3}|i_1\rangle|i_2\rangle|E_{i_3}\rangle. \tag{17}$$

The states $\{|E_{i_3}\rangle\}_{i_3=1}^{d_3} \in \mathcal{H}_{d_3}\otimes\mathcal{H}_{d_4}$ are orthonormal vectors in the subsystem $\{3,4\}$, hence the 2-RDM of $|\psi_{1234}\rangle$ agrees with that of $|\phi_{123}\rangle$ on particles $\{1,2\}$.

Note that for almost all states $|\psi_{1234}\rangle$, the set of vectors $\{\sum_{i_1=1}^{d_1}\sum_{i_2=1}^{d_2} c_{i_1i_2i_3}|i_1\rangle|i_2\rangle\}_{i_3=1}^{d_3}$ will be linearly independent.

Let us write $|E_{i_3}\rangle = \sum_{j_3=1}^{d_3}|j_3\rangle|e_{i_3j_3}\rangle$. Here $|j_3\rangle$ are orthonormal vectors in $\mathcal{H}_{d_3}$ and $|e_{i_3j_3}\rangle$ are vectors in $\mathcal{H}_{d_4}$ but in general unnormalized.

For any $1 \leq j_3 \leq d_3$, we will have

$$|\psi_{1234}\rangle = \sum_{i_1=1}^{d_1}\sum_{i_2=1}^{d_2}\sum_{j_3,i_3=1}^{d_3} c_{i_1i_2i_3}|i_1\rangle|i_2\rangle|j_3\rangle|e_{i_3j_3}\rangle. \quad (18)$$

Now let us consider the subsystem $\{1,3\}$. Since $|\phi\rangle_{123}$ and $|\psi\rangle_{123}$ have the same RDMs for particles $\{1,3\}$, this gives

$$\mathrm{tr}_2\,|\phi\rangle\langle\phi| = \mathrm{tr}_{\{2,4\}}\,|\psi\rangle\langle\psi|. \quad (19)$$

Substituting Eqs. (16) and (17) into Eq. (19) and comparing each matrix element results in the following equalities (for all i_1, i_1', j_3, j_3'):

$$\sum_{i_2=1}^{d_2} c_{i_1i_2j_3}c^*_{i_1'i_2j_3'} = \sum_{i_2=1}^{d_2}\sum_{i_3,i_3'=1}^{d_3} c_{i_1i_2i_3}c^*_{i_1'i_2i_3'}\langle e_{i_3'j_3'}|e_{i_3j_3}\rangle. \quad (20)$$

Now let us define $x_{i_3'j_3'i_3j_3} = \langle e_{i_3'j_3'}|e_{i_3j_3}\rangle$. Then Eq. (20) is a linear system of equations in the variables $x_{i_3'j_3'i_3j_3}$. It is not hard to verify that

$$x_{i_3'j_3'i_3j_3} = \begin{cases} 1 & \text{if } i_3' = j_3' = i_3 = j_3 \\ 0 & \text{otherwise} \end{cases} \quad (21)$$

is a solution of the system of equations, which corresponds to the state $|\phi_{123}\rangle$.

Now we need to show that when $d_1 \geq d_3$, generically Eq. (20) has only one solution which is given by Eq. (21). It turns out that this is indeed the case which then proves Theorem 3. In fact, the linear equations above are generically linearly independent. Therefore, $d_1^2d_3^2$ linear equations are sufficient to determine d_3^4 variables, which proves Theorem 3.

However, we do not know whether the sufficient condition given by Theorem 3 for almost all three-particle pure state to be UDA by its 2-RDMs of particle pairs $\{1,2\}$ and $\{2,3\}$ is also necessary. This still leaves a gap between the result of Theorem 3 for UDA, and the result for UDP in [13]. The results only coincide when $d_1 = d_2 = d_3$, i.e., the three qubit case. Whether UDP can imply UDA remains open in other cases.

Similar to the discussion in Sec. II, our discussion in this section also extends to uniqueness of low rank quantum states. In particular, we have the following theorem.

Theorem 4. *Almost every tripartite density operator ρ acting on the Hilbert space $\mathcal{H}_{d_1}\otimes\mathcal{H}_{d_2}\otimes\mathcal{H}_{d_3}$ with rank no more than $\min\{\lfloor\frac{d_1}{d_2}\rfloor,\lfloor\frac{d_1}{d_3}\rfloor\}$ can be uniquely determined among all states by its 2-RDMs of particle pairs $\{1,2\}$ and $\{1,3\}$.*

Obviously Theorem 4 implies Theorem 3 for $\mathrm{rank}\,\rho = 1$. This result is to our knowledge, the first one for uniqueness of mixed states with respect to RDMs. The proof is a direct extension of that is of Theorem 3, but with more lengthy details that we will include in Appendix B.

Let us look at some consequences of Theorem 4. Consider a four qubit system with qubits $1,2,3,4$, and look at the qubits $3,4$ as a single systems $3'$. Then Theorem 4 says also that almost all four qubit states of rank 2 are UDA by their RDMs of particles $\{1,2\}$ and $\{1,3'\} = \{1,3,4\}$, or one can say that almost all four qubit states of rank 2 are UDA by their 3-RDMs. This is indeed consistent with the multipartite result in [14] which states that almost all four-qubit pure states are UDA by their 3-RDMs, and our result is indeed stronger. This then demonstrates that our analysis naturally extends to systems of more than 3 particles. We also remark that the rank of a state ρ which could be UDA by its k-RDMs needs to be relatively low, otherwise one can always find another state ρ' with lower rank which has the same k-RDMs as those of ρ [19].

IV. THE CASE OF ONLY TWO OBSERVABLES

In Sec. II and Sec. III, we discussed the gap and coincidence between the two kinds of uniqueness for pure states, UDA and UDP, which in general are not the same thing. However, in certain interesting circumstances such as the three qubit case with respect to 2-RDMs, and in general the n-qubit case respect to $(n-1)$-RDMs, they do coincide. Starting from this section we would like to build some general understanding of the circumstances when UDP implies UDA for all pure states.

We start from the simplest case of $m = 2$, where only two observables are measured, i.e., $\mathbf{A} = (A_1, A_2)$. Intuitively, in this extreme case almost no pure state can be uniquely determined, either UDA or even UDP. However there are also exceptions. For instance, if one of the observables, say A_1, has a nondegenerate ground state $|\psi\rangle$, then $|\psi\rangle$ is UDA (hence, of course, UDP) even by measuring A_1 only. One would hope this is the only exception, that is, for a pure state $|\psi\rangle$, either it is UDA, or it is not UDP, when only two observables are measured. We make this intuition rigorous by the following theorem.

