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Variational approach to quantum state tomography based on maximal entropy formalism

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Quantum state tomography is an integral part of quantum computation and offers the starting point for the validation of various quantum devices. One of the central tasks in the field of state tomography is to reconstruct, with high fidelity, the quantum states of a quantum system. From an experiment on a real quantum device, one can obtain the mean measurement values of different operators. With such data as input, in this report we employ the maximal entropy formalism to construct the least biased mixed quantum state that is consistent with the given set of expectation values. Even though, in principle, the reported formalism is quite general and should work for an arbitrary set of observables, in practice we shall demonstrate the efficacy of the algorithm on an informationally complete (IC) set of Hermitian operators. Such a set possesses the advantage of uniquely specifying a single quantum state from which the experimental measurements have been sampled and hence renders the rare opportunity not only to construct a least-biased quantum state but even replicate the exact state prepared experimentally within a preset tolerance. The primary workhorse of the algorithm is reconstructing an energy function which we designate as the effective Hamiltonian of the system, and parameterizing it with Lagrange multipliers, according to the formalism of maximal entropy. These parameters are thereafter optimized variationally so that the reconstructed quantum state of the system converges to the true quantum state within an error threshold. To this end, we employ a parameterized quantum circuit and a hybrid quantum-classical variational algorithm to obtain such a target state, making our recipe easily implementable on a near-term quantum device.

1 Introduction

The method of uniquely characterizing the quantum mechanical state of a quantum system based on a series of measurements of an informationally complete (IC) set of Hermitian operators is called quantum state tomography (QST)[1–5] and forms an important basis for testing and validating quantum devices. However, traditional approaches to QST are being exhausted to their limits[6] because of certain limitations that accompany those approaches. Some of these limitations correspond to the exponential scaling of traditional QST techniques with the system size, which in turn require exponential amounts of storage and processing power to carry out the computations. Along with this, since we are in the era of noisy intermediate-scale quantum (NISQ)[7] devices, the fidelity of measurements is also a limiting factor for performing state tomography efficiently since noisy measurements can lead to low fidelity of the reconstructed quantum state.[8] Another challenging task within the domain of QST is to reconstruct high fidelity quantum states[9] that can be used as a starting point while addressing problems in the field of condensed-matter physics and also in the validation of quantum technologies.[10] Several research approaches have already been proposed that attempt to address one or other limitation, which have paved the way for further advancements in this field. Some of these tomographic techniques include maximum likelihood estimation (MLE),[11,12] Bayesian mean estimation (BME),[13,14] quantum overlap tomography,[15] shadow tomography,[16,17] neural network tomography,[18–22] and others.[23–26] In our previous work we proposed a method of QST based on the formalism of maximal entropy from an incomplete set of measurements.[27,28] With that motivation, this research is an attempt to address the challenge of quantum state preparation in the field of QST based on a variational approach that can be easily implemented on a near-term quantum device.

The maximal entropy formalism[24,29,30] provides the most unbiased probability distribution, and is based on maximization of the von Neumann entropy of the system, subject to the constraints of the problem.[23,31–33] As a natural consequence,

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when combined with the method of Lagrange multipliers it leads to an expression of the density operator, given by eqn (1), that can serve as an optimal candidate for variational Gibbs sampling.[9] Inspired by this, the current work focuses on reconstructing the quantum state of a system, represented by the quantum Gibbs state and based on the formalism of maximal entropy, from the mean measurement values of an IC set of Hermitian operators. Sampling from a probability distribution corresponding to the quantum Gibbs state plays an important role in a variety of diverse fields within and not limited to many-body physics,[10,34] quantum simulations,[35] quantum optimization,[36] and quantum machine learning.[37,38] However, preparing the Gibbs state of a given Hamiltonian at arbitrary low temperature is not an easy task[39] and various approaches have been proposed, both classical and quantum,[40–43] to prepare the Gibbs state under certain specified conditions. Some of these techniques include algorithms based on quantum rejection sampling,[44] dynamics simulation,[45,46] and dimension reduction,[47] but the overhead quantum resource cost of implementing these approaches is very high and thus not suitable for execution on near-term quantum devices. In order to find applications of quantum algorithms on NISQ devices the underlying quantum circuit should be shallow with a low circuit depth and a low number of qubits. Variational quantum algorithms (VQAs)[48] are one such class of hybrid quantum-classical algorithms that follow a heuristic approach based on the variational principle, and they have been quite popular in the recent years[49–54] owing to their implementation on NISQ devices with shallow quantum circuits.

