Quantum State Tomography via Reduced Density Matrices

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Quantum state tomography via local measurements is an efficient tool for characterizing quantum states. However, it requires that the original global state be uniquely determined (UD) by its local reduced density matrices (RDMs). In this work, we demonstrate for the first time a class of states that are UD by their RDMs under the assumption that the global state is pure, but fail to be UD in the absence of that assumption. This discovery allows us to classify quantum states according to their UD properties, with the requirement that each class be treated distinctly in the practice of simplifying quantum state tomography. Additionally, we experimentally test the feasibility and stability of performing quantum state tomography via the measurement of local RDMs for each class. These theoretical and experimental results demonstrate the advantages and possible pitfalls of quantum state tomography with local measurements.

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Introduction.—Quantum state tomography (QST) is one of the most famous double-edged swords in quantum information science. On the one hand, QST provides a complete description of an arbitrary quantum state, which is essential for benchmarking and validating quantum devices [1–5]. On the other hand, the exponential resources QST requires make scaling it to large systems infeasible in practice. In the past decade, tremendous effort has been devoted to boosting the efficiency of QST [6–12]. QST via reduced density matrices (RDMs) [13–18] is one especially promising approach, as it is significantly less resource intensive and many experimental setups are able to perform local measurements conveniently and accurately. One criterion for adopting this approach is that the global state has to be the only state which is compatible with its RDMs; that is, it must be uniquely determined (UD) by its RDMs.

The UD criterion can be further classified into two categories: uniquely determined among all states (UDA) and uniquely determined among pure states (UDP) by local RDMs. (In this work, UD refers to UD by its RDMs unless otherwise specified. For the background of UD via general measurements, see Appendix A in Ref. [19] for more details.) The quantum states of many physically realistic quantum systems usually belong to the UDA category. These systems involve only few-body interactions [24] and possess ground states which exhibit special properties [25–28]. To reconstruct states of this type, experimentalists need only measure RDMs and search for the global state which is compatible with these RDMs. This saves an exponential number of measurements [29].

In the case of states which satisfy the UDP criterion, two assumptions must be made if one wishes to reconstruct such states via RDMs. First, the experimentally prepared states must be (nearly) pure. Second, the search space of possible reconstructions must be limited to pure states; otherwise, the searching procedure may return incorrect mixed states with the same RDMs. Despite these assumptions, searching for UDP states has the advantage of significantly reducing the number of search parameters since the search space is pure. Traditionally, this has been the approach for dealing with many related problems, for instance, the famous Pauli problem and its finite dimensional versions [30,31].

In this Letter, we resolve the relation between the UDP and UDA criteria, and it is shown that there are states that are UDP but not UDA. Therefore, one should classify many-body quantum states into three different nontrivial classes: (A) neither UDP nor UDA, (B) UDA, or (C) UDP but not UDA. One may argue that the existence of states of class C is trivial as the set of pure states is of a much lower dimension then that of the mixed states. We emphasize, however, that this is not the case: when constructing examples of states of class C, one is working with pure

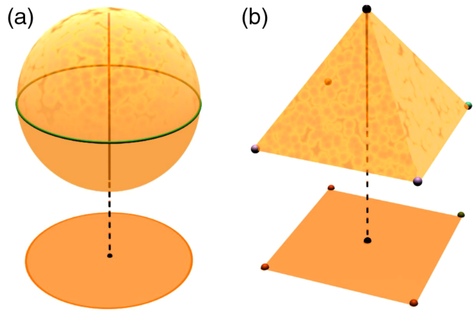

FIG. 1. Three-dimensional caricatures of the possible shapes of state space and the space of reduced density matrices as projections. Pure states are given by the extreme points. (a) A sphere, for which all boundary points are extreme points. Only the points on the boundary of the projected circle have a unique preimage in the state space, and so are UDA. All the interior points have multiple extreme points in their preimage, so they are not UDP. Thus, UDP implies UDA. (b) A polytope, for which the five vertices are extreme points. The four corner points have a unique preimage in the state space, and so are UDA. However, one interior point located at the center has multiple preimages where only one is an extreme point, so it is UDP but not UDA.

states that are already UDP, a strong restriction on the states under consideration, and the dimension argument does not work. In fact, to the contrary, it was known that for all three-qubit states, UDP equals UDA, and there are no states in class C. It is indeed a surprise that, when considering four and more qubit systems, nontrivial examples emerge in class C. In particular, we present a class of four-qubit states that are UDP by their two-particle RDMs (2-RDMs) but fail to be UDA. This is the first separation between UDA and UDP in the setting of RDMs.

