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 natural language for representing the spectrum of the Anderson insulator is that of product states over the single-particle modes. We show that product states over Matrix Product Operators of small bond dimension is the corresponding natural language for describing the MBL phases. In this language all of the many-body eigenstates are encoded by Matrix Product States (i.e. DMRG wave function) consisting of only two sets of low bond-dimension matrices per site: the $G_i$ matrix corresponding to the local ground state on site $i$ and the $E_i$ matrix corresponding to the local excited state. All $2^L$ eigenstates can be generated from all possible combinations of these matrices.

An Anderson insulator is a non-interacting system that is driven into the insulating phase by quenched disorder [1]. In one dimension, or for the case of strong disorder in higher dimensions, it is known that all single particle eigenstates can become localized [2]. When this occurs an Anderson insulator is a perfect insulator even at finite temperature. This should be contrasted with conventional insulators like band and Mott insulators that always display some form of activated behavior at finite temperatures.

The interacting analogue of the Anderson insulator is called many-body localization whose presence was originally suggested by a diagrammatic calculation [3][4]. Significant recent interest has gone to understanding whether many-body localized (MBL) phases exist as well as determining their properties [5][10]. Many-body localized phases are believed to have a number of unusual properties including: (a) zero conductivity at finite temperature, (b) failure to thermalize, and (c) a large number of local constants of motion and corresponding conserved quantities. For MBL systems with a thermally-driven (or more precisely energy-density-driven) transitions these features persist all the way to the critical energy density.

The MBL phase transition is unique in that the phase transition is dynamical and, therefore, not simply a feature of the ground state wave-function or finite temperature density matrix. Instead, the MBL phase transition is believed to be caused by a qualitative change in the finite energy density eigenstates of the Hamiltonian. In fact, it is known that MBL eigenstates are special with evidence accumulating that they obey an area law and exhibit poisson statistics. Understanding of these MBL eigenstates have come from exact-diagonalization studies of small (up to 16 sites [11][14]), T-DMRG (time dependent density matrix renormalization group [15][17]) and real space strong disorder renormalization group analysis [18][19].

In contrast to the MBL eigenspectrum, the many-body eigenstates of a typical many-body Hamiltonian have essentially the same properties as arbitrary states sampled from the Hilbert space. In fact, the eigenstate thermalization hypothesis (ETH) [20][22] suggests that typical eigenstates must locally look the same as the thermal density matrix at the temperature corresponding to their respective energy density. This means they obey a volume law: the entanglement entropy of a small subsystem with the remaining system is proportional to the volume of the subsystem. Moreover, level repulsion causes gaussian orthogonal ensemble level statistics in the eigenstates of a typical Hamiltonian.

Like MBL eigenstates, the many-body eigenstates in an Anderson insulator have atypical properties. In addition, though, they have a very simple form: a product state over localized single-particle eigenstates. Importantly, this means that for an $L$-site lattice, $L$ single particle localized orbitals is 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?

In this letter we use the language of matrix-product states to identify a simple form for MBL eigenstates. To manifest this structure, we describe the case of an Anderson insulator 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

$$\Psi_{Anderson} = \prod_i (|\psi_i e_i \rangle + \phi_i g_i\rangle). \tag{1}$$

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 $E_{i,j,k}^{\sigma_i}$ and $G_{i,j,k}^{\sigma_i}$, 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 can then write

$$\Psi_{\text{MBL}} = \prod_i (|\psi_iE_i^{r_i} + \phi_iG_i^{r_i})|\sigma_i\rangle.$$  

(2)

Hence, the MBL ground state corresponds to the Matrix Product State (MPS) representation. From our numerical results we describe a numerical procedure for constructing an MPO representation of system size in the MBL phase. To show this, we will argue that this MPO representation is compact – the system can all be encoded in the structure of Eq. (2). Then, the Hamiltonian. This will imply that the eigenstates of the finite value even as the system size becomes larger.

The full many-body spectrum can be obtained by composing all combinations of $G_i^{r_i}$’s and $E_i^{r_i}$’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 MBL phases this MPO is efficiently representable: the typical bond dimension of the tensors $G_i^{r_i}$ and $E_i^{r_i}$ saturates at a finite value even as the system size becomes larger.