Theorem 5. *When only two observables are measured, i.e., $\mathbf{A} = (A_1, A_2)$, UDP implies UDA for any pure state $|\psi\rangle$, regardless of the dimension d.*

To prove this theorem, recall that measuring $\mathbf{A}$ (i.e., measuring every observable in $\mathbf{A}$) for all quantum states ρ returns the set $C_m(\mathbf{A})$ given by Eq. (3). We know that $C_m(\mathbf{A})$ is a convex set, meaning for any $\vec{x},\vec{y} \in C_m(\mathbf{A})$, we have $(1-s)\vec{x} + s\vec{y} \in C_m(\mathbf{A})$ for any $0 < s < 1$.

For pure states, the corresponding set of average values is given by $W_m(\mathbf{A})$ as defined in Eq. (5). Unlike $C_m(\mathbf{A})$, $W_m(\mathbf{A})$ in general is not convex. Nevertheless, it is easy to see that $W_m(\mathbf{A}) = C_m(\mathbf{A})$ when $W_m(\mathbf{A})$ is convex.

For $m = 2$, the Hausdorff–Toeplitz theorem [20, 21] gives convexity of the numerical range of any operator, which in turn shows that $W_2(\mathbf{A})$ is convex. We explain briefly here. For any operator B acting on a Hilbert space $\mathcal{H}_d$, the numerical range of B is the set of all complex numbers $\langle\psi|B|\psi\rangle$, where $|\psi\rangle$ ranges over all pure states in $\mathcal{H}_d$.

Note that one can always write B as

$$\begin{aligned} B &= \frac{1}{2}[(B+B^\dagger)+(B-B^\dagger)] \\ &= \frac{1}{2}[(B+B^\dagger)+i(-iB+iB^\dagger)]. \end{aligned} \tag{22}$$

If we define $A_1 := (B+B^\dagger)/2$ and $A_2 := (-iB+iB^\dagger)/2$ then clearly both A_1 and A_2 are Hermitian. Then $W_2(\mathbf{A})$ is nothing but the numerical range of $B = A_1 + iA_2$ and hence is convex.

Furthermore, by studying the properties of the numerical range, it was shown in [22] (using different terminology) that if a pure state $|\psi\rangle$ is UDP, the point $\vec{x} := \mathbf{A}(|\psi\rangle)$ must be an extreme point of $W_2(\mathbf{A})$. Here $\vec{x}$ is an extreme point of the convex set $W_2(\mathbf{A})$ if there do not exist $\vec{y}, \vec{z} \in W_2(\mathbf{A})$, such that $\vec{x} = (1-s)\vec{y} + s\vec{z}$ for some $0 < s < 1$.

Because $W_2(\mathbf{A}) = C_2(\mathbf{A})$, $\vec{x}$ is also an extreme point of $C_2(\mathbf{A})$. One can further show that for any extreme point $\vec{x}$ of $C_2(\mathbf{A})$, and any quantum state ρ with $\mathbf{A}(\rho) = \vec{x}$, any pure quantum state $|\phi\rangle$ in the range of ρ will also have $\mathbf{A}(|\phi\rangle) = \vec{x}$. This then implies that if a pure state $|\psi\rangle$ is UDP by measuring $\mathbf{A}$, it must also be UDA, which proves the theorem.

Again, all the technical details of the proof will be presented in Appendix C.

In an attempt to extend Theorem 5 to the $m \geq 3$ case, a natural question that one could ask is whether or not UDP implies UDA whenever $W_m(\mathbf{A})$ is convex. Unfortunately this is not the case, as demonstrated by the following example.

For the qutrit case ($d = 3$), consider the observables $\mathbf{A} = (M_1, M_2, M_3)$, where the M_is are the Gell-Mann matrices given in Eq. (9). These are the Pauli operators embedded in the qutrit space. It is easily verified that in this case, $W_m(\mathbf{A})$ is the Bloch sphere together with its interior and is thus convex. Nonetheless, the unique pure state compatible with measurement result $(0,0,0)$ is the state $|2\rangle$, even though there are many mixed states sharing this measurement result, such as $\frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|)$.

Therefore, although the Hausdorff–Toeplitz theorem is famous for showing the convexity of numerical range of any operator, there is indeed a deeper reason than just the convexity of the numerical range which governs the validity of Theorem 5, which we discuss in more detail in Appendix C.

V. SYMMETRY OF THE STATE SPACE

In this section, we discuss some circumstances where UDP implies UDA in a more general context where more than two observables are measured, i.e., $m > 2$. Our focus is on the symmetry of the set of all quantum states. For a d-dimensional Hilbert space $\mathcal{H}_d$ we denote this set of states by K_d, that is

$$K_d = \{\rho \mid \rho \text{ acts on } \mathcal{H}_d\}. \tag{23}$$

Note that K_d is convex, as we know that for any $\rho_1, \rho_2 \in K_d$, $(1-s)\rho_1 + s\rho_2 \in K_d$ for all $0 < s < 1$. Furthermore, the extreme points of K_d are all the pure states. K_d is also called the state space for all the operators acting on $\mathcal{H}_d$.

We now explain the intuition. If K_d has a certain symmetry, then two pure states $|\psi_1\rangle$ and $|\psi_2\rangle$ that are 'connected' by the symmetry will give the same measurement results, and states $|\psi\rangle$ fixed by the symmetry will also be fixed by the projection onto the space of observables. In this situation, UDP implies UDA for all pure states.

To make this intuition concrete, let us first consider an example for $d = 2$, i.e., the qubit case. We know that K_d can be parameterized as in Eq. (10), where for $d = 2$, $\lambda_1 = X, \lambda_2 = Y, \lambda_3 = Z$ are chosen as Pauli matrices given in Eq. (8). Here K_d is the Bloch ball as shown in FIG. 1. The Bloch ball is clearly a convex set and the extreme points are those pure states on the boundary, which give the Bloch sphere.

