

## Reconstructing Complex States of a 20-Qubit Quantum Simulator

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A prerequisite to the successful development of quantum computers and simulators is precise understanding of the physical processes occurring therein, which can be achieved by measuring the quantum states that they produce. However, the resources required for traditional quantum state estimation scale exponentially with the system size, highlighting the need for alternative approaches. Here, we demonstrate an efficient method for reconstruction of significantly entangled multiqubit quantum states. Using a variational version of the matrix-product-state ansatz, we perform the tomography (in the pure-state approximation) of quantum states produced in a 20-qubit trapped-ion Ising-type quantum simulator, using the data acquired in only 27 bases, with 1000 measurements in each basis. We observe superior state-reconstruction quality and faster convergence compared to the methods based on neural-network quantum state representations: restricted Boltzmann machines and feed-forward neural networks with autoregressive architecture. Our results pave the way toward efficient experimental characterization of complex states produced by the quench dynamics of many-body quantum systems.

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### I. INTRODUCTION

Quantum computers and simulators have the potential to solve computationally difficult problems by utilizing the controllable dynamics of engineered quantum systems [1–4]. The latest programmable quantum simulators—in particular, those based on cold atoms [5] and trapped ions [6]—have been used to explore quantum many-body phenomena close to the threshold of what it is possible to simulate using classical resources [7–14]. The development of such technology hinges on our understanding of the physical processes within the quantum device at the level of both individual qubits and the entire system. In order to deepen this understanding, we ought to be able to

measure, characterize, and reconstruct the states produced in that device—i.e., to master the art known as quantum state tomography (QST) [15].

QST becomes increasingly challenging due to the exponential scaling of the number of required measurements and computational resources with the size (number of qubits) of a quantum system. This gives rise to a qualitatively new requirement: to reconstruct the state using incomplete measurement data in a computationally efficient manner. Addressing this challenge is of importance for further progress in quantum simulation and, as a consequence, understanding complex and nontrivial quantum many-body phenomena.

Large quantum systems can be tackled by means of so-called variational approaches. Their idea is to represent a high-dimensional quantum state with an ansatz that is dependent on much fewer parameters than the dimension of the Hilbert space under consideration. By using standard iterative optimization methods, these parameters can be adjusted such that the corresponding quantum state becomes optimal with respect to a criterion of interest,

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which in the context of QST would be the likelihood of the measurement data acquired.

In this work, we apply variational approaches to perform tomography of complex multiqubit quantum states produced in a  $N = 20$ -qubit trapped-ion quantum simulator, which corresponds to a Hilbert space of dimension  $2^{20} \approx 10^6$ . The system evolves under the action of an engineered many-body Hamiltonian [10] generating highly entangled states. Efficiently characterizing these states poses a current challenge due to their nonsymmetrical nature, which distinguishes them from highly symmetric states such as Greenberger-Horne-Zeilinger (GHZ) or  $W$  states, for which effective tomographic methods are available. Nevertheless, successful state reconstruction is achieved in spite of very limited data (statistics collected over 27 bases, with 1000 measurements in each basis).

In our present work, we compare the performance of three methods that belong to the following two classes: the matrix-product states (MPS) ansatz and two neural-network quantum state (NNQS) ansätze, a restricted Boltzmann machine and an autoregressive neural network. Both classes have their advantages and shortcomings. The MPS ansatz is easier to train but works best on chains of qubits with short-range one-dimensional (1D) correlations (more generally, area-law entanglement scaling) and a limited degree of entanglement [16,17]. In fact, a version of the MPS ansatz has been shown to fail on the specific system studied here [10]. On the other hand, NNQSs are more expressive [18] and have been shown to work well on states with volume-law entanglement scaling [19–21]. However, they are more difficult to train: they require sampling and, furthermore, transforming the sampled state into the measurement basis results in the emergence of an exponential number of terms. Therefore, there is no obvious answer to the question of which ansatz is more suitable in our case.

Our results unequivocally demonstrate that MPS surpasses both neural networks in terms of likelihood for the experimental data and in terms of fidelity for simulated ones. We believe this to be a consequence of the 1D geometry and short-range character of interactions in our trapped-ion simulator. To illustrate this point, at the end of the paper we provide an example of a volume-law scaling state the tomography of which can be successfully achieved with NNQS but fails with MPS.

## II. SETUP AND MEASUREMENT BASES

We study quantum states of a 20-qubit trapped-ion system, which is described in Ref. [10], at eight different time points during its evolution. We briefly recap the description of the experiment. The setup is based on the controllable 1D array of  $^{40}\text{Ca}^+$  ions, which are confined in a linear Pauli trap with an axial (radial) center-of-mass vibrational

frequency of 220 kHz (2.712 MHz) [22]. More information about the state preparation and measurement process can be found in Ref. [10]. The computational qubit basis consists of the states  $|S_{J=1/2; m_j=1/2}\rangle$  and  $|D_{J=5/2; m_j=5/2}\rangle$ , connected by an electric quadrupole transition at 729 nm. The leakage rates outside this qubit manifold are on a scale of 1 Hz [23], i.e., negligible in comparison with the time scales with which we are working here.

The qubit interactions under the influence of laser-induced forces are well described by the  $XY$  model in a dominant transverse field  $B$ , with the following Hamiltonian:

$$\hat{\mathcal{H}} = \hbar \sum_{i < j} J_{ij} (\sigma_i^+ \sigma_j^- + \sigma_i^- \sigma_j^+) + \hbar B \sum_j \sigma_j^z, \quad (1)$$

where  $J_{ij}$  is the  $N \times N$  qubit-qubit coupling matrix,  $\sigma_i^+$  ( $\sigma_i^-$ ) is the qubit raising (lowering) operator for qubit  $i$ , and  $\sigma_j^z$  is the Pauli  $Z$  matrix for qubit  $j$ . The coupling strengths fall approximately according to a power law  $J_{ij} \propto 1/|i-j|^\alpha$  with the distance  $|i-j|$ , where  $\alpha \approx 1.1$ . The 20-qubit register is initiated to a Néel-ordered product state  $|\Psi(0)\rangle = |1, 0, 1, \dots\rangle$ . It is then expected to evolve according to the Schrödinger equation

$$|\Psi_{\text{th}}(t)\rangle = e^{-i\hat{\mathcal{H}}t} |\Psi(0)\rangle. \quad (2)$$

The interaction initially gives rise to entanglement among neighboring qubits, which then spreads over the entire quantum register [24]. This evolution is affected by experimental imperfections and decoherence. However, the chosen experimental regime creates a decoherence-free subspace during the evolution [25]. Residual decoherence from imperfections in the laser-ion interaction is much slower than the evolution time scales studied here; hence it is fair to assume that the state purity does not degrade on these time scales.

