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Convergence of a Reconstructed Density Matrix to a Pure State Using the Maximal Entropy Approach

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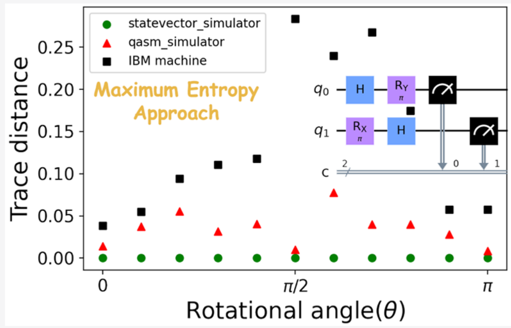
ABSTRACT: Impressive progress has been made in the past decade in the study of technological applications of varied types of quantum systems. With industry giants like IBM laying down their roadmap for scalable quantum devices with more than 1000-qubits by the end of 2023, efficient validation techniques are also being developed for testing quantum processing on these devices. The characterization of a quantum state is done by experimental measurements through the process called quantum state tomography (QST) which scales exponentially with the size of the system. However, QST performed using incomplete measurements is aptly suited for characterizing these quantum technologies especially with the current nature of noisy intermediate-scale quantum (NISQ) devices where not all mean measurements are available with high fidelity. We, hereby, propose an alternative approach to QST for the complete reconstruction of the density matrix of a quantum system in a pure state for any number of qubits by applying the maximal entropy formalism on the pairwise combinations of the known mean measurements. This approach provides the best estimate of the target state when we know the complete set of observables, which is the case of convergence of the reconstructed density matrix to a pure state. Our goal is to provide a practical inference of a quantum system in a pure state that can find its applications in the field of quantum error mitigation on a real quantum computer that we intend to investigate further.



1. INTRODUCTION

The rapid advancements toward the development of large scale quantum computing devices in recent years require efficient methods that can validate information processing on these devices. Quantum state tomography (QST) is one such standard data-driven technique that can characterize the quantum mechanical state of the system based on the information on the expectation values of a complete set of observables.[1−5] However, the increase in the size of quantum systems poses a critical limitation on QST due to the exponential scaling of the number of parameters required to reconstruct a quantum state that is a tensor product of qubits. In practice, full QST for large quantum systems has been performed on not more than 10-qubits.[6]

We are currently in the era of noisy intermediate-scale quantum (NISQ) computing[7] which restricts the use of a large quantum device for practical purposes such as recovering the true quantum state, owing to the inherent noise in the result. Measurements on these NISQ devices are therefore of limited fidelity, and in certain cases, we have access to only a limited number of observations. This along with the scaling problem makes QST intractable in real experiments except for small quantum systems. Various techniques have been suggested to address the underlying scaling problem as well as to mitigate against imperfect measurements.[8] Some of the proposed tomography methods are matrix product state tomography,[5] neural network tomography,[9−12] quantum overlapping tomography,[13] shadow tomography.[14,15] Apart from the conventional tomography techniques, there have been approaches that try to estimate the quantum state based on incomplete measurements.[16−18] Some of these methods include quantum state estimation using the maximum likelihood estimation[19,20] and Bayesian state estimation.[21,22]

In our previous work,[23] we proposed an alternative approach to QST based on the maximal information entropy formalism[17,24,25] using a finite but incomplete set of measurements that serve as the constraints of the problem. These are special kinds of constraints that correspond to the mean values of populations and coherences. We showed that using the maximal entropy approach we can obtain an accurate prediction of an unknown mean measurement (a probability) using a pair of known mean measurements (a probability and a

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coherence). In addition to the validation of the results of quantum calculations performed on NISQ devices using QST, there are a variety of further circumstances where the mean values of populations and coherences are of primary interest.[26−28] With an incomplete set of known mean measurements, maximizing the von Neumann entropy[16,29−31] of the system provides an additional constraint to obtain a unique solution for the state determination. In this paper, we extend this approach to reconstruct the complete density matrix of an n-qubit quantum system with a special reference to a pure state using the expectation values of N observables where $N = 2^n$. The unique feature of our approach is that we consider pairwise combination of the known probability with the known coherence to predict an unknown probability using the maximal entropy formalism and repeat this process until all the probabilities for all the n qubits have been determined. Once all the probabilities have been calculated, we employ the same approach on the pairwise combinations of the probabilities to determine all the unknown coherences. The detailed description of the method is provided in section 2. To validate and support our theoretical proposition, we conducted numerical simulations in IBM's qiskit.[32] We also implemented our approach on the IBM quantum computing chip that can be easily accessed through the IBM quantum experience.[33] The results in section 3 show the accuracy of our approach when we use the expectation values of observables obtained from noise-free *statevector_simulator* backend in Qiskit for the reconstruction of the complete density matrix for quantum systems ranging from 2 to 10 qubits using the proposed approach. We intend to further analyze this approach for applications in the field of quantum error correction and compare it with the available error correction codes.[34,35]

