# 16 Entanglement in correlated quantum systems: A quantum information perspective

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## Contents



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# 1 Introduction

Understanding the behavior of large interacting quantum systems is essential in quantum chemistry, in the study of exotic condensed matter phenomena such as high-Tc superconductivity or the fractional quantum Hall effect, and beyond. For sytems with only weak interactions, mean field approaches have been applied successfully. However, this approach breaks down when the interactions between parts of the system become sufficiently strong – interactions give rise to quantum correlations, i.e., entanglement, in the system, which is not captured by a mean field approach. The study of entanglement, on the other hand, is one of the core topics of Quantum Information Theory, where an extensive framework for the characterization, quantification, and manipulation of entanglement has been developed. This suggests to apply quantum information concepts, and in particular the theory of entanglement, to the description of quantum many-body systems. Indeed, an active field of research has grown during the last decade at the interface of quantum information theory and quantum many-body physics, and the aim of this lecture is to give an introduction to this area.

For clarity of the presentation, we will initially restrict to quantum spin systems on a lattice (such as a line or a square lattice in 2D), with a corresponding Hilbert space $(\mathbb{C}^d)^{\otimes N}$ (where each spin has $d$ levels, and the lattice has $N$ sites); generalizations to fermionic systems and beyond lattices will be discussed later. Also, we will for the moment focus on ground state problems, i.e., given some Hamiltonian $H$ acting on our spin system, we will ask about properties of its ground state $|\Psi\rangle$. The approach we pursue will be variational – we will try to obtain a family of states which gives a good approximation of the ground state, for which quantities of interest can be evaluated efficiently, and where the best approximation to the ground state can be found efficiently. For instance, mean-field theory is a variational theory based on the class of product states (for spin systems) or Slater determinants (for electronic systems).

Of course, one could simply parametrize the ground state as

$$|\Psi\rangle = \sum_{i_1,\ldots,i_N} c_{i_1\ldots i_N} |i_1,\ldots,i_N\rangle \,, \tag{1}$$

and use the $c_{i_1\ldots i_N}$ as variational parameters. Unfortunately, the number of parameters $c_{i_1\ldots i_N}$ grows exponentially with $N$, making it impossible to have an efficient description of $|\Psi\rangle$ for growing system sizes. On the other hand, we know that efficient descriptions exist for physical Hamiltonians: Since $H = \sum_i h_i$ is a sum of few-body terms (even if we don't restrict to lattice systems), a polynomial number $N^k$ of parameters (with $k$ the bodiness of the interaction) allows to specify $H$, and thus its ground state. This is, while a general $N$-body quantum state can occupy an exponentially large Hilbert space, all physical states live in a very small "corner" of this space. The difficulty, of course, is to find an efficient parametrization which captures the states in this corner of Hilbert space, while at the same time allowing for efficient simulation methods.

# 2 Matrix product states (MPS)

## 2.1 The area law

In order to have a guideline for constructing an ansatz class, let us look at the entanglement properties of ground states of interacting quantum systems. To this end, we consider a ground state $|\Psi\rangle$ on a lattice and cut a contiguous region of length $L$ (in one dimension) or an area $A$ (in two dimensions), cf. Fig. 1. It is a well-known result from quantum information theory [1]


**Fig. 1:** *Area law: The entropy of the reduced states of a block $A$ scales like the length of its boundary $\partial A$; in one dimension, this implies that the entropy is bounded by a constant.*

that the von Neumann entropy of the reduced density matrix $\rho_A$ of region $A$,

$$S(\rho_A) = -\rho_A \log \rho_A \ ,$$

quantifies the entanglement between region $A$ and the rest of the system. For a random quantum state, we expect this entanglement to be almost maximal, i.e., on the order of $|A| \log d$ (where $|A|$ is the number of spins in region $A$). Yet, if we study the behavior of $S(\rho_A)$ for ground states of local Hamiltonians, it is found that $S(\rho_A)$ essentially scales like the *boundary* of region $A$, $S(\rho_A) \propto |\partial A|$, with possible corrections for gapless Hamiltonians which are at most logarithmic in the volume, $S(\rho_A) \propto |\partial A| \log |A|$. This behavior is known as the *area law* for the entanglement entropy and has been observed throughout for ground states of local Hamiltonians (see, e.g., Ref. [2] for a review); for gapped Hamiltonians in one dimension, this result has been recently proven rigorously [3].

## 2.2 Matrix product states

Since the entropy $S(\rho_A)$ quantifies the entanglement between region $A$ and its complement, the fact that $S(\rho_A)$ scales like the *boundary* of $\rho_A$ suggests that the entanglement between region $A$ and the rest is essentially located around the boundary between the two regions, as illustrated in Fig. 2. We will now construct an ansatz for many-body quantum systems, starting from the

**Fig. 2:** *The area law suggests that the entanglement between two regions is located around the boundary.*

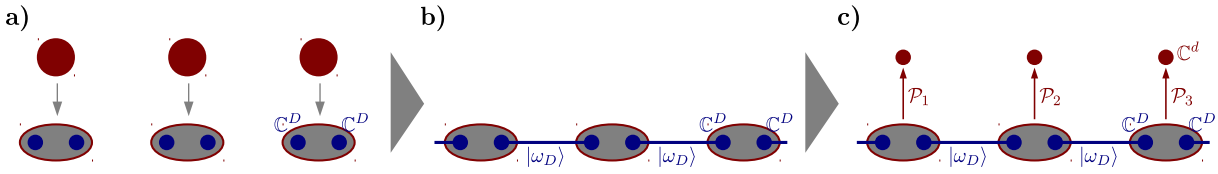



**Fig. 3:** *Construction of MPS:* ***a)*** *Each site is composed of two virtual subsystems.* ***b)*** *The virtual subsystems are placed in maximally entangled states.* ***c)*** *Linear maps $\mathcal{P}_s$ are applied which map the two virtual systems to the physical system.*

insight that the entanglement is concentrated around the boundary of regions; for the moment, we will focus on one-dimensional systems. Clearly, since we want to have this property for any partitioning of the lattice, we cannot just place entangled pairs as in Fig. 2, but we have to choose a more subtle strategy. To this end, we consider the system at each site as being composed of two "virtual" subsystems of dimension $D$ each, as illustrated in Fig. 3a. Then, each of the two subsystems is placed in a maximally entangled state

