Advanced Computational Physics

Time Evolution of one-dimensional spin systems, using Matrix Product States

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1 Matrix Product States (MPS)

The state space of many-particle models grows exponentially with the number of particles involved. Such models can therefore be treated exactly only for very small systems.
In recent years, a new representation for the states of one-dimensional systems has been developed, so-called Matrix Product States (MPS), which permit very precise and efficient approximations even for very large systems. They have allowed for, e.g., calculations of the ground state energy of Heisenberg models on several hundred sites to 10 digit precision. Recently, the non-equilibrium time evolution of such models has also become accessible.
This chapter provides a first introduction and examples for MPS.

1.1 Heisenberg spin chain and equivalent particle model

Throughout we shall treat the one-dimensional spin $\frac{1}{2}$ Heisenberg model with open boundary conditions:

$$\hat{H} = \sum_{j=1}^{L-1} J_{xy} \left(\hat{S}_j^x \hat{S}_{j+1}^x \; + \; \hat{S}_j^y \hat{S}_{j+1}^y \right) \; + \; J_z \, \hat{S}_j^z \hat{S}_{j+1}^z \tag{1.1}$$

$$= \sum_{j=1}^{L-1} \frac{1}{2} J_{xy} \left(\hat{S}_j^+ \hat{S}_{j+1}^- \; + \; \hat{S}_j^- \hat{S}_{j+1}^+ \right) \; + \; J_z \, \hat{S}_j^z \hat{S}_{j+1}^z \tag{1.2}$$

with $\hat{S}_j^{\pm} = \hat{S}_j^x \pm i \hat{S}_j^y$, thus $\hat{S}_j^+ |\downarrow\rangle_j = |\uparrow\rangle_j$ and $\hat{S}_j^- |\uparrow\rangle_i = |\downarrow\rangle_j$. The representation of $\hat{S}_j^\alpha$ in the z-Basis at site j is $\frac{1}{2}\sigma^\alpha$ (we leave out $\hbar$). Site L and site 1 do not interact, i.e. we have open boundary conditions.
A chain of L sites has 2^L basis states, which are $|s_1, s_2, \ldots, s_L\rangle$ with $s_j = \uparrow, \downarrow$ in the z-basis.
In case of isotropic couplings $J_{xy} = J_z =: J$ we get $\hat{H} = J \sum_j \vec{\hat{S}}_j \vec{\hat{S}}_{j+1}$. This model is also a good approximation of the strongly repulsive Hubbard model ($U \gg t$) at half filling.
On a one-dimensional chain, the Heisenberg model is equivalent to a model of "spinless fermions", if one identifies a down-spin at site j with an empty site, and an up spin with an occupied site:

$$|0\rangle_j = |\downarrow\rangle_j \quad \text{and} \quad |1\rangle_j = |\uparrow\rangle_j \; .$$

The Hamiltonian then becomes

$$\hat{H} = \sum_{j=1}^{L-1} t \left(c_j^\dagger c_{j+1} \; + \; c_j c_{j+1}^\dagger \right) \; + \; V \, \hat{n}_j \hat{n}_{j+1} - \frac{V}{2} (\hat{n}_j + \hat{n}_{j+1}) + \frac{1}{4} \tag{1.3}$$

with hopping $t = J_{xy}/2$, occupation number operator $\hat{n}_j = \hat{S}_j^z + \frac{1}{2}$, and "Coulomb repulsion" $V = J^z$. When one has a fixed particle number, the last 2 terms in $\hat{H}$ add up to a constant, i.e. they are just a shift of energy.

The models are equivalent since there is only next-nearest neighbor hopping, so that particles never switch places and thus the Pauli fermion-sign never appears.[1]
We will occasionally switch between the spin-language and the particle language.

