Unsupervised detection of decoupled subspaces: Many-body scars and beyond

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Highly excited eigenstates of quantum many-body systems are typically featureless thermal states. Some systems, however, possess a small number of special, low-entanglement eigenstates known as quantum scars. We introduce a quantum-inspired machine-learning platform based on a quantum variational autoencoder (QVAE) that detects families of scar states in spectra of many-body systems. Unlike a classical autoencoder, QVAE performs a parametrized unitary operation, allowing us to compress a single eigenstate into a smaller number of qubits. We demonstrate that the autoencoder trained on a scar state is able to detect the whole family of scar states sharing common features with the input state. We identify families of quantum many-body scars in the PXP model beyond the \mathbb{Z}_2 and \mathbb{Z}_3 families and find dynamically decoupled subspaces in the Hilbert space of disordered, interacting spin-ladder model. The possibility of an automatic detection of subspaces of scar states opens new pathways in studies of models with a weak breakdown of ergodicity and fragmented Hilbert spaces.

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I. INTRODUCTION

Recent progress in noisy, intermediate-scale quantum (NISO) computers [1-3] lead to a fast development of algorithms suited for use on these machines [4] with the purpose of achieving a quantum advantage in various areas: physics, machine learning, quantum chemistry, and combinatorial optimization. Of particular importance are variational quantum algorithms [5], in which quantum circuits are applied to quantum states, whose parameters are optimized with classical feedback loops. Physical applications include variational quantum eigensolvers [6-8], algorithms for groundstate preparation [9], time-evolution simulations [10-12], or quantum variational autoencoders (QVAE) [13-15]. The autoencoders encode the input data into a reduced representation and then use it to reconstruct the data with the optimal fidelity. As such, autoencoders are basic tools for data compression in machine learning. In turn, the task of QVAE is to realize the unitary transformation that transfers the input entangled n-qubits state into a product state of k, relevant, entangled qubits and n - k "trash" separable qubits [see Eq. (1) below]. QVAE have been realized experimentally in a photonic device [16] and recently employed in investigation of quantum phase transitions [17]. In this work we demonstrate the applicability of QVAE in an analysis of properties of highly excited eigenstates in quantum many-body systems.

According to eigenstate thermalization hypothesis (ETH) [18–20], a small subsystem of an isolated, interacting quantum many-body system is described by a thermal density

matrix after a long-time evolution, irrespectively of the initial nonequilibrium state. However, some systems violate this paradigm of quantum ergodicity and exhibit a longtime behavior dependent on the initial state. Examples of such nonergodic systems include integrable systems [21] and many-body localized phases in the presence of quenched disorder [22–26]. Another mechanism of ergodicity breaking in a form of persistent oscillations for particularly chosen initial states has been discovered in the experiment with ultracold Rydberg atoms [27]. This behavior arises due to the presence of few atypical, almost equally spaced eigenstates with low entanglement entropy, the so-called quantum many-body scars (QMBS) [28,29] that are embedded in the otherwise thermal spectrum of a quantum many-body system. For initial states with high overlap with a few QMBS, one observes longlived oscillations of observables, whereas for generic initial conditions the system quickly approaches the thermal equilibrium state. Several theories explaining the emergence of QMBS were proposed starting long time ago with the notion of "scars of symmetries" [30] (see also [31]): a spectrum generating algebra [32,33], Krylov restricted thermalization [34], projector embedding [35], and the presence of symmetric, coupled subspaces [36]. The QMBS occur in PXP model [37], describing Rydberg atoms chain, but also in Affleck-Kennedy-Lieb-Tasaki (AKLT) model [38,39], quantum local random networks [40], frustrated magnetic lattices [41], lattice gauge theories [42–44], optical lattices [45], or spin systems [46,47].

The aim of this work is to provide a scheme to detect families of QMBS based on QVAE. A *family* of QMBS is formed by eigenstates which (a) have an increased overlap with some "parent" state, (b) are characterized by a sub-volume-law entanglement entropy. The property (a) enables our algorithm

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to implicitly extract the features of the parent state from a single eigenstate in the training and encode them in QVAE. The probability that training succeeds is enhanced by the property (b). The performance of the trained autoencoder on other eigenstates serves as a measure of similarity between the eigenstates. The other representatives of the family of QMBS are found as eigenstates for which the performance of QVAE is significantly better than the typical behavior. In the following, we first describe details of the scheme. Then we apply it to detect the \mathbb{Z}_2 family and to discover different families of QMBS in the PXP model [28,37] and to identify subspaces of decoupled eigenstates in the spin ladder of [46].

