↓ Lecture 21 [10.07.25]

8.3. Reminder: Entanglement entropy

The entanglement entropy is (one of many) measures that quantify the "amount" of entanglement between two or more subsystems of a quantum mechanical system. It is crucial to understand certain ground state properties of quantum-many-body systems.

Entanglement in many-body systems is a complex phenomenon that *cannot* be fully captured by a single quantity (like entanglement entropy) [211].

1 | ◁ Bipartite quantum system with Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$

◁ *Pure* state $\rho = |\Psi\rangle\langle\Psi|$

"Bipartite" simply means that we can split the system into two subsystems, e.g., two halves of a spin chain with each $L/2$ spin-$\frac{1}{2}$.

→ ↓ *Reduced density matrix* $\rho_A := \mathrm{Tr}_B[\rho]$

The reduced density matrix ρ_A is computed by "tracing out" the "environment" B via the ↓ *partial trace* Tr_B [•] and encodes the expectation values of all observables localized on A.

$$S[A] := -\mathrm{Tr}\left[\rho_A \log_2(\rho_A)\right] \quad \geq 0 \qquad ⁂ \textit{ Entanglement entropy of } A \tag{8.18}$$

The entanglement entropy of subsystem A quantifies its entanglement with the environment (here: subsystem B) and is given by the ↓ *Von Neumann entropy* of the reduced density matrix ρ_A.

- It is always $S[A] = S[\bar{A}] = S[B]$ where $\bar{A} = B$ denotes the complement of A (→ *below*).
- ¡! A non-vanishing value of Eq. (8.18) only indicates entanglement if ρ_A is the reduced density matrix of a *pure state*. If ρ is already mixed, $S[A] \neq 0$ does *not* necessarily indicate entanglement between the subsystems.
- We use the base-2 logarithm $\log_2$ for convenience (in the literature, the natural logarithm is often used). With this choice, $S[A]$ measures the information in bits shared between subsystems A and B via entanglement:

$$\mathcal{H} = \mathbb{C}^2_A \otimes \mathbb{C}^2_B \ni |\Psi\rangle = \tfrac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \quad \overset{\circ}{\Rightarrow} \quad S[A] = 1 \tag{8.19}$$

Without the base-2 logarithm, it would be $S[A] = \log(2)$. The result $S[A] = 1$ for the Bell pair $|\Psi\rangle$ means that you gain one bit of information about the subsystem (qubit) B by measuring the subsystem (qubit) A.

- If $|\Psi\rangle = |\Psi_A\rangle \otimes |\Psi_B\rangle$ is a *product state* (= not entangled), the reduced density matrix $\rho_A = |\Psi_A\rangle\langle\Psi_A|$ is again pure ($\mathrm{Tr}[\rho_A^2] = 1$) and consequently $S[A] = 0$, indicating that there is no entanglement shared between subsystems A and B.

2 | ↑ *Schmidt decomposition*:

◁ Arbitrary state $|\Psi\rangle = \sum_{i,j} \Psi_{ij} |i\rangle_A \otimes |j\rangle_B \in \mathcal{H}_A \otimes \mathcal{H}_B$

$|i\rangle_X$: orthonormal basis (ONB) of $\mathcal{H}_X$
(Note that the dimensions of $\mathcal{H}_A$ and $\mathcal{H}_B$ are not necessarily equal.)

$\overset{\circ}{\to}$ $\exists$ ONB $\{|\Psi_k\rangle_X\}$ of $\mathcal{H}_X$ $(X = A, B)$ such that

$$|\Psi\rangle = \sum_{k=1}^{R} \lambda_k |\Psi_k\rangle_A \otimes |\Psi_k\rangle_B \qquad \text{⁂ Schmidt decomposition} \tag{8.20}$$

- $0 < \lambda_R \leq \ldots \leq \lambda_1$: ⁂ *Schmidt coefficients* (unique up to re-ordering)
- $|\Psi_k\rangle_A$ ($|\Psi_k\rangle_B$): left (right) ⁂ *Schmidt vectors*
- $1 \leq R \leq \min\{\dim \mathcal{H}_A, \dim \mathcal{H}_B\}$: ⁂ *Schmidt rank*