To prepare a quantum Gibbs state on a NISQ device using VQAs, several methods have been proposed.[55–60] In this work, we employed the approach of Wang *et al.*[39] wherein the loss function for preparing the Gibbs state on the quantum circuit involves the truncation of the Taylor series for the entropy, and which has been shown to prepare the Gibbs state for a given Hamiltonian with a fidelity of over 99%. The physical Hamiltonian of the system is unknown and is in fact unnecessary in this protocol. One only has access to the expectation values of the arbitrary set of Hermitian operators. In principle, using the formalism one can generate a least-biased quantum state that is consistent with such an arbitrary and even incomplete set of mean measurements, yet in this report we use an IC set for testing and validation with the hope of affording a near-exact reconstruction of the unknown pure quantum state used for sampling. This is attained by constructing a Hermitian matrix **H**, parameterized by Lagrange multipliers. The latter serve as a proxy Hamiltonian for the construction of the Gibbs state that represents the tomographic reconstruction of the state of the quantum system.

The hybrid quantum-classical tomographic protocol presented in this paper involves the application of shallow parameterized quantum circuits and is experimentally realizable on current-to-near-term quantum hardware. This in itself is advantageous over certain other tomographic protocols[11–14] as, upon optimization, the state is directly prepared on the quantum circuit and can be used further for quantum applications as per the requirement. Also, certain neural network-based state tomographic models work really well for real and entangled many-body quantum states, although their performance suffers for quantum states generated from random unitary operations.[18,19] As opposed to this, our variational approach to tomography is able to reconstruct, with high fidelity, not just real quantum states but also complex states with varying levels of entanglement as shown later in Fig. 6. The methodology is elaborately discussed in Section 2. To validate the proposed approach, the formalism is implemented in the IBM Qiskit[61] software development kit, and the results corresponding to the fidelity and trace distance between the reconstructed quantum state and the true state are shown in Section 3.

2 Methodology

The reconstruction of an unknown quantum state requires the information of a complete set of observables that are obtained through experimental measurements of Hermitian operators – usually defined as positive-operator-valued measures (POVMs). The formalism of maximal entropy provides a unique characterization of the quantum state subject to the expectation values of a given set of operators that serve as the constraints of the problem. It also ensures that the Von Neumann entropy of the proposed distribution is maximum under the given constraints. The maximal entropy formalism when combined with the method of Lagrange multipliers $\lambda_k \in \mathbb{C}^2$,[24,30] yields the following expression for the density operator of the unknown quantum state:[23,33]

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

where $\hat{f}_k$ corresponds to the operators whose expectation values are known, and $Z(\lambda_1, \ldots, \lambda_k) = \mathrm{Tr}\left(\exp\left\{-\sum_k \lambda_k \hat{f}_k\right\}\right)$ ensures normalization as $\mathrm{Tr}(\hat{\rho}) = 1$. In general, the formalism of maximal entropy outputs a mixed state that is parameterized by the Lagrange multipliers as shown in eqn (1). In our approach, since the target state is pure, these Lagrange multipliers are optimized such that the initial mixed state from the recipe gradually approaches idempotence during the training process and hence converges within an ε-neighborhood of the pure target state with ε being the error tolerance specified by the user. For example, consider the case a 2-qubit quantum system that can be uniquely described by the informationally complete (IC) set of Hermitian operators given by:

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

The expectation values of the four initial operators correspond to the probabilities, and the rest are the coherences of the 2-qubit quantum system.[32] The IC set of these operators can be obtained using linear combinations of Pauli string operators (σ_x, σ_y, σ_z, and σ_i):[27,62,63]

$$x_{11} = \langle|1\rangle\langle 1|\rangle = \frac{1}{4}(\sigma_z{}^2\sigma_z{}^1 + \sigma_z{}^2\sigma_i{}^1 + \sigma_i{}^2\sigma_z{}^1 + \sigma_i{}^2\sigma_i{}^1)$$

$$x_{12} = \langle|1\rangle\langle 2| + |2\rangle\langle 1|\rangle = \frac{1}{2}(\sigma_z{}^2\sigma_x{}^1 + \sigma_i{}^2\sigma_x{}^1)$$

$$x_{22} = \langle|2\rangle\langle 2|\rangle = \frac{1}{4}(\sigma_z{}^2\sigma_z{}^1 - \sigma_z{}^2\sigma_i{}^1 + \sigma_i{}^2\sigma_z{}^1 - \sigma_i{}^2\sigma_i{}^1)$$

and so on.

Analogous to the maximal entropy formalism, parameterized by a single parameter $\beta = 1/k_BT$ where k_B is the Boltzmann's constant and T is the temperature, the quantum Gibbs state for a given Hamiltonian H is defined as:

$$\hat{\rho} = \frac{\exp\{-\beta H\}}{\mathrm{tr}(\exp\{-\beta H\})}. \tag{3}$$

Constructing the Gibbs state of a given Hamiltonian on a parameterized quantum circuit requires minimization of the Helmholtz free energy described by the function:

$$F(\rho) = \mathrm{tr}(\rho \mathrm{H}) - \beta^{-1}S(\rho) \tag{4}$$

where $S(\rho) = -\mathrm{tr}(\rho \ln \rho)$ corresponds to the von Neumann entropy of ρ. However, the most challenging part of constructing the loss function that minimizes the free energy of the Hamiltonian is estimating the entropy of the parameterized quantum state.[64] In this work, to address the problem we adopted the method proposed by Wang *et al.*[39] wherein they used the Taylor series of entropy and truncated it at order K and, therefore, the truncated free energy is set as the loss function of the variational quantum algorithm. This method is practical in its implementation on a near-term quantum device as, essentially, the loss function involves estimating higher-order state overlaps, $\mathrm{tr}(\rho^k)$, that correspond to the truncated von Neumann entropy and can be carried out on a quantum device using swap tests.[55,65–68]

The core idea of the current research work stems from the combination of eqn (1) and (3), since in eqn (1) we are interested in maximizing the entropy by optimizing the unknown Lagrange multipliers λ_k according to the constraints of the expectation values of the set of Hermitian operators, and in eqn (3) we want to optimize the parameters of the quantum circuit to minimize the free energy that yields the quantum Gibbs state for a particular Hamiltonian. In our methodology, the exponent term in eqn (1) is a Hermitian matrix **H** that constitutes the Hamiltonian for which the Gibbs state given by eqn (3) is constructed on a quantum circuit using a variational algorithm. Thus, the hybrid variational quantum algorithm that is employed basically involves two levels of optimization that are termed the inner and outer optimization levels, as shown in Fig. 1. For a fixed set of Lagrange multipliers λ_k, the Hamiltonian **H** is constructed and passed onto the inner optimization level where the circuit parameters are variationally optimized using the truncated free energy as the loss function to yield a quantum Gibbs state corresponding to **H**. The constructed Gibbs state is then sent to the outer optimization level where the expectation values of the set of Hermitian operators are computed using the generated Gibbs state and then the Lagrange multipliers λ_k are updated so as to minimize the mean square error between the generated and true expectation values of the POVMs. The updated Lagrange multipliers