II. QUANTUM VARIATIONAL AUTOENCODER

The QVAE aims to compress the *n*-qubit input state $|\psi\rangle$ into a *k*-qubit state $|\phi\rangle$ (where k < n), i.e., to perform a unitary transformation $U(\theta)$ parametrized by the circuit parameters θ ,

$$|\psi\rangle \to U(\theta)|\psi\rangle = |\phi\rangle \otimes |0\rangle^{\otimes (n-k)},\tag{1}$$

where the last $n - k \equiv N_{\text{trash}}$ qubits are called "trash" qubits. The QVAE circuit starts with randomly initialized parameters θ which are variationally adjusted (here, using simultaneous) perturbation stochastic approximation optimizer [48-51]) to "optimal" value $\theta = \theta^*$ satisfying Eq. (1) for a given set of input states $\{|\psi_i\rangle\}$. At each optimization step, the unitary $U(\theta)$ is applied on $\{|\psi_i\rangle\}$ and the trash qubits are measured giving either "0" or "1." The total number of 1 defines the cost function that the optimizer tries to minimize in the next parameter update. (Cost function is the Hamming distance between the measured bit string of 1 and 0 on all trash qubits and the desired $|0\rangle^{\otimes (n-k)}$ trash qubit configuration.) Unlike for classical autoencoders, training a unitary encoder $U(\theta)$ automatically provides the decoder $U^{\dagger}(\boldsymbol{\theta})$ that can be applied to the compressed state $|\phi\rangle \otimes |0\rangle^{\otimes (n-k)}$ to reconstruct the input state $|\psi\rangle$. The cost function fulfills the requirement of locality on the trash qubits which is critical for circumventing the "barren plateaus" of the cost landscape and trainability of the model (see [52,53] for further details).

The architecture of the quantum circuit has to be expressible (i.e., able to encode a large class of quantum states with a few trainable parameters θ) and to possess a large entangling capability to transfer the entanglement of the whole system out of the trash qubits [54]. Building on the previous results [52,54] we choose alternating layered ansatz consisting of layers with single-qubit rotations around the *y* axis by an angle $\theta \in [0, 2\pi]$, $R_y(\theta) = \exp(-i\sigma_y\theta/2)$, and two-qubit controlled-Z (CZ) gates that apply a σ_z operator on one of the qubits if the other one is in the state $|1\rangle$ and act as an identity if the other qubit is in the state $|0\rangle$. Each of *L* layers of QVAE consists of $R_y(\theta)$ rotations of all qubits and CZ entangling operations between the neighboring qubits, with the pairs of entangled qubits alternating from layer to layer following a checkerboard pattern (see [55]).

In our scheme, as an input state $|\psi\rangle$ to train QVAE we take a single scar state that belongs to a given family of QMBS in a considered many-body system. To identify the other scars from the same family, we evaluate the performance of QVAE on eigenstates from the spectrum of the model. The numerical complexity of the procedure is thus $O(\mathcal{D})$ times

the number of iterations for QVAE training and $O(D^2)$ for the comparison of eigenstates where D is the dimension of the Hilbert space. This is lower than the exact diagonalization cost $O(D^3)$ required for generation of the input data.

III. SCARS IN THE PXP MODEL

The PXP Hamiltonian reads

$$\hat{H} = \sum_{i} \hat{P}_{i-1} \sigma_i^x \hat{P}_{i+1} \tag{2}$$

with periodic boundary conditions, where the projectors $\hat{P}_i = (1 - \sigma_i^z)/2$ ensure that neighboring spin-up states are separated at least by one lattice site, hence implementing the Rydberg blockade phenomenon [56] as a constraint on the Hilbert space. Certain specific initial states like $\mathbb{Z}_2 =$ $|0101...\rangle$, $\mathbb{Z}_3 = |001001...\rangle$ and product states that contain domain walls between \mathbb{Z}_2 and \mathbb{Z}_3 configurations give rise to persistent long-time oscillations of the local observables and the revivals of the wave function, while other states like $|\mathbb{Z}_0\rangle = |0000...\rangle$ and $|\mathbb{Z}_4\rangle = |00010001...\rangle$ show fast relaxation without revivals. The presence of families of \mathbb{Z}_2 and \mathbb{Z}_3 quantum scars gives rise to this behavior [57–65]. Some of the scarred states in the PXP model were constructed exactly as matrix product state (MPS) with a finite bond dimension [66], from which the family of \mathbb{Z}_2 scars was generated as quasiparticle excitations.