2. METHODS

A unique characterization of a quantum state requires measuring the expectation values of a complete set of observables. For the state vector of a quantum state with N entries, this complete set is defined by $2N - 1$ independent parameters whose knowledge is required to uniquely characterize the quantum state. For example, measurements of expectation values of 16 operators are required to completely describe a 2-qubit quantum system in a pure state:

$$\{|1\rangle\langle 1|, |2\rangle\langle 2|, |3\rangle\langle 3|, |4\rangle\langle 4|, (|1\rangle\langle 2|, |2\rangle\langle 1|), (|1\rangle\langle 3|, |3\rangle\langle 1|), (|1\rangle\langle 4|, |4\rangle\langle 1|), (|2\rangle\langle 3|, |3\rangle\langle 2|), (|2\rangle\langle 4|, |4\rangle\langle 2|), (|3\rangle\langle 4|, |4\rangle\langle 3|)\} \tag{1}$$

The expectation values of the above operators correspond to the probabilities and coherences in the 2-qubit system.[30] The maximal entropy formalism[24] seeks to determine a probability distribution that is consistent with the known average values of certain operators $\hat{f}_k$ as well as ensuring that the von Neumann entropy of the distribution be maximal. Combining it with the method of Lagrange multipliers, λ_k[17,25] yields the following form of the density operator:[16,31]

$$\hat{\rho} = \frac{1}{Z(\lambda_1, ..., \lambda_k)} \exp\left\{-\sum_k \lambda_k \hat{f}_k\right\} \tag{2}$$

where $Z(\lambda_1, ..., \lambda_k) = \mathrm{Tr}(\exp\{-\sum_k \lambda_k \hat{f}_k\})$ insures the normalization as $\mathrm{Tr}(\rho) = 1$. Thus, even when a complete set of observables is not available, the maximal entropy formalism provides a unique characterization of the quantum state consistent with the given constraints. In this current work, we start by reconstructing the density matrix of maximal entropy that corresponds to the case when only two measurements are available, specifically, a probability and a coherence. In general, the coherence will be a complex number so it is equivalent to two Hermitian observables. Based on the maximal entropy formalism, we can write the Hermitian density operator in terms of the operators corresponding to the available observables as

$$\hat{\rho} = \frac{1}{Z(\lambda_{11}, \lambda_{12}, \lambda_{21})} \exp\{-\lambda_{11}|1\rangle\langle 1| - \lambda_{12}|1\rangle\langle 2| - \lambda_{21}|2\rangle\langle 1|\} \tag{3}$$

where the Lagrange multipliers λ_k satisfy $\lambda_{21} = \lambda_{12}^*$ so that the density matrix is Hermitian. One can satisfy this by writing the Lagrange multiplier of the coherences in terms of an amplitude and a phase, $\lambda_{12} = |\lambda_{12}| \exp i\theta_{12}$. The details of the prediction of an unknown probability from a known probability and a coherence are presented in our previous work.[23] The operators in the exponent of eq 3 do not commute, so to obtain an explicit form for the density matrix, we first diagonalize the Hermitian matrix **A** corresponding to the exponent term in eq 3 and then express the density operator in terms of the eigenvalues and eigenvectors of **A**:

$$\hat{\rho} = \frac{1}{Z(\lambda_{11}, \lambda_{12}, \lambda_{21})} \sum_i \exp\{\epsilon_i\}|\phi_i\rangle\langle\phi_i| \tag{4}$$

where $\{\epsilon_i, \phi_i\}$ are the eigenvalues and eigenvectors of **A** expressed as a function of the unknown Lagrange multipliers in eq 3. For a 2-qubit system, the density operator, upon reconstruction from a known probability and a coherence so that there is only one phase, was shown to take the explicit form:

$$\begin{aligned}\hat{\rho} &= \frac{1}{Z}\sum_i \exp\{\epsilon_i\}|\phi_i\rangle\langle\phi_i| \\ &= \frac{1}{Z}\left(|4\rangle\langle 4| + |3\rangle\langle 3| + (a + b)|1\rangle\langle 1| + \left(\frac{a}{k_3^*} + \frac{b}{k_4^*}\right)|1\rangle\langle 2| \right. \\ &\left. + \left(\frac{a}{k_3} + \frac{b}{k_4}\right)|2\rangle\langle 1| + \left(\frac{a}{|k_3|^2} + \frac{b}{|k_4|^2}\right)|2\rangle\langle 2|\right)\end{aligned} \tag{5}$$

