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Encoding the structure of many-body localization with matrix product operators

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Anderson insulators are non-interacting disordered systems which have localized single particle eigenstates. The interacting analogue of Anderson insulators are the Many-Body Localized (MBL) phases. The spectrum of the many-body eigenstates of an Anderson insulator is efficiently represented as a set of product states over the single-particle modes. We show that product states over Matrix Product Operators of small bond dimension is the corresponding efficient description of the spectrum of an MBL insulator. In this language all of the many-body eigenstates are encode by Matrix Product States (i.e. DMRG wave function) consisting of only two sets of low bond-dimension matrices per site: the $G_i$ matrices corresponding to the local ground state on site $i$ and the $E_i$ matrices corresponding to the local excited state. All $2^n$ eigenstates can be generated from all possible combinations of these sets of matrices.

The primary result of this letter is to show that the matrix product operators of many-body localization with matrix product operators. Importantly, this means that for an $L$-site lattice, $L$ single particle localized orbitals are sufficient knowledge to generate every many-body eigenstate. From this simple form, many of the properties of Anderson insulators can be understood. This leads us to a simple question: Do the many-body eigenstates of a MBL phase also share a simple and concise form?

The primary result of this letter is to show that the matrix product states which represent MBL eigenstates have a simple uniform structure over the whole spectrum. To manifest this structure, we describe Anderson insulators and then show a natural generalization of the Anderson insulator case for the MBL case. Consider the specific example of one dimensional disordered spin-1/2 chains. In the non-interacting case, we can work in the basis of single particle eigenfunctions. Moreover, since all eigenfunctions are localized we can assign each eigenfunction to a lattice site $i$. Hence, each state of the many-body spectrum corresponds to a product state in which we assign each site of the lattice either $|\psi_i = 0, \phi_i = 1\rangle$ if the corresponding single particle state is empty or $|\psi_i = 1, \phi_i = 0\rangle$ if it is occupied

$$\Psi_{\text{Anderson}} = \prod_i (\psi_i |e_i\rangle + \phi_i |g_i\rangle).$$

A natural extension of these product states to the interacting but localized regime is obtained by replacing the the localized single particle orbitals $e_i$ and $g_i$ by tensors of finite bond dimension $E_{i,j,k}$ and $G_{i,j,k}$, where the indices $j$ and $k$ are dummy indices that are summed over when contracting the tensors. The index $\sigma_i$ corresponds to the local spin state on site $i$, which we will choose to be defined in the original Fock basis. While these tensor states can encode some short distance entanglement, just like product states, they cannot encode long distance entanglement. We give evidence that in the MBL phase all eigenstates can be compactly represented in the from

$$\Psi_{\text{MBL}} = \prod_i (\psi_i E_{i,j}^{\sigma_i} + \phi_i G_{i,j,k}^{\sigma_i})|\sigma_i\rangle.$$  

Hence, the MBL ground state corresponds to the Matrix Product State (i.e. DMRG wave function)

$$\Psi_{\text{MBL, 000...}} = \sum_{j,k,l} G_{i,j,k}^{\sigma_1} G_{2,j,k}^{\sigma_2} G_{2,k,l}^{\sigma_3} \cdots |\sigma_1 \sigma_2 \sigma_3 \cdots \rangle.$$  

Swapping $G_{i,j,k}^{\sigma_i}$ for $E_{i,j,k}^{\sigma_i}$ creates a local excitation of the system.

$$\Psi_{\text{MBL, 010...}} = \sum_{j,k,l} G_{i,j,k}^{\sigma_1} E_{2,j,k}^{\sigma_2} G_{2,k,l}^{\sigma_3} \cdots |\sigma_1 \sigma_2 \sigma_3 \cdots \rangle.$$  

The full many-body spectrum can be obtained by composing all combinations of $G_{i,j,k}^{\sigma_i}$'s and $E_{i,j,k}^{\sigma_i}$'s on all sites, thus mapping product states onto matrix product states. We show that these matrices can be directly identified from the Matrix Product Operator (MPO) derived from the unitary transformation that diagonalizes the Hamiltonian of our MBL system. Remarkably, we find strong numerical evidence that inside the

\[\text{Encoder} (\text{Matrix Product Operator})\]
MBL phases this MPO is efficiently representable: the typical bond dimension of the tensors $G_{i,j,k}^\sigma$ and $E_{i,j,k}^\sigma$ saturates at a finite value even as the system size increases.

An introduction to Matrix Product States and Operators – Here we review the essential aspects of MPS/MPO (for a more in-depth review see, e.g., Ref. 24). A convenient way to depict matrix product states and operators is shown in Fig. 1. For the case of spin-1/2 chains, the external indices can take on two values $\sigma_i, \chi_i \in \{\uparrow, \downarrow\}$. On the other hand the internal indices can span the range $[1, \ldots, D_i]$, where $D_i$ is the “bond dimension” for the bond between site $i$ and $i+1$. The value of $D_i$ is a tuning parameter that controls how much entanglement can be carried by the internal index linking neighboring sites. To describe eigenstates of strongly disordered systems we allow each internal bond to have a different bond dimension as dictated by the disorder realization.