$$|\omega_D\rangle = \sum_{i=1}^{D} |i,i\rangle$$

with the corresponding subsystems at the adjacent sites, as shown in Fig. 3b. The maximally entangled states are called "bonds", with $D$ the "bond dimension". This construction already satisfies the area law: For any region we cut, there are exactly two maximally entangled states crossing the cuts, bounding the entanglement by $2\log D$. Finally, we apply at each site $s$ linear maps $\mathcal{P}_s : \mathbb{C}^D \otimes \mathbb{C}^D \to \mathbb{C}^d$, which creates a description of a state on a chain of $d$-level systems, cf. Fig. 3c. (Note that the rank of the reduced density operator of any region cannot be increased by applying the linear maps $\mathcal{P}_s$.) The construction can be carried out either with periodic boundary conditions, or with open boundary conditions by omitting the outermost virtual subsystems at the end of the chain. The total state of the chain can be written as

$$|\Psi\rangle = (\mathcal{P}_1 \otimes \cdots \otimes \mathcal{P}_N)|\omega_D\rangle^{\otimes N} , \tag{2}$$

where the maps $\mathcal{P}_s$ act on the maximally entangled states as illustrated in Fig. 3c.
This class of states can be rewritten as follows: For each site $s$, define a three-index tensor $A^{[s]}_{i,\alpha\beta}$, $i = 1,\ldots,d$, $\alpha,\beta = 1,\ldots,D$, where the $A^{[s]}_i$ can be interpreted as $D \times D$ matrices, such that

$$\mathcal{P}_s = \sum_{i,\alpha,\beta} A^{[s]}_{i,\alpha\beta} |i\rangle\langle\alpha,\beta| . \tag{3}$$

Then, the state (2) can be rewritten as

$$|\Psi\rangle = \sum_{i_1,\ldots,i_N} \mathrm{tr}\left[A^{[1]}_{i_1} A^{[2]}_{i_2} \cdots A^{[N]}_{i_N}\right] |i_1,\ldots,i_N\rangle , \tag{4}$$

i.e., the coefficient $c_{i_1\ldots i_N}$ in (1) can be expressed as a product of matrices.[1] For this reason, these states are called *Matrix Product States* (MPS). For systems with open boundary conditions, the

[1] The equivalence of (2) and (4) can be proven straightforwardly by noting that for two maps $\mathcal{P}_1$ and $\mathcal{P}_2$, and

matrices $A^{[1]}_{i_1}$ and $A^{[N]}_{i_N}$ are $1 \times D$ and $D \times 1$ matrices, respectively, so that the trace can be omitted. More generally, $D$ can be chosen differently across each link.

As it turns out, MPS are very well suited to describe ground states of one-dimensional quantum systems. On the one hand, we have seen that by construction, these states all satisfy the area law. On the other hand, it can be shown that all states which satisfy an area law, such as ground states of gapped Hamiltonians [3], as well as states for which the entanglement of a block grows slowly (such as for critical 1D systems), can be well approximated by an MPS [4, 3]: Given a state $|\Phi\rangle$ on a chain of length $N$ for which the entropy of any block of length $L$ is bounded by $S_{\max}$, $S(\rho_L) \leq S_{\max}$, there exists an MPS $|\Psi_D\rangle$ which approximates $|\Phi\rangle$ up to error[2]

$$\big\| |\Phi\rangle - |\Psi_D\rangle \big\| =: \epsilon \leq \text{const} \times \frac{N \;\; e^{cS_{\max}}}{D^c} \,. \tag{5}$$

Note that even if $S_{\max}$ grows logarithmically with $N$, the numerator is still a polynomial in $N$. This is, in order to achieve a given accuracy $\epsilon$, we need to choose a bond dimension $D$ which scales polynomially in $N$ and $1/\epsilon$, and thus, the total number of parameters (and, as we will see later, also the computation time) scales polynomially as long as the desired accuracy is at most $1/\mathrm{poly}(N)$.

## 2.3 Tensor network notation

The defining equation (4) for Matrix Product States is a special case of a so-called *tensor network*. Generally, tensor networks are given by a number of tensors $A_{i_1,i_2,\ldots,i_K}$, $B_{i_1,i_2,\ldots,i_K}$, etc., where each tensor usually only depends on a few of the indices. Then, one takes the product of the tensors and sums over a subset of the indices,

$$c_{i_1\ldots i_k} = \sum_{i_{k+1},\ldots,i_K} A_{i_1,i_2,\ldots,i_K} B_{i_1,i_2,\ldots,i_K} \cdots \,.$$

For instance, in (4) the tensors are the $A^{[s]} \equiv A^{[s]}_{i,\alpha\beta}$, and we sum over the virtual indices $\alpha, \beta, \ldots$, yielding

$$c_{i_1\ldots i_N} = \mathrm{tr}\big[A^{[1]}_{i_1} A^{[2]}_{i_2} \cdots A^{[N]}_{i_N}\big] \,.$$

the bond $|\omega_D\rangle$ between them, it holds that

$$\mathcal{P}_1 \otimes \mathcal{P}_2 |\omega_D\rangle = \sum_{i_1,i_2,\alpha,\beta} (A^{[1]}_{i_1} A^{[2]}_{i_2})_{\alpha\beta} |i_1, i_2\rangle\langle\alpha,\beta| \,,$$

and iterating this argument through the chain.

[2] Stricly speaking, this bound only follows from an area law for the *Rényi entropy*

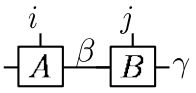
$$S_\alpha = \frac{\log \mathrm{tr}[\rho^\alpha]}{1-\alpha}$$

for $\alpha < 1$, with $c$ in (5) depending on $\alpha$ [4], which also holds for gapped Hamiltonians [3]. The proof uses the fact that a bound on the area law implies a fast decay of the Schmidt coefficients (i.e., the eigenvalues of the reduced density operator), and thus, one can construct an MPS by sequentially doing Schmidt decompositions of the state and discarding all but the largest $D$ Schmidt coefficients [5, 4].