The set of measurement bases is defined by the observables of the form  $\sigma_a \otimes \sigma_b \otimes \sigma_c \otimes \sigma_a \otimes \dots \otimes \sigma_c$  of periodicity  $k = 3$  and length 20, with  $a$ ,  $b$ , and  $c$  being all 27 possible sequences of  $X$ ,  $Y$ , and  $Z$ . This choice of the basis set has been made in Refs. [10,24], motivated by its sufficiency to observe genuine multipartite entanglement in groups of up to five qubits. By increasing the periodicity of the basis pattern, one could capture the entanglement in longer groups. This would become necessary for longer evolution times under the nearest-neighbor Hamiltonian, since the correlation length grows with time. Given knowledge of the speed at which the correlations propagate through the system, one can theoretically predict the correlation length and hence the period of the measurement basis sufficient for reliable characterization of the quantum state [26].

In this work, we use the same measurement data set as in Ref. [10], which includes 1000 measurements per basis

(limited by the stability of the experimental setup). As we show here, this set is sufficient for QST of the 20-qubit system.

### III. VARIATIONAL MANY-BODY STATE TOMOGRAPHY

The complete description of any pure quantum system constituting  $N$  qubits is given by  $|\Psi\rangle = \sum_{\mathbf{s}} \Psi(\mathbf{s})|\mathbf{s}\rangle$ , where  $\Psi(\mathbf{s})$  represents the probability amplitude corresponding to the computational basis element  $\mathbf{s} \equiv (s_1, s_2, \dots, s_N)$ , where  $s_i = 0$  or  $1$ , which we refer to as the bit configuration. Our goal is to reconstruct a useful many-body pure quantum state  $|\Psi_W\rangle$ , which maximizes the probability (likelihood) of having acquired the given measurement data. For numerical stability of gradient descent, it is more convenient to minimize the negative logarithm of that probability, which we hereafter refer to as the loss function:

$$\Xi = - \sum_{p=1}^K \sum_{m=1}^{M_p} \ln \left( |\langle \psi_m^p | \Psi_W \rangle|^2 + \varepsilon \right), \quad (3)$$

where  $K = 27$  is the number of measurement bases,  $M_p = 1000$  is the number of measurements per basis, and  $|\psi_m^p\rangle$  is the outcome of the  $m$ th projection measurement in  $p$ th basis. A small term  $\varepsilon = 10^{-10}$  is added to improve the reconstruction stability, as discussed in the Supplemental Material [27]. The subscript  $W$  in  $|\Psi_W\rangle$  defines the set of parameters of the variational ansatz used. In this study, the size of  $W$  has been chosen to be approximately 4000 in each ansatz. At first, the parameters  $W$  are randomly initialized and then they are adjusted (trained) to minimize the negative log-likelihood (see Eq. (3)) by gradient descent.

To prevent overfitting, we split the measurement data into two sets, training and test, in the ratio 4:1 [28]. Specifically, we consider the first 800 measurements in each basis to be the training data and the remaining 200 measurements to be the test data. The loss function is optimized on the training set and the test set is used to validate the performance of different methods. The training process is stopped as soon as the loss on the test set reaches its minimum.

An essential component of multiqubit tomography is the transformation (rotation) of the variational state  $|\Psi_W\rangle$  into the measurement basis required to compute the probability of each measurement outcome. We can express this mathematically as

$$\langle \psi_m^p | \Psi_W \rangle = \langle \mathbf{j}_m^p | \hat{U}_p | \Psi_W \rangle, \quad (4)$$

where  $|\mathbf{j}_m^p\rangle$  is the state in the computational basis defined by the bit string yielded by the measurement and  $\hat{U}_p$  is the rotation between the computational basis and the  $p$ th measurement basis. The problem is that an arbitrary rotation

can, in principle, lead to a vector with exponentially many terms, even if the initial state contains only a polynomial number of nonzero components. We address this problem differently for the MPS and NNQS ansätze.

### IV. MATRIX-PRODUCT STATES

A matrix-product state is a tensor network, which represents each amplitude in a quantum state as a product of matrices,

$$|\Psi_{\text{mps}}\rangle = \sum_{\mathbf{s}} \left[ A_{s_1}^1 A_{s_2}^2 \cdots A_{s_N}^N \right] |s_1 s_2 \dots s_N\rangle, \quad (5)$$

where  $A_{s_i=0}^i$  and  $A_{s_i=1}^i$  are the complex matrices corresponding to the  $i$ th qubit. The sizes of these matrices are hyperparameters of the MPS ansatz, which are referred to as bond dimensions. In our work, the matrices  $A_{s_1}^1$  and  $(A_{s_N}^N)^\top$  are of size  $1 \times 2$ ,  $A_{s_2}^2$  and  $(A_{s_{N-1}}^{N-1})^\top$  are of size  $2 \times 4$ ,  $A_{s_3}^3$  and  $(A_{s_{N-2}}^{N-2})^\top$  are of size  $4 \times 8$ ,  $A_{s_4}^4$  and  $(A_{s_{N-3}}^{N-3})^\top$  are of size  $8 \times 10$ , and all others are of size  $10 \times 10$  [29]. The maximal bond size of 10 is chosen as a hyperparameter.