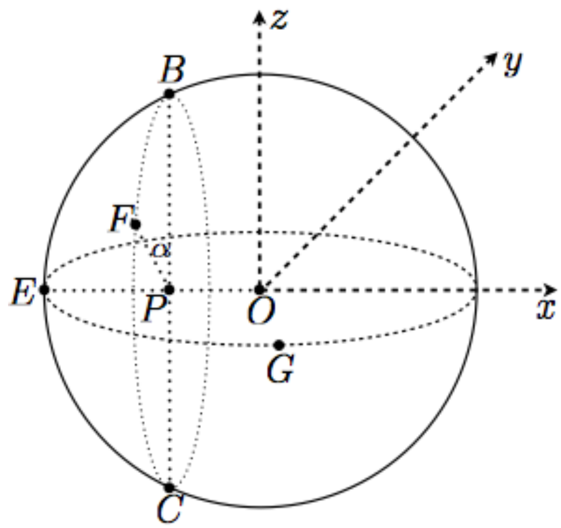

FIG. 1: Symmetry of the Bloch ball

We know that geometrically, measuring the observables in $\mathbf{A}$ corresponds to the projection onto the plane spanned by $\mathbf{A}$. For example, if we measure the Pauli X and Y operators, then geometrically this corresponds to the projection of the Bloch ball onto the xy plane. Since the Bloch ball has reflection symmetry with respect to the xy plane, two pure states (e.g. points B and C) connected by that symmetry will project onto the same measurement result P, as will all mixtures of B and C. Hence neither UDP nor UDA hold for such pure states for measuring X and Y. On the other hand, pure states fixed by the reflection symmetry are also fixed by the projection onto the xy plane. These are precisely the points on the Bloch sphere that are in the xy plane (e.g. the points E and G in

FIG. 1), and for such pure states both UDP and UDA hold. Therefore, for the observables X, Y we conclude that UDP = UDA.

Now let us look at another case where we only measure the Pauli X operator. Consider the group of symmetries of the Bloch ball consisting of rotation around the x axis. (Rotation by angle α, is shown in FIG. 1. In that figure, point B will become point F after this particular rotation, and indeed both points B and F yield the same measurement result, which is represented by point P on the x axis). Note that two points on the Bloch sphere will project to the same measurement result on the x axis if and only if they are in the same orbit under the rotation group. Thus a measurement result will come from a single pure state exactly when that pure state is a fixed point, and hence either both or neither of UDP and UDA hold for each pure state. For example, the point E is fixed by the rotation, and is uniquely determined by the measurement of X among all states. E corresponds to the -1 eigenstate of the Pauli X operator. Therefore, the rotational symmetry of the Bloch ball along the x axis gives UDP =UDA for any pure state when measuring the Pauli X operator, which corresponds to the x axis.

Mathematically, a symmetry of K_d is an affine automorphism of K_d. If $U \in M_d$ is unitary, the map taking ρ to $U\rho U^\dagger$ is such an affine automorphism (which for $d = 2$ will just be rotation around some axis of the Bloch ball). For instance, the rotation symmetry along the x axis by an angle α is given by conjugation by the unitary operator $\exp(-iX\alpha/2)$. If V is the conjugate linear map given by complex conjugation in the computational basis ($V|\psi\rangle = |\psi^*\rangle$), then the map taking ρ to $V\rho V^\dagger$ is the transpose map. For $d = 2$, this map is reflection of the Bloch ball in the xy-plane.

Recall that for a set of observables $\mathbf{A}$, we denote the real linear span by $\mathcal{S}(\mathbf{A})$. When discussing the uniqueness problems, it makes no difference if we append the identity operator to $\mathbf{A}$. Let us then assume $\mathbf{A} = (I, A_1, \ldots, A_m)$. We are now ready to put our intuition into a theorem.

Theorem 6. *Assume there exists a compact group G of affine automorphisms of K_d whose fixed point set is $K_d \bigcap S(\mathbf{A})$. Then each pure state acting on $\mathcal{H}_d$ which is UDP for measuring $\mathbf{A}$ is also UDA.*

In the first example above, the group for the reflection consists of the two element group generated by the reflection. In the rotation example, we can take the group to consist of all rotations around the given axis. We will leave the detailed mathematical proof of Theorem 6 to Appendix D, where operator algebras are one ingredient of the proof.

To motivate some further consequences of Theorem 6, consider a simple example. If $\mathbf{A}$ consists of a basis of diagonal matrices (i.e., a set of mutually commuting observables), then for any pure state, UDP implies UDA by Theorem 6. Here the group of symmetries can be taken to be conjugation by all diagonal unitaries. This group has fixed point set $K_d \bigcap S(\mathbf{A})$. In a more general case, if the complex span of $S(\mathbf{A})$ is a *-subalgebra of the operators acting on $\mathcal{H}_d$, then UDP = UDA for all pure states for measuring $\mathbf{A}$. This is a natural corollary of Theorem 6 that we will also discuss in detail in Appendix D.

VI. CONCLUSION AND DISCUSSION

In this work, we have discussed the uniqueness of quantum states compatible with given results for measuring a set of observables. For a given pure state, we consider two different types of uniqueness, UDP and UDA. We have taken the first step to study their relationship systematically. In doing so we have established a number of results, but also leave with many open questions.

First of all, although in general UDP and UDA are evidently different concepts, their difference is surprisingly 'not that large'. Specifically in the sense of general counting of the number of variables one needs to measure to uniquely determine all pure states in a d dimensional Hilbert space. Compared to full quantum tomography which requires $d^2 - 1$ variables measured to uniquely determine any quantum state, the $5d-7$ observables we have constructed to uniquely determine any pure state among all states is a significant improvement. It is indeed larger than the $4d - 5$ observables given in [1] to uniquely determine any pure state among all pure states, but the difference is only linear in d. We do not know whether there could be another construction for which we could further close the linear difference between UDA and UDP, to leave only a constant gap for large d.

When the Hilbert space is a multipartite quantum system, and the observables correspond to the RDMs, we focused on the situation when 'almost all pure states' are uniquely determined. We considered a 3-particle system with Hilbert space $\mathcal{H}_d = \mathcal{H}_{d_1} \otimes \mathcal{H}_{d_2} \otimes \mathcal{H}_{d_3}$, and showed that if $d_1 \geq \min(d_2, d_3)$, then almost all pure states are UDA by their 2-RDMs of particle pairs $\{1, 2\}$ and $\{1, 3\}$. This improves the results of [12], where $d_1 \geq d_2 + d_3 - 1$ is required; however it still leaves a gap compared to the Diosi UDP result which states that for $d_1 \geq 2$, almost all pure states are UDP by their 2-RDMs of particle pairs $\{1, 2\}$ and $\{1, 3\}$. Because our proof only gives a sufficient condition for UDA, we do not know whether it can be further improved. We also do not have an example showing there is indeed gap between UDA and UDP for almost all three-particle pure states to be uniquely determined by 2-RDMs of particle pairs $\{1, 2\}$ and $\{1, 3\}$.