The paper is structured as follows. First, we give a brief description of MPS’s and MPO’s showing how an MPO can be used to represent the unitary transformation that diagonalizes the Hamiltonian. This will imply that the eigenstates of the system can all be encoded in the structure of Eq. [2]. Then, we will argue that this MPO representation is compact – the bond-dimension of a typical bond of the MPO is constant as a function of system size in the MBL phase. To show this, we describe a numerical procedure for constructing an MPO representation of the unitary transformation and apply this procedure to construct the MPOs for a large number of disorder strengths, system sizes, and disorder realizations. We devise an approach to match product states to eigenstates so as to minimize the ‘locality mismatch’. From our numerical results we find that MPOs are indeed an efficient way to represent the many-body spectrum of an MBL system. At the same time we uncover strong Griffiths effects that arise from rare regions of weak disorder. To conclude, we discuss how a description in terms of MPOs naturally leads to the conjectured properties of MBL phases, and comment on the limitations on using MPO representation for numerical diagonalization of strongly disordered Hamiltonians.

**An introduction to Matrix Product States and Operators** – A MPS represents a quantum state and a MPO represents an operator. A convenient way to depict matrix product states and operators is using pictures composed of boxes and lines, see Fig. 1. For the case of spin-1/2 chains, the external indices can take on two values $\sigma_i,j_i \in \{|\uparrow\rangle_i, |\downarrow\rangle_i\}$. 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. In practice, to describe eigenstates of strongly disordered systems we allow each internal bond to have a different bond dimension as dictated by the disorder realization.

In summary, a MPS for an $L$-site chain is parameterized by $2L$ matrices – two matrices per site $M_i^{\uparrow \downarrow} \ldots$ and $M_i^{\downarrow \uparrow} \ldots$. Analogously, an MPO contains four matrices for each site $i$: $O_i^{\uparrow \downarrow} \ldots$, $O_i^{\downarrow \uparrow} \ldots$, $O_i^{\uparrow \uparrow} \ldots$, and $O_i^{\downarrow \downarrow} \ldots$.

We can represent the composition of operators and states in the matrix product language. As an example consider performing a basis transformation on the single site spin raising operator $\hat{\sigma}_i^\uparrow$. $\hat{\sigma}_i^\uparrow$ can be represented as an MPO of $D = 1$ with $O_i^{\uparrow \downarrow} \delta_{a,b}$ if $j \neq i$ and $O_i^{\uparrow \uparrow} = \sigma_{a,b}$. If the unitary transformation is also represented as an MPO, we obtain a new MPO with $O_i^{\uparrow \downarrow} = (U^{\gamma})^{\uparrow \downarrow} O_i^{\uparrow \downarrow} U_{\gamma}$. [See Fig. 1(c)].

When the unitary operator $U$, which diagonalizes a Hamiltonian, acts on one of the $2^L$ product states it returns the corresponding eigenstate of the Hamiltonian. In the MPS language a product state is a MPS of $D = 1$ and therefore when a product state is acted on by a MPO, the resulting MPS simply selects two of the four MPO matrices per site. Therefore, if we represent $U$ as an MPO, all the eigenstates of the Hamiltonian are encoded by matrix product states generated from all combinations of the matrices $O_i^{\uparrow \downarrow}$ and $O_i^{\uparrow \uparrow}$. We then choose $G_i$ and $E_i$ to be $O_i^{\uparrow \downarrow}$ or $O_i^{\uparrow \uparrow}$ depending on whether the product state which maps to the ground state has down or up on site $i$. Notice that all eigenstates of the system are represented by 4$L$ matrices (those that make up the MPO). The key question, which we shall now address, is whether the MPO which represents the unitary operator can be represented by matrices with a finite bond dimension independent of the system length $L$.