Our ansatz differs from a previous study on the applicability of MPSs for QST of trapped-ion qubits [24]. In that work, Lanyon *et al.* have implemented full mixed-state tomography of each neighboring qubit triplet in ion chains of sizes up to  $N = 14$  and then found a pure-state MPS that approximates the combined set of these three-qubit density matrices. This approach has been motivated by the existence of a lower bound on the fidelity between the reconstruction and the true state [30]. For 20-ion chains, this bound has been found to be low, leading to the conclusion that ‘‘MPS tomography failed to produce a useful pure-state description in our present 20-qubit system’’ [10]. However, this conclusion only applies to the specific QST strategy of Ref. [24]. This strategy, while allowing for full characterization of each triplet of neighboring qubits and hence estimating the lower bound on fidelity, does not account for the information on long-range correlations, which can be acquired through simultaneous measurements on all qubits. Our present ansatz addresses this shortcoming.

A significant benefit of the MPS approach to QST is the simplicity of rotating the state to the measurement basis (provided that the basis is local, i.e., is obtained from the computational basis by means of single-qubit rotations, as it is in our case). The matrices  $(A_{s_i}^i)$  and  $(A_{s_i}^i)'$  defining the states  $|\Psi_{\text{mps}}\rangle$  and  $\hat{U}_p |\Psi_{\text{mps}}\rangle$  are related according to

$$(A_{s_i}^i)' = \sum_{s_i'=0}^1 \hat{V}^i_{s_i s_i'} A_{s_i'}^i, \quad (6)$$

where  $\hat{V}^i = e^{i\pi/4\hat{\sigma}^i}$  is the  $2 \times 2$  matrix defining the SU(2) rotation to the measurement basis of the  $i$ th qubit,

which corresponds to the observable  $\hat{\sigma}^i$  [16], and the measurement-basis index  $p$  is omitted for brevity. Consequently, the likelihood given in Eq. (3) can be directly expressed in terms of the ansatz parameters and the bit strings with the measurement results.

## V. NEURAL NETWORKS

Here, we utilize two different NNQS ansätze, specifically, a restricted Boltzmann machine (RBM) and an autoregressive neural network (ARN). Both neural networks have two functions: inference and sampling. When used for inference, the neural network outputs the probability amplitude  $\Psi(\mathbf{s})$  for an input bit configuration  $\mathbf{s}$ . When used for sampling, the neural network outputs bit-configuration samples of the probability distribution  $|\Psi(\mathbf{s})|^2$ . The network has to be run multiple times to produce a large ensemble of samples, which approximates the state vector  $|\Psi\rangle = \sum_{\mathbf{s}} \Psi(\mathbf{s})|\mathbf{s}\rangle$ . The loss function in Eq. (3) can then be computed from this vector and the neural-network parameters can be adjusted to minimize it. The two networks are different in construction and functionality; here, we present a brief literature overview for both types of NNQS and the details of our implementation thereof. A more detailed introductory discussion is provided in the Supplemental Material [27].

RBM has been used for a large variety of quantum state analysis problems [19,31–38]; in particular, for QST in both discrete- and continuous-variable settings [39–42]. However, RBMs have their limitations: there is a known class of physically interesting quantum states that cannot be efficiently approximated by this ansatz [43]. In addition, the probability amplitudes output by the RBM are unnormalized, requiring a special procedure for estimating the partition function during training.

In contrast, the ARN approach gives normalized amplitudes explicitly [44], leading to an effective and unbiased sampling procedure. The ARN method has recently been used for solving quantum many-body problems [45]; in particular, in quantum chemistry [46]. A further advantage of ARN is its ability to generate nonredundant samples only, which greatly reduces the required computational resources [46].

We use two RBMs of identical architectures for the amplitudes and phases of qubit configurations, as proposed in the original work by Carleo and Troyer [31]. Each RBM has 100 hidden units, with the sampling implemented via one-step persistent contrastive divergence [47,48], i.e., such that the samples from each previous iteration are reused in the next one. Our ARN consists of two hidden layers with the size of each layer equal to  $N = 20$  as required by the autoregressive architecture (see the Supplemental Material [27]). To enhance the expressibility of the network, each unit in the hidden layers is a cluster of three numbers *à la* Refs. [49–51]. Each unit of the output layer is

a cluster of two numbers corresponding to the conditional amplitude and phase of the spin configuration. The ADAM optimizer [52] with the learning rate  $\gamma = 0.005$  is used for reconstructions. Convergence of the ARN ansatz is typically achieved in less than 1000 epochs, with a run time of around 30 min, using a single NVIDIA V100 Volta-based card, and a memory requirement of no more than 4 GB. Under the same conditions, 10 000 epochs are needed to reach the same level of convergence of the RBM ansatz.

To address the qubit-rotation issue in the NNQS ansatz, we again use the fact that all measurement bases are local. Denoting  $\mathbf{j}_m^p = j_1 \dots j_N$  and  $\hat{U}_p = \hat{V}_1 \otimes \dots \otimes \hat{V}_N$  and recalling that  $|\Psi\rangle = \sum_{\mathbf{s}} \Psi(\mathbf{s})|\mathbf{s}\rangle$  with  $|\mathbf{s}\rangle = |s_1 \dots s_N\rangle$  (where the  $|\mathbf{s}\rangle$  in this case are the sampled bit configurations), the overlap in Eq. (4) can be written as

$$\begin{aligned} \langle \mathbf{j}_m^p | \hat{U}_p | \Psi_w \rangle &= \sum_{\mathbf{s}} \Psi(\mathbf{s}) \langle j_1 \dots j_N | \hat{V}_1 \otimes \dots \otimes \hat{V}_N | s_1 \dots s_N \rangle \\ &= \sum_{\mathbf{s}} \Psi(\mathbf{s}) \langle j_1 | \hat{V}_1 | s_1 \rangle \times \dots \times \langle j_N | \hat{V}_N | s_N \rangle. \end{aligned} \quad (7)$$

We see that the overlap is a product of  $N$  complex numbers, which must be calculated  $K \times M_p \times |\{\mathbf{s}\}|$  times, where  $K$  represents the number of measurement bases and  $|\{\mathbf{s}\}|$  is the number of unique samples produced by NNQS. This calculation becomes tractable provided that the NNQS with the given  $|\{\mathbf{s}\}|$  is expressive enough to represent the optimal state of interest.

