Gaussian state approximation of quantum many-body scars

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Quantum many-body scars are atypical, highly nonthermal eigenstates of kinetically constrained systems embedded in a sea of thermal eigenstates. These special eigenstates are characterized, for example, by a bipartite entanglement entropy that scales as most logarithmically with subsystem size. We use numerical optimization techniques to investigate if quantum many-body scars of the experimentally relevant PXP model are well approximated by Gaussian states. These states are described by a number of parameters that scales quadratically with system size, thereby having a much lower complexity than generic quantum many-body states. We find that this is a good description for the quantum many-body scars away from the center of the spectrum.

I. INTRODUCTION

Typical isolated quantum many-body systems thermalize under their own internal dynamics [1–3]. Under time evolution, such systems loose information about their initial condition, leading to the emergence of statistical mechanics. Recent times show a keen interest in quantum many-body systems that fall out of this paradigm. By now, several mechanisms leading to the breakdown of thermalization have been identified, among them many-body localization [4–6], quantum many-body scarring [7–9], and Hilbert space fragmentation [10, 11].

Quantum many-body scarring is a form of ergodicity breaking that can be observed in constrained quantum systems [12]. In contrast to many-body localized systems, quantum many-body scarred systems do not thermalize only when being initialized in certain highly polarized out-of-equilibrium states [13]. These systems show long-living approximate periodic revivals to their initial state, which can be related to a small number of special, highly nonthermal eigenstates embedded in a sea of thermal eigenstates [14]. These special eigenstates are known as quantum many-body scars, in loose analogy to the single-body quantum scars first observed by Heller in 1984 [15]. Quantum many-body scars have attracted tremendous attention both theoretically [7–9] and experimentally [12, 16–18] in recent years. Several models capturing the phenomenon of quantum many-body scarring have been introduced, with the so-called PXP model for a chain of Rydberg atoms being arguably the most paradigmatic example [13, 14, 19].

For a number of models, quantum many-body scarred eigenstates can be constructed analytically [9, 20]. For quantum many-body scars without a known exact form, approximate matrix product states can be obtained [21–24]. Other works used for example mean-field like methods to approximate quantum many-body scars [25–27], and it has been suggested that they occur due to proximity of the model to to an integrable point [28–30].

Quantum many body scars have an entanglement entropy which grows at most logarithmically with subsystem size [13, 14]. Since ground states of local quadratic Hamiltontians scale similarly with system size [31], in this work, we consider if quantum many-body scars can be well approximated by ground states of non-interacting systems. These states belong to the a family of Gaussian states (also known as *coherent states*) and are fully described by a number of parameters that scales quadratically with the system size, thereby having a much lower degree of complexity than generic quantum many-body states [32]. Gaussian states have been found to provide an effective description of many-body states in a broad range of settings, for example in the context of the mean-field theory of superconductivity [33], or many-body localization [34–41].

In this work, we numerically optimize the parameters of a general non-interacting fermionic system towards a maximum overlap of a symmetrized ground state with a given quantum many-body scar of the PXP model, which is a paradigmatic toy model of quantum many-body scars. Related optimization procedure for a complimentary problem have been recently proposed [42, 43].

The outline of this work is as follows. In Section II, we introduce the model and the properties utilized in the remainder of this work. Section III outlines the approximation procedure, and in Section IV we present our results. In Section V, we conclude and outline some possible directions for future investigations.

II. MODEL

We consider the PXP model with open boundary conditions,

$$\hat{H}_{\mathrm{PXP}} = \sum_{i=1}^{L-2} \left(\hat{P}_i \, \hat{X}_{i+1} \, \hat{P}_{i+2} \right) + \hat{X}_1 \hat{P}_2 + \hat{P}_{L-1} \hat{X}_L, \quad (1)$$

where $\hat{X}_i = \hat{\sigma}_i^x$ and $\hat{P}_i = \frac{1}{2}\left(1 - \hat{\sigma}_i^z\right)$ with $\hat{\sigma}_i^x$ and $\hat{\sigma}_i^z$ denoting the Pauli x and z operators acting on site i, respectively. Motivated by experiments for which this model results as an effective description [12], up and down spin states are referred to as "ground" and "excited" states,