1.2 Matrix Product State ansatz

A general state of the Heisenberg chain is

$$\boxed{|\psi\rangle = \sum_{s_1,s_2,\ldots,s_L} c_{s_1,s_2,\ldots,s_L} \quad |s_1, s_2, \ldots, s_L\rangle} \tag{1.4}$$

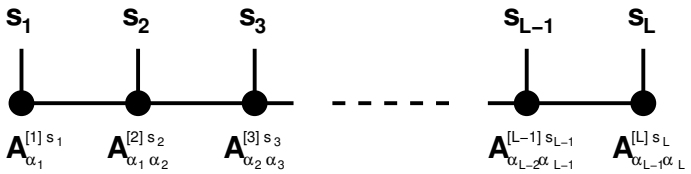
with 2^L complex numbers as coefficients.
We will now write the coefficents in a different way, as a product of matrices, with one matrix for every lattice-site. This can always be done exactly (see later) when the matrices are chosen big enough, namely up to $2^{L/2} \times 2^{L/2}$. We will later see that much smaller matrices ($O(100) \times O(100)$) already provide an extremely good approximation to physically relevant states.

Ansatz:

$$\boxed{|\psi\rangle \;=\; \sum_{s_1,s_2,\ldots,s_L} \sum_{\alpha_1,\alpha_2,\ldots,\alpha_{L-1}} A^{[1]s_1}_{\alpha_1} A^{[2]s_2}_{\alpha_1,\alpha_2} A^{[3]s_3}_{\alpha_2,\alpha_3} \ldots A^{[L-1]s_{L-1}}_{\alpha_{L-2},\alpha_{L-1}} A^{[L]s_L}_{\alpha_{L-1}} \quad |s_1, s_2, \ldots, s_L\rangle \; .} \tag{1.5}$$

- The A can be taken to be square matrices (except for the first and last A, which are vectors).
- Matrix size: $\chi \times \chi$, where χ is some number.
- $\alpha_j = 1 \ldots \chi$ are the matrix indices.
- The upper index $[j]$ numbers the lattice sites. There can be different matrices A at each site.
- At each site j, there are two matrices, $A^{[j]\uparrow}$, and $A^{[j]\downarrow}$, corresponding to the values $s_j =\uparrow$ and "$s_j =\downarrow$ in the basis vector $|s_1, s_2, \ldots, s_L\rangle$.
- Note that for a given state, **the matrices A are not unique**: one can replace any pair of matrices $A^{[j]}A^{[j+1]}$ by $(A^{[j]}X)\,(X^{-1}A^{[j+1]})$, with any invertible matrix X.

It is very helpful to denote this ansatz for the coefficients in a graphical way:



[1] A difference does however appear when one calculates fermionic observables like $\langle c_i c_j^\dagger \rangle$, which can be different from $\langle \hat{S}_i^- \hat{S}_j^+ \rangle$. Such observables will not appear in these lecture notes.

1.2.1 Examples

• Single basis state (Product state)

A basis state like $|\downarrow\downarrow\uparrow\downarrow\rangle$ is called "product state", since it can be written as a product $|\downarrow\rangle_1 |\downarrow\rangle_2 |\uparrow\rangle_3 |\downarrow\rangle_4$ and it does not contain any linear combination.

$$\begin{array}{rcccccccc} |\psi\rangle & = & | & \downarrow & \downarrow & \uparrow & \downarrow & \uparrow & \downarrow & \rangle \\ j & = & & 1 & 2 & 3 & 4 & 5 & 6 & \\ A_j^{\uparrow} & = & & 0 & 0 & 1 & 0 & 1 & 0 & \\ A_j^{\downarrow} & = & & 1 & 1 & 0 & 1 & 0 & 1 & \end{array}$$

The "matrices" A are just single numbers here. (In the numerical project, we will do time evolutions starting from such simple product states).

• Singlet, L=2 sites

$$\begin{array}{rcccccc} |\psi\rangle & = \frac{1}{\sqrt{2}} & (& | & \uparrow & \downarrow & \rangle \\ & & - & | & \downarrow & \uparrow & \rangle \ ) \end{array}$$

$$\begin{array}{rcccc} A_j^{\uparrow} & = & (1,0), & -\begin{pmatrix}0\\1\end{pmatrix}/\sqrt{2} \\ A_j^{\downarrow} & = & (0,1), & \begin{pmatrix}1\\0\end{pmatrix}/\sqrt{2} \end{array}$$