## VI. RESULTS

The central column of Fig. 1 shows the qubit values and their correlations obtained from the states  $|\Psi_w(t)\rangle$  reconstructed by the MPS corresponding to eight moments in time ranging from  $t = 0.0$  to 3.5 ms with a 0.5 ms interval, for which the measurements are performed. For comparison, we show the results corresponding to the theoretically expected evolution according to the Hamiltonian of Eq. (2) [10] (left column) and the direct measurement results (right column). We see that the agreement between the reconstructed state and the data is much better than that between either of the two and the theoretical model. In the Supplemental Material [27], we estimate the statistical uncertainty of our reconstruction and find that the deviation from the theoretical state is statistically significant [53].

Figure 2 shows the comparison between the loss given in Eq. (3) on the test sets for the states reconstructed via MPS and the two NNQS ansätze. We observe that the ARN and RBM exhibit comparable performance, while the MPS generally performs better.

The above results do not yet present compelling evidence of the reconstruction quality, as the states that generated the measurement data—the *ground truth* for

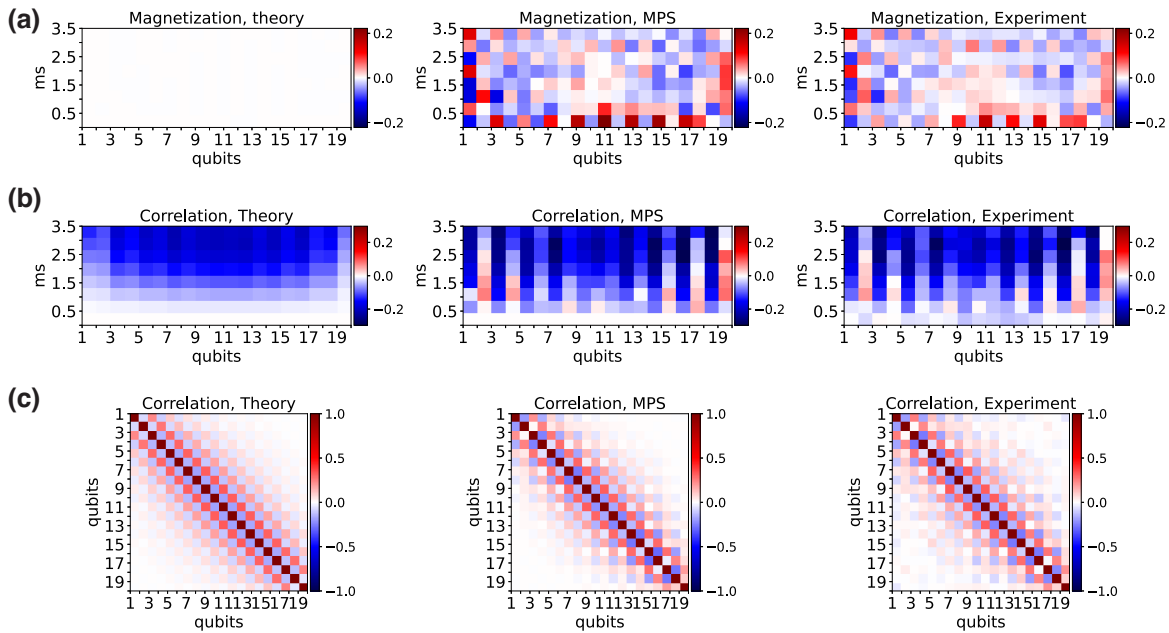


FIG. 1. The estimation of observables in the experimental and reconstructed states. For the observable  $\hat{\sigma}_Y$ , (a) single-qubit expectation values ( $Y_i$ ), (b) correlations for neighboring qubits ( $Y_i Y_{i-1}$ ), and (c) full pairwise correlations ( $Y_i Y_j$ ) are shown. The vertical axes in (a) and (b) enumerate the eight moments in time for which the measurements have been made; the data in (c) correspond to  $t = 3$  ms. The left columns show the theoretically expected evolution given in Eq. (2), the central column the experimental MPS reconstruction, and the right column is obtained directly from the experimental data. The empty rectangle in the left column of (a) means that the theoretically expected magnetization is constantly zero.

the machine-learning problem—are not known. Hence, in addition to QST based on experimental data, we perform a series of independent numerical experiments in which we

reconstruct a state from simulated measurement data generated from the theoretically expected state according to Eq. (2) in the given 27 measurement bases. This allows us to quantify the fidelity of the reconstructed states with the true underlying state, as shown in Fig. 3. We observe again that the reconstruction fidelity  $|\langle \Psi_{th}(t) | \Psi_W(t) \rangle|^2$  obtained with the MPS consistently surpasses the neural-network methods for all evolution times. Importantly, Fig. 3 shows that despite the low number of experimental shots, the reconstruction fidelity of the NNQS ansatze improves significantly with an increased number of samples drawn from the neural network for each training step. For all methods, the fidelity also decreases with increasing time  $t$  as the evolving state becomes more complex.

As shown above, MPS outperforms NNQSs in terms of likelihood for the experimental data and in terms of fidelity for the simulated one. One can suspect two possible reasons for that: insufficient expressive power of NNQS methods or failure of training. To resolve this dichotomy, we test for insufficient expressivity by training the NNQSs to directly maximize the fidelity with the theoretical ground-truth states rather than the likelihood of the simulated measurement data. As a result, we have obtained fidelities exceeding 99% for all eight states of the time evolution. We note that the training on simulated data is merely for developing a better understanding of the behavior of the NNQSs and has not been used when reconstructing experimentally measured quantum states.

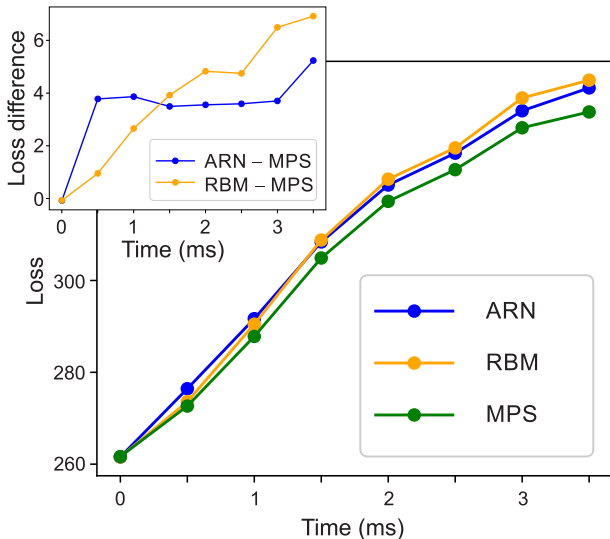


FIG. 2. A comparison of the loss (negative log-likelihood) on the test data for the experimentally reconstructed states. The data shown represent different evolution times in the experiment and different reconstruction methods. For each point, the number of samples drawn from the NNQS ansatze is 30 000. The inset shows the difference of the three methods.