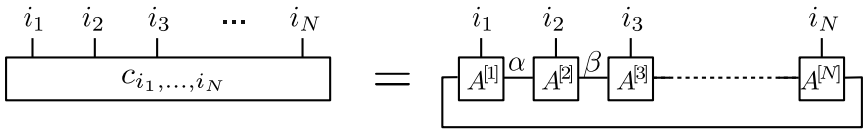
Tensor networks are most conveniently expressed in a graphical language. Each tensor is denoted by a box with "legs" attached to it, where each leg corresponds to an index – a three-index tensor $A^{[s]} \equiv A^{[s]}_{i,\alpha\beta}$ is then depicted as

$$A^{[s]}_{i,\alpha\beta} \equiv$$ 


Summing over a joint index is denoted by connecting the corresponding legs, e.g.,

$$\sum_\beta A_{i,\alpha\beta} B_{j,\beta\gamma} \equiv$$ 


In this language, the expansion coefficient $c_{i_1 \ldots i_N}$ [Eq. (1)] of an MPS (which we will further on use interchangably with the state itself) is written as :

$$|\Psi\rangle \equiv$$ 

(6)

We will make heavy use of this graphical language for tensor networks in the following.

## 2.4 Evaluating expectation values for MPS

As we have discussed at the end of Section 2.2, MPS approximate ground states of local Hamiltonians efficiently, as the effort needed for a good approximation scales only polynomially in the length of the chain and the desired accuracy. Thus, it seems appealing to use the class of MPS as a variational ansatz to simulate the properties of quantum many-body systems. However, to this end it is not sufficient to have an efficient description of relevant states – after all, the Hamiltonian itself forms an efficient description of its ground state, but it is hard to extract information from it! Rather, a good variational class also requires that we can efficiently extract quantities of interest such as energies, correlation functions, and the like, and that there is an efficient way to *find* the ground state (i.e., minimize the energy within the variational class of states) in the first place.

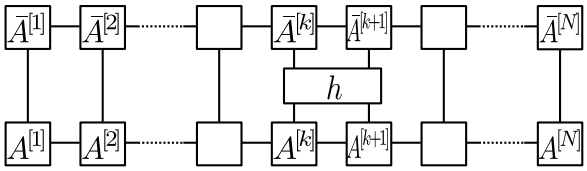
Let us start by discussing how to compute the expectation value a local operator $h$ (such as a term in the Hamiltonian) for an MPS. To this end, note that

$$\langle\Psi|h|\Psi\rangle = \sum_{\substack{i_1,\ldots,i_N \\ j_1,\ldots,j_N}} c^*_{i_1\ldots i_N} c_{j_1\ldots j_N} \delta_{i_1,j_1} \cdots \delta_{i_{k-1},j_{k-1}} h^{j_k j_{k+1}}_{i_k i_{k+1}} \delta_{i_{k+2},j_{k+2}} \cdots \delta_{i_N,j_N}$$

where

$$h = \sum_{\substack{i_k,i_{k+1} \\ j_k,j_{k+1}}} h^{j_k j_{k+1}}_{i_k i_{k+1}} |i_k, i_{k+1}\rangle\langle j_k, j_{k+1}|$$

acts on sites $k$ and $k+1$. Using the graphical tensor network notation, this can be written as

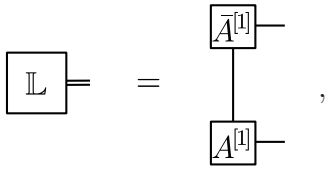
$\langle\Psi|h|\Psi\rangle =$ 

. (7)

In order to evaluate this quantity, we have to contract the whole diagram (7). In principle, contracting arbitrary tensor networks can become an extremely hard problem (strictly speaking, PP-hard [6]), as in some cases it essentially requires to determine exponentially big tensors (e.g., we might first have to compute $c_{i_1\ldots i_N}$ from the tensor network and from it determine the expectation value). Fortunately, it turns out that the tensor network of Eq. (7) can be contracted efficiently, i.e., with an effort polynomial in $D$ and $N$. To this end, let us start from the very left of the tensor network in Eq. (7) and block the leftmost column (tensors $A^{[1]}$ and $\bar{A}^{[1]}$). Contracting the internal index, this gives a two-index tensor

$$\mathbb{L}^{\alpha\alpha'} = \sum_i A^{[1]}_{i\alpha}\bar{A}^{[1]}_{i\alpha'} ,$$

which we interpret as a (bra) *vector* with a "double index" $\alpha\alpha'$ of dimension $D^2$. Graphically, this can be denoted as

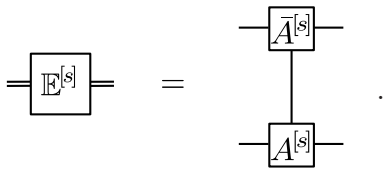


,

where we use a doubled line to denote the "doubled" index of dimension $D^2$. We can now continue this way, and define operators (called *transfer operators*)

$$(\mathbb{E}^{[s]})^{\beta\beta'}_{\alpha\alpha'} = \sum_i A^{[s]}_{i,\alpha\beta}\bar{A}^{[s]}_{i,\alpha'\beta'}$$

which we interpret as mapping the double index $\alpha\alpha'$ to $\beta\beta'$, and graphically write as



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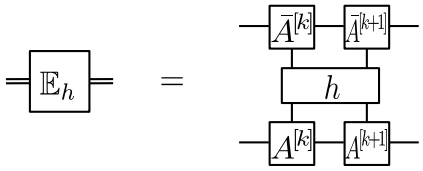
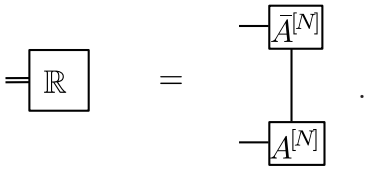
Similarly, we define operators



(8)

and



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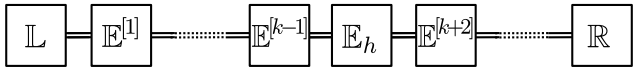
All of these operators can be computed efficiently (in the parameters $D$ and $N$), as they are vectors/matrices of fixed dimension $D^2$, and can be obtained by contracting a constant number of indices.
Using the newly defined objects $\mathbb{L}$, $\mathbb{E}$, $\mathbb{E}_h$, and $\mathbb{R}$, the expectation value $\langle\Psi|h|\Psi\rangle$, Eq. (7), can be rewritten as

$$\langle\Psi|h|\Psi\rangle = \mathbb{L}\mathbb{E}^{[2]}\cdots\mathbb{E}^{[k-1]}\mathbb{E}_h\mathbb{E}^{[k+2]}\cdots\mathbb{R}$$