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respectively. We consider the experimentally relevant subspace of the Hilbert space that does not contain two neighboring sites in the excited state. Due to the projector terms $\hat{P}_i$, this subspace is decoupled from the rest of the Hilbert space. The Hamiltonian is symmetric with respect to spatial inversion, governed by the operator $\hat{\pi}$, which maps site i to site $L-i+1$. The Hamiltonian also anti-commutes with the parity operator, $\hat{\mathcal{C}} = \prod_{i=1}^{L} \hat{\sigma}_i^z$, such that if $|\psi_E\rangle$ is an eigenstate of $\hat{H}_{\mathrm{PXP}}$ with eigenvalue E, then $\hat{\mathcal{C}}\,|\psi_E\rangle$ is an eigenstate with energy $-E$. The spectrum is, therefore, symmetric around energy zero and contains an exponentially (in system size) large number of zero-energy eigenstates [44–46]. Since the parity operator has eigenvalues ± 1, any eigenstate of the Hamiltonian can be decomposed as $|\psi_E\rangle = (\hat{P}_+ + \hat{P}_-)\,|\psi_E\rangle$, where $\hat{P}_\pm$ are the projectors on the corresponding subspaces of $\hat{\mathcal{C}}$. Applying the operator $\hat{\mathcal{C}}$ to this state gives, $\hat{\mathcal{C}}\,|\psi_E\rangle = (\hat{P}_+ - \hat{P}_-)\,|\psi_E\rangle$, which as mentioned above, corresponds to an eigenstate of energy $-E$. Therefore, for $E \neq 0$, $\langle\psi_E|\hat{\mathcal{C}}|\psi_E\rangle = \langle\psi_E|\hat{P}_+|\psi_E\rangle - \langle\psi_E|\hat{P}_-|\psi_E\rangle = 0$, and we see that $\langle\psi_E|\hat{P}_+|\psi_E\rangle = \langle\psi_E|\hat{P}_-|\psi_E\rangle = 1/2$.

Quantum many-body scars are eigenstates characterized by an anomalously high overlap with the $\mathbb{Z}_2$-ordered states $|\mathbb{Z}_2\rangle = |\bullet\circ\bullet\circ\cdots\bullet\circ\rangle$ and $|\mathbb{Z}_2'\rangle = |\circ\bullet\circ\bullet\cdots\circ\bullet\rangle$, where $\circ$ and $\bullet$ are pictorial representations of a site in the ground and excited state, respectively [13, 14]. These special eigenstates display a bipartite entanglement entropy that scales at most logarithmically with subsystem size. The null space of the Hamiltonian is also known to host a quantum many-body scar for certain system sizes [13, 21, 47]. As motivated below, we do not consider these zero-energy scars in this work. The quantum-many body scars have almost equal energy separations of $\Omega \approx 1.31$, which only weakly depends of the system size. This results in the appearance of long-lived periodic revivals to the initial state starting from a $\mathbb{Z}_2$-ordered state.

III. GAUSSIAN STATE APPROXIMATION

The most general quadratic Hamiltonian with L fermionic modes is given by

$$\hat{H} = \sum_{i,j=1}^{L} \left[A_{ij}\hat{c}_i^\dagger \hat{c}_j + \tfrac{1}{2}\big(B_{ij}\hat{c}_i^\dagger \hat{c}_j^\dagger - B_{ij}^* \hat{c}_i \hat{c}_j\big)\right], \qquad (2)$$

where A is Hermitian and B is antisymmetric and the operators $\hat{c}_i$ and $\hat{c}_j^\dagger$ obey the standard fermionic anticommutation relations $\{\hat{c}_i, \hat{c}_j\} = \{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} = 0$ and $\{\hat{c}_i, \hat{c}_j^\dagger\} = 1$. Fermions are created and annihilated in pairs, meaning that eigenstates can have either an even or an odd number of fermions. Hamiltonian (2) is diagonalized by a Bogoliubov transformation [32, 48, 49],

