Reconstructing quantum states efficiently

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Quantum state tomography, the ability to deduce the density matrix of a quantum system from measured data, is of fundamental importance for the verification of present and future quantum devices. It has been realized in systems with few components but for larger systems it becomes rapidly infeasible because the number of quantum measurements and computational resources required to process them grow exponentially in the system size. Here we show that we can gain an exponential advantage over direct state tomography for quantum states typically realized in nature. Based on singular value thresholding and matrix product state methods we introduce a state reconstruction scheme that relies only on a linear number of measurements. The computational resources for the postprocessing required to reconstruct the state with high fidelity from these measurements is polynomial in the system size.

It is one of the principal features distinguishing classical from quantum many-body systems, that for the former the specification of a state requires a parameter set whose size scales linearly in the number of subsystems, while in the latter this set scales exponentially. It is this difference that supports the observation that quantum devices appear to be fundamentally hard (exponential in the number of subsystems) to simulate on a classical computer and may in turn possess a computational power exceeding that of classical devices \cite{1}.

This presents us with the blessing of being able to construct information processing devices fundamentally superior to any classical device and the curse of their complexity, challenging our ability to verify efficiently that such a quantum information processing device or quantum simulator is actually functioning as intended. Such devices and, more generally, quantum simulators may be viewed as the preparation of elaborate quantum states on which we then carry out measurements. Verifying efficiently that an intended state—the ground or thermal state of a physical Hamiltonian for example—has indeed been prepared by a quantum information processor or a quantum simulator is essential.

The full determination of the quantum state of a system, that is quantum state tomography \cite{2}, can of course be achieved – one simply measures a complete set of observables whose expectation values fully determine the quantum state \cite{3-7}. In practice however, this approach is beset with several problems when applied to quantum-many party systems. Firstly, in quantum state tomography the size of the set of measurements scales exponentially with the number of subsystems. For moderately sized systems, such as the electronic states of 8 ions \cite{4}, tomography has been demonstrated but it rapidly becomes infeasible for larger systems thanks both to excessive time required to carry out the measurements and because the precision of those measurements has to increase exponentially to ensure that a function of the probability amplitudes of the state will not return an essentially random result. Secondly, making the connection between the measurement data on the one hand and the density matrix of a state best approximating these data on the other will usually require classical postprocessing that cannot be executed efficiently on a classical computer (see \cite{4}). Thirdly, writing out the full state of a physical system will be impossible for more than approximately 40 spin-1/2 particles and approximate representations from which one can extract expectation values efficiently to high precision need to be used.

Here, we address all of the above challenges at the same time and demonstrate the efficiency of the proposed approach with numerical examples. We present the case of general pure quantum states in some detail and outline generalizations to mixed states. To pave the way towards the general argument, we start the exposition with a discussion of unique ground states of local Hamiltonians.

Consider a \(k\)-local Hamiltonian acting on a set \(L\) of \(N\) spins arranged on some lattice equipped with the notion of a distance \(\text{dist}(i,j)\) between sites \(i\) and \(j\),

\[
\hat{H} = \sum_{i \in L} \hat{h}_i, \tag{1}
\]

where each Hamiltonian \(\hat{h}_i\) acts on spins that are at most at a distance \(k\) from spin \(i\). Let us collect these in the set \(I_i = \{j \in L : \text{dist}(i,j) \leq k\}\). The non-degenerate ground state of a \(k\)-local Hamiltonian is the state of lowest energy and therefore uniquely determined by the expectation values of the \(\hat{h}_i\). Indeed, if there was another state with the same expectation values, its energy would be the same, violating the uniqueness assumption. For an unknown \(k\)-local Hamiltonian we do not know the \(\hat{h}_i\), and cannot restrict measurements to these observables only. The ground state \(|gs\rangle\) is nevertheless uniquely determined by all its reductions to the sites \(I_i\), \(\hat{\varrho}_i = \text{tr}_{L\setminus I_i}[|gs\rangle\langle gs|]\), as these determine all possible expectation values of operators acting on \(I_i\), in particular those of the unknown \(\hat{h}_i\). Hence, if an experiment prepares the unique ground state of some unknown \(k\)-local Hamiltonian, we can determine that state fully by measuring the \(N\) reduced density matrices \(\hat{\varrho}_i\). In this setting we have hence overcome the first problem mentioned above as the state is fully determined by the \(\hat{\varrho}_i\), so \(N\) density matrices of size \(2^{|I_i|} \times 2^{|I_i|}\), where \(|I_i|\) is the cardinality of \(I_i\). For a nearest neighbour Hamiltonian on a \(d\)-dimensional lattice, e.g., \(|I_i| = 2d + 1\). Using these insights, we will discuss the case of general pure states later.