Finally, we considered situations for which we can show that UDP implies UDA. These include: (i) the general 2-qubit system; (ii) the 3-qubit system when we consider uniqueness for almost all pure states and the measurements corresponds to 2-RDMs; (iii) when only two observables are measured; and (iv) the observables measured correspond to some symmetry of the state space. However we do not know how far we are from enumerating all the possible situations that UDP implies UDA, when considering uniqueness for all pure states or almost all pure states. In principle one can even consider the relationship between UDP and UDA for special subsets of pure states.

We believe our systematic study of the uniqueness of quantum states compatible with given measurement results shed light on several aspects of quantum information theory and its connection to different topics in mathematics. These include quantum tomography and the space of Hermitian operators, unique ground states of local Hamiltonians and general solutions to certain linear equations, measurements and numerical ranges of operators, and the geometric meaning of measurements and the symmetry of state space. We thus believe that the previously-mentioned open questions warrant further investigation.

Appendix A: Proof of Theorem 1 and 2

Theorem 1 follows from the following lemma.

Lemma 1. *There exists a set of* $m = d^2 - 5d + 6$ *linearly independent Hermitian matrices* $H_1, H_2, \dots, H_m \in M_d(\mathbb{C})$, *such that the Hermitian matrix*

$$\sum_{j=1}^{m} r_j H_j$$

has at least two positive eigenvalues for any nonzero real vector $r = (r_j) \in \mathbb{R}^m$.

Proof. We prove the statement by giving an explicit construction. Our proof is motivated by and similar to the diagonal filling technique used in Ref. [18], but along the other direction of the diagonals.

We will need Lemma 9 from Ref. [18] about totally nonsingular matrices, which we restate as Lemma 3 in the following. For simplicity, we also assume that the totally nonsingular matrix is real. Therefore, for any length $L \in \mathbb{N}$ and $L \geq 2$, there are $L-1$ linearly independent real vectors such that every nonzero linear combination of them has at least 2 nonzero entries.

Let $H = (H_{jj'}) \in M_d(\mathbb{C})$ be a matrix. We will always fix the diagonal to be zero, namely $H_{jj} = 0$ for $0 \leq j \leq d-1$. In the strictly upper triangular part of the matrix, there are $2d-3$ lines of entries parallel to the antidiagonal. That is, each line contains entries $H_{jj'}$ with $j < j'$ and $j + j' = k$ where k goes from 1 to $2d-3$. We will call this the k-th line of the matrix in the following. We also call the set of entries $H_{jj'}$ with $j + j' = k$ the k-th antidiagonal. It is easy to see that the length L_k of the k-th line is

$$L_k = \begin{cases} \left\lceil \dfrac{k+1}{2} \right\rceil & \text{for } k \leq d-1, \\ \left\lceil \dfrac{2d-1-k}{2} \right\rceil & \text{otherwise.} \end{cases}$$

So the length $L_k \geq 2$ for $3 \leq k \leq 2d-5$, and we can find $L_k - 1$ real vectors for which every nonzero linear combination has at least 2 nonzero entries. For each of the $L_k - 1$ vectors, we can form two Hermitian matrices. One of them is the symmetric one whose k-th line is filled with the vector, and the lower triangular part determined by the Hermiticity condition. Such a matrix is real, symmetric, and has nonzero entries only on its k-th antidiagonal. We will call it a real k-th line matrix. The other is the one with k-th line filled with the vector multiplied by $i = \sqrt{-1}$, and lower part is determined by the Hermiticity condition. This is a matrix consisting of purely imaginary entries on the k-th antidiagonal and we call it an imaginary k-th line matrix.

Now we prove that the constructed matrices satisfy our requirement. First we prove that the matrices are linearly independent. It suffices to show that the matrices of nonzero k-th line is linearly independent. Let $\{v_j\}$ be the set of linearly independent real vectors chosen for the k-th line. We need to show that $\{(v_j, v_j), (iv_j, -iv_j)\}$ is linearly independent over $\mathbb{C}$. If the contrary is true, that is, there exists complex numbers c_j, d_j not all zero such that

$$\sum_j c_j (v_j, v_j) + \sum_j d_j (iv_j, -iv_j) = 0.$$

This is equivalent to

$$\sum_j c_j v_j + i \sum_j d_j v_j = 0$$
$$\sum_j c_j v_j - i \sum_j d_j v_j = 0.$$

From the above two equations, we get $\sum_j c_j v_j = 0$ and $\sum_j d_j v_j = 0$ which is a contradiction.

Next, we prove that for any nonzero real coefficient $r \in \mathbb{R}^m$, the matrix $H = \sum r_j H_j$ has at least two positive eigenvalues. Let k_0 be the largest k such that there is a k-th line matrix H_j whose coefficient r_j is nonzero. Then, either the real k_0-th line matrices or the imaginary ones have nonzero coefficients. By the construction, this implies that there are at least two nonzero entries on the k_0th line of the matrix H. Let the nonzero entries be $a, b \in \mathbb{C}$. We then have a principle submatrix of the form

$$\begin{pmatrix} 0 & x & y & a \\ \bar{x} & 0 & b & 0 \\ \bar{y} & \bar{b} & 0 & 0 \\ \bar{a} & 0 & 0 & 0 \end{pmatrix},$$

where x, y are two unknown number and $\bar{a}$ represents the complex conjugate of a. This matrix has trace 0 and determinant $|ab|^2$. Therefore, it has exactly two positive eigenvalues. As it is a principle submatrix of matrix H, it follows from Theorem 7 that H has at least two positive eigenvalues.

The number of matrices constructed in this way is the summation

$$m = \sum_{k=3}^{2d-5} 2(L_k - 1),$$

which can be computed to be

$$d^2 - 5d + 6.$$

□

We note that our construction will also imply that the matrix has at least two negative eigenvalues, and thus has rank at least 4. But our bound is even better than the $(d-3)^2$ bound on the dimension of subspaces in which every matrix has rank ≥ 4. This is not a contradiction, as we are considering only real linear combinations. For example, the case of $d=4$ has two matrices for our purpose, namely

$$H_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \text{ and } H_2 = \begin{pmatrix} 0 & 0 & 0 & i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix}.$$

These two matrices do satisfy our requirements, but their span over $\mathbb{C}$ contains the rank 2 matrix $H_1 + iH_2$.

Lemma 1 generalizes naturally to the case where we want all matrices to have at least $q+1$ positive eigenvalues. If we consider lengths $L_k \geq q+1$ for $2q+1 \leq k \leq 2d-2q-3$, we can find $L_k - q$ real vectors for which every nonzero linear combination has at least $q+1$ nonzero entries. For each of the $L_k - q$ vectors, we can also form two Hermitian matrices. Such constructed matrices are linearly independent and any real linear combination has at least $q+1$ positive eigenvalues.