**Small bond dimension MPO** – The strategy that we employ for testing whether MPOs can efficiently describe the unitary

**FIG. 1.** Box and line depiction of (a) a matrix product state $|\psi\rangle$, (b) a matrix product operator $U$, and (c) the product of three matrix product operators $U^\gamma \hat{\sigma}_i^\uparrow U$. The boxes correspond to tensors and lines to tensor indices. Lines that connect two boxes correspond to indices that are contracted while dangling lines correspond to external indices. The matrix product state $|\psi\rangle$ “eats” the external indices $|\sigma_1 \sigma_2 \sigma_3 \ldots\rangle$ (these are the configurations of our spin-1/2 chain) and “spits” out a complex number – the amplitude of that configuration. Similarly, the matrix product operator “eats” one set of external indices $|\sigma_2 \sigma_3 \sigma_4 \ldots\rangle$ corresponding to the “ket” and a second set of external indices $\langle \chi_1 \chi_2 \chi_3 \ldots\rangle$ corresponding to the “bra” and “spits” out the value of the corresponding matrix element.
transition from the localized to the delocalized phase. Inset: Local-
chain length keeps grows. The change of regime corresponds to the
order the bond dimension saturates at a finite value, even as the
For systems with weak disorder the bond dimension grows linearly
Disorder. The solid lines represent fits to the numerical data (see text).
Chain Length for a number of values of disorder strength. The points
FIG. 2. Bond Dimension of the Matrix Product Operator represent-
imation into a matrix product operator. The Hamiltonian we
maximally preserves locality, and (3) we compress the trans-
ion using exact diagonalization, (2) we identify a correspon-
dence to eigenstates to product states within the same total
sector.
Having performed the bipartite matching, we move on to
the second numerical challenge: finding the MPO represent-
ation of our unitary transformation. Here, we can take ad-
vantage of the spatial information extracted in the previous step: we rewrite the unitary operator as a wave function by
collapsing the two sets of external indices \( \sigma \) for the eigen-
state spins and \( \chi \) for the product state spin into a single index
\( \mu \). This glues together indices that are spatially
close, meaning little entanglement exists between \( \mu_i \) and \( \mu_j \) if
i and j are far apart. We then compress this state into a MPS.
Finally, we convert the MPS into an MPO by splitting the \( \mu \)
indices into the \( \sigma \) and \( \chi \) constituents.

The bond dimension of the resulting MPO is set by a tun-
ing knob contained in the compression step where we select
a cut-off for the smallest singular value we keep. If we se-
lect a lower cut-off, then we keep more singular values and
hence obtain an MPO with a higher bond dimension which
more faithfully matches the exact unitary. Consider fixing the
cut-off to a small value. If the unitary is indeed local, i.e. the
Hamiltonian giving rise to it is many-body localized, we find
that there are very few singular values above the cut-off and
hence the resulting MPO has a small bond dimension. On the
other hand if the unitary is non-local, i.e. the parent Hamilto-
subspace independently. Having obtained a list of eigenvectors
we move onto the first of the two numerical challenges:
how to relate the list of eigenvectors \( P_E \) to the list of product
states \( P_P \).

The conjecture for why the unitary should be compressible
into an MPO of low bond dimension is that all of the exci-
tations of the system in the MBL phase must be spatially lo-
calized and the unitary therefore only needs to connect these
spatially local sub-systems. This can be performed using a
unitary with bond dimension \( D \leq 4^l \), where \( l \) is the charac-
teristic lengthscale. However, to take advantage of this fact
we must extract the locations of these localized excitations in
each eigenvector and hence map the eigenvector onto the cor-
responding product state.

In principle, we could try every possible match between the
two lists \( P_E \) and \( P_P \) and select the one that produces the MPO
with the lowest bond dimension; this procedure, however, is
numerically intractable and therefore we use the following
heuristic approach. Consider the function \( M(i) \) which speci-
fies a unique matching of product states labelled by \( i \) to eigen-
states \( M(i) \). Then define the objective function \( \sum_i |(M(i))| i \|^2 \).
We maximize this objective function over functions \( M \); this
will have high overlap with the product states to which it should
be mapped. We further optimize the matching task by matching
only eigenstates to product states within the same total \( \sigma \)
sector.

Having performed the bipartite matching, we move on to
the second numerical challenge: finding the MPO representa-
tion of our unitary transformation. Here, we can take ad-
vantage of the spatial information extracted in the previous step: we rewrite the unitary operator as a wave function by
collapsing the two sets of external indices \( \sigma \) for the eigen-
state spins and \( \chi \) for the product state spin into a single index
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Hamiltonian giving rise to it is many-body localized, we find
that there are very few singular values above the cut-off and
hence the resulting MPO has a small bond dimension. On the
other hand if the unitary is non-local, i.e. the parent Hamilto-
nian is ergodic, there are many more singular values above the cut-off and hence the bond dimension of the resulting MPO is large.