To overcome the second problem, we require an efficient method to find a pure state \(|\psi\rangle\) whose reduced density matrices \(\hat{\sigma}_i = \text{tr}_{L\setminus I_i}[|\psi\rangle\langle \psi|]\) coincide with the \(\hat{\varrho}_i\). The method of choice is singular value thresholding (SVT) \cite{8,9} (see the Appendix for technical details), which has been developed very
recently in the context of classical compressive sampling or matrix completion [10] and may also be applied to the quantum setting [11][12]. SVT provides a recursive algorithm that converges provably towards a low rank solution satisfying a set of linear constraints such as the requirement to match reduced density matrices. SVT converges rapidly to the solution especially so when it has low rank. Unfortunately, SVT as originally proposed is not scalable as it requires a full representation of a matrix of the same size as the density matrix describing the system and a singular value decompositions of this matrix. Hence, both the requirement for memory and time scale exponentially in the number of sub-systems and the straightforward application of SVT is restricted to well below 20 spin-1/2 particles. However, as we will see, a modification of the algorithm allows us to overcome this problem.

Denote by $|\phi\rangle$ the unknown target state and by $\hat{\rho}_n$, $n = 1, \ldots, N$, its reduced density matrices as described above. The following modification of the standard SVT algorithm (see appendix) will yield a state $|\psi\rangle$ whose reduced density matrices $\hat{\sigma}_i$ closely matches those of $|\phi\rangle$. Let $\hat{\sigma}_j$, $j = x, y, z, 0$, the Pauli spin matrices acting on site $j$ and by $\hat{P}_k$ denote all the possible operators $\prod_{j \in I_k} \sigma_j^{\alpha_j}$, $i = 1, \ldots, N$, of which there are $\sum_{j \in L} A^{[I_j]} = K$. From $\hat{\rho}_n$ we know the expectation values $\langle \hat{\rho}_n \prod_{j \in I_k} \sigma_j^{\alpha_j} | \phi \rangle = \text{tr}[\hat{\rho}_n \prod_{j \in I_k} \sigma_j^{\alpha_j}]$ and hence the numbers $p_k = \langle \phi | \hat{P}_k | \phi \rangle$, $k = 1, \ldots, K$. The algorithm may then be described as follows. First set up the operator $\hat{R} = \sum_{k=1}^{K} p_k \hat{P}_k / 2^N$ and initialize $\hat{Y}_0$ (e.g., by the zero matrix). Then proceed inductively by finding the eigenstate $|y_n\rangle$ with largest eigenvalue, $y_n$, of $\hat{Y}_n$ and set

$$\hat{X}_n = y_n \sum_{k=1}^{K} \frac{\langle y_n | \hat{P}_k | y_n \rangle}{2^N} \hat{P}_k, \quad \hat{Y}_{n+1} = \hat{Y}_n + \delta_n (\hat{R} - \hat{X}_n).$$  

A rigorous proof of convergence of $\hat{\sigma}_i = \text{tr}[\hat{Y}_n | y_n\rangle \langle y_n |]$ to $\hat{\rho}_i$ (equivalently of $\langle y_n | \hat{P}_k | y_n \rangle$ to $p_k$) will be presented elsewhere. Heuristically, convergence is suggested by the extensive numerics below and can be expected from the fact that SVT possesses a convergence proof for small $\delta_n \in \mathbb{R}$ [9], see Appendix.

So far, this algorithm still suffers from the fact that in every step the $2^N \times 2^N$ matrix $\hat{Y}_n$ needs to be diagonalized. However, the $\hat{Y}_n$ are of the form $\sum_{k=1}^{K} a_k \hat{P}_k$, $a_k \in \mathbb{R}$, i.e., they have the form of a local “Hamiltonian”. In one spatial dimension, the ground states of local Hamiltonians are well approximated by matrix product states (MPS) [13][14]. Hence, $|y_n\rangle$ can be determined employing MPS algorithms [15][16], for which the number of parameters scale polynomially in the system size and converge rapidly [17][18]. Hence, for one spatial dimension, we have overcome the second and third problem mentioned above: This postprocessing is efficient as MPS algorithms are and a MPS provides an efficient representation of the state as it depends only on linearly many parameters. Any general pure state may be represented by a MPS and generic MPS are unique ground states of local Hamiltonians [14]. Hence, the above algorithm will produce a state that is close to the target state if the MPS dimension and the size of the reduced density matrices is chosen sufficiently large.