This is, $\langle\Psi|h|\Psi\rangle$ can be computed by multiplying a $D^2$-dimensional vector $O(N)$ times with $D^2 \times D^2$ matrices. Each of these multiplication takes $O(D^4)$ operations, and thus, $\langle\Psi|h|\Psi\rangle$ can be evaluated in $O(ND^4)$ operations. There are $O(N)$ terms in the Hamiltonian, and thus, the energy $\langle\Psi|\sum_i h_i|\Psi\rangle/\langle\Psi|\Psi\rangle$ can be evaluated in time $O(N^2D^4)$, and thus efficiently; in fact, this method can be easily improved to scale as $O(ND^3)$.[3] Similarly, one can see that e.g. correlation functions $\langle\Psi|P_i \otimes Q_j|\Psi\rangle$ or string order parameters $\langle\Psi|X \otimes X \otimes \cdots \otimes X|\Psi\rangle$ can be reduced to matrix multiplications and thus evaluated in $O(ND^3)$. Exactly the same way, evaluating expectation values for MPS with periodic boundary conditions can be reduced to computing the trace of a product of matrices $\mathbb{E}$ of size $D^2 \times D^2$. Each multiplication scales like $O(D^6)$, and using the same tricks as before, one can show that for systems with periodic boundary conditions, expectation values can be evaluated in time $O(ND^5)$.
In summary, we find that energies, correlations functions, etc. can be efficiently evaluated for MPS, with computation times scaling as $O(ND^3)$ and $O(ND^5)$ for open and periodic boundary conditions, respectively.

## 2.5 Variational optimization of MPS

As we have seen, we can efficiently compute the energy of an MPS with respect to a given local Hamiltonian $H = \sum_i h_i$. In order to use MPS for numerical simulations, we still need to figure out an efficient way to find the MPS which minimizes the energy for a given $D$. To this end, let us first pick a site $k$, and try to minimize the energy as a function of $A^{[k]}$, while keeping all other MPS tensors $A^{[s]}$, $s \neq k$, fixed. Now, since $|\Psi\rangle$ is a linear function of $A^{[k]}$, we have that

$$\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\vec{A}^{[k]\dagger} X \vec{A}^{[k]}}{\vec{A}^{[k]\dagger} Y \vec{A}^{[k]}}$$

is the ratio of two quadratic forms in $A^{[k]}$. Here, $\vec{A}^{[k]}$ denotes the vectorized version of $A^{[k]}_{i,\alpha\beta}$, where $(i,\alpha,\beta)$ is interpreted as a single index. The matrices $X$ and $Y$ can be obtained by contracting the full tensor network (7) except for the tensors $A^{[k]}$ and $\bar{A}^{[k]}$, which can be done

[3] Firstly, one uses that the products $\mathbb{L}\cdots\mathbb{E}^{[s]}$ and $\mathbb{E}^{[s]}\cdots\mathbb{R}$ need to be computed only once (this can be simplified even further by choosing the appropriate gauge [7, 8]), reducing the $N$-scaling to $O(N)$. Secondly, one slightly changes the contraction order: Starting from the left, one contracts $A^{[1]}$, $\bar{A}^{[1]}$, $A^{[2]}$, $\bar{A}^{[2]}$, $A^{[3]}$, etc.: This involves multiplications of $D \times D$ matrices with $D \times dD$ matrices, and $D \times Dd$ matrices with $Dd \times D$ matrices, yielding a $O(dD^3)$ scaling.

efficiently. The $\vec{A}^{[k]}$ which minimizes this energy can be found by solving the generalized eigenvalue equation

$$X\vec{A}^{[k]} = E\,Y\vec{A}^{[k]}$$

where $E$ is the energy; again, this can be done efficiently in $D$. For MPS with open boundary conditions, we can choose a gauge[4] for the tensors such that $Y = \mathbb{1}$ [7, 8] – this reduces the problem to a usual eigenvalue problem, and avoids problems due to ill-conditioned $Y$.

This shows that we can efficiently minimize the energy as a function of the tensor $A^{[k]}$ at an individual site $k$. In order to minimize the overall energy, we start from a randomly chosen MPS, and then sweep through the sites, sequentially optimizing the tensor at each site. Itering this a few times over the system (usually sweeping back and forth) quickly converges to a state with low energy. Although in principle, such an optimization can get stuck [10, 11], in practice it works extremely well and generally converges to the optimal MPS (though some care might have to be put into choosing the initial conditions).

In summary, we find that we can use MPS to efficiently simulate ground state properties of one-dimensional quantum systems with both open and periodic boundary conditions. This simulation method can be understood as a reformulation of the Density Matrix Renormalization Group (DMRG) algorithm [12, 13], which is a renormalization algorithm based on keeping the states which are most relevant for the entanglement of the system, and which since its invention has been highly successful in simulating the physics of one-dimensional quantum systems (see Refs. [7, 14] for a review of the DMRG algorithm and its relation to MPS).

# 3 Projected entangled pair states (PEPS)

## 3.1 PEPS for two-dimensional systems

As we have seen, MPS are very well suited for simulating ground state properties of one-dimensional systems. But what if we want to go beyond one-dimensional systems, and, e.g., study interacting spin systems in two dimensions? Two-dimensional systems can exhibit a rich variety of phenomena, such as topologically ordered states [15, 16], which are states distinct from those in the trivial phase, yet which do not break any (local) symmetry. Moreover, two-dimensional spin systems can be highly frustrated due to the presence of large loops in the interaction graph, and even classical two-dimensional spin glasses can be hard to solve [17]. In the following, we will focus on the square lattice without loss of generality.

[4] MPS have a natural gauge degree of freedom, since for any $X_s$ with a right inverse $X_s^{-1}$, we can always replace

$$A_i^{[s]} \leftrightarrow A_i^{[s]} X_s$$
$$A_i^{[s+1]} \leftrightarrow X_s^{-1} A_i^{[s+1]}$$

without changing the state; this gauge degree of freedom can be used to obtain standard forms for MPS with particularly nice properties [9, 8].