To summarize, an MPS for an $L$-site chain is parametrized by $2L$ matrices – two matrices per site $M_{i,k,k+1}^\sigma$ and $M_{i,k,k+1}^{\sigma\tau}$. Analogously, an MPO contains four matrices for each site $i$: $O_{i,k,k+1}^{\sigma\tau\sigma\tau}, O_{i,k,k+1}^{\sigma\tau\sigma\sigma}, O_{i,k,k+1}^{\sigma\tau\tau\tau}$, and $O_{i,k,k+1}^{\sigma\tau\tau\sigma}$.

A unitary operator $U$, which diagonalizes a Hamiltonian, maps the eigenstates of the Hamiltonian to the product states (i.e. bit strings of length $L$). Consider the action of the MPO representing $U$ on the MPS representing the product state $|p\rangle$. The MPS has $D = 1$, thus the resulting MPS, $U|p\rangle$, simply selects two of the four MPO matrices per site. Hence, all the eigenstates of the Hamiltonian are encoded by matrix product states generated from all combinations of the matrices $O_{i,k,k+1}^{\sigma\tau\sigma\tau}$ and $O_{i,k,k+1}^{\sigma\tau\tau\tau}$. We then choose $G_i$ and $E_i$ to be $O_i^{\sigma\tau\sigma\tau}$ or $O_i^{\sigma\tau\tau\tau}$ depending on whether the product state which maps to the ground state has $\downarrow$ or $\uparrow$ on site $i$. Notice that all eigenstates of the system are represented by $4L$ matrices (those that make up the MPO). The key question that we address is whether the MPO which represents the unitary operator can be represented by matrices with a fixed bond dimension that is independent of the system length $L$.

Small bond dimension MPO – The strategy that we employ for testing whether MPOs can efficiently describe the unitary transformation that takes product states to eigenstates consists of three steps: (1) we construct the exact unitary transformation using exact diagonalization, (2) we identify a correspondence between the exact eigenstates and product states which maximally preserves locality, and (3) we compress the transformation into a matrix product operator. We test this approach on a spin 1/2 chain with the Hamiltonian

$$H = \sum_{(i,j)} S_i \cdot S_j + \sum_i h_i S_i^z$$

where $h_i$ is a random field chosen from a distribution $h_i \in [-\Delta, \Delta]$. The location of the MBL transition in $H$, as a function of $\Delta$, is still not fully established. The current best lower bound is at $\Delta \geq 4.25$. In our strategy, there is a clear notion of optimality: the procedure that produces an MPO with the smallest bond dimension. This hinges on correctly identifying the spatial position of the excitations in each exact eigenstate and matching these locations to the corresponding product state. Finding the optimal matching is a numerically challenging task and hence we use a heuristic procedure. The bond dimensions we obtain are therefore an upper bound to the best MPO bond dimensions.

To find the matching between the list of eigenvectors $|e\rangle$ and product states $|p\rangle$ we use the intuition that each eigenstates of the strongly localized interacting system should have a considerable overlap with its parent state – an eigenstate of the non-interacting system. In our case, the non-interacting system corresponds to Hamiltonian (5) without the Heisenberg coupling, hence the parent states are the product states. For the case of weak interactions (large $\Delta$) this heuristic gives a one-to-one and onto mapping $f(|e\rangle) = |p\rangle$ between eigenstates and product states. However, generically, the heuristic can map multiple eigenstates to the same product state – a sit-
Hamiltonian of reference\textsuperscript{10}. In the product basis, the Hamiltonian (5) acquires the form
\[ H_{\text{eff}} = \sum_i J_{i,i} \sigma_i^z + \sum_{i,j} J_{i,j} \sigma_i^x \sigma_j^x + \sum_{i,j,k} J_{i,j,k} \sigma_i^x \sigma_j^x \sigma_k^x + \ldots \] (6)

We generate \( H_{\text{eff}} \) by solving \( Ax = b \) for \( x = \{1, h_1, h_2, \ldots, J_{12}, J_{13}, \ldots\} \) and \( A \) is the matrix that relates this set of couplings to the exact eigenvalues via the l-bit configurations. In the MBL phase all couplings \( J_{i,j}, J_{i,j,k}, \ldots \) must decay as a function of the separation (\( |i - j| \)). We use this fact to our advantage to extract \( \xi \) from the decay of \( J_{i,j} \). We find that, up to a fixed rescaling by the factor 8.7, the two definitions of \( \xi \) seem to match [see Inset Fig 2].