For higher spatial dimensions MPS are not efficient representations and for optimal performance they need to be replaced by other variational classes. A variety of MPS generalization have been proposed of which the most promising are perhaps the tensor-tree ansatz [19] and MERA-approach [20], PEPS [21] and weighted graph states [22]. For each of these, numerical algorithms have been developed that determine the largest eigenvalue of a local Hamiltonian. Being the key ingredient in our modified SVT method developed here, these more general variational classes may be combined naturally in the way we have described for MPS.

Let us now consider numerical examples for different target states $|\phi\rangle$ to demonstrate the feasibility and efficiency of the proposed algorithm. We start with ground states of nearest-neighbor Hamiltonians on a chain, i.e., the $|\phi\rangle = |gs\rangle$ are completely determined by all the reductions to two adjacent spins as outlined above and the above algorithm not only produces states that match the reduced density matrices of the ground states but, in fact, states that are themselves close to the ground states. Among ground states of one-dimensional nearest-neighbor Hamiltonians the critical ones are the most challenging to approximate by MPS as they violate the entanglement-area law [23] and we test our algorithm for such an example: the critical Ising model. In order for the local operators in the Hamiltonian not to be exactly the ones that are measured, we also rotate the Ising model locally by $\pi/4$ around each spin axis. This model is solvable and in order to show that we do not consider a pathological case, we also consider one-dimensional random Hamiltonians of the form

$$\hat{H} = \sum_{i=1}^{N-1} \hat{r}_i^{(i)} \hat{r}_{i+1}^{(i)}$$

where the $\hat{r}_i^{(i)}$, $\hat{r}_{i+1}^{(i)}$ act on spin $i$ and $i + 1$, respectively, and are hermitian matrices with entries that have real and imaginary part picked from a uniform distribution over $[-1, 1]$. For each Hamiltonian, we first determine the ground state $|gs\rangle$ exactly (i.e., the target state $|\phi\rangle$) and its reductions and then computed the fidelity $\langle |gs\rangle | y_n\rangle^2$ after $n$ iterations of the MPS-SVT algorithm, see Fig. 1.

Our method is of interest for all situations in which standard tomography will not be feasible. This is the case for the verification of state preparation in experiments with too many particles. An example is the recent ion trap experiment [4] for the preparation of W-states, $|\phi\rangle = (|10\cdots0\rangle + |01\cdots0\rangle + \cdots + |00\cdots1\rangle)/\sqrt{N}$, that were limited to 8 qubits principally because the classical postprocessing of data became prohibitive for longer chains. Here we demonstrate the efficiency of our approach (we are not limited to few ions and demonstrate convergence for up to 20 ions – even higher number of ions are easily accessible due to the MPS alteration of the SVT method) by illustrating how one would postprocess experimentally obtained reduced density matrices to guarantee the generation of $|\phi\rangle$ or a state very close to it. We mimic experimental noise by adding Gaussian distributed random numbers with zero mean to the $p_k$. After initializing the MPS algorithm with the MPS representation of $|\phi\rangle$ and $\hat{Y}_0 = \hat{R}$, we use
\( x_n \):= \( \sum_k |p_k - \langle y_n | \hat{P}_k | y_n \rangle | \) as a figure of merit for convergence, i.e., after a given number of iterations, we pick the \( |y_n\rangle \) with minimum \( x_n \). The result of such a procedure is shown in Fig. 1.