To show the existence of Eq. (8.20), use a ↓ *singular value decomposition* of the complex $N_A \times N_B$ matrix $M_\Psi = (\Psi_{ij})$ where $N_A = \dim \mathcal{H}_A$ and $N_B = \dim \mathcal{H}_B$,

$$M_\Psi \overset{\text{SVD}}{=} U \Lambda V^\dagger, \tag{8.21}$$

with $N_A \times N_A$ unitary U, $N_B \times N_B$ unitary V, and $N_A \times N_B$ positive semidefinite diagonal matrix Λ. The diagonal entries of Λ are the ↓ *singular values* of M_Ψ and the non-zero ones correspond to the Schmidt coefficients λ_k. The unitaries U and V determine the basis change from $|i\rangle_A$ to $|\Psi_k\rangle_A$ and from $|j\rangle_B$ to $|\Psi_k\rangle_B$, respectively.

Normalization $\langle\Psi|\Psi\rangle = 1 \to \sum_{k=1}^{R} \lambda_k^2 = 1$

This means that one can think of $\{\lambda_k^2\}$ as a probability distribution over $\{1, \ldots, R\}$!

3 | We can use a Schmidt decomposition to compute the reduced density matrix:

$$\rho_A = \mathrm{Tr}_B\,[|\Psi\rangle\langle\Psi|] \overset{\text{def}}{=} \sum_{k=1}^{R} \lambda_k^2\, |\Psi_k\rangle_A \langle\Psi_k|_A \tag{8.22}$$

Here we used the right Schmidt basis $|\Psi_k\rangle_B$ to evaluate the partial trace over B.

→ Entanglement entropy:

$$S[A] \triangleq -\sum_{k=1}^{R} \lambda_k^2 \log_2 \lambda_k^2 \tag{8.23}$$

Evaluate the logarithm and the trace in the Schmidt basis $|\Psi_n\rangle_A$.

Eq. (8.23) is the ↓ *Shannon entropy* of the probability distribution $\{\lambda_k^2\}$.

$\overset{\circ}{\to}$ Upper bound:

$$S[A] \leq \log_2 R \tag{8.24}$$

To show this:

$$S[A] = -\sum_{k=1}^{R} \lambda_k^2 \log_2 \lambda_k^2 = \sum_{k=1}^{R} \lambda_k^2 \log_2 \frac{1}{\lambda_k^2} \overset{*}{\leq} \log_2 \sum_{k=1}^{R} \lambda_k^2 \frac{1}{\lambda_k^2} = \log_2 R \tag{8.25}$$

The inequality follows from ↓ *Jensen's inequality* and that $\log_2(x)$ is a concave function.

- The upper bound (8.24) is sharp. To see this, consider again the Bell pair

$$|\Psi\rangle = \tfrac{1}{\sqrt{2}}(|00\rangle + |11\rangle) = \tfrac{1}{\sqrt{2}}|0\rangle_A \otimes |0\rangle_B + \tfrac{1}{\sqrt{2}}|1\rangle_A \otimes |1\rangle_B \tag{8.26}$$

with Schmidt coefficients $\lambda_1^2 = \frac{1}{2}$ and $\lambda_2^2 = \frac{1}{2}$ and Schmidt rank $R = 2$ so that

$$S[A] = -\tfrac{1}{2}\log_2 \tfrac{1}{2} - \tfrac{1}{2}\log_2 \tfrac{1}{2} = 1 = \log_2 2\,. \tag{8.27}$$

Such states are called ⁂ *maximally entangled*.