where $Z = \sum_i \exp\{\epsilon_i\}$, $k_3 = -\frac{\epsilon_3}{\lambda_{12}^*}$, $k_4 = -\frac{\epsilon_4}{\lambda_{12}^*}$, a = $a = \frac{|k_3|^2}{\sqrt{(k_3^2+1)(k_3^{*2}+1)}} \exp \epsilon_3$, and $b = \frac{|k_4|^2}{\sqrt{(k_4^2+1)(k_4^{*2}+1)}} \exp \epsilon_4$. Since the basis operators are orthogonal, the mean measurements correspond to the coefficients of the operators in the reconstructed density matrix. Therefore,

$$x_{11} = f(\lambda_{11}, \lambda_{12}, \lambda_{21}) = \langle |1\rangle\langle 1| \rangle = \frac{a + b}{Z} \tag{6}$$

$$x_{22} = g(\lambda_{11}, \lambda_{12}, \lambda_{21}) = \langle |2\rangle\langle 2| \rangle = \left(\frac{a}{|k_3|^2} + \frac{b}{|k_4|^2}\right) \Big/ Z \tag{7}$$

$$x_{12} = h(\lambda_{11}, \lambda_{12}, \lambda_{21}) = \langle |1\rangle\langle 2| \rangle = \left(\frac{a}{k_3^*} + \frac{b}{k_4^*}\right) \Big/ Z \tag{8}$$

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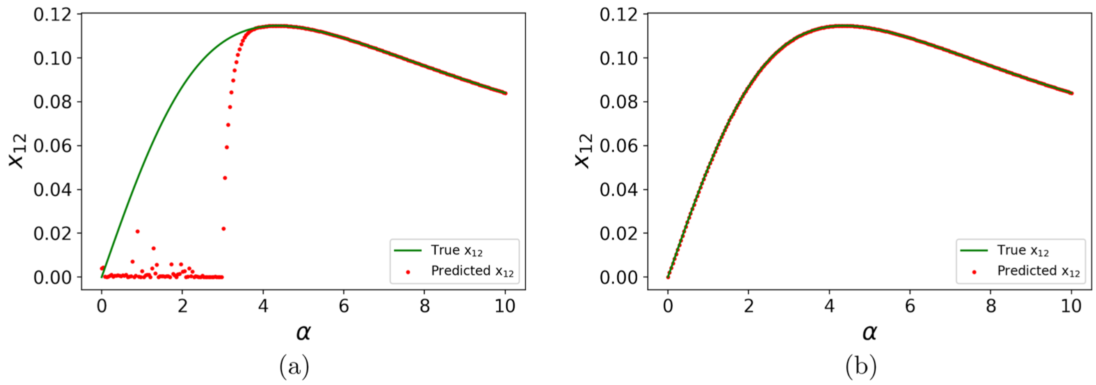

Figure 1. Plot of the predicted and true mean measurement x_{12} versus the coefficient α of the state $|\psi\rangle = \frac{1}{\sqrt{N}}(|00\rangle + \alpha|01\rangle + \beta|10\rangle + \gamma|11\rangle)$ for fixed $\beta = 3$ and $\gamma = 3$, using the maximal entropy formalism from (a) two known probabilities x_{11} and x_{22} and prediction of x_{12} using maximal entropy formalism and (b) two known probabilities x_{11} and x_{22} and also employing the scaling approach; prediction of x_{12} using maximal entropy formalism combined with the scaling technique.

The state defined in eq 5 is a mixed state. This is to be expected since we only provided information sufficient to define a pure state of the first qubit. In our previous work, we have already established that from eq 5 the information about x_{22} can be obtained using x_{11} and x_{12} following the determination of the unknown Lagrange multipliers in eq 3. However, in the case that the density matrix is real valued, we can also propose that the mean measurement value x_{12} can be determined using the same expression if we know x_{11} and x_{22} as the mean measurements in (eqs 6−8) are functions of the Lagrange multipliers (λ_{11}, λ_{12}, λ_{21}) that can be determined using the expectation values of x_{11} and x_{22}.

After determining x_{12} using the proposed approach, we can similarly determine x_{ij}, for real valued coherences, using the corresponding two probabilities, x_{ii} and x_{jj}, at a time. The full density matrix of a quantum system can be deduced if we have determined all the coefficients c_{ij} in the definition of density operator in eq 9:

$$\hat{\rho} = \sum_{ij} c_{ij}|i\rangle\langle j| \tag{9}$$

The coefficient c_{ij} is the expectation value of the corresponding operator $|i\rangle\langle j|$ which can be determined, if the density matrix is real valued, by applying the maximal entropy approach on the pair of known mean measurements for the operators: $|i\rangle\langle i|$ and $|j\rangle\langle j|$:

$$c_{ij} = \langle|i\rangle\langle j|\rangle \tag{10}$$

Therefore, if the density matrix is real valued, by considering all the pairwise combinations of the N probabilities $|i\rangle\langle i|$ and $|j\rangle\langle j|$ and applying the maximal entropy approach over each such combination, we can determine all the real valued coherences and determine the state. The number of times the maximal entropy approach is applied on the pairwise combinations of the N probabilities to determine all the coherences is $N(N-1)/2$, which is the number of unknown coherences. In section 2.2.1, we show a more general result, namely, that also when the coherences are complex valued, it follows from the representation $\lambda_{12} = |\lambda_{12}|\exp i\theta_{12}$ with $\theta_{21} = -\theta_{12}$ that it is sufficient to know the phases of half of the coherences in order to construct the phases of the other half. We show the application of this approach first by reconstructing the density matrix for the maximally entangled 2-qubit Bell state followed by the reconstruction of a 3-qubit multipartite entangled wave function. Thereby, we propose a scheme to also reconstruct the phases of the coherences and combine it with the maximal entropy approach to reconstruct the full density matrix for a quantum system in the pure state. To summarize the method, we start with a certain number of known mean measurements (for example, N probabilities if the target state is real; 1 probability and $N-1$ coherences if the target state is complex) and apply the formalism of maximal entropy on each pairwise combination of the known mean measurements. Each time we consider a pair of known mean measurements and apply the maximal entropy formalism, we get a mixed state with an accurate description of an unknown mean measurement that is the coefficient of the corresponding operator term in eq 5. We repeat this process for all the different pairs of the known mean measurements and determine all the unknown coefficients c_{ij} in eq 10 and thereby combine everything together to reconstruct the complete density matrix of the quantum system in a pure state. To verify that such a process gives us a pure state in the absence of noise as well as the known mean measurements belonging to a pure state, we calculate the entropy and trace of the square of the density matrix at each step of the process as a measure of its convergence to a pure state in the Results and Discussion.

2.1. Bell State. To reconstruct the density matrix of the 2-qubit Bell state: $|B> = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, we just need to determine the amplitude of the coherences as the target state is real. Following the approach of considering two probabilities at a time and applying the maximal entropy formalism to predict a coherence and repeating this process for all the six pairwise probability combinations for Bell state, we determine each of the coherence and combine it as per eq 9 to obtain the following density matrix:

$$\rho_{\mathrm{rec}} = \begin{bmatrix} 0.5 & 0 & 0 & 0.5 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0.5 \end{bmatrix}$$

The predicted coherences match exactly with the coherences of the original Bell state density matrix and, therefore, support our approach of reconstruction of the density matrix.

2.2. Reconstructing Density Matrix for Multipartite Entangled States. Moving forward, we consider a system

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with more than two nonzero coefficients in the maximally entangled state. For example, let us consider a 3-qubit entangled state: $|\psi> = \frac{1}{\sqrt{3}}(|100\rangle + |010\rangle + |001\rangle)$. Clearly, in the true density matrix defined for this state, all the coherence terms will be zero except for the cross terms ($\langle|010\rangle\langle 100|\rangle$, $\langle|001\rangle\langle 100|\rangle$, $\langle|001\rangle\langle 010|\rangle$, and their complex conjugate) that will be 0.3333. However, when we reconstruct the density matrix as per the above approach, we obtained the following density matrix:

$$\rho_{rec} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.3333 & 0.3286 & 0 & 0.3286 & 0 & 0 & 0 \\ 0 & 0.3286 & 0.3333 & 0 & 0.3286 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.3286 & 0.3286 & 0 & 0.3333 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

We see that some errors show up in the determination of coherences using the maximal entropy approach. The predicted coherence values further diverge from the true value if we have more nonzero coefficients of the basis states defining the maximally entangled state. To further demonstrate this, we consider a general 2-qubit quantum state with real amplitudes: $|\psi\rangle = \frac{1}{\sqrt{N}}(|00\rangle + \alpha|01\rangle + \beta|10\rangle + \gamma|11\rangle)$ and try to predict the coherence x_{12} using the probabilities x_{11} and x_{22} for various values of α and for fixed values for β and γ. As can be seen in Figure 1a, the prediction of the unknown mean measurement is highly inaccurate for smaller coefficient values of α and it improves considerably for larger values. This is primarily because upon solving the transcendental eqs 6 and 7, the determined value of the Lagrange multiplier λ_{12} is close to zero that leads to a numerical singularity while reconstructing the density matrix as λ_{12} is in the denominator when we calculate the projection operators in the eigen basis. To address this problem, we used a simple scaling approach described in detail in the Supporting Information. We then apply the maximal entropy formalism to determine the unknown coherence. The maximal entropy approach is invariant under this scaling technique, and it is done to make sure that the trace of the scaled pairwise density matrix is unity. Figure 1b shows the accuracy of the prediction of the coherence using the maximal entropy formalism combined with the scaling technique for a general 2-qubit quantum system.