So far we have presented the method for pure states and one-dimensional systems. The SVT algorithm as described above works for higher-dimensional systems as well and may be made efficient by adopting higher dimensional analogues of MPS methods as outlined above. The extension to mixed states is also straightforward as its treatment can be reduced to that of pure states by using the fact that every mixed state on \( N \) qubits can be purified to a pure state on \( 2N \) qubits. Hence we may ask for a globally pure state on \( 2N \) qubits that matches the reduced density on all contiguous sites of \( k \) qubits on the first \( N \) qubits. While the reduced density matrices do not uniquely determine the mixed state, approximations of better and better quality can be obtained by increasing \( k \). As an example, suppose the state is the Gibbs state corresponding to a \( k \)-local Hamiltonian \( \hat{H} \), i.e., the state \( \hat{\varrho} \) minimizing the free energy

\[ \text{tr} [\hat{\varrho} \hat{H}] - TS(\hat{\varrho}). \]  

The first term is, as before, for a \( k \)-local Hamiltonian, determined by the reduced density matrices. The entropy of the total state however can only be learnt exactly from the complete density matrix. However, for essentially all reasonable physical systems, the entropy density \( \lim_{k \to \infty} (\text{tr}_{k+1,...}(\rho))/k \) in the thermal state of a Hamiltonian exists [24] and as a consequence the total entropy of the state can be estimated efficiently from the knowledge of reduced density matrices.

Our algorithm described above may also be adapted straightforwardly to determine hypothesis states in recently proposed algorithms for quantum learning [25]. Here, a small given set of randomly chosen observables is measured and on the basis of the measurement outcomes a quantum state closely approximating the measured expectation values needs to be found. This state will, with large probability, predict the expectation values of all observables. Present approaches to determine such states are based on semi-definite programming and are therefore inherently non-scalable, they are limited to perhaps 12 qubits [25].

Our algorithm will be essential for efficient tomography and verification of medium to large scale quantum information devices. Already today they are beginning to reach scales for which standard tomography is not feasible anymore. Furthermore, it may also be applied to problems in condensed matter physics where the system has too many components to achieve tomography by standard means.

Hence our combination of singular value thresholding with the matrix product state representation is expected to become a useful tool in a wide variety of physical settings and algorithms.

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**Appendix**

In singular value thresholding [8, 9] one seeks a solution for the minimization of the trace norm of a matrix $X$ subject to some linear constraints, i.e.

\[
\begin{align*}
\text{minimize} & \quad \text{tr}|X| \\
\text{subject to} & \quad \mathcal{P}_\Omega(X) = \mathcal{P}_\Omega(M)
\end{align*}
\]

where $\mathcal{P}_\Omega(M)$ is a matrix whose elements are non-zero only on the entries belonging to the index set $\Omega$. For a value $\tau > 0$ and a sequence $\{\delta_k\}_{k \geq 1}$ one inductively defines

\[
\begin{align*}
X^{(k)} &= \text{shrink}(Y^{(k-1)}, \tau) \\
Y^{(k)} &= Y^{(k-1)} + \delta_k \mathcal{P}_\Omega(M - X^{(k)}),
\end{align*}
\]

where, in standard SVT,

\[
\text{shrink}(Y, \tau) = U \text{diag}(\max\{0, \sigma_i - \tau\}) V^\dagger
\]

with the singular value decomposition $Y = U \text{diag}(\{\sigma_i\}) V^\dagger$.

If it is our goal to reconstruct pure states compatible with given reduced density matrices we may adapt SVT and in the process make it suitable for application to matrix product states. To this end we introduce a small but crucial variation of the shrink operation. Rather than introducing a threshold $\tau$ we retain only the largest singular value $\sigma_1$ and the corresponding matrix $U \text{diag}(\max_i \sigma_i \cdot 0 \ldots 0) V^\dagger$. If the target state is pure, i.e., a matrix with rank equal to one, this can be expected to converge rapidly, an expectation that is confirmed by extensive numerics.

While $\mathcal{P}_\Omega(M - X^{(k)})$ is not itself positive, initializing the recursion with a positive operator, e.g., a pure state, and choosing sufficiently small $\delta_k$ will ensure that in the second step of the recursion a matrix is generated whose largest eigenvalue is positive and equal to the largest singular value.

Crucially, this largest eigenvalue and corresponding eigenstate can then be computed efficiently via the maximization of the expectation value of a matrix product state solving the multi-quadratic optimization problem by a succession of quadratic optimization problems each of which can be solved by extensive numerics.

Reduced density matrices are obtained by measuring the set of strings of Pauli operators $\hat{P}_k$, $k = 1, \ldots, K$. Then $\mathcal{P}_\Omega(Y) = \sum_{k=1}^K \text{tr}(Y \hat{P}_k)\hat{P}_k/2^N$ and is hermitian.