Our findings have important consequences to the RDM approach to state tomography but are also illuminating to other areas of related research. First, the existence of states in class C must reveal interesting geometry of the many-body quantum state space. Our usual intuition about the state space looks more like the picture in Fig. 1(a)—the Bloch sphere. In this simple situation, one easily verifies that UDP equals UDA. However, in higher dimensional state spaces, projections of the state space could possibly look like Fig. 1(b), where UDP may not imply UDA. Second, the UDA versus UDP problem, originated from the study of ground states of local Hamiltonians, also sheds light on the structure of many-body entanglement as the local determination problem of entangled state is of fundamental importance.

Our construction is based on the study of four-qubit symmetric (i.e., bosonic) states. Note that the properties of bosonic states have recently been extensively studied theoretically [32–34] and experimentally [35,36] due to their significant roles in characterizing cold atomic systems.

To illustrate the validity of our construction, we experimentally demonstrate the reconstruction of a series of four-qubit states by measuring their 2-RDMs. We examine the differences among states of the three possible classes. We test the robustness (stability) against experimental errors of our construction.

Three classes.—We classify four-qubit pure states into three classes according to how they are UD by their 2-RDMs and present some examples for each class.

Class A: Neither UDP nor UDA. Consider GHZ-type state:$\alpha|0000\rangle + \beta|1111\rangle$, whose 2-RDMs are

$$|\alpha|^2|00\rangle\langle 00| + |\beta|^2|11\rangle\langle 11|. \quad (1)$$

It is not UDP (thus not UDA) since any pure state $\alpha|0000\rangle + e^{i\phi}\beta|1111\rangle$ or mixed state $|\alpha|^2|0000\rangle\langle 0000| + |\beta|^2|1111\rangle\langle 1111|$ has the same 2-RDMs. Therefore, to reconstruct four-qubit GHZ-type states experimentally, it is insufficient to only measure its 2-RDMs, even if assuming the prepared state is pure.

Class B: UDP and UDA. The W-type state

$$|W\rangle = a|0001\rangle + b|0010\rangle + c|0100\rangle + d|1000\rangle \quad (2)$$

is known to be UDA [37] and also UDP. Unlike the GHZ-type state, to reconstruct the global state, one needs only know its 2-RDMs.

Class C: UDP but not UDA. The existence of this type of states is the main theoretical result of this Letter. Up until now, no such states are known. This is likely due to the fact that analytically determining the uniqueness properties of quantum states is notoriously difficult in general.

The outline of our approach is as follows. We focus on the four-qubit bosonic (symmetric) state $|\psi_S\rangle = \sum_{j=0}^{4} c_j|w_j\rangle$, where the normalized Dicke state $|w_j\rangle$ is defined to be proportional to $P_{\rm sym}(|0\rangle^{\otimes j} \otimes |1\rangle^{\otimes 4-j})$ with $P_{\rm sym}$ being the projection onto the four-qubit symmetric subspace. This symmetry assumption significantly simplifies the analysis since all the 2-RDMs are the same. To further simplify the analysis, we assume $c_1 = c_3 = 0$ and that c_0, c_2, and c_4 are all real:

$$|\psi_S\rangle = c_0|w_0\rangle + c_2|w_2\rangle + c_4|w_4\rangle. \quad (3)$$

To determine the parameter regions of c_0, c_2, c_4 where $|\psi_S\rangle$ is UDP but not UDA, we take three steps.

Step 1: First, we prove that there is no other pure bosonic state which has the same 2-RDMs as $|\psi_S\rangle$ when $|\psi_S\rangle$'s 2-RDMs have three distinct nonzero eigenvalues.

Step 2: Next, we observe that any pure bosonic state which is uniquely determined among all other pure bosonic states is also UDP.

Step 3: Finally, we provide the region where the 2-RDMs of $|\psi_S\rangle$ are separable. $|\psi_S\rangle$ is guaranteed not to be UDA in this region. Therefore, within this parameter region, $|\psi_S\rangle$ is UDP but not UDA as long as its 2-RDMs are nondegenerate and not rank one.