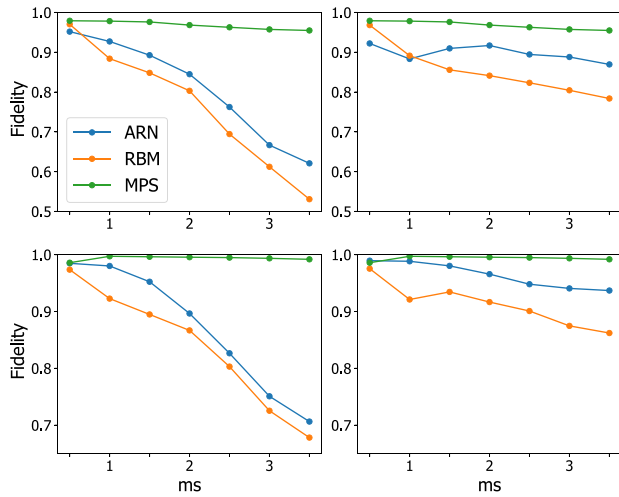


FIG. 3. The fidelities of the states reconstructed from the simulated data generated from the theoretical states given in Eq. (2), with respect to these states. The performance of the NNQS ansatz improves with the number of samples drawn from the NN during training: left, 25 000 samples; right, 300 000 samples. For all methods, the performance improves with the number of experimental shots: top, 1000 shots; bottom, 10 000 shots.

These results indicate that the neural-network ansatz are in principle sufficiently expressive, meaning that there exists a parameter set for which the NNQS is able to approximate the ground-truth state to within 1% fidelity, at least for the simulated data. This is consistent with the conclusion of Refs. [19,54] that neural networks are able to represent a wide range of quantum states. Moreover, these states demonstrate lower loss on the simulated data sets than the NNQSs trained to maximize the likelihood. These observations lead us to conclude that the poorer performance of the NNQS is likely attributed to their challenging training. We assume that this is due to a complex loss-function landscape in the NNQS parameter space. The

improvement of NNQS fidelity with more data could then be due to this landscape getting smoother with fewer local optima, so the neural network becomes easier to train.

Figure 4 shows the analysis of overfitting in our training process. The loss on the training set monotonically decreases with training [Fig. 4(a)], while the loss on the test set, previously unseen by the reconstruction algorithm, starts to increase at some point during training [Fig. 4(b)]. This is because the measurement data are samples of a statistical distribution associated with the quantum state. Maximizing the likelihood for a specific set of samples may result in a reconstructed state that is overfitted to this sample [55,56]. Validating the reconstructed state on the test data set enables us to control this overfitting.

As seen in Fig. 4(b), the lowest loss on the test set corresponds to the maximum of the fidelity curve [Fig. 4(c)]. This indicates that monitoring the loss on the test set is a good independent indicator for deciding when to stop the training to prevent overfitting, particularly in the case of the ARN, which shows a pronounced dip (peak) in the loss on the test set (fidelity with the true states) in Fig. 4.

We observe that MPS trains significantly faster than NNQSs.

## VII. MPS IS NOT ALWAYS BETTER

The above results demonstrate the advantage of the MPS ansatz, which is made manifest in both faster convergence and a higher reconstruction quality. This advantage is a consequence of our system being a 1D qubit chain with area-law entanglement scaling dynamics, which falls within the scope of this ansatz. One should keep in mind, however, that this scope is quite limited. For example, its performance can drop significantly if the entanglement of the state scales according to the volume law, in which case exponential bond dimension scaling is required [16]. To illustrate this point, we apply QST to a 1D state with

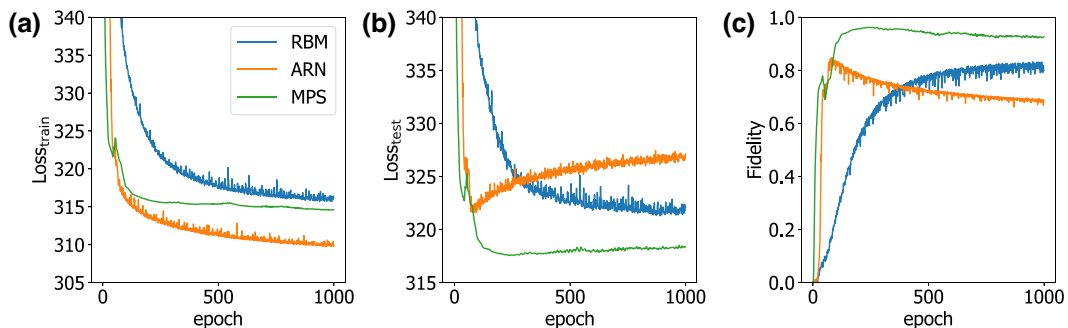


FIG. 4. The learning curves (the progress in the loss function and fidelity in the process of learning) for different ansatz reconstructing  $|\Psi_{\text{th}}(t = 2.5 \text{ ms})\rangle$  from simulated data with 1000 measurements per basis. Losses on the (a) training and (b) test sets are shown, as well as (c) the fidelity between the reconstructed and ground-truth states. The number of samples drawn from the NNs during training is 300 000. The observed kinks are a consequence of automatic adjustment of the learning rate by the ADAM optimizer.