- From the Schmidt coefficients one can compute the ⁂ *entanglement spectrum* $\{\xi_k\}$

$$\lambda_k^2 \equiv e^{-\xi_k} \quad \Leftrightarrow \quad \xi_k = -2\ln\lambda_k \tag{8.28}$$

with $0 \leq \xi_k < \infty$. The idea is that the entanglement structure is encoded in the reduced density matrix ρ_A which – as a non-negative Hermitian matrix – can be interpreted as Gibbs state $\rho_A \equiv e^{-H_E}$ of an artificial "entanglement Hamiltonian" $H_E = -\ln\rho_A$ [212]. With Eq. (8.22) it follows that the spectrum of H_E is exactly the entanglement spectrum $\{\xi_k\}$ defined above. The entanglement spectrum contains much more information about the entanglement structure than the entanglement entropy and can be used to identify topological phases [213].

4 | Example:

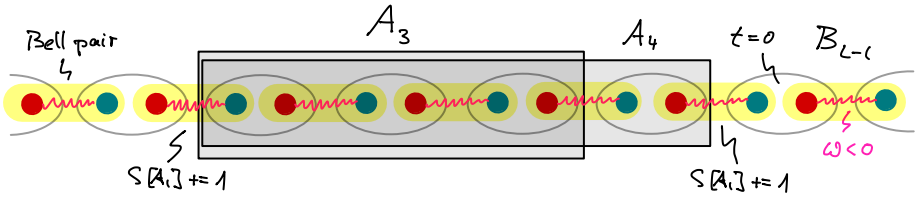
≺ Bosonic SSH chain (8.6) and split chain in two contiguous Segments A_l and B_{L-l}

We consider a chain with periodic boundaries, the segments comprise l and $L-l$ unit cells.

≺ Fixpoints of the two gapped phases:

- Phase A ($t = 0$ and $w < 0$):

(The sign of t and w is not important for this example.)



→ Ground state: (we omit the normalization)

$$|A\rangle = \bigotimes_{i=1}^{L} (|0\rangle_{2i}|1\rangle_{2i+1} + |1\rangle_{2i}|0\rangle_{2i+1}) \tag{8.29}$$

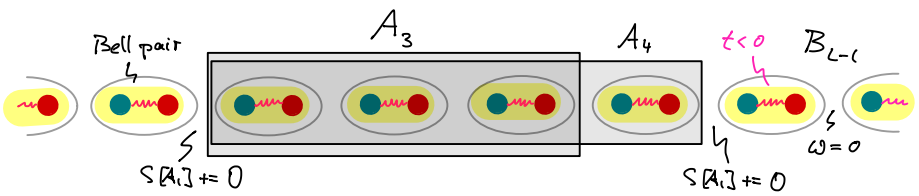
The ground state is a product of spin-triplets *between* adjacent sites of the chain.

→ Entanglement entropy:

$$S[A_l] = \langle \#\text{ of Bell pairs connecting } A_l \text{ and } B_{L-l}\rangle = 2 \tag{8.30}$$

¡! The entanglement entropy of A_l is *independent* of the size of the segment A_l.
This is a crucial observation and becomes important → *below*.

- Phase B ($t < 0$ and $w = 0$):



→ Ground state:

$$|B\rangle = \bigotimes_{i=1}^{L} (|0\rangle_{2i-1}|1\rangle_{2i} + |1\rangle_{2i-1}|0\rangle_{2i}) \tag{8.31}$$

Now the ground state forms triplets of spins *within* sites.

→ Entanglement entropy:

$$S[A_l] = \langle \#\text{ of Bell pairs connecting } A_l \text{ and } B_{L-l} \rangle = 0 \tag{8.32}$$

Again, the entanglement entropy of A_l is size-independent (here: zero).

¡! The point of this example is *not* to suggest that the fact that $S[A_l] \neq 0$ in phase A and $S[A_l] = 0$ in phase B can be used to distinguish the two phases. The vanishing entanglement entropy in phase B is a fine-tuned feature of the fixpoint wave function $|B\rangle$. For $0 < |w| \ll |t|$ there will be (weak) couplings of spins between adjacent sites so that one should expect $S[A_l] > 0$ even in phase B. The crucial observation is that in both phases the entanglement does not grow with the size of the segment A_l.