$$\hat{d}_i = \sum_j \big(U_{ij}\hat{c}_j + V_{ij}\hat{c}_j^\dagger\big) \qquad (3)$$

$$\hat{d}_i^\dagger = \sum_j \big(V_{ij}^*\hat{c}_j^\dagger + U_{ij}^*\hat{c}_j\big), \qquad (4)$$

where U and V are required to obey $UV^T + VU^T = 0$ and $UU^\dagger + VV^\dagger = 1$ in order for $\hat{d}_i$, $\hat{d}_j^\dagger$ to obey the fermionic anti-commutation relations. The eigenstates of Hamiltonian (2) are thus given by product states in the basis of the quasi-particles created by $\hat{d}_i^\dagger$ on top of a quasi-particle vacuum, $|\psi_0\rangle$.

In this work, we focus on the question whether quantum many-body scars can be well approximated by symmetrized ground state of a non-interacting Hamiltonian,

$$|\psi_\pm\rangle = \mathcal{N}\left(|\psi_0\rangle \pm \hat{\pi}|\psi_0\rangle\right). \qquad (5)$$

Here $\mathcal{N}$ is a normalization factor, and $|\psi_0\rangle$ is the groundstate of (2). The states are symmetrized to follow the inversion symmetry of the scars, which results in a better approximation (see the Appendix for details). For quantum many-body scars which are symmetric with respect to inversion we take $|\psi_+\rangle$, and for quantum many-body scars which are antisymmetric we take $|\psi_-\rangle$.

We look for matrices A and B characterizing the quadratic Hamiltonian (2), which give maximal overlap between $|\psi_\pm\rangle$ and a given quantum many-body scar. To compute the overlap, we take the state $|\psi_\pm\rangle$ in the basis where $\hat{n}_i = \hat{c}_i^\dagger \hat{c}_i$ is diagonal, and the quantum many-body scar in the basis where $\hat{\sigma}_i^z$ is diagonal. The PXP model is time-reversal symmetric, therefore we lower the computational costs by restricting A and B to be real. Since the quantum many-body scars have considerable overlap with the $\mathbb{Z}_2$ state, for the initial guess of the matrices A and B we use

$$A = \mathrm{diag}\,(1, 1, -1, 1, \ldots, -1, 1) \qquad B = 0, \qquad (6)$$

such that the initial ground state of (2) is given by the $\mathbb{Z}_2$ state. The number of fermions in this ground state corresponds to the number of (-1)'s on the main diagonal of A. Since in the fermionic language the parity operator is given by $\hat{\mathcal{C}} = (-1)^{\hat{N}}$, where $\hat{N}$ is the operator counting the number of fermions, a state with an even (odd) number of fermions is an eigenstate of the parity operator with eigenvalue $+1$ (-1). By changing the sign of the first element on the main diagonal of the initial guess for A we can control the evenness of the fermion number and as such the parity of the ground state. We have found empirically that the best optimized output is obtained by changing the sign of the first (or last) diagonal element of A, instead of changing the sign of other diagonal elements of A. Taking the diagonal elements of A as ± 1 in a random fashion leads to significantly lower optimized overlaps.

For the optimization procedure we use the Limited-Memory Broyden-Fletcher-Goldfarb-Shanno (also known as LM-BFGS) algorithm [50], which we terminate when the gradient of the overlap with respect to the optimization parameters is equal to zero up to numerical precision. We remark that it is generically impossible to analytically find the optimal parameters of a Gaussian state approximating a given many-body state [51].

We consider relatively modest system sizes due to the high computational costs of the optimization procedure. Typically, optimization requires several thousands, or with outliers, several tens of thousands evaluations of the overlap. For each such overlap the *many-body* ground-state of the quadratic system has to be re-calculated. We note that, while the single-particle states of a quadratic model can be computed in time polynomial with the system size, the computation of the *many-body* ground state scales exponentially with the system size.

We note in passing, that the outlined procedure does *not* typically correspond to the calculation of the natural orbitals from the diagonalization of the single-particle density matrix. In fact, it is known that a ground state constructed in the basis of natural orbitals produces optimal results only for states with two fermions [51, 52].