This approach can be followed to reconstruct the full density matrix of a quantum system with any number of qubits. In the case of quantum states with real coherences, for the prediction of an unknown coherence from two known probabilities, we just need to determine the unknown Lagrange multipliers (λ_{11}, λ_{12}, λ_{21}) and apply this approach. We repeat this procedure to consider all possible pairwise combinations of probabilities and predict all the unknown coherences. Once we determine all the unknowns, we combine everything together to obtain the reconstructed density matrix given by eq 9. Therefore, we can reconstruct the complete density matrix of an N-qubit quantum system in the case of real coherences from N probabilities.

2.2.1. Complex Coherence and Phase Estimation. So far, we have established that the maximal entropy formalism combined with the scaling technique accurately predicts the amplitude of coherence from the known probabilities. However, in the case of complex coherence, we need more information than just the probabilities as we also need to determine the phase of coherence which is specific to a quantum system. To estimate the phase of every coherence term in the reconstruction of the density matrix, the following phase estimation algorithm is employed. To demonstrate it, let us consider a 2-qubit quantum system defined by

$$|\psi\rangle = \frac{1}{\sqrt{N}}(\alpha \exp\{i\theta_1\}|00\rangle + \beta \exp\{i\theta_2\}|01\rangle + \gamma \exp\{i\theta_3\}|10\rangle + \delta \exp\{i\theta_4\}|11\rangle) \tag{11}$$

where α, β, γ, and δ are real coefficients. The coherences are then defined as

$$\begin{aligned} x_{12} &= \langle|00\rangle\langle 01|\rangle = \alpha\beta \exp\{i(\theta_1 - \theta_2)\} = \alpha\beta \exp ip_{12} \\ x_{13} &= \langle|00\rangle\langle 10|\rangle = \alpha\gamma \exp\{i(\theta_1 - \theta_3)\} = \alpha\gamma \exp ip_{13} \\ x_{14} &= \langle|00\rangle\langle 11|\rangle = \alpha\delta \exp\{i(\theta_1 - \theta_4)\} = \alpha\delta \exp ip_{14} \end{aligned} \tag{12}$$

and so on. p_{12}, p_{13}, and p_{14} correspond to the phases of the coherences x_{12}, x_{13}, and x_{14}:

$$\begin{aligned} p_{12} &= \theta_1 - \theta_2 \\ p_{13} &= \theta_1 - \theta_3 \\ p_{14} &= \theta_1 - \theta_4 \end{aligned} \tag{13}$$

Now, the phase of the remaining coherence terms of the density matrix can be estimated if we have information about the phases p_{12}, p_{13}, and p_{14}:

$$\begin{aligned} p_{23} &= \theta_2 - \theta_3 = p_{13} - p_{12} \\ p_{24} &= \theta_2 - \theta_4 = p_{14} - p_{12} \\ p_{34} &= \theta_3 - \theta_4 = p_{14} - p_{13} \end{aligned} \tag{14}$$

Thus, we can determine the phases of all the remaining coherences using the above approach and then combine it with the determined amplitudes from maximal entropy approach to reconstruct the entire density matrix.

Therefore, in the case of complex coherences, for the prediction of an unknown coherence from two known probabilities, apart from the determination of the unknown Lagrange multipliers (λ_{11}, λ_{12}, λ_{21}), we also need to determine the phase (θ) of coherence. For determining the phase of all the coherence terms of the density matrix, we need information about the phase of $N - 1$ coherence terms as seen in eq 14. In our previous work, we have shown that we can accurately predict an unknown probability from a known probability and a coherence. Therefore, given $N - 1$ coherences and a probability, we can construct all the probabilities using the pairwise combination of the known probability with the known coherences and applying the maximal entropy approach. After the determination of all the probabilities, we take the pairwise combination of all the probabilities and using the above approach for phase estimation and amplitude determination using maximal entropy formalism, we construct all the unknown coherences

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and combine everything to obtain the complete density matrix for a general pure state with complex amplitudes from N observables ($N - 1$ coherences and 1 probability).

3. RESULTS AND DISCUSSION

In this current work, we propose to reconstruct the complete density matrix for a general pure state with complex amplitudes from N observables ($N - 1$ coherences and 1 probability) using the method discussed in section 2. The approach that we follow can work for a quantum system with any number of qubits. To test and validate the proposed theory, we conducted numerical experiments in IBM's Qiskit,[32] which is an open-source quantum computing platform with prototype quantum devices to run and simulate quantum programs. We also implemented the theory on IBM's quantum computing chip[36] and used the measurement data to reconstruct the density matrix and then compare it with the true result.