We restate our result as Lemma 2 which will lead to Theorem 2.

Lemma 2. *There exists a set of $m = d^2 - (4q+1)d + (4q^2+2q)$ linearly independent Hermitian matrices $H_1, H_2, \ldots, H_m \in M_d(\mathbb{C})$, such that the Hermitian matrix*

$$\sum_{j=1}^{m} r_j H_j$$

has at least $q+1$ positive eigenvalues for any nonzero real vector $r = (r_j) \in \mathbb{R}^m$.

We just follow the lines of the proof of Lemma 1. To complete our argument, we need to show that any $2(q+1)$ by $2(q+1)$ invertible, traceless, Hermitian, upper left triangular matrix has exactly $q+1$ positive eigenvalues.

We prove this claim by induction. When $q=1$, it is already known. Let's assume this claim holds true for all $q \leq r$. Then for $q = r+1$, we can write such matrix A in the following form

$$\begin{pmatrix} 0 & x_1 & x_2 & \cdots & x_{2r+1} & x_{2r+2} & a \\ \bar{x_1} & 0 & y_1 & \cdots & y_{2r} & b & 0 \\ \bar{x_2} & \bar{y_1} & 0 & \cdots & c & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\ \bar{a} & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

One may observe that, by deleting the first and the last rows/columns, we will have a $2r$ by $2r$ invertible, traceless, Hermitian, upper left triangular submatrix.

From our assumption, this submatrix has exactly r positive eigenvalues which means A has at least r positive eigenvalues and at least r negative eigenvalues.

Note that its determinant equals $(-1)^{q+1}|ab\cdots|^2$. It follows that A has exactly $r+1$ positive eigenvalues, which completes the argument.

The number of matrices constructed in this way is given by the summation

$$\begin{aligned} m &= 2\sum_{k=2q+1}^{2d-2q-3}(L_k - q) \\ &= 2\sum_{k=2q+1}^{d-1}(\Big\lceil\frac{k+1}{2}\Big\rceil - q) + 2\sum_{k=d}^{2d-2q-3}(\Big\lceil\frac{2d-1-k}{2}\Big\rceil - q) \\ &= d^2 - (4q+1)d + (4q^2+2q). \end{aligned}$$

Lemma 3 (Lemma 9, [18]). *Let M be a d by d totally non-singular matrix, with $d \geq n$. Let v be any linear combination of n of the columns of M. Then v contains at most $n-1$ zero elements.*

Theorem 7 (Theorem 4.3.15, [23]). *Let A be a n by n Hermitian matrix, let r be an integer with $1 \leq r \leq n$, and let A_r denote any r by r principle submatrix of A (obtained by deleting $n-r$ rows and the corresponding columns from A). For each integer k such that $1 \leq k \leq r$ we have*

$$\lambda_k^{\uparrow}(A) \leq \lambda_k^{\uparrow}(A_r) \leq \lambda_{k+n-r}^{\uparrow}(A).$$

Appendix B: Proof of Theorem 4

Theorem 4 *Almost every tripartite density operator ρ acting on the Hilbert space $\mathcal{H}_{d_1} \otimes \mathcal{H}_{d_2} \otimes \mathcal{H}_{d_3}$ with rank no more than $\min\{\lfloor\frac{d_1}{d_2}\rfloor, \lfloor\frac{d_1}{d_3}\rfloor\}$ can be uniquely determined among all states by its 2-RDMs of particle pairs $\{1,2\}$ and $\{1,3\}$.*

Proof. For any $\rho_{123} \in \mathcal{B}(\mathcal{H}_{d_1} \otimes \mathcal{H}_{d_2} \otimes \mathcal{H}_{d_3})$, we can choose $|\phi_{1234}\rangle$ to be the pure state whose 3-RDM of particles $\{1,2,3\}$ is exactly ρ_{123}. We can further assume $d_4 \leq \operatorname{rank}\rho_{123}$.

Without loss of generality, we can assume

$$|\phi_{1234}\rangle = \sum_{i_1,i_2,i_3,i_4} c_{i_1i_2i_3i_4}|i_1\rangle|i_2\rangle|i_3\rangle|i_4\rangle.$$

If there is another σ_{123} that agrees with ρ_{123} on subsystems $\{1,2\}$ and $\{1,3\}$ then we can find some pure state $|\psi\rangle_{12345}$ whose 3-RDM of the particle set $\{1,2,3\}$ is σ_{123}.

Generically, the vectors $\sum_{i_1i_2} c_{i_1i_2i_3i_4}|i_1\rangle|i_2\rangle$ are linearly independent and they will span the range of $\rho_{12} = \operatorname{tr}_3\rho_{123}$.

Hence, any pure state $|\psi_{12345}\rangle$ that agrees with $|\phi_{1234}\rangle$ on subsystem $\{1,2\}$ can be expanded as

$$|\psi_{12345}\rangle = \sum_{i_3,i_4}\sum_{i_1,i_2} c_{i_1i_2i_3i_4}|i_1\rangle|i_2\rangle|E_{i_3i_4}\rangle,$$

where $\{|E_{i_3i_4}\rangle\}$s are orthonormal vectors in $\mathcal{H}_{d_3}\otimes\mathcal{H}_{d_4}\otimes\mathcal{H}_{d_5}$.

We can write

$$E_{i_3 i_4} = \sum_{j_3,j_4} |j_3\rangle|j_4\rangle|e_{i_3i_4,j_3j_4}\rangle,$$

where $|e_{i_3i_4,j_3j_4}\rangle$ are vectors on $\mathcal{H}_{d_5}$ which are in general unnormalized. Now $|\psi_{12345}\rangle$ becomes

$$|\psi_{12345}\rangle = \sum_{i_1,i_2,i_3,i_4,j_3,j_4} c_{i_1i_2j_3j_4}|i_1\rangle|i_2\rangle|j_3\rangle|j_4\rangle|e_{i_3i_4,j_3j_4}\rangle.$$

Recall that $|\psi_{12345}\rangle$ and $|\phi_{1234}\rangle$ agree on subsystem $\{1,3\}$, so we have

$$\mathrm{tr}_{\{2,4,5\}}(|\psi\rangle\langle\psi|) = \mathrm{tr}_{\{2,4\}}(|\phi\rangle\langle\phi|).$$

Firstly, let's look into the left hand side.