IV. RESULTS

Since the quadratic Hamiltonian (2) conserves the evenness of the number of fermions, we have to approximate the projections of the scars onto different parity sectors, $\hat{P}_\pm|\psi_{\rm scar}\rangle$, separately. We note, that for system sizes dividable by 4, the $\mathbb{Z}_2$ state lies in the positive parity sector and in the negative parity sector otherwise. On the other hand, as shown in Section II, all eigenstates of the PXP model (with nonzero eigenvalue), including the scars, have the same overlap with both sectors. We denote by $|\psi_{\rm init}\rangle$ the symmetrized ground state of Hamiltonian (2) which corresponds to the initial choice of matrices A and B according to (6). The resulting optimized symmetrized state will be denoted by $|\psi_{\rm opt}\rangle$. For convenience, in Fig. 1 we plot $4|\langle\psi_{\rm opt}|\hat{P}_\pm|\psi_{\rm scar}\rangle|^2$, which is bounded from above by unity, since $\langle\psi_{\rm scar}|\hat{P}_\pm|\psi_{\rm scar}\rangle = 1/2$ (see Section II). We focus only on scars with positive energies, $E_{\rm scar} > 0$, since the spectrum of the PXP model is symmetric around zero. We do not consider quantum many-body scars at zero energy, since scars are not uniquely defined due to numerous degeneracy at zero energy.

Fig. 1 shows the initial $4|\langle\psi_{\rm init}|\hat{P}_\pm|\psi_{\rm scar}\rangle|^2$ and optimized overlaps $4|\langle\psi_{\rm opt}|\hat{P}_\pm|\psi_{\rm scar}\rangle|^2$ for system sizes $L = 8$ to $L = 14$ as a function of the energies of the scars, $E_{\rm scar}$. We observe that the optimized overlap is close to unity for the two quantum many-body scars closest to the edge of the spectrum. In fact, the highest-energy scars are the highest excited eigenstates (or, equivalently, the ground states). We also note that the optimization leads to a significant improvement of the overlap for quantum many-body scars away from the center of the spectrum,

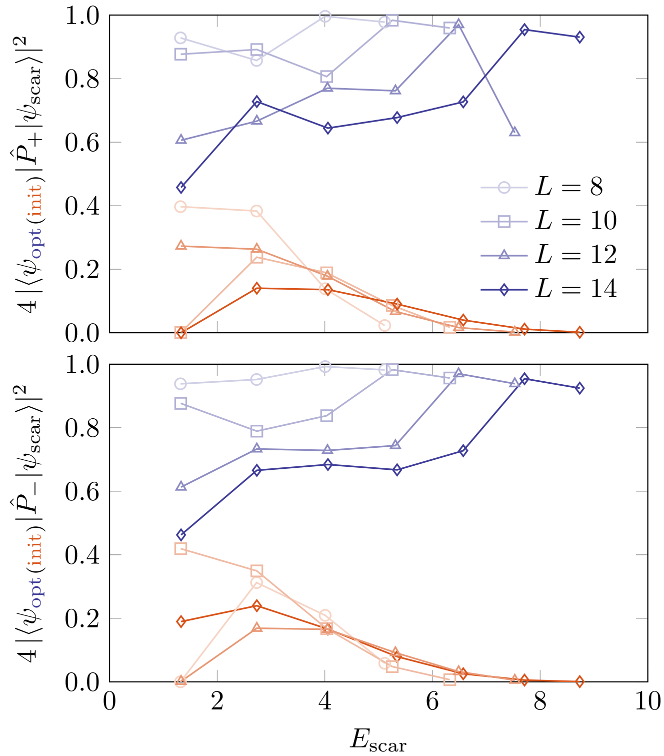

FIG. 1. Blue lines (upper sets of curves) show the optimized overlaps $4|\langle\psi_{\rm opt}|\hat{P}_+|\psi_{\rm scar}\rangle|^2$(upper panel) and $4|\langle\psi_{\rm opt}|\hat{P}_-|\psi_{\rm scar}\rangle|^2$ (lower panel) for several system sizes as a function of the energy of the quantum many-body scars. Red lines (lower sets of curves) show the overlap $4|\langle\psi_{\rm init}|\hat{P}_+|\psi_{\rm scar}\rangle|^2$ (upper panel) and $4|\langle\psi_{\rm init}|\hat{P}_-|\psi_{\rm scar}\rangle|^2$ (lower panel). The largest possible overlap with this normalization is unity.