• Nonlocal singlet

$$\begin{array}{rcccccccccc} |\psi\rangle & = \frac{1}{\sqrt{2}} & (& | & \downarrow & \downarrow & \uparrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \rangle \\ & & - & | & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \uparrow & \downarrow & \downarrow & \rangle \ ) \end{array}$$

$$\begin{array}{rcccccccc} A_j^{\uparrow} & = & 0, & 0, & (1,0), & \begin{pmatrix}0&0\\0&0\end{pmatrix}, & \begin{pmatrix}0&0\\0&0\end{pmatrix}, & -\begin{pmatrix}0\\1\end{pmatrix}/\sqrt{2}, & 0, \quad 0 \\ A_j^{\downarrow} & = & 1, & 1, & (0,1), & \begin{pmatrix}1&0\\0&1\end{pmatrix}, & \begin{pmatrix}1&0\\0&1\end{pmatrix}, & \begin{pmatrix}1\\0\end{pmatrix}/\sqrt{2}, & 1, \quad 1 \end{array}$$

2 Singular Value Decomposition (SVD)

The Singular Value Decomposition (SVD) is an extremely important and versatile tool from linear algebra. It is related to the familiar eigenvalue decomposition (see below). However, it is in general a different decomposition, and it is valid **for every real or complex matrix !**
Unfortunately, the SVD is often unknown to physicists, whereas it is extremely widespread elsewhere and used for e.g. image processing, signal processing, optimizations, etc. For this reason, we will treat it in some detail.

2.1 Basic SVD

Every real or complex $n \times m$ matrix M can be decomposed like

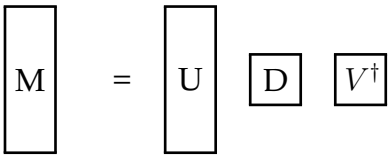
$$\boxed{M \;=\; U\; D\; V^\dagger} \tag{2.1}$$

with a diagonal matrix D that contains only *positive real numbers* (or zero), which are called the *singular values* of M. It is of dimension $N = \min(n, m)$. Furthermore,

$$U^\dagger U = \mathbb{1},\; V^\dagger V = \mathbb{1},\; D = \begin{pmatrix} \lambda_1 & & & & \\ & \ddots & & & \\ & & \lambda_r & & \\ & & & 0 & \\ & & & & \ddots \\ & & & & & 0 \end{pmatrix},\quad \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r > \lambda_{r+1} = \cdots = \lambda_N = 0. \tag{2.2}$$

The number r of non-zero entries λ is called the *rank* of the matrix M.

- Case $m \leq n$: 

- Case $m \geq n$: 

- When M is real, then U and $V^\dagger$ can also be chosen real.
- When M is real and quadratic, then U and $V^\dagger$ are rotations (basis transformations), and D scales the directions in the intermediate basis.
- This version of the SVD, with (in general) non-square matrices U and $V^\dagger$, is called a "thin SVD".
- When two or more singular values are equal, then the SVD in this subspace is non-unique.
- In addition, for every direction j, one can multiply U by a phase factor $\exp(i\varphi_j)$ and $V^\dagger$ by $\exp(-i\varphi_j)$ without changing M.
- The values λ_i are uniquely determined.
- The matrices U and $V^\dagger$ are only determined up to phase factors:

  $$\lambda_j \;=\; e^{i\varphi_j}\, \lambda_j\, e^{-i\varphi_j}$$

  which can be moved into U and $V^\dagger$ [1]

[1] When several λ_j are identical, the phase factors become unitary matrices.

2.2 SVD as a sum of outer products

The singular value decomposition $M = UDV^\dagger$ can equivalently be written as

$$M_{ij} = \sum_k \lambda_k U_{ik} \left(V^\dagger\right)_{kj} = \sum_k \lambda_k \, u_i^{(k)} \, v_j^{(k)}. \tag{2.3}$$

Here $u_i^{(k)} = U_{ik}$ and $v_i^{(k)} = V_{ik},\ i = 1, \ldots, m;\ \ k = 1, \ldots, N = \min(m, n)$ are the column vectors of U and V (not of $V^\dagger$). The property $U^\dagger U = V^\dagger V = \mathbb{1}$ implies that they are orthonormal. In vector notation, the SVD reads

$$M_{ij} = \sum_k \lambda_k \, \vec{\mathbf{u}}^{(k)} \times \vec{\mathbf{v}}^{(k)T} \quad = \sum_k \Bigg(\Bigg) \times \big(\quad \big) \tag{2.4}$$