Input data to QVAE correspond to the eigenstates of the PXP model obtained through exact diagonalization for the system size N = 24 in the inversion-symmetric and zeromomentum sector with the Hilbert space dimension $\mathcal{D} =$ 2359 ($D \ll 2^L$ due to constraints and periodic boundary conditions). Local constraints of the PXP model allow to reduce the computational cost of the procedure by considering only the projection of OVAE onto the constrained subspace of Hilbert space. To that end, it suffices to substitute $R_{y}(\theta) \rightarrow$ $\tilde{R}_{v}(\theta), CZ_{i} \rightarrow E_{i}$ in the circuit, with $\tilde{R}_{v}(\theta)$ rotating qubit *i* only if qubits i - 1, i + 1 are in the $|0\rangle$ state (identity otherwise), and E_i acting on four qubits $i - 1, \ldots, i + 2$, performing the entangling operation of qubits *i* and i + 1 if qubits i - 1, i + 2are in the state $|0\rangle$ (identity otherwise). Exact matrix forms of these operators are given in [55]. This version of the QVAE will be referred to as the CQVAE. We should note that the translational and inversion symmetries of the original Hamiltonian are not exploited in the CQVAE because these symmetries are manifestly broken by the considered few-qubit gates. Thus, for N = 24, the CQVAE still acts on 2359 eigenstates but each of them is expressed in a 103 682-dimensional Hilbert space.

We select a \mathbb{Z}_2 scar at energy $E \approx -2.67$ as the training input state $|\chi_0\rangle$. This state has a significant overlap with the \mathbb{Z}_2 configuration, i.e., $|\langle\chi_0|\mathbb{Z}_2\rangle|^2 = 0.15$ (cf. with a value expected in the high-temperature thermal ensemble $1/\mathcal{D} \approx$ 0.0004). Figure 1(a) shows performance of a trained autoencoder on eigenstates from the PXP Hamiltonian spectrum. Indeed, we see that the \mathbb{Z}_2 scars are characterized by a significant drop in the CQVAE cost. Plots of CQVAE reconstruction fidelity (not shown) also reveal high-fidelity peaks on \mathbb{Z}_2 scars. In this way, the family of \mathbb{Z}_2 scars can be identified in an automatic way. Interestingly, the \mathbb{Z}_3 family has the largest



FIG. 1. (a) Performance of the CQVAE with $N_{\text{trash}} = 8$ and L = 7 trained on the strongest \mathbb{Z}_2 scar of the PXP model with N = 24 close to the middle of the spectrum, applied to all eigenstates. Best performance is observed in the eigenstates from the \mathbb{Z}_2 scars family that have an increased overlap with the $|\mathbb{Z}_2\rangle$ state, as presented in (b). Lines serve as a guide to the eye. Error bars come from averaging over 32 independent trainings.

cost even though it has low entanglement entropy showing that CQVAE learned to distinguish the real-space patterns \mathbb{Z}_3 scar states from the dominant configurations of \mathbb{Z}_2 family [see Fig. 1(b)]. Interestingly, at smaller system sizes, e.g., N = 12, we can recover the "parent" state $|\chi\rangle \approx |\mathbb{Z}_2\rangle$ for the family by optimizing the *input* of the trained CQVAE to minimize cost (see [55] for details).