3.1. Trace Distance and Fidelity. We considered different quantum circuits comprising of 2−10 qubits with random quantum gates as shown in Figure 2 for one sample 6-qubit circuit and tried to reconstruct the density matrix followed by its comparison with the true density matrix. The mean measurements necessary for reconstruction of the density matrix are obtained from simulating the quantum circuits. We used the *statevector_simulator* backend in IBM's Qiskit that simulates the quantum circuit without the consideration of errors and noise.

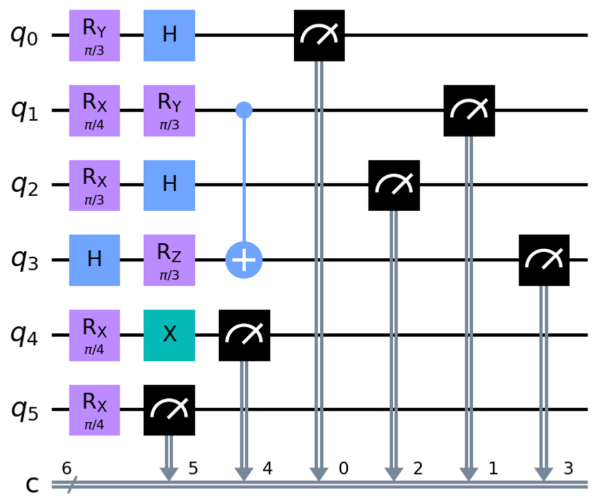

Figure 2. Sample 6-qubit quantum circuit with random quantum gates considered for testing and validating the reconstruction of the density matrix.

To distinguish between the two states, the trace distance and fidelity between the reconstructed density matrix and true density matrix are calculated for different numbers of qubits. The results in Figure 3 show that the states match exactly as the trace distance between the reconstructed state and the true state is zero and the fidelity is one even for a quantum system with a higher number of qubits.

3.2. Convergence to Pure State. Two of the most common parameters to characterize a pure state from its density matrix (ρ) are entropy(ρ) = 0 and Tr(ρ^2) = 1. Our approach is to reconstruct the density matrix of a quantum system using two observables at a time and then repeat the process with different known mean measurements until all the observables have been determined. At each step, we have more information about the system which means that we get closer to reconstructing the pure state, and therefore, the entropy of the reconstructed density matrix at each step should approach toward zero and the trace of ρ^2 should approach toward one. The number of repetitions required for complete reconstruction of the n-qubit quantum system is $N(N - 1)/2$ where $N = 2^n$. Figure 4 shows the plots of entropy (ρ) and trace (ρ^2) at each step for a 6-qubit system for the sample circuit shown in Figure 2. The plots validate the convergence of the reconstructed density matrix to a pure state at the end of the complete procedure.

4. ERROR ANALYSIS

As we saw in the previous section, we considered trace distance, between the reconstructed state and the true state, as a measure to test the performance of our approach. The first step toward the reconstruction of the density matrix is to obtain the mean measurement values of the minimum number of observables required to reproduce the quantum state. These expectation values can be obtained by running the quantum circuit on a quantum computing chip or using an efficient simulator to simulate the expected results. An online platform for cloud-based quantum computing is provided by IBM Quantum Experience on which we conducted numerical experiments to validate our work.

Figure 6 shows a 2-qubit quantum circuit along with a plot of the trace distance between the true and the reconstructed

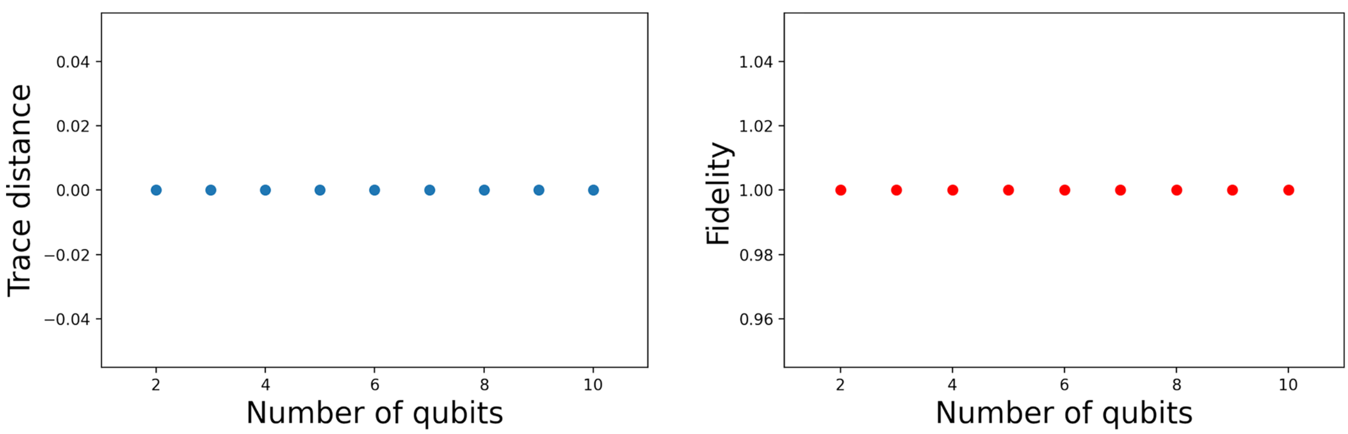

Figure 3. Plots of the trace distance and fidelity between the reconstructed density matrix and the true density matrix.