This a sum of *outer products* of the vectors $\vec{u}^{(k)}$ and $\vec{v}^{(k)}$, weighted with λ_k.
The vectors $\vec{u}^{(k)}$ and $\vec{v}^{(k)}$ are called left and right *singular vectors* of M. The SVD together with $V^\dagger V = \mathbb{1}$ implies

$$M \, \vec{v}^{(k)} = \lambda_k \, \vec{u}^{(k)} \quad \text{and} \quad M^\dagger \, \vec{u}^{(k)} = \lambda_k \, \vec{v}^{(k)} \, .$$

2.3 Connection to the eigenvalue decomposition

- An SVD exists for every matrix, with positive singular values, whereas an eigenvalue decomposition does not exist for every matrix, and eigenvalues need not be real or positive.
- When M is quadratic and all eigenvalues are ≥ 0, then the eigenvalue decomposition $M = UDU^\dagger$ is the same as the SVD.
- The SVD of an arbitrary matrix M provides the eigenvalue decomposition for the hermitian matrices $M^\dagger M$ and $MM^\dagger$:

$$M^\dagger M = \left(UDV^\dagger\right)^\dagger UDV^\dagger = VD^\dagger U^\dagger \ UDV^\dagger = V \begin{pmatrix} |\lambda_1|^2 & & \\ & |\lambda_2|^2 & \\ & & \ddots \end{pmatrix} V^\dagger.$$

  Similarly,

$$MM^\dagger = UDV^\dagger \left(UDV^\dagger\right)^\dagger = UDV^\dagger \ VD^\dagger U^\dagger = U \begin{pmatrix} |\lambda_1|^2 & & \\ & |\lambda_2|^2 & \\ & & \ddots \end{pmatrix} U^\dagger.$$

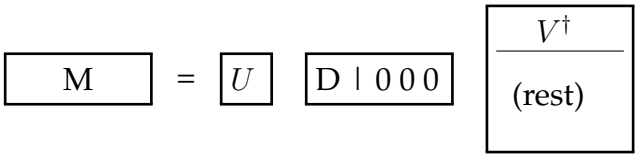
2.4 Representation of the SVD with square matrices

When M is not quadratic, then either U or $V^\dagger$ is not quadratic in the SVD $M = UDV^\dagger$. Alternatively, one can write the SVD with *unitary* quadratic matrices $\tilde{U}$ and $\tilde{V}$:

$$M = UDV^\dagger \quad = \quad \tilde{U}\tilde{D}\tilde{V}^\dagger \tag{2.5}$$

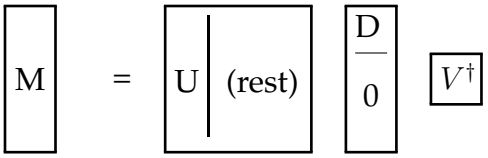
This can be interpreted as a basis transformation by $\tilde{V}^\dagger$, a weighting of directions by $\tilde{D}$, and another basis transformation by $\tilde{U}$. When M is $m \times n$ dimensional, then $\tilde{U}$ is $m \times m$, $\tilde{D}$ is $m \times n$, and $\tilde{V}^\dagger$ is $n \times n$.

- Case $m \leq n$:



  In this case, $\tilde{U} = U$. The lower rows of $\tilde{V}^\dagger$ contain extra eigenvectors, beyond those in $V^\dagger$. They do not contribute to M because of the zeroes in $\tilde{D}$. Since the eigenvectors in $\tilde{V}^\dagger$ are orthogonal, the application of M to such a vector gives zero, i.e. they belong to the *null space* of M. (The directions j beyond the rank r, with vanishing singular value $\lambda_{j>r} = 0$ also belong to the null space). When considering the action of M on the full vector space, this null space can be ignored (see below).

- Case $m \geq n$:



  Now $\tilde{V} = V$.