9. Primer on matrix product states

Matrix product states (and their generalization as → *tensor network states*, Section 9.3) are a *generic framework* to encode and describe many-body quantum states. This framework is not specific to the description of topological phases, but a versatile tool applied in most fields of modern condensed matter physics (and quantum information), for example, as the theoretical underpinning of the powerful → *density matrix renormalization group (DMRG)* algorithm (→ Section 9.2).

Relevant literature (including reviews/introductions) is provided throughout the following sections.

9.1. Matrix product states

Here we introduce the matrix product representation of quantum states on *general grounds*, without specialization to symmetry-protected topological phases. As an application, we will use the methods developed in this section later in Chapter 10 to classify SPT phases in 1D interacting spin systems:

1 | ◁ System of L d-dimensional quantum systems: $\mathcal{H} = \bigotimes_{i=1}^{L} \mathbb{C}_i^d$

◁ Arbitrary quantum state: $|\Psi\rangle = \sum_{\boldsymbol{i}} \Psi_{\boldsymbol{i}} |\boldsymbol{i}\rangle$ [here $\boldsymbol{i} = (i_1, \ldots, i_L)$ is a multi-index]

In total there are d^L complex number $\Psi_{\boldsymbol{i}}$ needed to describe the state.

2 | Matrix Product Expansion:

The following discussion is based on Ref. [214].

Our goal is to construct a novel encoding of $\Psi_{\boldsymbol{i}}$ that becomes efficient for states with "low" entanglement:

i | ◁ Subsystems $A = [1]$ and $B = [2, \ldots, L]$

→ Schmidt decomposition:

$$|\Psi\rangle = \sum_{k_1=1}^{R_1} \lambda_{k_1}^{[1]} |\Psi_{k_1}^{[1]}\rangle \otimes |\Psi_{k_1}^{[2\ldots L]}\rangle \tag{9.1}$$

ii | Expand left Schmidt state into local basis: $|\Psi_{k_1}^{[1]}\rangle = \sum_{i_1=1}^{d} \Gamma_{k_1}^{[1]i_1} |i_1\rangle$

Here, $\Gamma^{[1]}$ denotes the matrix that encodes the basis change from the standard basis into the Schmidt basis on site 1.

$$\rightarrow \qquad |\Psi\rangle = \sum_{i_1=1}^{d} \sum_{k_1=1}^{R_1} \Gamma_{k_1}^{[1]i_1} \lambda_{k_1}^{[1]} |i_1\rangle \otimes |\Psi_{k_1}^{[2\ldots L]}\rangle \tag{9.2}$$

iii | Expand the right Schmidt state as follows:

$$|\Psi_{k_1}^{[2\ldots L]}\rangle = \sum_{i_2=1}^{d} |i_2\rangle \otimes |\tilde{\Psi}_{k_1 i_2}^{[3\ldots L]}\rangle \tag{9.3}$$

Note that the states $|\tilde{\Psi}^{[3\ldots L]}_{k_1 i_2}\rangle$ are not Schmidt vectors and not normalized!

$$\rightarrow \qquad |\Psi\rangle = \sum_{i_1,i_2=1}^{d} \sum_{k_1=1}^{R_1} \Gamma^{[1]i_1}_{k_1} \lambda^{[1]}_{k_1} |i_1\rangle \otimes |i_2\rangle \otimes |\tilde{\Psi}^{[3\ldots L]}_{k_1 i_2}\rangle \tag{9.4}$$

iv | ◁ Subsystems $A = [1, 2]$ and $B = [3, \ldots, L]$

→ Schmidt decomposition:

$$|\Psi\rangle = \sum_{n=1}^{R_2} \lambda^{[2]}_n |\Psi^{[1,2]}_n\rangle \otimes |\Psi^{[3\ldots L]}_n\rangle \tag{9.5}$$

→ $|\tilde{\Psi}^{[3\ldots L]}_{k_1 i_2}\rangle$ can be expanded in $|\Psi^{[3\ldots L]}_n\rangle$