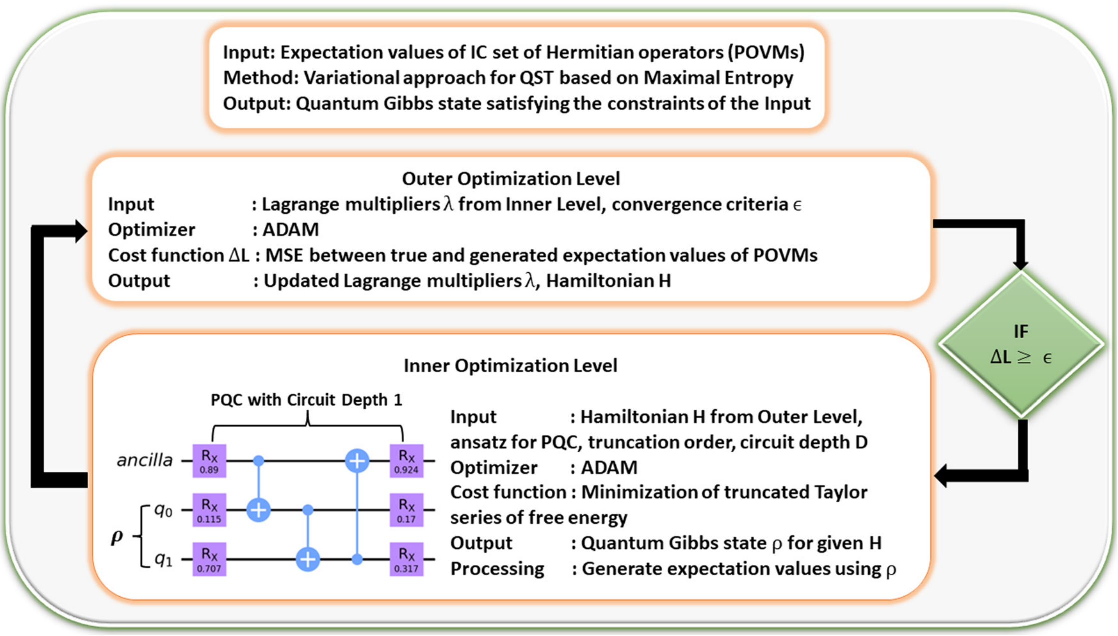

Fig. 1 Hybrid quantum–classical variational algorithm for quantum state tomography based on the formalism of maximal entropy.

yield the new proxy Hamiltonian **H** that is again sent back to the inner optimization level, and this process continues until convergence of the generated expectation values to the true values. This variational approach to QST based on maximal entropy is theoretically generalizable to any number of qubits.

The variational quantum circuit comprises of n-qubits that correspond to the size of the quantum system and also an additional ancilla qubit. The circuit incorporates a series of parameterized single qubit rotational gates on every qubit, and each qubit is entangled to the next qubit using controlled-NOT (CNOT) gates. This sequence of rotation and CNOT gates is repeated depending on the expressivity that is required to obtain high fidelity of the prepared quantum states. The scaling of the algorithm in terms of quantum resource allocation is strictly polynomial, since to reconstruct a generic n-qubit pure quantum state we require $n + 1$ qubits and $\mathcal{O}(Dn)$ quantum gates wherein D is the depth (number of repeating layers) of the circuit ansatz used.

Using the aforesaid procedure, in this work, we were able to obtain a high fidelity of 0.99 by setting $D = 2$ for a two-qubits system and $D = 6$ for a six-qubits quantum system. The choice of the single qubit rotational gates depends on whether the reconstructed state needs to be real or complex. In the case of real quantum states, parameterized R_y gates can be used; otherwise, for generalized complex states, one can choose R_x gates in the sequence.

3 Results and discussion

In this work we propose a variational approach based on maximal entropy formalism to perform quantum state tomography on a near-term quantum device. This procedure outputs a reconstructed quantum state that is prepared on a parameterized quantum circuit using the expectation values of an IC set of Hermitian operators as input. The approach is tested and validated through numerical simulations conducted on IBM's Qiskit[61] framework using its prototype quantum simulators for quantum systems consisting of up to 6 qubits. There are various backends available in Qiskit, and we used the noise-free statevector_simulator backend to corroborate the theory.

Different quantum circuits ranging from 2 to 6 qubits and consisting of one and two qubit quantum gates, such as rotational, Hadamard, CNOT gates, *etc.*, are used to prepare the sample states whose measurement statistics are reproduced using the reconstructed quantum state from the proposed maximal entropy based variational approach. Sample 4-qubit and 6-qubit quantum circuits are shown in Fig. 2. As discussed in Section 2, at the end of full execution of the inner optimization level, a quantum Gibbs state is generated that is used to calculate the expectation values of the considered Hermitian operators. The mean square error (MSE) between the generated and the true expectation values serve as the loss function for updating the Lagrange multipliers in the outer optimization level. The MSE loss is plotted as a function of the number of epochs in Fig. 3 for one example quantum state in each case of n-qubits (n = 2–6). As can be seen in Fig. 3, the MSE loss converges to zero faster for smaller systems and the convergence becomes more erratic as the size of the quantum system increases.