as can be seen by comparing to the overlap with the initial guess, $|\psi_{\rm init}\rangle = (|\mathbb{Z}_2\rangle \pm |\mathbb{Z}_2'\rangle)/\sqrt{2}$.

Quantum many-body scars distinguish themselves from other types of non-ergodic many-body states by their anomalously high overlap with the $|\mathbb{Z}_2\rangle$ and $|\mathbb{Z}_2'\rangle$ states. This can be seen at the lower (red) set of lines in Fig. 1, which shows the overlap, $4|\langle\psi_{\rm init}|\hat{P}_+|\psi_{\rm scar}\rangle|^2$, where $|\psi_{\rm init}\rangle = (|\mathbb{Z}_2\rangle \pm |\mathbb{Z}_2'\rangle)/\sqrt{2}$. In Fig. 2, we see that also the optimized state has a qualitatively similar overlap with the $|\mathbb{Z}_2\rangle$ and $|\mathbb{Z}_2'\rangle$ states, by plotting $|\langle\psi_{\rm init}|\psi_{\rm opt}\rangle|^2$ as a function of the energy of the quantum many-body scars for the system sizes considered above. It is interesting to note that at the edges of the spectrum where the approximation of the scars is the best, the optimized and initial states are almost orthogonal to each other.

The structure of the optimized matrices A and B could provide insight on the structure of the quantum many-body scars. Fig. 3 shows color plots of the optimized matrices for the scar with the second-highest (the highest-energy scar is the ground state) energy at system size $L = 14$. The optimized Hamiltonian is not translationally invariant (even in the bulk) and exhibits a notion

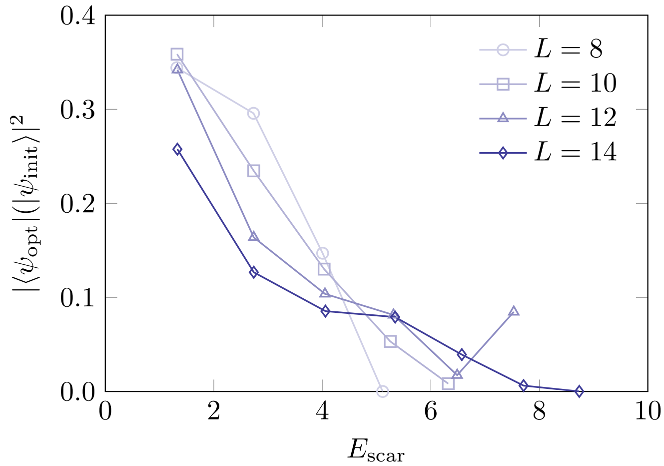

FIG. 2. The overlap $|\langle\psi_{\rm opt}|\psi_{\rm init}\rangle|^2$ as a function of the energy of the quantum many-body scars at several system sizes.