→ Choose coefficients $\Gamma^{[2]i_2}_{k_1 k_2}$ such that

$$|\tilde{\Psi}^{[3\ldots L]}_{k_1 i_2}\rangle \equiv \sum_{k_2=1}^{R_2} \Gamma^{[2]i_2}_{k_1 k_2} \lambda^{[2]}_{k_2} |\Psi^{[3\ldots L]}_{k_2}\rangle \tag{9.6}$$

This is an implicit definition of the three-index symbol ("tensor") $\Gamma^{[2]i_2}_{k_1 k_2}$; that we extracted the Schmidt coefficients $\lambda^{[2]}_{k_2}$ is our choice!

Eq. (9.4) →

$$|\Psi\rangle = \sum_{i_1,i_2=1}^{d} \sum_{k_1,k_2=1}^{R_1,R_2} \left(\Gamma^{[1]i_1}_{k_1} \lambda^{[1]}_{k_1} \Gamma^{[2]i_2}_{k_1 k_2} \lambda^{[2]}_{k_2}\right) |i_1\rangle \otimes |i_2\rangle \otimes |\Psi^{[3\ldots L]}_{k_2}\rangle \tag{9.7}$$

v | Iterate steps **iii** | and **iv** | for every site $\overset{\circ}{\rightarrow}$ (9.8)

$$|\Psi\rangle = \sum_{i_1\ldots i_L=1}^{d} \overbrace{\sum_{k_1\ldots k_{L-1}=1}^{R_1\ldots R_{L-1}} \left(\Gamma^{[1]i_1}_{k_1} \lambda^{[1]}_{k_1} \Gamma^{[2]i_2}_{k_1 k_2} \lambda^{[2]}_{k_2} \ldots \Gamma^{[L-1]i_{L-1}}_{k_{L-2} k_{L-1}} \lambda^{[L-1]}_{k_{L-1}} \Gamma^{[L]i_L}_{k_{L-1}}\right)}^{\Psi_i} \times |i_1\rangle \otimes |i_2\rangle \otimes \ldots \otimes |i_{L-1}\rangle \otimes |i_L\rangle$$

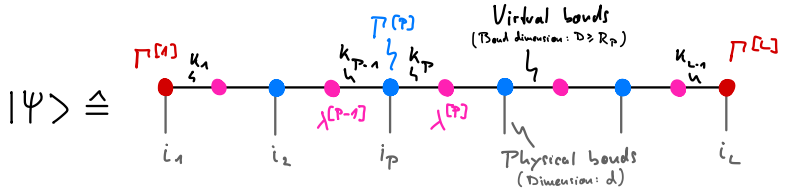
This form is called ⁂ *Canonical form* of a matrix product state (MPS)

- $i_1, \ldots, i_L$: ⁂ *Physical indices/bonds*
- d: ⁂ *Physical dimension*
- $k_1, \ldots, k_{L-1}$: ⁂ *Virtual indices/bonds*
- $R_1, \ldots, R_{L-1}$: ⁂ *Bond dimensions*

  Strictly speaking, the bond dimensions are *lower bounded* by the Schmidt rank. Nothing prevents us to use larger bond dimensions than the Schmidt rank to find an exact description of a given state.

  → Replace $R_1, \ldots, R_{L-1}$ by Uniform bond dimension $D := \max\{R_1, \ldots, R_{L-1}\}$

→ Pictorial representation:



3 | Why "matrix product state"?

→ Define matrices: $(p = 2, \ldots, L-1)$

$$M_i^{[1]} := \left(\Gamma_k^{[1]i}\sqrt{\lambda_k^{[1]}}\right)_k \qquad d \times (1 \times R_1)\text{-matrices} \tag{9.9a}$$

$$M_i^{[p]} := \left(\sqrt{\lambda_k^{[p-1]}}\Gamma_{kl}^{[p]i}\sqrt{\lambda_l^{[p]}}\right)_{kl} \qquad d \times (R_{p-1} \times R_p)\text{-matrices} \tag{9.9b}$$

$$M_i^{[L]} := \left(\sqrt{\lambda_k^{[L-1]}}\Gamma_k^{[L]i}\right)_k \qquad d \times (R_{L-1} \times 1)\text{-matrices} \tag{9.9c}$$