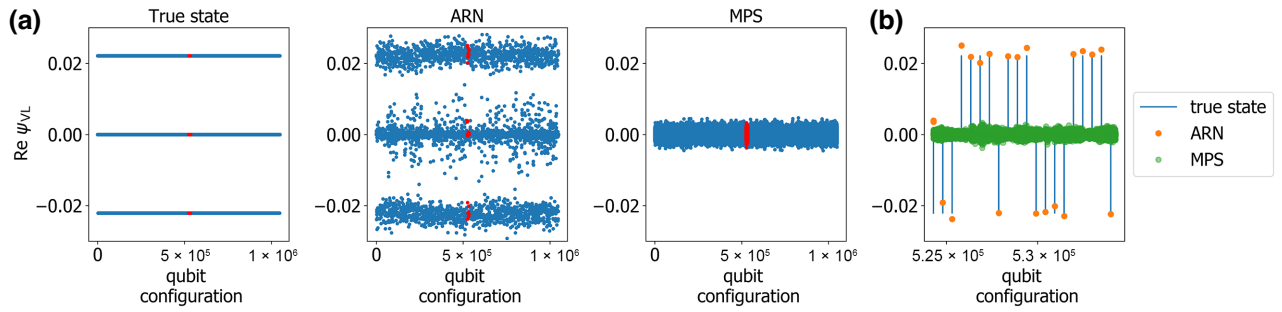


FIG. 5. QST reconstruction of the volume-law state of Eq. (8) from simulated data. The horizontal axis indexes bit configurations from 1 to  $2^{20}$ , while the vertical axis shows the real part of the corresponding amplitude. (a) The amplitudes for the entire set of possible spin configurations. (b) The data for a small interval of bit strings, showing consistency between the true state and reconstructions. The corresponding points in (a) are shown in red.

volume-law scaling discussed in Ref. [19]:

$$|\Psi_{\text{VL}}\rangle = \frac{1}{2^{N/4}} \sum_{\mathbf{s}} (-1)^s |\mathbf{s}\mathbf{s}\rangle, \quad (8)$$

where the summation is over all possible bit strings  $\mathbf{s}$  of length  $N/2$  and the allowed configurations of the  $N$  qubits are such that the first half of the string is identical to the second. We artificially generate 1000 outcomes per basis for the same set of 27 measurement settings and reconstruct the state via MPS and ARN, resulting in fidelities of 0.000081% and 88.1%, respectively. The amplitudes of the underlying ideal state of Eq. (8) and of the reconstructed states are depicted in Fig. 5. Hence, the results presented in this work ought not to be viewed as an argument against the ability of NNQS to represent complex multidimensional entangled states.

## VIII. CONCLUSIONS

We have performed quantum state reconstruction of a 20-qubit state (in the pure-state approximation), which, to our knowledge, is the largest experimental system to which QST has been applied [24,42,57]. The state that has been reconstructed is the result of quench dynamics under an  $XY$  Hamiltonian. The  $XY$  model is an archetypal model for the study of quantum many-body phenomena, including phase transitions, quasiparticle dynamics, and entanglement propagation. The  $XY$  model is known to be a universal simulator of Hamiltonians in two dimensions and thus has broad significance for the field of quantum simulation [58].

Here, we have focused on the time evolution of many-body quantum systems following a quench, which is a challenging problem, even in one dimension [4]. By examining the growth of entanglement in quantum dynamics, we have been able to not only gain valuable insights into the underlying microscopic processes but also explore the complexity of quantum states. This information is

directly connected to the efficiency of simulations conducted on classical computers [26]. As, using quantum quench dynamics, one can generate states that contain a substantial amount of entanglement, they can be used as a test bed to understand the underlying dynamics of challenging quantum many-body problems from various domains including condensed-matter physics, quantum statistical mechanics, high-energy physics, atomic physics, and quantum chemistry.

The number of variational parameters (approximately 4000) in all methods is very low compared to the Hilbert-space dimension ( $2^{20} \approx 10^6$ ). More importantly, the number of measurement bases (27) is far below the QST quorum ( $\geq 2^{20} + 1$ ) and the number of measurements in each basis is far below the dimension of the Hilbert space. Nonetheless, the reconstructed states reproduce the true state of the system very well. This demonstrates that under the right circumstances, state reconstruction remains possible even from highly incomplete data sets.

Among the methods used, RBM and ARN show comparable reconstruction quality, while MPS outperforms both NNQSs in terms of both the experimental data likelihood and fidelity with ideal simulated states. Moreover, the MPS converges faster and generalizes better (overfits less) on average than the neural networks.

Inquiring into the reasons for this disparity in performance, we have found that it is not the expressive power of NNQSs that limits their fidelity but the complexity of their training. One can identify two issues here. The first is the transformation (rotation) of the state into different measurement bases. A rotated MPS can be readily expressed as another MPS with a different parameter set, whereas rotating an NNQS is much more complicated. Second, the data likelihood can be directly expressed in terms of MPS parameters, whereas NNQSs require an expensive and imprecise sampling procedure. Both of these features complicate the training of neural-network ansätze for quantum state representation.

On the other hand, the superiority of MPS is linked to the physical nature of quantum states that are produced by the 1D quantum simulator, in particular, the dominance of nearest-neighbor correlations. Such states are known to be well described by MPS. The class of states for which NNQS may show superior performance in QST is states with volume-law entanglement scaling, as shown in Fig. 5.

A natural next step would be to extend our method to mixed states. A challenge associated with that is the quadratic increase in the number of parameters in a density matrix as compared to a pure-state vector. This can be mitigated by combining machine-learning methods with quantum state tomography by compressed sensing [59]. An alternative is to directly apply the MPS formalism to mixed states [60].

The code and data used in this paper are available on Zenodo [61].