2.5 Pseudoinverse

We first discuss the case of a square matrix M. Formally, the inverse is

$$M^{-1} = \left(\tilde{U}\tilde{D}\tilde{V}^\dagger\right)^{-1} = \tilde{V}\tilde{D}^{-1}\tilde{U}^\dagger, \tag{2.6}$$

since $\tilde{U}$ and $\tilde{V}$ are unitary. But the matrix M can contain singular values $\lambda_{j>r} = 0$. In these directions j, M does not act, and the inverse $\tilde{D}^{-1}$ would contain infinity.
It is much better to *exclude this null space* competely also from the inverse, i.e. to set $\tilde{D}^{-1}$ to zero there. This is called the *pseudoinverse*:

$$\lambda_j \mapsto \frac{1}{\lambda_j}, \quad \text{but} \quad 0 \mapsto 0. \tag{2.7}$$

In practice, one maps singular values to zero when they are below some threshold (e.g. 10^{-15}). Using the pseudoinverse, $M^{-1}M$ becomes

$$M^{-1}M = \tilde{V}\tilde{D}^{-1}\tilde{U}\tilde{U}^\dagger\tilde{D}\tilde{V}^\dagger = \begin{pmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & & 0 & \\ & & & & \ddots \\ & & & & & 0 \end{pmatrix} = \ldots = M\,M^{-1} \tag{2.8}$$

in which only (up to) the first r components correspond to the unity matrix, while the rest vanishes.
The same considerations apply when M is not square, $n > m$ or $m > n$. Then $M^{-1}M$ is an $n \times n$ matrix. and MM^{-1} is $m \times m$. They are both of the form eq. 2.8.

2.6 Applications

The computational cost of the SVD is $\mathcal{O}(\max(n, m)^3)$, similar to a matrix diagonalization.

Many applications of the SVD involve *truncation*: one replaces small singular values by zero. This provides an *approximation* to M, which is usually very good. Yet it often contains *far* fewer components, providing for much lower computational cost.
Applications include image processing, signal processing, optimizations, strongly correlated many body systems, and many more.

3 Schmidt decomposition of a quantum state; Entanglement

3.1 Schmidt decomposition

Consider any quantum-mechanical system and two arbitrarily chosen subsystems A and B, for instance the left and right side of a one dimensional chain with some arbitrary split.
Let $|j\rangle_A$ be the orthonormal basis states of subsystem A, and $|k\rangle_B$ those of subsystem B. Then a general state of the total system is

$$|\Psi\rangle = \sum_{j,k} c_{jk} \, |j\rangle_A \, |k\rangle_B, \tag{3.1}$$

where c_{jk} are coefficients.
We now regard c_{jk} as a matrix and look at its singular value decomposition:

$$c_{jk} = \tilde{U}\tilde{D}\tilde{V}^\dagger, \quad \text{with } \tilde{U} \text{ and } \tilde{V} \text{ unitary.} \tag{3.2}$$

Written in matrix components, this becomes $c_{jk} = \sum_{\alpha=1}^{\chi} \lambda_\alpha \, \tilde{U}_{j\alpha} \left(\tilde{V}_{\alpha k}\right)^\dagger$, where χ is the rank of the matrix c_{jk}, the so called Schmidt-rank. Since $\tilde{U}$ and $\tilde{V}$ are unitary it is possible to perform two basis transformations: $|A\rangle_\alpha := \sum_j \tilde{U}_{j\alpha}|j\rangle_A$ and $|B\rangle_\alpha := \sum_k (\tilde{V}^\dagger)_{\alpha k}|k\rangle_B$ and express the state $|\Psi\rangle$ in the new basis:

$$\boxed{|\Psi\rangle = \sum_{\alpha=1}^{\chi} \lambda_\alpha \, |A\rangle_\alpha \, |B\rangle_\alpha, \quad \text{with } \chi \leq \min(\dim(A), \dim(B)).} \tag{3.3}$$

This Schmidt-decomposition of a general state $|\Psi\rangle$ always exists!
The normalization $\langle\Psi\,|\,\Psi\rangle = 1$ implies

$$\boxed{\sum_\alpha \lambda_\alpha^2 = 1\,.} \tag{3.4}$$

3.2 Reduced Density Matrix of a pure state

The total density matrix of a *pure* state is just: $\hat{\rho} = |\Psi\rangle\langle\Psi|$
With the results from the previous section this can be written as:

$$\hat{\rho} = \sum_{\alpha=1}^{\chi} \sum_{\beta=1}^{\chi} \lambda_\alpha \lambda_\beta |A\rangle_\alpha |B\rangle_\alpha \, {}_\beta\langle A| \, {}_\beta\langle B|$$

The *reduced density matrix* for the subsystem A is defined by taking the trace over the subsystem B:

$$\boxed{\hat{\rho}_A = \text{ tr}_B\, \hat{\rho} = \sum_\gamma {}_\gamma\langle B|\hat{\rho}|B\rangle_\gamma} \tag{3.5}$$

and since the bases $|A\rangle$ and $|B\rangle$ are orthonormal, one gets:

$$\boxed{\hat{\rho}_A = \sum_{\gamma=1}^{\chi} \lambda_\gamma^2\, |A\rangle_{\gamma\,\gamma}\langle A|} \tag{3.6}$$

This is a sum over eigenvalues[1] λ_γ^2 times a corresponding projection operator $|A\rangle_{\gamma\,\gamma}\langle A|$.