**Numerical Results** – The main result of our manuscript is depicted in Fig. 2. In this figure, we plot the bond dimension \( D \) of the Matrix Product Operator representing the unitary that diagonalizes the Hamiltonian \( H \) as a function of system size \( L \) for various disorder strengths \( \Delta \). In producing the plot, we have averaged the \( \log[D] \) over many disorder realizations. As we are averaging the logarithm of the bond dimension, rare regions do not have a disproportionate affect on the average. From the figure, we observe that for systems with weak disorder (\( \Delta \lesssim 3 \)) the bond dimension grows linearly with system size, while for those with strong disorder (\( \Delta \gtrsim 15 \)) the bond dimension has saturated by the time the chain length has reached \( L = 12 \). For disorder strengths \( 3 \lesssim \Delta \lesssim 15 \) we do not have access to long enough chains to make a qualitative statement.

We can, however, quantify the saturation effect by fitting the \( D \) vs. \( L \) curves with a generic saturation function:

\[
\log[D(L)] = a \tanh(L/\xi) \quad \text{where} \quad a \quad \text{and} \quad \xi \quad \text{are the fitting parameters.}
\]

In the inset of Fig. 2, we plot the saturation length scale \( \xi \) as a function of the bond dimension. We observe that for systems with strong disorder the saturation length-scale is indeed very short. As the disorder becomes weaker, \( \xi \) increases, becoming divergent for \( \Delta \lesssim 3 \). The \( \xi \) we obtain matches that of Ref. [23] [see caption Fig. 2].

To summarize, our main result is that for systems in the MBL phase the full spectrum of eigenvectors in the localized phase can be described using an MPO of low bond dimensions. This observation dictates the structure of the many-body eigenstates. The properties of this structure can be used to identify the unusual properties, both static and dynamic, of MBL matter. Specifically, the MPO representation quantifies the notion of localized excitations and therefore dictates such properties as lack of thermalization, entanglement, emergent integrability, etc. We shall explicitly come back to these points in the discussion section, but first we explore how the MPO representation breaks down as we approach the delocalization critical point.

To understand the nature of the break down of the MPO representation, we look at the distribution of bond dimensions at fixed disorder strength. Specifically, we ask whether the distribution of bond dimensions is sharply peaked or not, and if not how does it behave. We summarize the behavior of bond dimensions in 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 \( \approx 1 \). As the disorder strength decreases the Griffiths regions become less rare and begin to resonate. At the transition point we see a drastic change in the distribution of \( D \) as it becomes extremely broad. This broadening, which has also been observed in the entanglement entropy of single eigenstates [14], culminates in the shift of the maximum of the distribution to 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 \( U \sigma_k^+ U^\dagger \). Note this is the l-bit raising operator [23] in the MPO language. The application of the MPO composed from \( UU^\dagger \) and the MPO composed from \( U \sigma_k^+ U^\dagger \) differ only on a single site [see Fig. 2]. As the matrix on this site has a bond dimension which doesn’t grow with system size, it will connect single eigenstates to a sub-extensive number of eigenstates all of which must have similar matrices far from the operator application. This fact tells us that \( 1 \) there is no thermalization as a local kick to the system remains local; \( 2 \) there is no electrical conductivity as an excitation injected into the system at site \( i \) remains put for very long times; and \( 3 \) there is no level repulsion as excitations from spatially distant operators \( \sigma_k^+ \) and \( \sigma_k^- \) have no overlap.

Finally, this 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

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

where \( |p\rangle \) is a product state over all the sites. Applying the MPO \( U \) to this operator gives us \( U\rho_{\text{product}} U^\dagger = \sum_i \alpha_i |e_i\rangle\langle e_i| \) 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, we see the MPO \( U_{\text{product}} U^\dagger \) 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. 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 ef-
effects will control the success of this endeavor. Specifically, each disorder realization will have rare regions of lower than typical disorder that will require an exponentially large bond dimension. The probability to find a rare region of length $l$ in a chain of length $L$ scales as $\exp(-l/\xi)$. Therefore, with probability 1 a chain will contain a rare region that requires $D \propto L/\xi$, which is a much softer constraint than the typical exponential scaling for exact diagonalization. Although we save the construction of these MPOs for larger systems for a future work, we point out that having the complete spectrum will allow for efficient evaluation of finite energy density and dynamical properties of these systems.

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 very natural language to understand the property 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. [25].

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