We direct the reader to Appendix B for steps 1 and 2 and to Appendix C for step 3 in the Supplemental Material [19]. Note that for $|\psi_S\rangle$ in this class, all the mixed states which share the same RDMs with $|\psi_S\rangle$ form a convex set. This set, with $|\psi_S\rangle$ as an extreme point, has infinite states.

Experiment.—We experimentally inspect all three classes of state using nuclear magnetic resonance (NMR) and test their stability against experimental noise. The four-qubit sample is ^{13}C-labeled transcrotonic acid dissolved in d6-acetone, where the molecular structure and Hamiltonian form are shown in Appendix E [19]. All experiments were carried out on a Bruker DRX 700 MHz spectrometer at room temperature.

The experiments are divided into three steps: (i) prepare the initial state $|0000\rangle$, (ii) evolve $|0000\rangle$ to the desired state in each class, and (iii) measure the final state by full QST and 2-RDMs, reconstruct the original state via the measured 2-RDMs, and compare it with the full QST result. We describe each step briefly as follows. For more experimental details, see Appendixes E and F in Ref. [19].

(i) In the majority of experiments in quantum information, $|0\rangle^{\otimes n}$ is chosen as the input state. In NMR, we instead generate a so-called pseudopure state (PPS) from the thermal equilibrium state. This initialization step is realized by the spatial averaging technique [38–40], which involves both unitary and nonunitary (realized by z-gradient pulses) transformations. The form of four-qubit PPS is

$$\rho_{0000} = \frac{1-\epsilon}{16}\mathbb{I} + \epsilon|0000\rangle\langle 0000|, \tag{4}$$

where $\mathbb{I}$ is identity and $\epsilon \approx 10^{-5}$ is the polarization. Although the PPS is highly mixed, the large $\mathbb{I}$ does not evolve under any unital propagator, nor is it observed in NMR spectra. Hence, only the deviated part $|0000\rangle$ contributes to the experimental results and the PPS is able to serve as an input state.

(ii) The next step is to create the desired states of the different UD classes. The radio-frequency (rf) pulses during this procedure are optimized by the gradient ascent pulse engineering (GRAPE) algorithm [41,42] and are designed to be robust to the static field distributions (T_2^* process) and rf inhomogeneity. The designed fidelity for each pulse exceeds 0.99, and all pulses are rectified via a feedback-control setup in the NMR spectrometer to minimize the discrepancies between the ideal and implemented pulses [43,44].

Class A: States belonging to this class are neither UDP nor UDA by their 2-RDMs. The following states are in class A:

$$\begin{aligned} |\mathrm{GHZ}\rangle_+ &= \alpha|0000\rangle + \beta|1111\rangle, \\ |\mathrm{GHZ}\rangle_- &= \alpha|0000\rangle - \beta|1111\rangle, \\ \rho^G_{\mathrm{mix}} &= |\alpha|^2|0000\rangle\langle 0000| + |\beta|^2|1111\rangle\langle 1111|, \end{aligned} \tag{5}$$

and ρ^G_+ and ρ^G_- are the density matrices of $|\mathrm{GHZ}\rangle_+$ and $|\mathrm{GHZ}\rangle_-$, respectively. All of these states have the same 2-RDMs, which means that the 2-RDMs are not sufficient to reconstruct these states. To verify this, we first need to prepare each state in Eq. (5) from $|0000\rangle$. For ρ^G_+, qubit one first undergoes a rotation around the y axis that $R_y(\theta) = e^{-i\theta\sigma_y/2}$ with $\theta = 2\arccos(\alpha)$. Then three controlled-NOT (CNOT) gates CNOT_{12}, CNOT_{13}, and CNOT_{14} are applied consecutively, where qubit one is the control and others are targets. The single-qubit rotation $R_y(\theta)$ is realized by a 1 ms GRAPE pulse, and the three CNOT gates are realized by a 30 ms GRAPE pulse. We can similarly construct ρ^G_- by instead employing a single-qubit rotation of $R_y(-\theta) = e^{i\theta\sigma_y/2}$. For ρ^G_{mix}, we simply prepare a classical distribution of two pure states $|0000\rangle$ and $|1111\rangle$. In these experiments, we prepare nine distinct states by varying α from 0.1 to 0.9 with 0.1 increment.

Class B: States belonging to this class are both UDP and UDA, with the W-type state in Eq. (2) being a typical example. In experiment, we simply set $a = b$ and $c = d$, and then prepare six inputs $|W\rangle$ by changing a from 0.1 to 0.6 with 0.1 increment. This state preparation is directly realized by a state-to-state GRAPE pulse with a duration of 20 ms.