To perform quantum state tomography it is imperative that the reconstructed quantum state should be in close agreement with the true state. To demonstrate this, in the state preparation circuit, we also change the parameters of the single-qubit unitaries randomly for 20 different quantum states of n-qubits (n = 2–5) and 5 different quantum states for n = 6 qubits, keeping the number of CNOT gates fixed in each case. Observables from these states were subsequently used to train our algorithm and the corresponding fidelity of reconstruction was recorded. The latter is plotted as a function of the number of qubits (n) in Fig. 4. The variance associated with the reconstruction is indicated by the error bars of the box plots. In all cases we see that the lowest fidelity attained is 0.93. To show the convergence of fidelity with the number of epochs, a plot of fidelity between the reconstructed quantum state and the true state as a function of the number of epochs is shown in Fig. 5 for the different quantum systems with varying numbers of qubits for a single quantum state in each case. The figure shows the convergence of the reconstructed state to the true

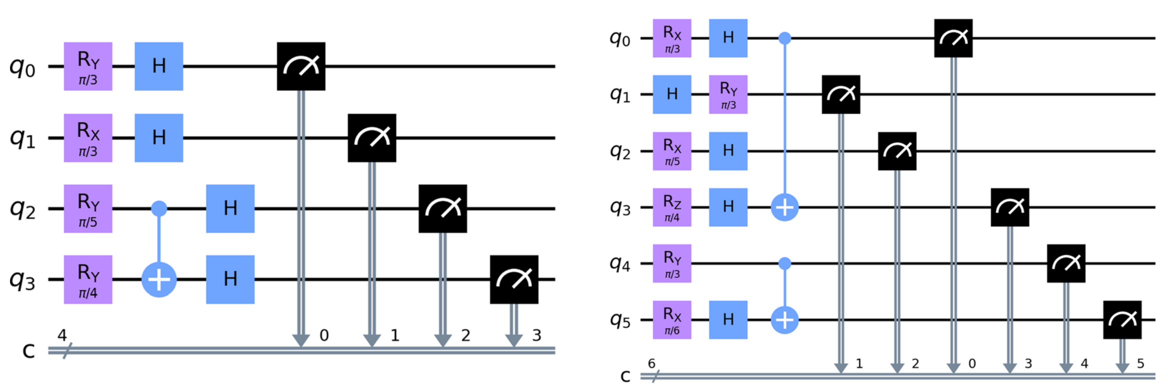

Fig. 2 Sample 4-qubit (left) and 6-qubit (right) quantum circuits for which the quantum states are reconstructed using the proposed approach based on maximal entropy formalism.

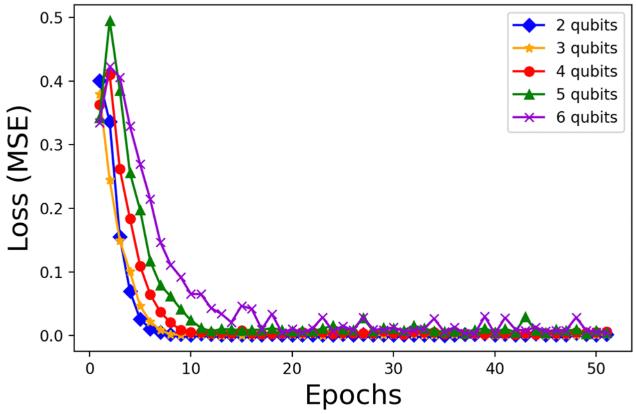

Fig. 3 For qubits ranging from 2 to 6, this plot shows the mean square error (MSE) loss as a function of the number of epochs between the true expectation values and the generated expectation values of the IC set of Hermitian operators, obtained using the reconstructed quantum state upon each step of optimization.