The next step is to find other scarred families. We select eigenstates with a low entanglement entropy S = $-\text{Tr}\rho_A \ln \rho_A < 2.7$, where ρ_A is the reduced density matrix of the half of the spin chain, train the CQVAE on each of them, and calculate the cost on other eigenstates. Pairs of eigenstates that have a low cost when training on both of them are regarded as belonging to the same scar family. This property is transitive, i.e., if eigenstates $|E_1\rangle$, $|E_2\rangle$ have a small cost and $|E_2\rangle$, $|E_3\rangle$ as well, then a set $|E_1\rangle$, $|E_2\rangle$, $|E_3\rangle$ is regarded as one family. Figure 2 shows five families discovered by the CQVAE in the PXP model for N = 24, with an example of the training results on one representative of the family No. 1 [Fig. 2(a)]. The eigenstates from the family No. 1 are characterized by increased overlaps with several Fock states, the example of $|i_1\rangle = |1010100100100100100100\rangle$ state is shown in Fig. 2(b). Other Fock states with high overlaps with the family No. 1 contain a mixture of the same number of rearranged three \mathbb{Z}_2 and six \mathbb{Z}_3 patterns. The same holds true for families No. 2–No.5 of scar states found for N = 24. Patterns with a larger period can be found, e.g., family No. 2 has increased overlaps with four \mathbb{Z}_3 and three \mathbb{Z}_4 configurations. In that way, our QVAE-based scheme allows to explain the presence and identify relations between eigenstates with low entanglement entropy of the PXP model [see Fig. 2(c)]. Since the families of scar states do not have a single simple representative Fock state, their classification, especially in system-size independent manner is more involved; in [55] we show the details of the families for N = 24.



FIG. 2. (a) CQVAE cost of eigenstates of the PXP model, N = 24, reveals a scar "family No. 1" upon training on one of its representatives. Similar plots for other scarred families found by the algorithm are given in [55]. (b) Overlaps of the eigenstates with state $|i_1\rangle$. (c) Entanglement entropy vs energy.

IV. DISORDERED SPIN LADDER

Consider a spin ladder with Hamiltonian

$$H = H^{\parallel} + H^{\perp} = \frac{1}{4} \sum_{k=1}^{L-1} h_{k,k+1}^{\parallel} + \frac{1}{4} \sum_{k=1}^{L} h_k^{\perp}, \qquad (3a)$$

where

$$h_{k,k+1}^{\parallel} = \sigma_k^{x} \sigma_{k+1}^{x} + \sigma_k^{y} \sigma_{k+1}^{y} + \tau_k^{x} \tau_{k+1}^{x} + \tau_k^{y} \tau_{k+1}^{y},$$

$$h_k^{\perp} = J \left(\sigma_k^{x} \tau_k^{x} + \sigma_k^{y} \tau_k^{y} \right) + \Delta_k \sigma_k^{z} \tau_k^{z} + h_k \left(\sigma_k^{z} + \tau_k^{z} \right).$$
(3b)

k = 1, ..., N labels the rungs of the ladder, and spins on the left and right legs of the ladder are represented by Pauli matrices σ_k^{α} and τ_k^{α} ($\alpha = x, y, z$), respectively. Values of h_k are drawn from a uniform distribution in the interval [-h, h], and we set J = 1, h = 0.1, $\Delta_k = 1$. The model has a U(1) symmetry associated with the total magnetization $Z = \sum_{k=1}^{N} (\sigma_k^z + \tau_k^z)$ and a \mathbb{Z}_2 symmetry associated with the exchange of the ladder legs $\sigma_k^{\alpha} \leftrightarrow \tau_k^{\alpha}$. Even though this model has signatures of quantum ergodicity (e.g., energylevel spacings follow the Wigner-Dyson distribution), one can analytically construct exact invariant subspaces of the Hamiltonian (3) that are not related to any local conserved quantity as shown in [46]. It is first noticed that the eigenstates of h_k^{\perp} on a single rung are $|S\rangle = (|_1^0\rangle - |_0^1\rangle)/\sqrt{2}$ ("singlet"), $|T\rangle =$ $(|_{1}^{0}\rangle + |_{0}^{1}\rangle)/\sqrt{2}$ ("triplet"), $|D\rangle = |_{0}^{0}\rangle$ ("doublon"), $|H\rangle = |_{1}^{1}\rangle$ ("holon"), where the first (second) row of the vector corresponds to the left (right) leg of the ladder. Product of such states is an eigenstate of the total leg Hamiltonian H^{\perp} . By examining the action of the remaining H^{\parallel} on the two-rung