Class C: States belonging to this class are UDP but not UDA. The type of state we prepare $|\psi_S\rangle$ is described in Eq. (3) and conforms to the following parametrization:

$$\begin{aligned} c_0 &= \frac{\sin t - \sin\theta\cos t}{\sqrt{2}}, \\ c_2 &= \cos\theta\cos t, \\ c_4 &= -\frac{\sin\theta\cos t + \sin t}{\sqrt{2}}, \end{aligned}$$

where we fix $\theta = \pi/12$ and choose t from $\pi/6 + \pi/18$ to $5\pi/6 - \pi/18$, and increment by $\pi/18$. With the exception of the point $t = \pi/2$, this curve lies within the region of states that are UDP but not UDA, as outlined in Appendixes A and B. All these states are prepared by state-to-state GRAPE pulses with a fixed duration of 20 ms. In order to demonstrate that these states are not UDA, we also prepare corresponding mixed states with the same 2-RDMs as outlined in Appendix D in Ref. [19].

(iii) After preparing these states, we perform four-qubit QST [45,46], which includes measuring the 2-RDMs. To determine the original four-qubit state, a maximum likelihood approach [47] is adopted to reconstruct the most likely state based on the measured 2-RDMs.

Results.—Now, we discuss the effectiveness and stability of QST via 2-RDMs for each class of states.

Class A: In Fig. 2(a), it is clear that any two of ρ^G_+, ρ^G_-, and ρ^G_{mix} have completely different fidelities in the four-qubit form (blue and yellow), but they share the same 2-RDMs up to minor experimental errors (red and green). Therefore, these states are neither UDP nor UDA, and it is insufficient to rely only on their 2-RDMs for QST.

Class B: The W-type state in Eq. (2) is known to be UDA. In Fig. 3(a), the blue triangles represent the fidelities $F(\rho^W_{\mathrm{QST}}, \rho^W_{\text{2-RDM}})$ between the prepared four-qubit state ρ^W_{QST} via full QST and the reconstructed four-qubit state $\rho^W_{\text{2-RDM}}$ via 2-RDMs. For every tested W-type state, the worst fidelity is still about 97% as shown by the triangles in

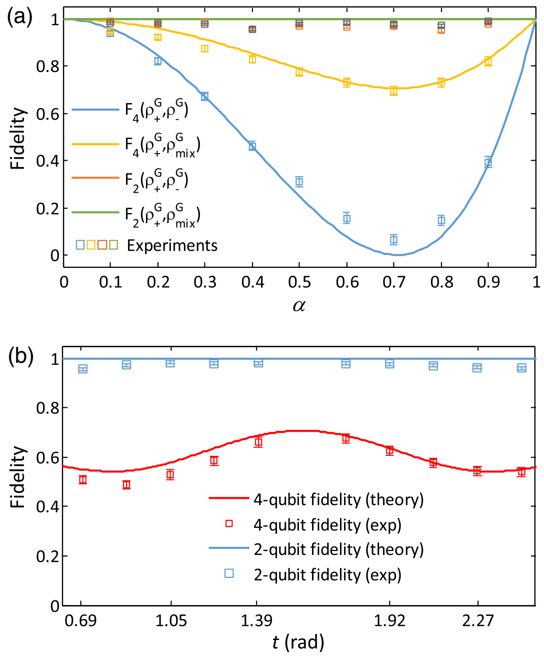

FIG. 2. (a) GHZ-type states (class A) such as ρ_+^G in Eq. (5) are neither UDP nor UDA. The four-qubit fidelities between ρ_+^G and ρ_-^G (blue) and ρ_+^G and ρ_{mix}^G (yellow) are completely different, but they do have the same 2-RDMs (red and green, where the worst-case fidelity out of six possible 2-RDM fidelities is shown) up to minor experimental errors. The error bars are calculated from the imperfection of the GRAPE pulses and fitting procedure. (b) States in class C are not UDA, so there can exist mixed states between which they have very low four-qubit fidelity (red) but the same 2-RDMs (blue). However, these types of states are UDP, so there do not exist any other four-qubit pure states with the same 2-RDMs.