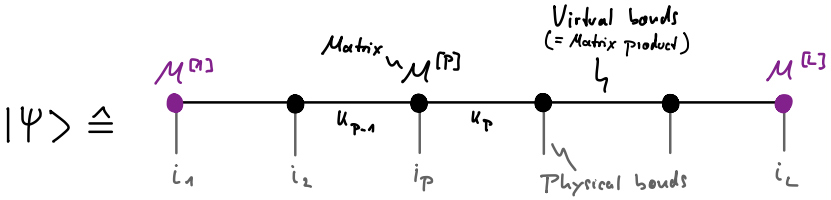
Eq. (9.8) →

$$|\Psi\rangle = \sum_{\boldsymbol{i}} \overbrace{\underbrace{M_{i_1}^{[1]} \cdot M_{i_2}^{[2]} \cdot \ldots \cdot M_{i_{L-1}}^{[L-1]} \cdot M_{i_L}^{[L]}}_{\text{Matrix product}}}^{\Psi_{\boldsymbol{i}}} |i_1 i_2 \ldots i_{L-1} i_L\rangle \tag{9.10}$$

→ Sums over virtual indices become matrix products

→ ⁂ *Matrix product state (MPS)*

→ Pictorial representation:



The matrices on the first and last site are actually row and column vectors, respectively.

- Our choice in Eq. (9.9c) to distribute the Schmidt coefficients evenly on the matrices is arbitrary. The matrix expansion of the wave function $\Psi_{\boldsymbol{i}}$ in Eq. (9.10) is therefore *not* unique.
- This "gauge freedom" is actually much larger: You can apply any invertible transformation T via $TT^{-1} = \mathbb{1}$ between any of the matrix products in Eq. (9.10) without changing the state $\Psi_{\boldsymbol{i}}$. Such transformations can be used to tailor the properties of the matrices $M_{i_p}^{[p]}$ to specific tasks.

4 | Preliminary summary:

- We have shown that *any* quantum state on L d-level quantum systems can be written *exactly* as a matrix product state of the form Eq. (9.10).

  This means that matrix product states are not a particular type of quantum state; they are a particular way of *encoding* a quantum state. This encoding is beneficial for states with *low entanglement* (→ *below*).

- To encode $\Psi_{\boldsymbol{i}}$, one needs $L \cdot d$ matrices $M_{i_p}^{[p]}$; these matrices have dimensions $R_{p-1} \times R_p$ where R_p denotes the Schmidt rank between site p and $p+1$.
- Any given MPS of the form Eq. (9.10) can be brought into its canonical form Eq. (9.8). This form is convenient because it explicitly contains the Schmidt decomposition (and Schmidt coefficients) for *every* cut of the system into two subsystems. It also shows how the bond dimension at every bond is determined by the entanglement between the subsystems connected by this bond.

5 | Comments on Complexity:

i | If one chooses a uniform bond dimension $D = \max\{R_1, \ldots, R_{L-1}\}$, the number of complex matrix entries needed to encode $\Psi_{\boldsymbol{i}}$ scales like

$$\begin{aligned} \text{Complexity}(\Psi) &\equiv \langle \#\,\text{Complex numbers to encode } \Psi_{\boldsymbol{i}} \rangle \\ &\sim \underbrace{L \cdot d}_{\#\,\text{Matrices}} \cdot \underbrace{D^2}_{\text{Size of matrices}} \end{aligned} \tag{9.11}$$

ii | On first glance, Eq. (9.11) might suggest that the complexity scales *linearly* with the system size L (which would be remarkable). Of course, this cannot be true; the hitch is that the bond dimension D depends on the entanglement which, in turn, can depend on the system size as well:

$$\text{Complexity}(\Psi) \overset{9.11}{\geq} D = \max\{R_1, \ldots, R_{L-1}\} = R_{\max} \overset{8.24}{\geq} 2^{S_{\max}} \tag{9.12}$$

$S_{\max}$: maximal entanglement entropy of $|\Psi\rangle$ over all partitions A_l of the 1D system

iii | Note that the entanglement entropy is always upper bounded by the system size (times some constant): $S_{\max} \leq \text{const} \cdot L$.