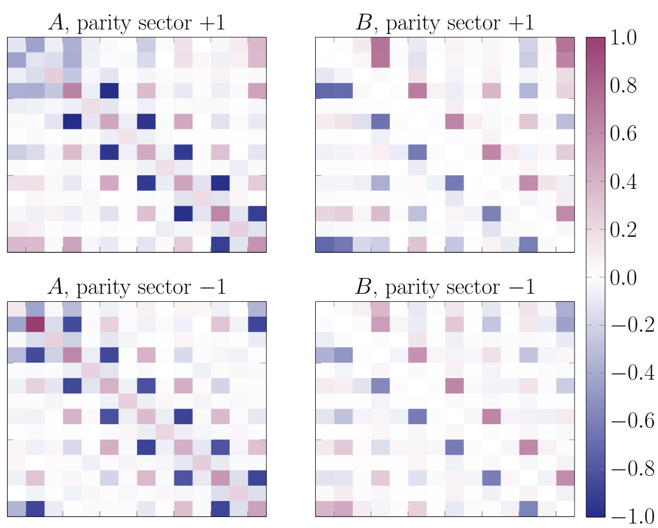

FIG. 3. Color plots of the matrices A (left) and B (right) of the quadratic Hamiltonian (2), whose ground-state has the largest overlap with the scar with the second-highest energy for $L = 14$. The top panels correspond to optimization with respect to $\hat{P}_+ |\psi_{\rm scar}\rangle$ and the bottom panels with respect to $\hat{P}_- |\psi_{\rm scar}\rangle$. The scale has been chosen such that the largest absolute value is unity.

of locality, reflected in the band-like structure. This observation is presumably related to the low-entanglement property of the quantum many-body scars.

V. CONCLUSIONS AND OUTLOOK

We have studied to what extent quantum many-body scars in the PXP model can be described by inversion symmetrized Gaussian state, which corresponds to a ground-state of a quadratic Hamiltonian with no particle number conservation. For this, we numerically optimized a quadratic fermionic Hamiltonian whose ground-state has a maximal overlap with the quantum many-body scar under consideration. We found that quantum many-body scars away from the center of the spectrum can be well described by states of this form. This holds in particular for the highest (or equivalently, lowest) energy quantum many-body scar. We also showed, that the optimal quadratic Hamiltonian is local, has a non-negligible pairing and is *not* translationally invariant. In fact, enforcing translation invariance in the optimization procedure, provides considerably lower overlaps (not shown). Since entanglement entropy of ground-states of local quadratic Hamiltonians scales logarithmically with the system size [31], our result suggests that similar scaling will hold also for quantum many-body scars, at least not too close to the center of the spectrum.

In this work, we have used a distinct quadratic Hamiltonian for each quantum many-body scar. In future studies, it would be interesting to see if a single optimal quadratic Hamiltonian can be used to reasonably capture the structure of each of the scars, as also to understand the origin of such an effective single-particle description. It would be also interesting to investigate further if similar results can be obtained for other quantum many-body scarred models.

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Appendix: Optimization results for Gaussian states

Here, we study the overlap of quantum many-body scars with optimized Gaussian states, here denoted by $|\psi_{\rm opt,0}\rangle$, instead of the symmetrized version $|\psi_{\rm opt}\rangle$ [see (5)]. As this investigation is only for illustrative purposes, we restrict the analysis to optimization with respect to the parity sector containing the $\mathbb{Z}_2$ state, which is arguably physically the most interesting. Fig. 4 shows the optimized overlaps as a function of the energy of the quantum many-body scar for several system sizes. Comparing the results with those shown in Fig. 1, we observe a substantially lower overlap, which highlights the importance of symmetrization.

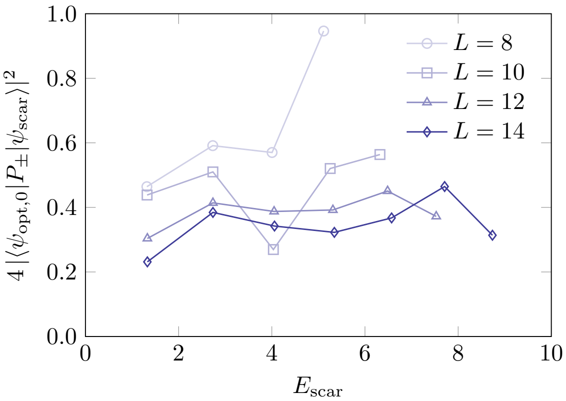

FIG. 4. The optimized overlaps $4|\langle\psi_{\rm scar}|\hat{P}_\pm|\psi_{\rm opt,0}\rangle|^2$ for several system sizes as a function of the energy of the quantum many-body scars. The sign of the projector $P_\pm$ is chosen such that it projects on to the parity sector containing the $\mathbb{Z}_2$ state. The largest possible overlap with this normalization is unity.

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