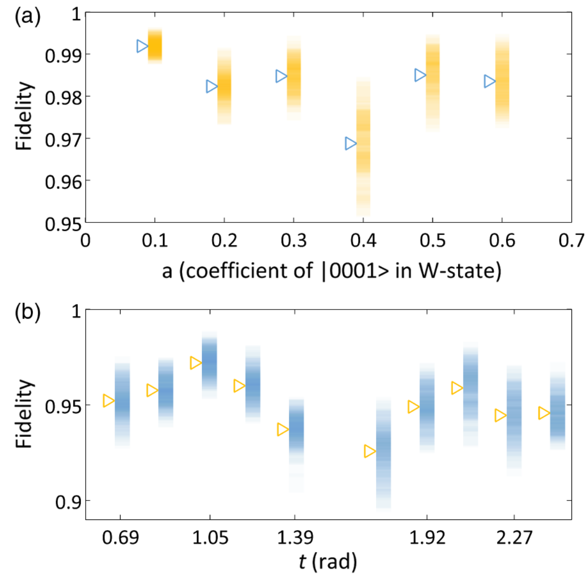

FIG. 3. Stability test against experimental noise for $|W\rangle$ and $|\psi_S\rangle$. The noise is artificially added in Gaussian distribution to the measured 2-RDMs under experimental conditions, by randomly sampling 90 distinct sets of 2-RDMs. The arrows indicate the mean for each sampled results. (a) Fidelities of the $|W\rangle$ (class B) in a noisy environment. The x axis is the coefficient a defined in Eq. (2). (b) Fidelities of the $|\psi_S\rangle$ (class C) in a noisy environment, as a function of t defined in Eq. (3).

Fig. 3(a). This indicates that the 2-RDMs are indeed sufficient for the reconstruction of the original four-qubit state.

However, under realistic experimental conditions, the prepared state ρ_{QST}^W unavoidably deviates from the desired state. This may drive it outside the UDA region, so that it is no longer UDA. To test if this is the case, we simulate different outputs of 2-RDMs by adding Gaussian distributed noise and repeating the reconstruction of the four-qubit state via the 2-RDMs, as outlined in Appendix F in Ref. [19]. From the yellow bars in Fig. 3(a), it can be seen that even with artificial noise, QST via 2-RDMs is stable, since the fidelity is always over 0.95.

Class C: This class is UDP, which means we do not have any other pure state that gives the same 2-RDMs other than the target state. However, it is not UDA, so there do exist some mixed states (see Appendix D in Ref. [19]) with the same 2-RDMs. Figure 2(b) illustrates such results. Both in theory and experiment, we see that the target state $|\psi_S\rangle$ and a corresponding mixed state have low fidelity with one another (yellow) but the same 2-RDMs (blue). Therefore, when reconstructing this type of four-qubit state via its 2-RDMs, we need to assume that the original state is pure. Otherwise, it is likely to obtain some mixed state which will not necessarily be the true state of the system.

Similarly to the W-type state, we test whether the UDP property of $|\psi_S\rangle$ is stable against noise. As seen in Fig. 3(b), even under the application of Gaussian noise, as long as we assume our state is pure we can always reconstruct the correct four-qubit state with high fidelity (> 0.90) using only its 2-RDMs.

Conclusion.—In summary, we disprove the hypothesis that UDP implies UDA for RDMs [16] by demonstrating the existence of a family of four-qubit states that are UDP but not UDA by their 2-RDMs. This new finding allows us to classify pure states into three classes according to their UD properties, in order to improve the efficiency of QST: in class A, where the state is neither UDP nor UDA, full QST is necessary; in class B, where the state is UDP and UDA, the measurement of 2-RDMs is sufficient to determine the global state; and in class C, where the state is UDP but not UDA, the measurement of 2-RDMs combined with the assumption that the global state is pure is sufficient. This approach simplifies QST significantly, since full QST of n qubits requires $4^n - 1$ observables while 2-RDM measurement requires $\binom{n}{1} \times 3 + \binom{n}{2} \times 9$ observables (all weight-one and weight-two Pauli operators) only.

We check the feasibility of this protocol for each class with a four-qubit NMR quantum processor. The results indicate that for classes B and C, it is not necessary to implement the full QST—2-RDMs already enable the reproduction of the global state with high fidelities. As there are always experimental errors, we also demonstrate the stabilities of this protocol, namely, whether it is robust against experimental noise. The results reveal that the approach of doing QST solely via the measurement of 2-RDMs is robust to the noise under our experimental conditions and hopefully behaves the same in other experimental platforms.

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