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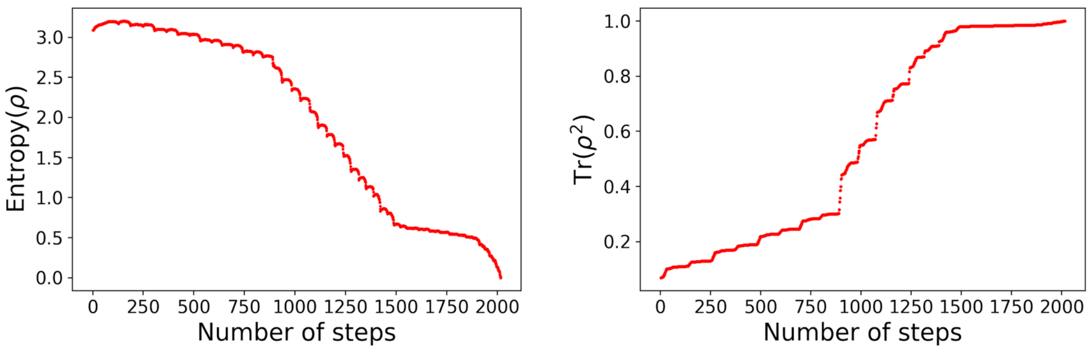

Figure 4. Entropy of the reconstructed density matrix (ρ) and trace of ρ^2 as a function of number of steps for reconstructing the full density matrix of a 6-qubit quantum circuit.

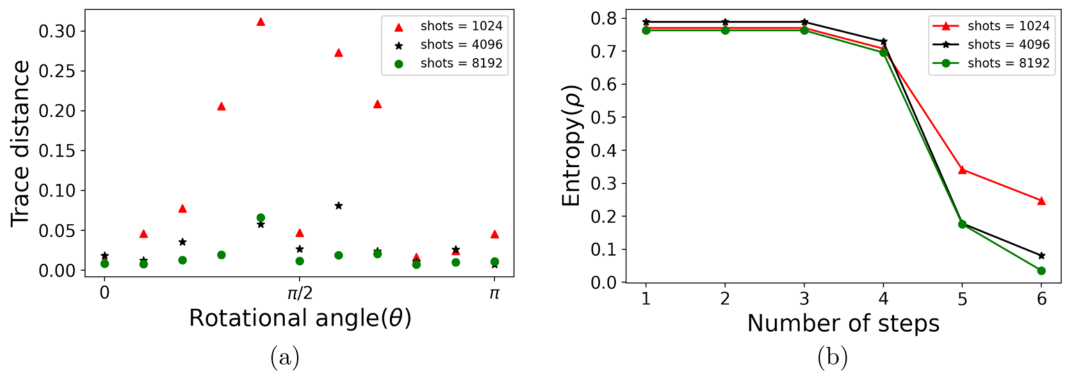

Figure 5. For the 2-qubit quantum circuit in Figure 6, these plots show that as the effect of statistical fluctuations in *qasm_simulator* is decreased upon increasing the number of shots, the reconstructed state is closer to the true state. (a) Trace distance between the true and the reconstructed state as a function of different rotational angles in R_x and R_y gates. (b) Entropy of the reconstructed density matrix as a function of the number of steps for complete reconstruction.

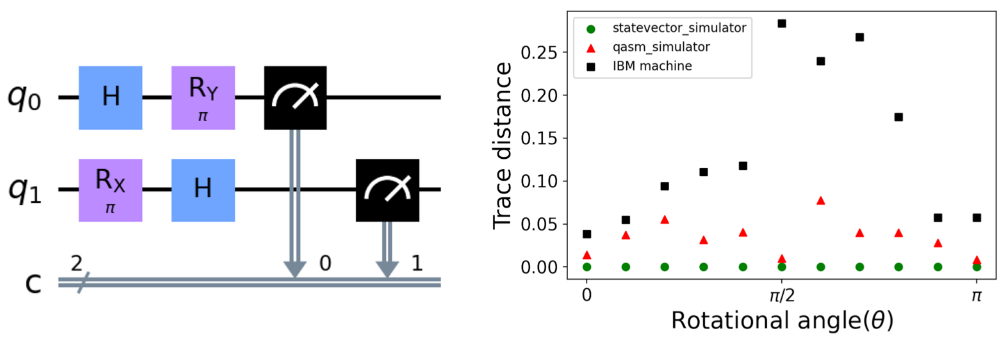

Figure 6. Trace distance between the true and the reconstructed state for the shown 2-qubit quantum circuit as a function of different rotational angles in the R_x and R_y gates for the three backends in Qiskit: *statevector_simulator*, *qasm_simulator*, and *IBM machine.*