This follows from Eq. (8.24) and the fact that the Schmidt rank is upper bounded by the total dimension d^L of the Hilbert space: $S[A] \leq L \log_2 d$.

For a generic state, this upper bound is tight (→ *below*) and we find the worst-case scaling:

$$\text{Complexity}(\Psi) \gtrsim 2^{\text{const} \cdot L} \tag{9.13}$$

→ Exponentially many matrix entries ☹

This should not surprise us. It is well-known that encoding generic quantum states requires exponential amounts of resources in the system size (that's why we try to build quantum computers after all). And this complexity does not go away by rewriting the wave function in a different form …

iv | So under which conditions *can* the MPS encoding be beneficial?

$$S_{\max} \sim \text{const} \xrightarrow[\text{Eqs. (9.11) and (9.12)}]{?} \text{Complexity}(\Psi) \sim L \cdot \text{const} \quad ☺ \tag{9.14a}$$

$$S_{\max} \sim \log L^{\text{const}} \xrightarrow[\text{Eqs. (9.11) and (9.12)}]{?} \text{Complexity}(\Psi) \sim L \cdot L^{\text{const}} \quad ☺ \tag{9.14b}$$

- ¡! The "?" indicates that these are *possibilities* allowed by the lower bound Eq. (9.12). These are *not* implications; for such we would need an *upper* bound on the bond dimension from the entanglement entropy (which we don't have).

It turns out that *in practice*, the arrows in Eq. (9.14) often *are* implications. The linear lower bound Eq. (9.14a) is not always achievable because approximations with a constant error often require a scaling $D \sim L^{\text{const}}$ of the bond dimension (→ *below*), but even then a polynomial scaling $\text{Complexity}(\Psi) \sim L^{\text{const}}$ is possible (which is the foundation for numerical methods like → *DMRG*, Section 9.2). Note that for some states with translational invariance [like the fixpoint ground states $|A\rangle$ and $|B\rangle$ of the bosonic SSH chain, Eqs. (8.29) and (8.31)], even $\text{Complexity}(\Psi) \sim \text{const}$ (independent of L!) is possible.

- Unfortunately, this favorable scaling of the complexity of MPS encodings cannot be proven for generic weakly entangled states because there are (rather artificial) counterexamples that, despite low entanglement entropy, do *not* allow for efficient MPS encodings (or even approximations) [215]. See also the → *next* point.
- Assume our system satisfies $S_{\max} \leq \text{const}$ independent of the system size L. [It satisfies a strict → *area law* like the two ground states in Eqs. (8.29) and (8.31) of the bosonic SSH chain.] Why does this not automatically imply an exact MPS encoding with constant bond dimension D? That is, why

$$D = \text{const} \quad \Rightarrow \quad S_{\max} \leq \text{const} \tag{9.15a}$$

$$\text{but} \quad S_{\max} \leq \text{const} \quad \not\Rightarrow \quad D = \text{const} \tag{9.15b}$$

for $L \to \infty$. [The first implication follows from the canonical form Eq. (9.8) in combination with Eq. (8.24).]

The crucial point is that $S[A] \leq \text{const}$ can be true even if Eq. (8.23) contains an exponential number of non-vanishing summands, i.e., $R \sim d^L$ is consistent with a bounded entanglement entropy! For example, the Schmidt coefficients can (and often do) decay exponentially in their index: $\lambda_k \sim \mu^k$ for some $0 < \mu < 1$. In this case, one cannot find an *exact* MPS representation with fixed bond dimension, although an *approximate* one with error that is exponentially suppressed in D is possible.