$$\begin{aligned}
&\mathrm{tr}_{\{2,4,5\}}(|\psi\rangle\langle\psi|_{12345}) \\
=\ &\mathrm{tr}_{\{2,4,5\}}(\sum_{\substack{i_1,i_2,i_3,i_4,j_3,j_4,\\ i_1',i_2',i_3',i_4',j_3',j_4'}} c_{i_1i_2i_3i_4}c^*_{i_1'i_2'i_3'i_4'}\cdot|i_1\rangle\langle i_1'| \\
&\otimes|i_2\rangle\langle i_2'|\otimes|j_3\rangle\langle j_3'|\otimes|j_4\rangle\langle j_4'|\otimes|e_{i_3i_4,j_3j_4}\rangle\langle e_{i_3'i_4',j_3'j_4'}|) \\
=\ &\sum_{\substack{i_1,i_2,i_3,i_4,j_3,\\ j_4,i_1',i_3',i_4',j_3'}} c_{i_1i_2i_3i_4}c^*_{i_1'i_2i_3'i_4'}\langle e_{i_3'i_4',j_3'j_4}|e_{i_3i_4,j_3j_4}\rangle \\
&\cdot|i_1\rangle\langle i_1'|\otimes|j_3\rangle\langle j_3'| \\
=\ &\sum_{i_1,j_3,i_1',j_3'}(\sum_{i_2,i_3,i_4,j_4,i_3',i_4'} c_{i_1i_2i_3i_4}c^*_{i_1'i_2i_3'i_4'}\cdot \\
&\langle e_{i_3'i_4',j_3'j_4}|e_{i_3i_4,j_3j_4}\rangle)|i_1\rangle\langle i_1'|\otimes|j_3\rangle\langle j_3'|.
\end{aligned}$$

Then, for the right hand side,

$$\begin{aligned}
&\mathrm{tr}_{\{2,4\}}(|\phi\rangle\langle\phi|_{1,2,3,4}) \\
=&\sum_{i_1,i_2,i_3,i_4,i_1',i_3'} c_{i_1i_2i_3i_4}c^*_{i_1'i_2i_3'i_4}|i_1\rangle\langle i_1'|\otimes|i_3\rangle\langle i_3'| \\
=&\sum_{i_1,j_3,i_1',j_3'}\sum_{i_2,j_4} c_{i_1i_2j_3j_4}c^*_{i_1'i_2j_3'j_4}|i_1\rangle\langle i_1'|\otimes|j_3\rangle\langle j_3'|.
\end{aligned}$$

Combining the above two equations, we have

$$\begin{aligned}
&\sum_{\substack{i_2,i_3,i_4,j_4,\\ i_3',i_4'}} c_{i_1i_2i_3i_4}c^*_{i_1'i_2i_3'i_4'}\langle e_{i_3'i_4',j_3'j_4}|e_{i_3i_4,j_3j_4}\rangle \\
=&\sum_{i_2,j_4} c_{i_1i_2j_3j_4}c^*_{i_1'i_2j_3'j_4}
\end{aligned}$$

for any i_1, i_1', j_3, j_3'.

Similarly, it follows from the fact that $|\psi_{12345}\rangle$ and $|\phi_{1234}\rangle$ agree on subsystem $\{1,2\}$ that we have the following:

$$\begin{aligned}
&\sum_{\substack{i_3,i_4,j_3,\\ j_4,i_3',i_4'}} c_{i_1i_2i_3i_4}c^*_{i_1'i_2'i_3'i_4'}\langle e_{i_3'i_4',j_3j_4}|e_{i_3i_4,j_3j_4}\rangle \\
=&\sum_{i_3,i_4} c_{i_1i_2i_3i_4}c^*_{i_1'i_2'i_3i_4}
\end{aligned}$$

for any i_1, i_2, i_1', i_2'.

Let us denote $x_{p_3,p_4,q_3,q_4,p_3',p_4',q_3'} = \langle e_{p_3p_4,q_3q_4}|e_{p_3'p_4',q_3'q_4}\rangle$ for any $p_3, p_4, q_3, q_4, p_3', p_4', q_3'$.

If there is only one solution $\{x_{p_3,p_4,q_3,q_4,p_3',p_4',q_3'}\}$ that satisfies the above two linear systems, then

$$\begin{aligned}
&\sigma_{123} \\
=\ &\mathrm{tr}_{\{4,5\}}\,|\psi\rangle\langle\psi|_{12345} \\
=\ &\mathrm{tr}_{\{4,5\}}(\sum_{\substack{i_1,i_2,i_3,i_4,j_3,j_4,\\ i_1',i_2',i_3',i_4',j_3',j_4'}} c_{i_1i_2i_3i_4}c^*_{i_1'i_2'i_3'i_4'}\cdot|i_1\rangle\langle i_1'| \\
&\otimes|i_2\rangle\langle i_2'|\otimes|j_3\rangle\langle j_3'|\otimes|j_4\rangle\langle j_4'|\otimes|e_{i_3i_4,j_3j_4}\rangle\langle e_{i_3'i_4',j_3'j_4'}|) \\
=\ &\sum_{\substack{i_1,i_2,i_3,i_4,j_3,j_4,\\ i_1',i_2',i_3',i_4',j_3'}} c_{i_1i_2i_3i_4}c^*_{i_1'i_2'i_3'i_4'}\langle e_{i_3'i_4',j_3'j_4}|e_{i_3i_4,j_3j_4}\rangle \\
&\cdot|i_1\rangle\langle i_1'|\otimes|i_2\rangle\langle i_2'|\otimes|j_3\rangle\langle j_3'|
\end{aligned}$$

is completely determined.

There are generically $d_1^2d_3^2 + d_1^2d_2^2$ linearly independent linear equations and $d_3^4d_4^2$ variables. $d_3^4d_4^2 \le d_3^4(\mathrm{rank}\,\rho)^2 \le d_3^4(\frac{d_1}{d_3})^2 < d_1^2d_3^2 + d_1^2d_2^2$ implies that there is at most one solution. Thus a generic low-rank density operator ρ_{123} is UDA by its 2-RDMs of particle pairs $\{1,2\}$ and $\{1,3\}$. □

Appendix C: Proof of Theorem 5

We begin by presenting without proof a result that was proved as Theorem 1(i) in [22]. Before we state the result, recall from Sec. IV that $W_2(A)$ is the numerical range of $A_1 + iA_2$ and is thus convex by the Hausdorff–Toeplitz theorem [20, 21]. It therefore makes sense to talk about extreme points of $W_2(A)$ in this case.