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- [1] R. P. Feynman, Simulating physics with computers, *Int. J. Theor. Phys.* **21**, 467 (1982).
- [2] R. P. Feynman, Quantum mechanical computers, *Found. Phys.* **16**, 507 (1986).
- [3] S. Lloyd, Universal quantum simulations, *Science* **273**, 1073 (1996).
- [4] J. I. Cirac and P. Zoller, Goals and opportunities in quantum simulation, *Nat. Phys.* **8**, 264 (2012).
- [5] C. Gross and I. Bloch, Quantum simulations with ultracold atoms in optical lattices, *Science* **357**, 995 (2017).
- [6] R. Blatt and C. F. Roos, Quantum simulations with trapped ions, *Nat. Phys.* **8**, 277 (2012).
- [7] A. Mazurenko, C. S. Chiu, G. Ji, M. F. Parsons, M. Kanász-Nagy, R. Schmidt, F. Grusdt, E. Demler, D. Greif, and M. Greiner, A cold-atom Fermi-Hubbard antiferromagnet, *Nature* **545**, 462 (2017).
- [8] H. Bernien, S. Schwartz, A. Keesling, H. Levine, A. Omran, H. Pichler, S. Choi, A. S. Zibrov, M. Endres, M. Greiner, *et al.*, Probing many-body dynamics on a 51-atom quantum simulator, *Nature* **551**, 579 (2017).
- [9] A. Keesling, A. Omran, H. Levine, H. Bernien, H. Pichler, S. Choi, R. Samajdar, S. Schwartz, P. Silvi, S. Sachdev, *et al.*, Quantum Kibble-Zurek mechanism and critical dynamics on a programmable Rydberg simulator, *Nature* **568**, 207 (2019).
- [10] N. Friis, O. Marty, C. Maier, C. Hempel, M. Holzäpfel, P. Jurcevic, M. B. Plenio, M. Huber, C. Roos, R. Blatt, *et al.*, Observation of entangled states of a fully controlled 20-qubit system, *Phys. Rev. X* **8**, 021012 (2018).
- [11] A. Omran, H. Levine, A. Keesling, G. Semeghini, T. T. Wang, S. Ebadi, H. Bernien, A. S. Zibrov, H. Pichler, S. Choi, *et al.*, Generation and manipulation of Schrödinger cat states in Rydberg atom arrays, *Science* **365**, 570 (2019).
- [12] S. Ebadi, T. T. Wang, H. Levine, A. Keesling, G. Semeghini, A. Omran, D. Bluvstein, R. Samajdar, H. Pichler, W. W. Ho, *et al.*, Quantum phases of matter on a 256-atom programmable quantum simulator, *Nature* **595**, 227 (2021).
- [13] D. Bluvstein, A. Omran, H. Levine, A. Keesling, G. Semeghini, S. Ebadi, T. T. Wang, A. A. Michailidis, N. Maskara, W. W. Ho, *et al.*, Controlling many-body dynamics with driven quantum scars in Rydberg atom arrays, [ArXiv:2012.12276](https://arxiv.org/abs/2012.12276) (2020).
- [14] P. Scholl, M. Schuler, H. J. Williams, A. A. Eberharter, D. Barredo, K.-N. Schymik, V. Lienhard, L.-P. Henry, T. C. Lang, T. Lahaye, *et al.*, Quantum simulation of 2D antiferromagnets with hundreds of Rydberg atoms, *Nature* **595**, 233 (2021).
- [15] M. Paris and J. Rehacek, *Quantum State Estimation* (Springer Science & Business Media, 2004), Vol. 649.
- [16] R. Orús, Tensor networks for complex quantum systems, *Nat. Rev. Phys.* **1**, 538 (2019).
- [17] A. M. Gomez, S. F. Yelin, and K. Najafi, Reconstructing quantum states using basis-enhanced born machines, [ArXiv:2206.01273](https://arxiv.org/abs/2206.01273) (2022).
- [18] O. Sharir, A. Shashua, and G. Carleo, Neural tensor contractions and the expressive power of deep neural quantum states, *Phys. Rev. B* **106**, 205136 (2022).
- [19] D.-L. Deng, X. Li, and S. Das Sarma, Quantum entanglement in neural network states, *Phys. Rev. X* **7**, 021021 (2017).
- [20] Y. Levine, O. Sharir, N. Cohen, and A. Shashua, Quantum entanglement in deep learning architectures, *Phys. Rev. Lett.* **122**, 065301 (2019).
- [21] M. Hibat-Allah, M. Ganahl, L. E. Hayward, R. G. Melko, and J. Carrasquilla, Recurrent neural network wave functions, *Phys. Rev. Res.* **2**, 023358 (2020).
- [22] C. Hempel, Ph.D. thesis, University of Innsbruck, Innsbruck, Austria, 2014.
- [23] P. Schindler, D. Nigg, T. Monz, J. T. Barreiro, E. Martinez, S. X. Wang, S. Quint, M. F. Brandl, V. Nebendahl, C. F. Roos, *et al.*, A quantum information processor with trapped ions, *New J. Phys.* **15**, 123012 (2013).
- [24] B. Lanyon, C. Maier, M. Holzäpfel, T. Baumgratz, C. Hempel, P. Jurcevic, I. Dhand, A. Buyskikh, A. Daley, M. Cramer, *et al.*, Efficient tomography of a quantum many-body system, *Nat. Phys.* **13**, 1158 (2017).
- [25] M. K. Joshi, F. Kranzl, A. Schuckert, I. Lovas, C. Maier, R. Blatt, M. Knap, and C. F. Roos, Observing emergent