To see this, one can show [216] that for every state $|\Psi\rangle \in \bigotimes_{p=1}^{L} \mathbb{C}_p^d$ there exists an MPS $|\Psi_D\rangle$ with uniform bond dimension D such that

$$\| |\Psi\rangle - |\Psi_D\rangle \|^2 \overset{*}{\leq} 2 \sum_{p=1}^{L-1} \epsilon_p(D) \tag{9.16}$$

where

$$\epsilon_p(D) = \sum_{k=D+1}^{R_p} \left(\lambda_k^{[p]}\right)^2 \tag{9.17}$$

is the error contribution from "cutting off" the Schmidt vectors of the partition between sites p and $p+1$ starting at $k = D+1$ (remember that Schmidt coefficients are sorted in decreasing order, i.e., we keep the D coefficients with highest weight in $|\Psi_D\rangle$).

This demonstrates that states that can be efficiently approximated by an MPS must have quickly decaying Schmidt coefficients. Unfortunately, this quick decay does not automatically follow from a bounded entanglement entropy $S_{\max} \leq \text{const}$ (although it does follow from a similar statement about certain ↑ *Rényi entropies*, → *below*).

Let us assume that the Schmidt coefficients decay exponentially: $\lambda_k^{[p]} \sim \mu^k$ for some $0 < \mu < 1$ (this is a situation one encounters quite often). Then

$$\epsilon_p(D) = \sum_{k=D+1}^{R_p} \mu^{2k} \leq \mu^{2D} \sum_{k=1}^{\infty} \mu^{2k} = \text{const} \cdot \mu^{2D}\,, \tag{9.18}$$

where we used the convergence of the geometric series for $0 < \mu < 1$. In this case, one can approximate the state by an MPS with the error

$$\| |\Psi\rangle - |\Psi_D\rangle \|^2 \lesssim \text{const} \cdot L \cdot \mu^{2D} \tag{9.19}$$

So while $|\Psi\rangle$ cannot be expressed exactly by an MPS with fixed bond dimension, it can be approximated by an MPS with constant error for $L \to \infty$ with only $D \sim \log L$ in the worst case. Plugging this into Eq. (9.11), one finds

$$\text{Complexity}(\Psi_D) \sim \text{const} \cdot L \cdot (\log L)^2 \tag{9.20}$$

for a constant-error approximation of $|\Psi\rangle$ (much better than the generic scaling d^L).

v | Comment:

Here we always assume that our many-body Hilbert space has a natural tensor product structure augmented by a natural *ordering* of tensor factors (subsystems). When we talk about "maximum entanglement entropy," we refer to the maximum of $S[A_l]$ for a contiguous subset starting at the first factor (with respect to the given ordering) and ending at the lth factor. Such orderings are naturally given for one-dimensional many-body systems with local Hamiltonians (which is the situation we are interested in).

However, without a Hamiltonian that "imprints" a one-dimensional spatial "meta-structure" on the Hilbert space, the ordering of subsystems becomes ambiguous. Note that if you maximize $S[A]$ not only over contiguous intervals but over *every* subset of subsystems, one generically obtains $S_{\max} \in \mathcal{O}(L)$, so that no efficient MPS encoding is possible. This means that the *ordering* of subsystems matters for an efficient MPS encoding!

A natural question is then: Given an arbitrary state in a Hilbert space with a given tensor product structure but *without* a prescribed *ordering* of these factors, how to identify the ordering that allows for the MPS representation with the lowest maximal bond dimension? Unfortunately, one can show (somewhere in my notes) that this problem (more precisely: its decision version) is NP-hard and therefore does not have an efficient solution (unless P = NP).

We conclude:

→ Every state can be written exactly as a matrix product state (with $D \sim d^L$).
→ States with *bounded entanglement* in 1D can* be represented (or at least approximated) by matrix product states with slowly increasing (or even constant) bond dimension.

The * reads "in practice" or "except for artificial counterexamples." (See discussion on MPS approximations ← *above* and → *below*.)

This insight will be crucial for the classification of SPT phases of interacting spin systems in 1D.