- When there is only one term in the sum, $\chi = 1$, then $\hat{\rho_A}$ is a pure state and the Schmidt decomposition is simply $|\Psi\rangle = |A\rangle|B\rangle$, i.e. the total system is in a product state.
  Example: $|\Psi\rangle = |\uparrow\rangle_A|\downarrow\rangle_B = |\uparrow\downarrow\rangle$
- When there is more than one term in the sum, $\chi > 1$, the reduced density matrix is a *mixed state*, and the eigenvalues λ_γ^2 correspond to the probability to be in the state $|A\rangle_\gamma$.
  Example: The total state is a singlet $|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$ (see below).

The reduced density matrix for sub-system B is defined completely analogous to the sub-system A case, which results in the same Schmidt rank χ.

$$\hat{\rho}_B = \sum_{\gamma=1}^{\chi} \lambda_\gamma^2 |B\rangle_{\gamma\,\gamma}\langle B| \tag{3.7}$$

3.3 Entanglement

The entanglement is similar in definition to the entropy of a statistical system which is

$$S = -\,\text{tr}(\hat{\rho}\ln\hat{\rho}). \tag{3.8}$$

Note that the entropy of a pure state is zero since:

$$\hat{\rho} = |\Psi\rangle\langle\Psi| \,\hat{=}\, \big(1\big) \quad \Rightarrow \quad \ln\hat{\rho} = 0 \quad \text{(see below)} \tag{3.9}$$

3.3.1 Von Neumann entanglement entropy

The von Neumann entropy of a subsystem A is defined as the entropy of its reduced density matrix:

$$\boxed{S_A := -\,\text{tr}_A(\hat{\rho}_A \ln\hat{\rho}_A)} \tag{3.10}$$

It is a measure of the entanglement of the two subsystems A and B.
Since the reduced density matrix ρ_A is diagonal in the basis $|A\rangle$:

$$\hat{\rho}_A = \sum_{\gamma=1}^{\chi} \lambda_\gamma^2\, |A\rangle_{\gamma\,\gamma}\langle A|,$$

[1] Note that the lecture notes for introductory quantum mechanics called the eigenvalues λ_{gamma}, without squares.

the von Neumann entropy reduces to

$$\boxed{S_A = -\sum_{\gamma=1}^{\chi} \lambda_\gamma^2 \ln \lambda_\gamma^2 = S_B} \tag{3.11}$$

Thus the entanglement entropy of subsystem A relative to B is the same as that of subsystem B relative to A.
S_A takes its maximum possible value when all λ_γ are of equal value, i.e. $\lambda_\gamma^2 = \frac{1}{\chi}$
(since $\sum_\gamma \lambda_\gamma^2 = 1$). Then the reduced density matrix is just a normalized identity matrix:

$$\hat{\rho}_A = \frac{1}{\chi} \begin{pmatrix} 1 & & \\ & 1 & \\ & & \ddots \\ & & & 1 \end{pmatrix} \tag{3.12}$$

and S_A is given by:

$$S_A = -\chi \left(\frac{1}{\chi} \ln \frac{1}{\chi} \right) = \ln \chi \tag{3.13}$$

3.3.2 Examples for a two site system

• **Product state** $|\Psi\rangle = |\uparrow_A \uparrow_B\rangle = |\uparrow\rangle_A |\uparrow\rangle_B$

- Schmidt decomposition: $|\Psi\rangle = |1\rangle_A |1\rangle_B = \sum_{\alpha=1}^{1} 1 |1\rangle_A |1\rangle_B$
- Reduced density matrix: $\hat{\rho}_A = |\uparrow\rangle_{A\,A}\langle\uparrow|$, which is a pure state.
- Entropy: $S_A = S_B = -1^2 \ln 1^2 = 0$, i.e. there is no entanglement!