Proposition 1. *Let $\vec{x} \in W_2(A)$. Then $\vec{x}$ is an extreme point of $W_2(A)$ if and only if*

$$M_x := \{\lambda|\psi\rangle : \lambda \in \mathbb{C}, \mathbf{A}(|\psi\rangle) = \vec{x}\}$$

is a linear subspace of $\mathcal{H}_d$.

We are now in a position to prove Theorem 5.

Proof of Theorem 5. Suppose that $|\psi\rangle$ is UDP and define $\vec{x} := (\langle\psi|A_1|\psi\rangle, \langle\psi|A_2|\psi\rangle)$. Then $M_x = \{\lambda|\psi\rangle : \lambda \in \mathbb{C}\}$, which is linear, so $\vec{x}$ is an extreme point of $W_2(A)$ by Proposition 1. Because $W_2(A) = C_2(A)$ in this case by convexity, $\vec{x}$ is also an extreme point of $C_2(A)$. Suppose now that there exists a mixed state $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$ with $\vec{x} = (\mathrm{Tr}(A_1\rho), \mathrm{Tr}(A_2\rho))$. Then $\vec{x} = \sum_i p_i(\langle\psi_i|A_1|\psi_i\rangle, \langle\psi_i|A_2|\psi_i\rangle)$. Since $\vec{x}$ is extreme in $C_2(A)$, it follows that $\vec{x} = (\langle\psi_i|A_1|\psi_i\rangle, \langle\psi_i|A_2|\psi_i\rangle)$ for all i, which contradicts the fact that $|\psi\rangle$ is UDP unless each $|\psi_i\rangle$ is the same up to global phase (i.e., $\rho = |\psi\rangle\langle\psi|$). □

Based on the proof of Theorem 5, we might expect that UDP implies UDA for all pure states whenever $W_m(\mathbf{A})$ is convex. However, the example provided in Sec. IV showed this not to be the case. We now expand upon the reason for this apparent discrepancy, which lies buried in the proof of Proposition 1.

In the case when $W_m(\mathbf{A})$ is convex, the "only if" implication of Proposition 1 still holds for arbitrary m. However, the proof of the "if" implication relies on the fact that if $\vec{x} := \mathbf{A}(|\phi\rangle)$ and $\vec{y} := \mathbf{A}(|\psi\rangle)$, then for any $s \in (0,1)$ we can find $\alpha, \beta \in \mathbb{C}$ such that $s\vec{x} + (1-s)\vec{y} = \mathbf{A}(\alpha|\phi\rangle + \beta|\psi\rangle)$. In other words, the proof of the proposition uses the fact that $W_m(\mathbf{A})$ is not only convex, but that convex combinations are in a sense well-behaved between the input and output of $\mathbf{A}(\cdot)$. For convenience, we refer to this property as *strong convexity* for the remainder of this section.

The standard proofs of the Hausdorff–Toeplitz theorem show that strong convexity, not just convexity itself, always holds when $m = 2$. To see how strong convexity can fail when $m > 2$ even when convexity holds, we again return to the example of Sec. IV. In this case, we have $\mathbf{A}(|0\rangle) = (0,0,1)$ and $\mathbf{A}(|1\rangle) = (0,0,-1)$. However, even though $W_3(A)$ is convex and thus there exists a pure state $|\psi\rangle$ with $\mathbf{A}(|\psi\rangle) = (0,0,0)$, the only such pure state is $|\psi\rangle := |2\rangle$, which is not contained in the span of $|0\rangle$ and $|1\rangle$.

We might hope that strong convexity, rather than convexity itself, provides the natural generalization of Theorem 5. That is, we might hope that if $W_m(\mathbf{A})$ is strongly convex, then UDP implies UDA for all pure states. It turns out that this is a true but vacuous statement – if $W_m(\mathbf{A})$ is strongly convex then it must be the case that $m \leq 2$, so Theorem 5 itself applies directly. This fact seems to be implicit in many papers on the joint numerical range, but we prove it here for completeness.

Before stating the result, we briefly note that we can assume without loss of generality that $\mathbf{A}$ contains I and is linearly independent, as adding the identity to $\mathbf{A}$ has no effect on convexity, UDA, or UDP, and furthermore these properties only depend on the span of the observables in $\mathbf{A}$.

Proposition 2. *Let $\mathbf{A} = (I, A_1, \ldots, A_m)$ be a linearly independent set. Then $W_{m+1}(\mathbf{A})$ is strongly convex if and only if $m \leq 2$.*

Proof. The "if" direction, as already mentioned, follows from any of the usual proofs of the Hausdorff–Toeplitz theorem.

For the "only if" direction, suppose that that $W_{m+1}(\mathbf{A})$ is strongly convex and assume (in order to get a contradiction) that $m \geq 3$. By [24, Theorem 4.1], there exists $X \in M_{d,2}$ with $X^*X = I$ such that $X^*\mathbf{A}X := \{I, X^*A_1X, \ldots, X^*A_mX\}$ spans all of M_2. By letting $|\phi\rangle$ and $|\psi\rangle$ be the column vectors of X, we see that strong convexity of $W_{m+1}(\mathbf{A})$ immediately implies convexity of $W_{m+1}(X^*\mathbf{A}X)$. Since convexity of $W_{m+1}(X^*\mathbf{A}X)$ depends only on the span of $X^*\mathbf{A}X$, it follows that $W_4(\mathbf{B})$ is also convex, where $\mathbf{B} := \{\lambda_0, \lambda_1, \lambda_2, \lambda_3\}$ is the Pauli basis given by Equation (8). However, it is easily verified that $W_4(\mathbf{B})$ is the Bloch sphere embedded in 4-dimensional space and hence is not convex, which gives the desired contradiction. □

It thus seems that numerical range and convexity arguments are not able to tell us anything non-trivial about the UDP/UDA problem beyond the $m = 2$ case of Theorem 5.

Appendix D: Symmetries and UDP/UDA: Proof of Theorem 6

We will see that if there is a compact group of symmetries whose fixed point set is the linear span of observables $(A_1, \ldots, A_m)$, then UDP for these observables implies UDA for any pure state. We start with the following result about fixed points of compact groups.