- hydrodynamics in a long-range quantum magnet, *Science* **376**, 720 (2022).
- [26] J. Schachenmayer, B. P. Lanyon, C. F. Roos, and A. J. Daley, Entanglement growth in quench dynamics with variable range interactions, *Phys. Rev. X* **3**, 031015 (2013).
- [27] See the Supplemental Material at <http://link.aps.org/supplemental/10.1103/PRXQuantum.4.040345> for a more detailed discussion about neural networks.
- [28] V. R. Joseph, Optimal ratio for data splitting, *Stat. Anal. Data Min.: ASA Data Sci. J.* **15**, 531 (2022).
- [29] U. Schollwöck, The density-matrix renormalization group in the age of matrix product states, *Ann. Phys.* **326**, 96 (2011).
- [30] M. Cramer, M. B. Plenio, S. T. Flammia, R. Somma, D. Gross, S. D. Bartlett, O. Landon-Cardinal, D. Poulin, and Y.-K. Liu, Efficient quantum state tomography, *Nat. Commun.* **1**, 1 (2010).
- [31] G. Carleo and M. Troyer, Solving the quantum many-body problem with artificial neural networks, *Science* **355**, 602 (2017).
- [32] I. Glasser, N. Pancotti, M. August, I. D. Rodriguez, and J. I. Cirac, Neural-network quantum states, string-bond states, and chiral topological states, *Phys. Rev. X* **8**, 011006 (2018).
- [33] B. Jónsson, B. Bauer, and G. Carleo, Neural-network states for the classical simulation of quantum computing, *ArXiv:1808.05232* (2018).
- [34] D.-L. Deng, X. Li, and S. Das Sarma, Machine learning topological states, *Phys. Rev. B* **96**, 195145 (2017).
- [35] Y. Nomura, A. S. Darmawan, Y. Yamaji, and M. Imada, Restricted Boltzmann machine learning for solving strongly correlated quantum systems, *Phys. Rev. B* **96**, 205152 (2017).
- [36] D. Luo and B. K. Clark, Backflow transformations via neural networks for quantum many-body wave functions, *Phys. Rev. Lett.* **122**, 226401 (2019).
- [37] J. Han, L. Zhang, and E. Weinan, Solving many-electron Schrödinger equation using deep neural networks, *J. Comput. Phys.* **399**, 108929 (2019).
- [38] H. Saito, Solving the Bose-Hubbard model with machine learning, *J. Phys. Soc. Jpn.* **86**, 093001 (2017).
- [39] G. Torlai, G. Mazzola, J. Carrasquilla, M. Troyer, R. Melko, and G. Carleo, Neural-network quantum state tomography, *Nat. Phys.* **14**, 447 (2018).
- [40] G. Torlai and R. G. Melko, Latent space purification via neural density operators, *Phys. Rev. Lett.* **120**, 240503 (2018).
- [41] E. S. Tiunov, V. Tiunova, A. E. Ulanov, A. Lvovsky, and A. Fedorov, Experimental quantum homodyne tomography via machine learning, *Optica* **7**, 448 (2020).
- [42] G. Torlai, B. Timar, E. P. L. van Nieuwenburg, H. Levine, A. Omran, A. Keesling, H. Bernien, M. Greiner, V. Vuletić, M. D. Lukin, R. G. Melko, and M. Endres, Integrating neural networks with a quantum simulator for state reconstruction, *Phys. Rev. Lett.* **123**, 230504 (2019).
- [43] X. Gao and L.-M. Duan, Efficient representation of quantum many-body states with deep neural networks, *Nat. Commun.* **8**, 1 (2017).
- [44] D. Wu, L. Wang, and P. Zhang, Solving statistical mechanics using variational autoregressive networks, *Phys. Rev. Lett.* **122**, 080602 (2019).
- [45] O. Sharir, Y. Levine, N. Wies, G. Carleo, and A. Shashua, Deep autoregressive models for the efficient variational simulation of many-body quantum systems, *Phys. Rev. Lett.* **124**, 020503 (2020).
- [46] T. D. Barrett, A. Malyshev, and A. Lvovsky, Autoregressive neural-network wavefunctions for ab initio quantum chemistry, *Nat. Mach. Intell.* **4**, 351 (2022).
- [47] M. A. Carreira-Perpinan and G. Hinton, in *International workshop on artificial intelligence and statistics* (PMLR, 2005), p. 33.
- [48] T. Tieleman, in *Proceedings of the 25th International Conference on Machine Learning* (2008), p. 1064.
- [49] M. Germain, K. Gregor, I. Murray, and H. Larochelle, in *International Conference on Machine Learning* (PMLR, 2015), p. 881.
- [50] H. Larochelle and I. Murray, in *Proceedings of the Fourteenth International Conference on Artificial Intelligence and Statistics* (JMLR Workshop and Conference Proceedings, 2011), p. 29.
- [51] G. Papamakarios, T. Pavlakou, and I. Murray, Masked autoregressive flow for density estimation, *Adv. Neural. Inf. Process. Syst.* **30**, (2017).
- [52] D. P. Kingma, J. Ba, Adam: A method for stochastic optimization, *arXiv:1412.6980* (2014).
- [53] Y. Bar-Shalom, X. R. Li, and T. Kirubarajan, *Estimation with Applications to Tracking and Navigation: Theory Algorithms and Software* (John Wiley & Sons, 2001).
- [54] O. Sharir, A. Shashua, and G. Carleo, Neural tensor contractions and the expressive power of deep neural quantum states, *arXiv:2103.10293* (2021).
- [55] D. Mogilevtsev, Z. Hradil, J. Rehacek, and V. S. Shchepochnikov, Cross-validated tomography, *Phys. Rev. Lett.* **111**, 120403 (2013).
- [56] A. Steffens, C. Riofrio, W. McCutcheon, I. Roth, B. A. Bell, A. McMillan, M. Tame, J. Rarity, and J. Eisert, Experimentally exploring compressed sensing quantum tomography, *Quantum Sci. Technol.* **2**, 025005 (2017).
- [57] C. A. Riofrio, D. Gross, S. T. Flammia, T. Monz, D. Nigg, R. Blatt, and J. Eisert, Experimental quantum compressed sensing for a seven-qubit system, *Nat. Commun.* **8**, 15305 (2017).
- [58] T. S. Cubitt, A. Montanaro, and S. Piddock, Universal quantum Hamiltonians, *Proc. Natl. Acad. Sci.* **115**, 9497 (2018).
- [59] D. Gross, Y.-K. Liu, S. T. Flammia, S. Becker, and J. Eisert, Quantum state tomography via compressed sensing, *Phys. Rev. Lett.* **105**, 150401 (2010).
- [60] F. Verstraete, J. J. Garcia-Ripoll, and J. I. Cirac, Matrix product density operators: Simulation of finite-temperature and dissipative systems, *Phys. Rev. Lett.* **93**, 207204 (2004).
- [61] M. K. Kurmapu, V. V. Tiunova, E. S. Tiunov, M. Ringbauer, C. Maier, R. Blatt, T. Monz, A. K. Fedorov, and A. I. Lvovsky, Data and code for “Reconstructing complex states of a 20-qubit quantum simulator”. <https://doi.org/10.5281/zenodo.7697376>.
- [62] Compute Canada: [www.computeCanada.ca](http://www.computeCanada.ca)