state as a function of the rotational angles of the R_x and R_y gates for the various methods used for getting the input mean measurements. For simplicity of the calculations, the R_x and R_y rotational angles are kept the same. However, there is no limitation on the choice of the rotation angle of the R_x and R_y gates. The first method that we employed to obtain the mean measurements was the *statevector_simulator* backend in Qiskit in which we can get the final wave function of the simulated state, and therefore, the probabilities and coherences can be calculated directly. Since no noise is accounted for in this procedure, the reconstructed state matches exactly with the true state, and hence, the trace distance is zero.

Next we considered the noisy quantum circuit simulator backend in Qiskit, which is the *qasm_simulator* that encompasses statistical errors inversely proportional to the square root of the number of shots given for the circuit to be simulated. As is reflected in Figure 5, the impact of these statistical fluctuations is mitigated when we consider higher number of shots for simulating the quantum circuit on *qasm_simulator*. As expected, the reconstructed density matrix is closer to the true density matrix when higher numbers of shots are considered for performing the calculations. Also, the operator for calculating coherence unlike probability is not directly available for *qasm_simulator* as well as for the IBM machine and so we decompose the coherence operator into tensor products of Pauli matrices as discussed in[23,37,38] and thereby, obtain the coherences.

Lastly, we implemented our approach to reconstruct the density matrix for the quantum system corresponding to the state obtained upon running the circuit shown in Figure 6 on

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the 5-qubit IBM quantum computing chip: IBM Q 5 Yorktown.[36] In order to mitigate the measurement errors, we also employed the Qiskit's *ignis.mitigation.measurement* module which does so by constructing a calibration matrix. Considering the presence of noise in the quantum chips, the trace distance plot corroborates our approach of carrying out quantum state tomography for a general pure state with any number of qubits.

The current approach assumes that the available mean measurements belong to a pure state and so, in the presence of noise, the density matrix constructed out of the noisy data corresponding to the true state no longer represents a pure state, and therefore, the reconstructed state (from the noisy input mean measurements) and the noiseless true state differ considerably (in certain cases as shown in Figure 6) from each other. However, the method in itself leads to a single solution even if we change the order of the pairwise iterations in the case of noisy inputs. Even in the presence of noise, the method is scalable for higher number of qubits systems as well. The noise in the input data affects the convergence of the reconstructed state to a pure state, and therefore, we would not get the same level of accuracy while reconstructing the density matrix with noisy mean measurements as the input for the calculations. The accuracy of the method is sensitive to the accuracy of the input mean measurements obtained from the various input methods considered for the density matrix reconstruction. Since the errors in the mean measurements obtained from a real prototype IBM quantum chip are completely random, these errors are reflected while calculating the trace distance between the reconstructed state and the true state in Figure 6.

5. CONCLUDING REMARKS

In this study, we have shown the reconstruction of the density matrix of a pure state using expectation values of N observables consisting of a probability and $N - 1$ coherences. Our approach is based on the formalism of maximal entropy where the constraints for state determination are mean values of populations and coherences. This method provides us with an inference of the quantum state which is then compared with the original state to demonstrate the accuracy of our approach. Our approach focuses on the maximal entropy formalism of the scaled pairwise combinations of the known mean measurements to construct the whole density matrix. It is worth noting that the pairwise maximum entropy approach is invariant under the proposed scaling technique and invites a future fundamental investigation to figure out the origin of this scaling. The simple nature of our proposed formalism can find its application in a variety of different areas where quantum state tomography is essential. We intend to further study this approach to characterize and mitigate quantum gate errors that occur when running circuits on IBM's quantum computing chips. Also, the current approach to reconstruct the density matrix is applied and tested for pure states but it can be a good starting point for the reconstruction of mixed states as well. This is because the maximum entropy formalism was developed with mixed states in mind. What we have done is emphasized applications to pure states because these are often of interest in quantum computing. However, there are other physical situations where mixed states are to be expected.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.jpca.1c05884.

Scaling approach for accurate prediction of coherence (PDF)

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Notes

The authors declare no competing financial interest.
Raw data leveraged in the present study is available by request to the authors.

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