To summarize, our main result is that for systems in the MBL phase the full spectrum of eigenvectors can be described using an MPO of low bond dimensions. This observation dictates the structure of the many-body eigenstates. The MPO representation quantifies the notion of localized excitations and therefore dictates such properties as lack of thermalization, entanglement, emergent integrability, etc.

To understand the nature of the break down of the MPO representation, we look at the distribution of bond dimensions at fixed disorder strength Fig. 3(a). In the strongly localized matter, we find that the distribution of bond dimensions tends to be strongly peaked around \( D = 1 \) (the minimum possible value for \( D \)). As the disorder strength decreases, we observe that (1) the peak in the distributions is starting to shift to small but finite values of \( D \) associated with a growing localization length, and (2) the emergence of a power law tail in the distributions [see Fig. 3(b)]. This power law tail signifies the onset of Griffiths physics: the system contains exponentially rare regions of the delocalized phase that give an exponentially strong contribution to the bond dimension. Griffiths physics have been seen in similar quantities such as the entanglement of individual eigenstates by ref.\textsuperscript{11,13,15}. As the disorder strength decreases the Griffiths regions become less rare. At the transition point we see a drastic change in the distribution of \( D \) as it becomes extremely broad. Similar broadening has been observed in entanglement entropies of single eigenstates\textsuperscript{15}. On the delocalized side of the transition the distribution again becomes sharply peaked, but this time around a system size dependent value. The broadening of the distribution at the transition point indicates that the mechanism that drives the delocalization transition is the formation of resonances between the rare regions.

Discussion – The fact that the unitary that diagonalizes the Hamiltonian can be compressed into an MPO of small bond dimension has direct consequences for the properties of the MBL phase. We begin by noting that the typical entanglement entropy of any of the eigenstates is finite as it is limited by \( \log[D] \) which contradicts ETH. Within our framework we can rule out thermalization without appealing to ETH. Consider a local operator such as \( U \sigma_1^y U^\dagger \). Note this is the l-bit raising operator\textsuperscript{10} in the MPO language. The application of the MPO composed from \( UU^\dagger \) and the MPO composed from \( U \sigma_1^x U^\dagger \) differ only on a single site [see Fig. 1(c)]. As the matrix on this site has a bond dimension which doesn’t grow with sys-
The MPO language lets us explicitly write the emergent local constants of motion. A constant of motion is a hermitian operator which commutes with the Hamiltonian. Consider operators of the form

$$\rho_{\text{product}} = I_1 \otimes \ldots I_{k-1} \otimes \sigma_i^z \otimes I_{k+1} \ldots I_n = \sum_p \alpha_p |p\rangle \langle p|$$

where $|p\rangle$ is a product state over all the sites. Applying the MPO $U$ to this operator gives us $U\rho_{\text{product}}U^\dagger = \sum \alpha_i |e_i\rangle \langle e_i|$ where $|e_i\rangle$ are eigenstates of the many-body system. Operators of this form commute with the Hamiltonian and consequently are constants of motion. Mirroring our previous argument, as $U\rho_{\text{product}}U^\dagger$ differ from $UU^\dagger$ by a single matrix they have an exponential weak effect on distant parts of the system and hence the constants of motion we’ve written down are local.

Finally we remark that the application of MPOs as a variational basis for diagonalizing many-body localized Hamiltonians has not escaped our notice. There has been considerable work on using MPS as a variational basis for individual eigenstates and the extension to MPOs is natural. Indeed, our numerics indicates that in the localized phase we can represent the entire spectrum of eigenstates of the Hamiltonian in a compact form using an MPO of low bond dimension. Due to the compact nature of the MPO representation it should be possible to diagonalize the Hamiltonian of rather large systems, significantly beyond the limits of exact diagonalization. The Griffiths effects will control the success of this endeavor.

We point out that having the complete spectrum will allow for efficient evaluation of finite energy density and dynamical properties of these systems. In fact, during the refereeing process of this paper two groups have made progress on the this program of variationally optimizing MPOs.

In this work, we have focused on elucidating a structure for the entire spectrum of eigenstates that is analogous to the structure that is seen in Anderson localization. We have additionally seen that the structure of these eigenstate gives us a way to understand the properties of the MBL phase. Although we have focused here primarily on one-dimensional system, there is every reason to believe that the natural generalization where PEPS replace MPS will hold for higher dimensions.

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Note added: during the preparation of this manuscript we became aware of a complementary work Ref. 35.
27. In constructing the MPO representation $U$ we used the standard singular value decomposition method with a threshold – singular values below the threshold were dropped. All data presented in the manuscript were collected with the threshold set to 0.01. We tested that decreasing the threshold to 0.001 did not significantly affect the data. Specifically, there was no quantifiable affect on the localization length nor the transition point.