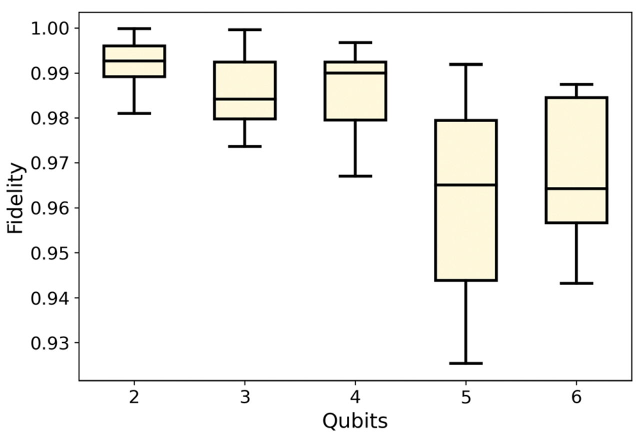

Fig. 4 Fidelity of the reconstructed quantum states with respect to the true states generated by randomly choosing the parameters of the rotational gates of the prototype quantum circuits for n-qubit (n = 2–6) systems.

state as the Lagrange multipliers are updated with each step, and the fidelity approaches 1.0 near the end of the optimization cycle. Another measure to test the performance of our approach is the trace distance between the true state (σ) and the reconstructed quantum state (ρ). The trace distance, which is given by $T(\rho,\sigma) = \frac{1}{2}\|\rho - \sigma\|_1$, is a measure of the closeness between two states. For the converged set of λ parameters for the same states considered for the fidelity plot, Fig. 5 shows the trace distance between the reconstructed quantum state and the true state, and as can be seen, the trace distance is below 0.05, which also validates the successful reconstruction of the quantum state.

To show the reconstruction accuracy of our model with respect to varying levels of entanglement within the system, we consider a 4-qubit system and vary the parameters of the rotational gates as well as the number of CNOT gates (*i.e.*, introducing different degrees of correlation among the sub-system qubits) in the state preparation unitary. A prototypical representative of such a quantum circuit for the validation of our approach is shown in Fig. 2(left). We compute the entanglement entropy of a 2-qubit reduced density matrix (2-RDM), defined by $S(^2\rho) = -\mathrm{Tr}(^2\rho\ln(^2\rho))/2\ln 2$, for each such quantum state. We also use observables sampled from each such quantum state to variationally train our algorithm and create a maximal-entropy representation of the target state. A plot for the fidelity of operation *vs.* $S(^2\rho)$ is displayed in Fig. 6. We see that the performance of our algorithm is a non-monotonic function of $S(^2\rho)$. The plot also explicitly shows that our algorithm is capable of correctly obtaining the target state with high fidelity, even when the sub-system entropy on the *abscissa* is high, indicating a higher degree of correlation.

4 Concluding remarks

In this research we have shown the successful reconstruction of the quantum state based on a variational approach to QST utilizing the formalism of maximal entropy, which can easily be implemented on a near-term quantum device. The reconstructed state can reproduce the measurement statistics of the IC set of Hermitian operators that are considered while formulating the cost function for updating the variational parameters of the Hamiltonian arising from maximal entropy. High levels of fidelity between the converged state and the true state for all the considered quantum systems, as well as low values for the trace distance, depict the validation of the proposed approach for QST. This proposed variational approach can be applicable to a variety of different directions where QST is essential. For example, we intend to study this approach further for analyzing, characterizing, and mitigating single- and double-qubit quantum gates' errors while running computations on prototype quantum devices. Recently, noise fingerprints developed on a prepared stationary state were used to identify and understand the underlying noise profile of NISQ devices that causes the state to develop non-stationary character.[69] This characterizes an effective bath generated by the noise that exhibits both colored noise and non-Markovian behavior, and therefore can be used for mitigating noise errors in quantum simulations. Although our variational approach has not yet been used for denoising, a possible extension of the above work in the context of the protocol presented in the paper could be as follows: given the power-spectral density (PSD) of the noise (from the analysis of the article cited), can one train our algorithm using noisy estimates of observables and yet reconstruct the true state with high precision? It is well-known that variational algorithms are robust against coherent/parametric types of noise,[70] but the PSD can include fingerprints of both incoherent (depolarizing errors) and coherent noise. Access to the spectral information as contained in the PSD can characterize the noise and could possibly enable us to reconstruct observables for the true state *via* appropriate