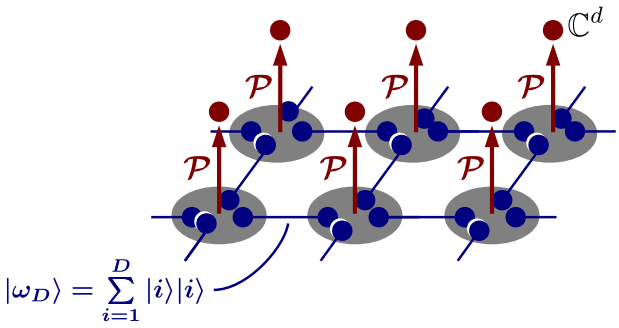



**Fig. 4:** *PEPS construction for a 2D square lattice, where we have omitted the site-dependence $\mathcal{P} \equiv \mathcal{P}_s$ of the maps $\mathcal{P}_s$.*

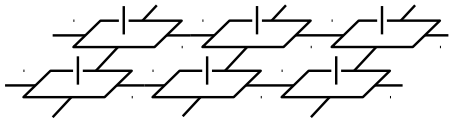
A first idea to simulate two-dimensional systems would be to simply use an MPS, by choosing a one-dimensional ordering of the spins in the two-dimensional lattice. While this approach has been applied successfully (see, e.g., Ref. [18]), it cannot reproduce the entanglement features of typical ground states in two dimensions as one increases the system size: As we have discussed in Section 2.1, two-dimensional systems also satisfy an area law, i.e., in the ground state we expect the entanglement of a region $A$ with its complement to scale like its boundary, $S(\rho_A) \sim |\partial A|$. To obtain an ansatz with such an entanglement scaling, we follow the same route as in the construction of MPS: We consider each site as being composed of *four* $D$-dimensional virtual subsystems, place each of them in a maximally entangled state $|\omega_D\rangle$ with the corresponding subsystem of each of the adjacent sites, and finally apply a linear map

$$\mathcal{P}_s : \mathbb{C}^D \otimes \mathbb{C}^D \otimes \mathbb{C}^D \otimes \rightarrow \mathbb{C}^d$$

at each site $s$ to obtain a description of the physical state on a 2D lattice of $d$-level sytems. The construction is illustrated in Fig. 4. Due to the way they are constructed, these states are called *Projected Entangled Pair States* (PEPS). Again, we can define five-index tensors $A^{[s]} = A^{[s]}_{i,\alpha\beta\gamma\delta}$, where now

$$\mathcal{P}_s = \sum_{i\alpha\beta\gamma\delta} A^{[s]}_{i,\alpha\beta\gamma\delta} |i\rangle\langle\alpha,\beta,\gamma,\delta| \,,$$

and express the PEPS in Fig. 4 graphically as a tensor network

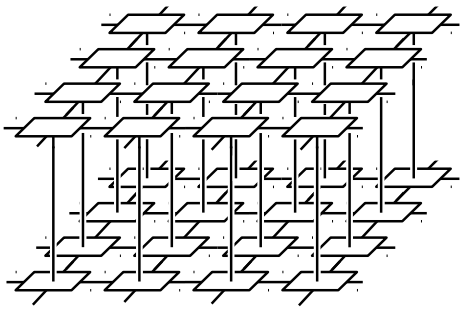


(where we have omitted the tensor labels). Similar to the result in one dimension, one can show that PEPS approximate ground states of local Hamiltonians well as long as the density of states grows at most polynomially with the energy [19, 20], and thereby provide a good variational ansatz for two-dimensional systems. (Note, however, that it is not known whether all 2D states which obey an area law are approximated well by PEPS.)

## 3.2 Contraction of PEPS

Let us next consider what happens if we try to compute expectation values of local observables for PEPS. For simplicity, we first discuss the evaluation of the normalization $\langle\Psi|\Psi\rangle$, which is obtained by sandwiching the ket and bra tensor network of $|\Psi\rangle$,

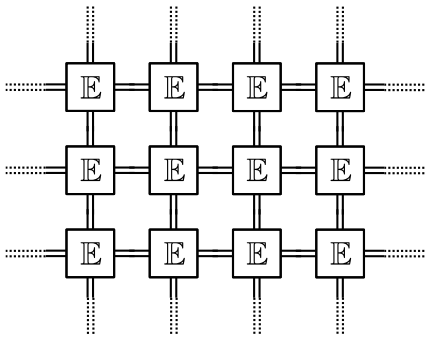
$\langle\Psi|\Psi\rangle$ =



. (9)

This can again be expressed using transfer operators


(the $\mathbb{E}$ should be thought of as being "viewed from the top"), leaving us with the task of contracting the network

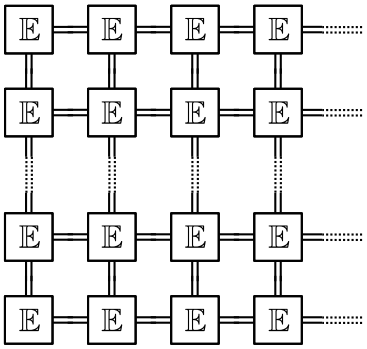



.

[This easily generalizes to the computation of expectation values, where some of the $\mathbb{E}$ have to be modified similarly to Eq. (8)]. Different from the case of MPS, there is no one-dimensional structure which we can use to reduce this problem to matrix multiplication. In fact, it is easy to see that independent of the contraction order we choose, the cluster of tensors we get (such as a rectangle) will at some point have a boundary of a length comparable to the linear system size. This is, we need to store an object with a number of indices proportional to $\sqrt{N}$ – and thus an *exponential* number of parameters – at some point during the contraction, making it impossible to contract such a network efficiently. (Indeed, it can be proven that such a contraction is a computationally hard problem [6].)