FIG. 3. Cost function of QVAE trained on an eigenstate from the one-holon subspace of the spin-ladder model with N = 8 (16 spins in total), evaluated on the eigenstates from Z = 1 symmetry sector. Color bar denotes the bipartite entanglement entropy for 4 rungs. Results averaged over 56 independent trainings of the QVAE with $N_{\text{trash}} = 5$ and L = 10.

states $|\{ST, SH, TH, HH ...\}\rangle$ one shows that H^{\parallel} annihilates configurations ST, TS, HH, DD, and moves H (or D) around if S or T are its neighbors. It follows that configurations $|STSTST...\rangle$ and $|TSTSTS...\rangle$ are annihilated by H^{\parallel} (they are a "vacuum background"). Upon inserting a given number of only holons (or doublons) between them, e.g., $|STSH_jTSH_kTS...\rangle$, one constructs an invariant subspace with a given number of the four letters that are conserved under the action of the total Hamiltonian H. Dimension of such a subspace after r insertions of doublons (or holons) is $\binom{N}{r}$.

Construction of invariant subspaces in this model required an involved theoretical insight [46]. Here, by employing the QVAE we can detect their presence in an automatic way. Let us restrict only to the Z = 1 symmetry sector of the Hamiltonian (3) with N = 8 rungs and a single disorder realization. We encode the ladder state onto the spatially one-dimensional quantum circuit, by mapping the left (right) leg of the ladder to odd (even) sites of the circuit. In this manner, the neighboring spins of the ladder are mapped to sites of the circuit that are close to each other. Training of the QVAE on a generic eigenstate and application to all others gives a featureless QVAE cost. However, if we train on an eigenstate from the invariant subspace represented by state $|STSTHSTS\rangle$ with 1 holon H, 4 singlets S, and 3 triplets T, we get a significantly lower error on all 8 eigenstates that span this subspace (see Fig. 3). The QVAE cost on the other invariant subspace $|TSTSHTST\rangle$ with a different number of singlets and triplets [but an identical entanglement entropy (notice the color scale in Fig. 3)] is comparable to the QVAE cost on generic, highly entangled, eigenstates. Similarly, a QVAE trained on an eigenstate from the subspace $|TSTSHTST\rangle$ yields small costs on eigenstates from this subspace whereas the cost on eigenstates from $|STSTHSTS\rangle$ is substantial (plot not shown). This is in a full analogy with results for PXP model and demonstrates how QVAE identifies and distinguishes families of scar states.

V. CONCLUSION

We proposed a scheme based on QVAE that allows to identify families of nonergodic eigenstates of quantum many-body systems. We validated our scheme on the \mathbb{Z}_2 family of scar states of the PXP model. Then, our scheme was employed to demonstrate presence of families of scar states in spectrum of PXP model beyond the \mathbb{Z}_2 and \mathbb{Z}_3 families. To confirm the generality of our approach, we used it to identify the family of scar states in the disordered spin ladder (3) as well as in a PXP-like model with a three-body blockade [55]. The use of QVAE is crucial in our scheme. QVAE learns from a single, high-dimensional measurement point (a single eigenstate), in contrast to classical autoencoders that require a larger set of training data. The flow of the entanglement entropy through the layers of the autoencoder has a physical meaning and results in a compression of the quantum state. By respecting the laws of quantum mechanics, QVAE becomes a versatile tool in studying eigenstates of many-body systems allowing, for instance, for a direct implementation of the local constraints of PXP model on the QVAE. Finally, we also point out that having the eigenstates one can try to identify scarred states by calculating the inverse participation ratio (IPR) with a negligible numerical cost instead of costly entanglement entropy. Moreover, instead of exact diagonalization used here, one may use an approximate algorithm, e.g., DMRG-X [67], to obtain a subset of eigenstates serving as an input to QVAE.

While all calculations performed here used classical machine, hardware implementation of QVAE on a physical quantum computer seems straightforward [17]. Although preparation of ground states of selected Hamiltonians is possible by the variational quantum eigensolvers, algorithms that provide excited states are more involved [4]. Hence, the preparation of the input states is the most challenging step of our scheme that is feasible only for limited system sizes. However, to navigate through the exponentially large Hilbert space one can use a prior knowledge about the scar states (e.g., their energy) which may extend the interval of system sizes accessible on current quantum hardware.

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