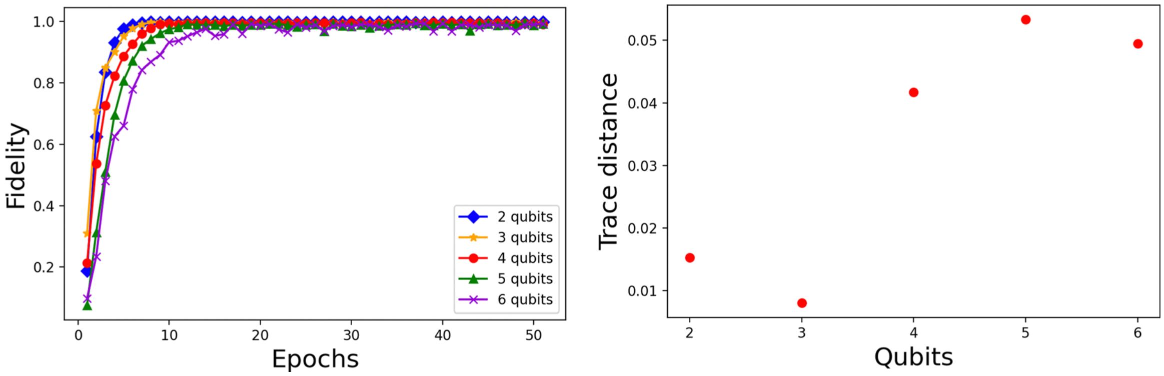

Fig. 5 As a measure of convergence, the fidelity between the true state and the final reconstructed quantum state is plotted as a function of the number of epochs (left), and the trace distance between the two states, obtained using the converged Lagrange multipliers at the end of the optimization process, is plotted against the number of qubits (right). The fidelity close to 1.0 and the trace distance close to 0.05 at the end of the optimization cycle show that the proposed method based on maximal entropy formalism is able to successfully reconstruct the quantum state using the experimental mean measurement values of the IC set of operators.

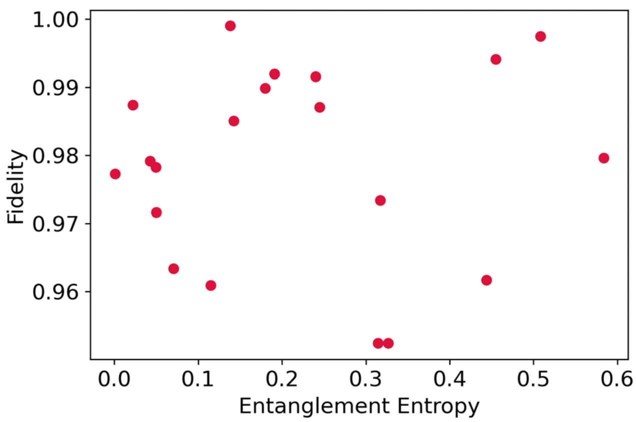

Fig. 6 For 4-qubit quantum states with varying levels of entanglement within the system as demonstrated by 2-qubit RDM entanglement entropy, the fidelity of the reconstructed quantum state is plotted. The high fidelity of reconstruction, even in the case of entangled quantum systems, validates the proposed tomographic approach for general state reconstruction.

averaging over the underlying distribution function from which the noise is sampled. This method can also be used as an efficient approach for sampling the Gibbs state and, therefore, can serve as a starting point for preparing targeted quantum states for quantum simulations.

Data availability

The data generated during the current study are available from the corresponding author upon reasonable request.

Author contributions

S. K. and R. D. L. designed the model and the computational framework. R. G. and M. S. developed the theory and performed the calculations. All authors analyzed and discussed the results and contributed to the final version of the manuscript.

Conflicts of interest

There are no conflicts to declare.

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