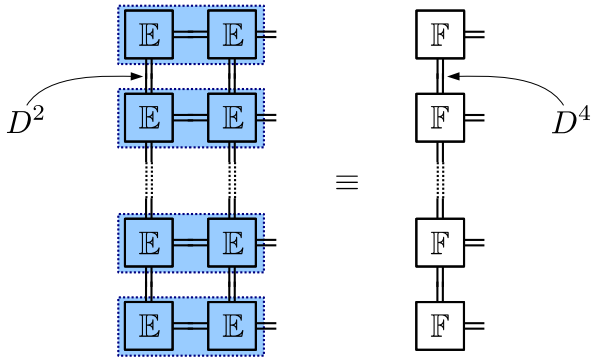
This means that if we want to use PEPS for variational calculations in two dimensions, we have to make use of some approximate contraction scheme, which of course should have a small and ideally controlled error. To this end, we proceed as follows [21]: Consider the contraction of a

two-dimensional PEPS with open boundary conditions,




. (10)

Now consider the first two columns, and block the two tensors in each column into a new tensor $\mathbb{F}$ (with vertical bond dimension $D^4$):




. (11)

This way, we have reduced the number of columns in (10) by one. Of course, this came at the cost of squaring the bond dimension of the first column, so this doesn't help us yet. However, what we do now is to approximate the right hand side of (11) by an MPS with a (fixed) bond dimension $\alpha D^2$ for some $\alpha$. We can then iterate this procedure column by column, thereby contracting the whole PEPS, and at any point, the size of our tensors stays bounded. It remains to be shown that the elementary step of approximating an MPS $|\Phi\rangle$ [such as the r.h.s. of (11)] by an MPS $|\Psi\rangle$ with smaller bond dimension can be done efficiently: To this end, it is sufficient to note that the overlap $\langle\Phi|\Psi\rangle$ is linear in each tensor $A^{[s]}$ of $|\Psi\rangle$, and thus, maximizing the overlap

$$\frac{\big|\langle\Phi|\Psi\rangle\big|^2}{\langle\Psi|\Psi\rangle}$$

can again be reduced to solving a generalized eigenvalue problem, just as the energy minimization for MPS in the one-dimensional variational method. Differently speaking, the approximate contraction scheme succeeds by reducing the two-dimensional contraction problem to a sequence of one-dimensional contractions, i.e., it is based on a dimensional reduction of the problem.

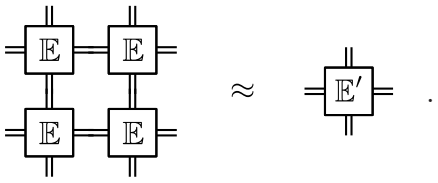
This shows that PEPS can be contracted approximately in an efficient way. The scaling in $D$ is naturally much less favorable than in one dimension, and for the most simple approach one finds a scaling of $D^{12}$ for open boundaries, which using several tricks can be improved down to $D^8$. Yet, the method is limited to much smaller $D$ as compared to the MPS ansatz. It should be

noted that the approximate contraction method we just described has a controlled error, as we know the error made in in each approximation step. Indeed, the approximation is very accurate as long as the system is short-range correlated, and the accuracy of the method is rather limited by the $D$ needed to obtain a good enough approximation of the ground state. Just as in one dimension, we can use this approximate contraction method to build a variational method for two-dimensional systems by successively optimizing over individual tensors [21].

## 3.3 Extensions of PEPS

The PEPS construction is not limited to square lattices, but can be adapted to other lattices, higher dimensions, and even arbitrary interaction graphs. Clearly, the approximate contraction scheme we just presented works for any two-dimensional lattice, and in fact for any planar graph. In order to approximately contract systems in more than two dimensions, note that the approximate contraction scheme is essentially a scheme for reducing the dimension of the problem by one; thus, in order to contract e.g. three-dimensional systems we can nest two layers of the scheme. In cases with a highly connected PEPS graph (e.g., when considering systems with highly connected interaction graphs such as orbitals in a molecule), one can of course still try to find a sequential contraction scheme, though other contraction methods might be more promising.

The contraction method described in Section 3.2 is not the only contraction scheme for PEPS. One alternative method is based on renormalization ideas [22–24]: There, one takes blocks of e.g. $2 \times 2$ tensors and tries to approximate them by a tensor with lower bond dimension by the appropriate truncation,




Finding the best truncation scheme requires exact knowledge of the environment, i.e., the contraction of the remaining tensor network. Since this is as hard as the original problem, heuristic methods to approximate the environment (such as to only contract a small number of surrounding tensors exactly, and imposing some boundary condition beyond that) have been introduced. While these approximations are in principle less accurate and the error is less controlled, their more favorable scaling allows for larger $D$ and thus potentially better approximations of the ground state.

Another approach to speed up PEPS contraction is using Monte Carlo sampling [25–27]: We can always write

$$\frac{\langle\Psi|O|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \sum_i p(i) \frac{\langle i|O|\Psi\rangle}{\langle i|\Psi\rangle} \,, \tag{12}$$

where the sum runs over an orthonormal basis $|i\rangle$, and $p(i) = |\langle i|\Psi\rangle|^2/\langle\Psi|\Psi\rangle$; in particular, we want to consider the local spin basis $i = (i_1, \ldots, i_N)$. If we can compute $\langle i|\Psi\rangle$ and $\langle i|O|\Psi\rangle$ (where the latter reduces to the former if $O$ is a local operator), then we can use Monte Carlo

sampling to approximate the expectation value $\langle\Psi|O|\Psi\rangle$. In particular, for PEPS $\langle i|\Psi\rangle$ can again be evaluated by contracting a two-dimension tensor network; however, this network now has bond dimension $D$ rather than $D^2$. Thus, we can apply any of the approximate contraction schemes described before, but we can go to much larger $D$ with the same computational resources; it should be noted, however, that the number of operations needs to be multiplied with the number $M$ of sample points taken, and that the accuracy of Monte Carlo sampling improves as $1/\sqrt{M}$.

# 4 Simulating time evolution and thermal states

Up to now, our discussion has been focused on ground states of many-body systems. However, the techniques described here can also be adapted to simulate thermal states as well as time evolution of systems governed by local Hamiltonians. In the following, we will discuss the implementation for one-dimensional systems; the generalization to to 2D and beyond is straightforward.