Theorem 8. *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 μ be Haar measure on G, and define $P : H \to H$ to be the linear map satisfying*

$$\langle P\xi, \eta\rangle = \int_G \langle g\xi, \eta\rangle \, d\mu(g) \tag{24}$$

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

Proof. Left and right invariance of Haar measure imply that $Pg = gP = P$ for all $g \in G$. The definition of P implies that $L \subset \operatorname{im} P$. Now $gP = P$ for all $g \in G$ implies $\operatorname{im} P \subset L$, and hence $\operatorname{im} P = L$. Next, $\operatorname{im} P = L$ and the definition of P give $P^2 = P$. To show that $P^\dagger = P$ we use the fact that the integrals of $f(g)$ and $f(g^{-1})$ are the same for Haar measure, together with the assumption that G is a group of unitaries:

$$\begin{aligned}
\langle \xi, P\eta\rangle = \langle P\eta, \xi\rangle^* &= \int_G \langle g\eta, \xi\rangle^* d\mu(g) \\
&= \int_G \langle \xi, g\eta\rangle d\mu(g) = \int_G \langle g^\dagger \xi, \eta\rangle d\mu(g) \\
&= \int_G \langle g^{-1}\xi, \eta\rangle d\mu(g) = \int_G \langle g\xi, \eta\rangle d\mu(g) \\
&= \langle P\xi, \eta\rangle
\end{aligned} \tag{25}$$

Finally, by the Alaoglu–Birkhoff mean ergodic theorem [25, Prop. 4.3.4] P is in the strong closure of the convex hull of G. Since H is finite dimensional, then the space of linear operators on H is also finite dimensional, so the convex hull of the compact set G is compact and hence closed.

□

Symmetries of K_d are given by conjugation by unitaries or by the transpose map or by composition of these two types of symmetries. (An affine automorphism of K_d preserves transition probabilities, cf. [26], so this is a consequence of Wigner's theorem [27, 233-236].)

If we view the space of observables in M_d as a real Hilbert space (with the usual inner product $\langle X, Y\rangle = \operatorname{tr}(XY)$), then conjugation by unitaries and the transpose map both preserve this inner product, so are given by unitaries on this Hilbert space.

If L is a (real) linear subspace of observables containing the identity, then L will be the real linear span of $L \cap K_d$. Thus any symmetry of K_d will fix $L \cap K_d$ if and only if that symmetry when extended to a map on M_d fixes L. If G is a compact group of symmetries whose fixed point set is $L \cap K_d$, then the corresponding maps on M_d will have fixed point set L.

Theorem 9. *Let A be a finite set of observables on H_d with real linear span L. Assume there exists a compact group G of affine automorphisms of K_d whose fixed point set is $L \cap K_d$. Then each pure state which is UDP for measuring A is also UDA.*

Proof. As discussed above, we may view G as a compact group of unitaries with fixed point set L. Define P as in Theorem 8. Fix a pure state ρ.

Suppose first that $\rho \notin L \cap K_d$. Then there is some $g \in G$ such that $g(\rho) \neq \rho$. Since $Pg = P$, both $g(\rho)$ and ρ are pure states with the same image in $L \cap K_d$ under the map P. Thus UDP fails for ρ (and hence trivially UDA fails).

Now suppose $\rho \in L \cap K_d$. Let $\sigma \in K_d$ be a pre image of ρ under P. Then

$$1 = \langle P\sigma, \rho \rangle = |\int_G \langle g\sigma, \rho \rangle \, d\mu(g)| \leq \int_G ||g\sigma|| \|\rho\| \, d\mu(g) \leq 1,$$

and equality can hold only if $g\sigma = \rho$ for all g, i.e., if and only if $\sigma \in L$. Then $\sigma = P\sigma = \rho$, so for such ρ both UDP and UDA hold.

□

Corollary 1. *For $d = 2$, for all pure states and all sets $\mathbf{A}$ of observables, UDP implies UDA.*

Proof. Let $A_1 = I, A_2, \ldots, A_m$ be observables in M_2 and let $L = S(A)$ be their real linear span. We will show that there is a finite group of affine automorphisms G of the state space K_d of M_2 with fixed point set $L \cap K_d$. There are three cases, depending on the dimension of the fixed point set. The fixed point set in the Bloch sphere will be the central point, a diameter of the Bloch sphere, or the intersection of a plane (through the center) with the Bloch sphere. In each case reflection of the Bloch sphere in the fixed point set generates an order 2 group of affine automorphisms with fixed point set $L \cap K_d$. Now the corollary follows from Theorem 9.

□

Corollary 2. *Let $\mathbf{A} = A_1, \ldots, A_p$ be observables in M_d. If the (complex) linear span of $\mathbf{A}$ is a *-subalgebra $\mathcal{A}$ of M_d, then UDP = UDA for pure states measured by these observables.*

Proof. UDP and UDA for a set of observables aren't affected if we include the identity among those observables, so hereafter we assume that $I_d \in \mathbf{A}$. Note that $\mathcal{A}$ is the linear span of the unitaries in $\mathcal{A}$. Furthermore, $\mathcal{A}$ is a von Neumann algebra containing the identity I_d, so by the bicommutant theorem [28, Thm. 2.77] $(\mathcal{A}')' = \mathcal{A}$, where for $X \subset M_d$, X' denotes the algebra of matrices that commute with all matrices in X. Combining these two statements shows that $\mathcal{A}$ is the set of matrices that commute with all unitaries in $\mathcal{A}'$, and thus is the set of fixed points of $G = \{\mathrm{Ad}_U \mid \text{U is a unitary in } \mathcal{A}'\}$. It follows that $L = \mathcal{A}_{sa}$ (the Hermitian matrices in $\mathcal{A}$) is the set of observables fixed by the compact group G. The corollary follows from Theorem 9.

□

Example 1. *Let $\mathbf{A} = \{E_{11}, \ldots, E_{dd}\}$. Then the complex linear span of $\mathbf{A}$ consists of the diagonal matrices. From Corollary 2 it follows that for each pure state on M_d, UDP for $\mathbf{A}$ implies UDA.*

We can generalize the last example by taking the *-algebra consisting of diagonal observables with the restriction that certain diagonal entries coincide. For example, if $d = 7$ we can look at diagonal matrices of the form $\mathrm{diag}(a, a, b, b, b, c, d)$ whose linear span will be 4 dimensional. The space of Hermitian members of this algebra is four dimensional. If we choose 4 observables including the identity spanning this space, then UDA = UDP for all pure states when measuring these observables. (We could drop the identity from this list if we wish.) In this way for any d we can find a set of k observables for any $k \leq d$ for which UDA = UDP.

We can also find many larger sets of observables for which UDA = UDP. For example, for any d we can consider the *-algebra of all block diagonal matrices with k blocks that are of size $d_i \times d_i$ for $1 \leq k \leq p$, where $d_1 + d_2 + \cdots d_p = d$. The subspace of Hermitian matrices in this algebra has dimension $\sum_i d_i^2$, so any such dimension is realizable as the number of observables in a set of observables for which UDA = UDP holds for all pure states.

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