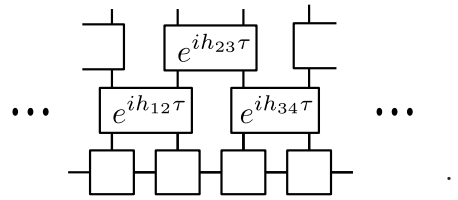
Let us start by discussing how to simulate time evolutions. (This will also form the basis for the simulation of thermal states.) We want to study how an initial MPS $|\Psi\rangle$ changes under the evolution with $e^{iHt}$; w.l.o.g., we consider $H$ to be nearest neighbor. To this end, we perform a Trotter decomposition

$$e^{iHt} \approx \left(e^{iH_{\text{even}}t/M} e^{iH_{\text{odd}}t/M}\right)^M$$

where we split $H = H_{\text{even}} + H_{\text{odd}}$ into even and odd terms (acting between sites $12$, $34$, …, and $23$, $45$, …, respectively), such that both $H_{\text{even}}$ and $H_{\text{odd}}$ are sums of non-overlapping terms. For large $M$, the Trotter expansion becomes exact, with the error scaling like $O(1/M)$. We can now write

$$e^{iH_{\text{even}}\tau} = \bigotimes_{i=1,3,5,\ldots} e^{ih_{i,i+1}\tau} = \boxed{e^{ih_{12}\tau}}\ \boxed{e^{ih_{34}\tau}}\ \cdots$$

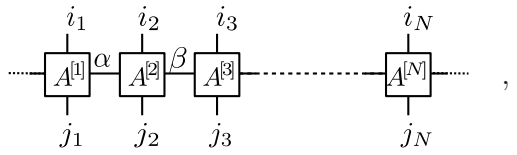
(with $\tau = t/M$), and similarly for $e^{iH_{\text{odd}}\tau}$. Thus, after one time step $\tau$ the initial MPS is transformed into




Here, the lowest line is the initial MPS, and the next two lines the evolution by $H_{\text{even}}$ and $H_{\text{odd}}$ for a time $\tau$, respectively. We can proceed this way and find that the state after a time $t$ is described as the boundary of a two-dimensional tensor network. We can then use the same procedure as for the approximate contraction of PEPS (proceeding row by row) to obtain an MPS description of the state at time $t$ [5]. A caveat of this method is that this only works well as long as the state has low entanglement at all times, since only then, a good MPS approximation of the state exists [4, 28]. While this holds for low-lying excited states with a small number of quasiparticles, this is not true after a quench, i.e., a sudden change of the overall

Hamiltonian of the system [29, 30]. However, this does not necessarily rule out the possibility to simulate time evolution using tensor networks, since in order to compute an expectation value $\langle\Psi|e^{-iHt}Oe^{iHt}|\Psi\rangle$, one only needs to contract a two-dimensional tensor network with no boundary, which can not only be done along the time direction (row-wise) but also along the space direction (column-wise), where such bounds on the correlations do not necessarily hold; indeed, much longer simulations times have be obtained this way [31].
In the same way as real time evolution, we can also implement imaginary time evolution; and since $e^{-\beta H}$ acting on a random initial state approximates the ground state for $\beta \to \infty$, this can be used as an alternative algorithm for obtaining MPS approximations of ground states.
In order to simulate thermal states, we use Matrix Product Density Operators (MPDOs) [32]

$$\rho = \sum_{\substack{i_1,\ldots,i_N \\ j_1,\ldots,j_N}} \mathrm{tr}[A^{[1]}_{i1,j1}\cdots A^{[N]}_{i_N,j_N}]|i_1,\ldots,i_N\rangle\langle j_1,\ldots,j_N|$$

$=$ 

,

where each tensor $A^{[s]}$ now has two physical indices, one for the ket and one for the bra layer. We can then write the thermal state as

$$e^{-\beta H} = e^{-\beta H/2}\,\mathbb{1}\,e^{-\beta H/2}$$

and use imaginary time evolution (starting from the maximally mixed state $\mathbb{1}$ which has a trivial tensor network description) and the Trotter decomposition to obtain a tensor network for $e^{-\beta H}$, which can again be transformed into an MPDO with bounded bond dimension using approximate contraction [32].

# 5 Other tensor network ansatzes

There is a number of other entanglement based ansatzes beyond MPS and PEPS for interacting quantum systems, some of which we will briefly sketch in the following.
Firstly, there is the Multiscale Entanglement Renormalization Ansatz (MERA) [33], which is an ansatz for scale invariant systems (these are systems at a critical point where the Hamiltonian is gapless, and which have algebraically decaying correlation functions), and which incorporates the scale-invariance in the ansatz. A first step towards a scale-invariant ansatz would be to choose a tree-like tensor network. However, such an ansatz will not have sufficient entanglement between different blocks. Thus, one adds additional *disentanglers* which serve to remove the entanglement between different blocks, which gives rise to the tensor network shown in Fig. 5. In order to obtain an efficiently contractible tensor network, one chooses the tensors to be unitaries/isometries in vertical direction, such that each tensor cancels with its adjoint. It is easy to see that this way for any local $O$, in the tensor network for $\langle\Psi|O|\Psi\rangle$ most tensors cancel, and one only has to evaluate a tensor network of the size of the *depth* of the MERA, which is

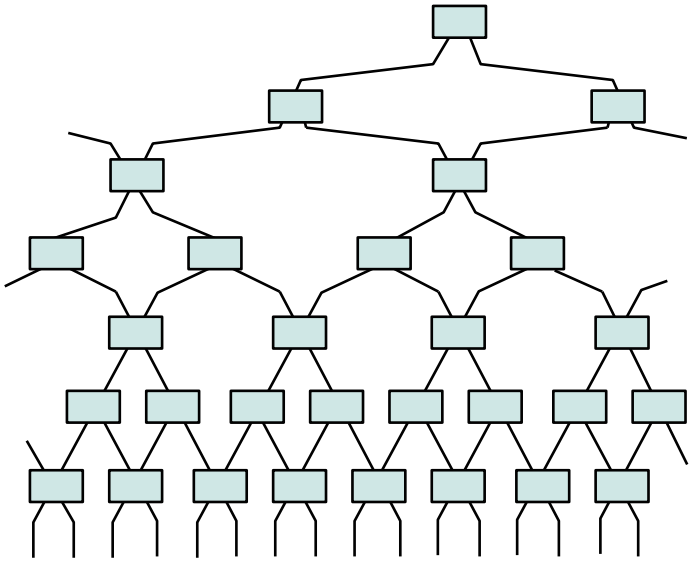


**Fig. 5:** *The Multi-Scale Entanglement Renormalization Ansatz (MERA) in 1D. (The left and right boundary are connected.)*

logarithmic in its length [33]. The MERA ansatz is not restricted to one dimension and can also be used to simulate critical system in 2D and beyond [34].

A different variational class is obtained by studying states for which expectation values can be computed efficiently using Monte Carlo sampling. Following Eq. (12), this requires (for local quantities $O$) that we can compute $\langle i|\Psi\rangle$ efficiently for all $i = (i_1, \ldots, i_N)$. One class of states for which this holds is formed by MPS, which implies that we can evaluate expectation values for MPS using Monte Carlo sampling [26, 25] (note that the scaling in $D$ is more favorable since $\langle i|\Psi\rangle$ can be computed in time $\propto ND^2$). This can be extended to the case where $\langle i|\Psi\rangle$ is a product of efficiently computable objects, such as products of MPS coefficients defined on subsets of spins: We can arrange overlapping one-dimensional strings in a 2D geometry and associate to each of them an MPS, yielding a class known as string-bond states [25, 35], which combines a flexible geometry with the favorable scaling of MPS-based methods. We can also consider $\langle i|\Psi\rangle$ to be a product of coefficients each of which only depends on the spins $i_k$ supported on a small plaquette, and where the lattice is covered with overlapping plaquettes, yielding a family of states known as Entangled Plaquette States (EPS) [36] or Correlator Product States (CPS) [37], which again yields an efficient algorithm with flexible geometries. In all of these ansatzes, the energy is minimized by using a gradient method, which is considerably facilitated by the fact that the gradient can be sampled directly without the need to first compute the energy landscape.

In order to simulate infinite lattices, it is possible to extend MPS and PEPS to work for infinite systems: iMPS and iPEPS. The underlying idea is to describe the system by an infinite MPS and PEPS with a periodic pattern of tensors such as ABABAB... (which allows the system to break translational symmetry and makes the optimization more well-behaved). Then, one fixes all tensors except for one and minimizes the energy as a function of that tensor until convergence is reached. For the optimization, one needs to determine the dependence of the energy on the

selected tensor, which can be accomplished in various ways, such as using the fixed point of the transfer operator, renormalization methods (cf. Section 3.3), or the corner transfer matrix approach. For more information, see, e.g., [38–40].

# 6 Simulation of fermionic sytems

Up to now, we have considered the simulation of spin systems using tensor networks. On the other hand, in many cases of interest, such as for the Hubbard model or the simulation of molecules, the underlying systems are fermionic in nature. In the following, we will discuss how tensor network methods such as MPS, PEPS, or MERA can be extended to the simulation of fermionic systems.

In order to obtain a natural description of fermionic systems, the idea is to replace each object (i.e., tensor) in the construction of MPS, PEPS, or MERA by fermionic operators [41–43]. This is, in the construction of MPS and PEPS, Fig. 3 and Fig. 4, both the maximally entangled bonds and the $\mathcal{P}_s$ are now built from fermionic operators and need to preserve parity; equally, in the MERA construction, Fig. 5, all unitaries and isometries are fermionic in nature. The resulting states are called fermionic PEPS (fPEPS) and fermionic MERA (fMERA).

Let us now have a closer look at a fermionic tensor network, and discuss how to compute expectation values for those states. E.g., the fPEPS construction yields a state

$$(\mathcal{P}_1 \otimes \mathcal{P}_2 \otimes \cdots)(\omega_1 \otimes \omega_2 \otimes \cdots)|\Omega\rangle \ ,$$

where $|\Omega\rangle$ is the vacuum state, the $\omega_i$ create entangled fermionic states between the corresponding auxiliary modes, and the $\mathcal{P}_s$ map the auxiliary fermionic modes to the physical fermionic modes at site $s$ (leaving the auxiliary modes in the vacuum). While the product of the $\omega_i$ contains only auxiliary mode operators in a given order, the product of the $\mathcal{P}_s$ contains the physical and auxiliary operators for each site grouped together. To compute expectation values, on the other hand, we need to move all the physical operators to the left and the virtual operators to the right in the product of the $\mathcal{P}_s$; additionally, the virtual operators have to be arranged such that they cancel with the ones arising from the product of the $\omega_i$. Due to the fermionic anti-commutation relations, this reordering of fermionic operators results in an additional complication which was not present for spin systems. Fortunately, it turns out that there are various ways how to take care of the ordering of fermionic operators at no extra computational cost: One can use a Jordan-Wigner transformation to transform the fermionic system to a spin system [41, 43]; one can map the fPEPS to a normal PEPS with one additional bond which takes care of the fermionic anticommutation relations [42]; or one can replace the fermionic tensor network by a planar spin tensor network with parity preserving tensors, where each crossing of lines [note that a planar embedding of a network such as the 2D expectation value in Eq. (9) gives rise to crossings of lines, which corresponds to the reordering of fermionic operators] is replaced by a tensor which takes care of the anticommutation rules [44, 45].

# 7 Summary

In this lecture, we have given an overview over entanglement-based ansatzes for the description and simulation of quantum many-body systems. We started by discussing the area law for the entanglement entropy which is obeyed by ground states of local interactions, and used this to derive the Matrix Product State (MPS) ansatz which is well suited to describe the physics of such systems. We showed that the one-dimensional structure of MPS allows for the efficient evaluation of expectation values, and that this can be used to build a variational algorithm for the simulation of one-dimensional systems. We have then discussed Projected Entangled Pair States (PEPS), which naturally generalize MPS and are well suited for the description of two-dimensional systems, and we have shown how approximation methods can be used to implement efficient PEPS based simulation. We have also demonstrated that MPS and PEPS can be used to simulate the time evolution and thermal states of systems governed by local Hamiltonians. Finally, we have discussed other tensor network based approaches, such as MERA for scale-invariant systems or iMPS and iPEPS for infinite sytems, and concluded with a discussion on how to apply tensor network methods to fermionic systems.

At the end, let us note that while we have focused on Tensor Networks in the context of numerical simulations, these ansatzes also serve as powerful analytical tools. To name just a few, MPS and PEPS can be used to build exactly solvable models (most prominently, the AKLT model [46]), where a given MPS or PEPS arises as the exact ground state of a local Hamiltonian [9, 47, 48], and they serve as a framework to understand entanglement properties of quantum states and thus to classify quantum phases, such as topological phases [49] and symmetry protected phases [50–53], thereby going beyond the framework of Landau theory which can be understood using product states, i.e., MPS with $D = 1$.

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