• **Singlet:** $|\Psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_A |\downarrow\rangle_B - |\uparrow\rangle_B |\downarrow\rangle_A)$

- Schmidt decomposition: already done! $|\Psi\rangle = \sum_{\alpha=1}^{2} \lambda_\alpha |A\rangle_\alpha |B\rangle_\alpha$, where

$$\begin{aligned} |A\rangle_1 &= |\uparrow\rangle_A & , \ |A\rangle_2 &= |\downarrow\rangle_A \\ |B\rangle_1 &= |\downarrow\rangle_B & , \ |B\rangle_2 &= -|\uparrow\rangle_B \\ \lambda_1 &= \frac{1}{\sqrt{2}} & , \ \lambda_2 &= +\frac{1}{\sqrt{2}} \end{aligned}$$

- Reduced density matrix:

$$\begin{aligned} \hat{\rho}_A &= \sum_{\alpha=1}^{2} \lambda_\alpha^2 |A\rangle_{\alpha\,\alpha}\langle A| = \frac{1}{2}(|\uparrow\rangle_{A\,A}\langle\uparrow| + |\downarrow\rangle_{A\,A}\langle\downarrow|) \\ &= \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}_A = \frac{1}{2} \mathbb{1}_A \quad \rightarrow \text{ mixed state} \end{aligned}$$

- Entropy: $S_A = -2(\frac{1}{2} \ln \frac{1}{2}) = \ln 2$

4 Derivation of MPS

4.1 Exact representation of a state by an MPS

The coeffients of any pure state

$$|\Psi\rangle = \sum_{s_1 \dots s_L} c_{s_1 \dots s_L} |s_1 \dots s_L\rangle$$

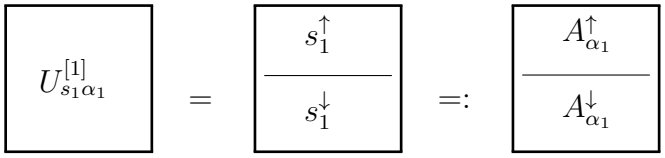
can be written as a "Matrix Product State" by going through the system site by site and performing Schmidt decompositions, i.e. basis transformations, at each site.

• First site

We treat the coefficients $c_{s_1,(s_2 \dots s_L)}$ as a matrix with row index s_1 and column index $(s_2 \dots s_L)$ and apply a SVD:

$$c_{s_1,(s_2 \dots s_L)} = \sum_{\alpha_1=1}^{2} \underbrace{U^{[1]}_{s_1 \alpha_1}}_{\text{2x2 matrix}} \lambda^{[1]}_{\alpha_1} V^{\dagger}_{\alpha_1 (s_2 \dots s_L)}$$

The upper index $[1]$ denotes the first lattice site. Since the index s_1 has only two values, $s_1 = \uparrow$ and $s_1 = \downarrow$, the matrix $U^{[1]}$ is (2×2) dimensional. We split it into two (1×2)-matrices $A^{[1]\uparrow}$ and $A^{[1]\downarrow}$ for the two spin components $\uparrow$ and $\downarrow$.



$\alpha_1 = 1, 2$ $\alpha_1 = 1, 2$ $\alpha_1 = 1, 2$

U is a unitary matrix. It contains a basis transformation from the basis $s_1 = \uparrow, s_1 = \downarrow$ to a new basis with indices $\alpha_1 = 1, 2$. Similarly, $V^{\dagger}$ defines a basis transformation on the vectors $|s_2, s_3, \dots, s_L\rangle$, i.e. we get the Schmidt decomposition

$$|\Psi\rangle = \sum_{\alpha_1=1}^{2} \lambda^{[1]}_{\alpha_1} |\Phi^L_{\alpha_1}\rangle |\Phi^R_{\alpha_1}\rangle, \tag{4.1}$$

where $L(R)$ denote the left(right) subsystem.

• Second site

We now regard $\lambda_{\alpha_1} V^{\dagger}_{\alpha_1 (s_2 \dots s_L)}$ (including the diagonal matrix λ !) as a matrix element $(\text{matrix})_{(\alpha_1 s_2)(s_3 \dots s_L)}$ with row index $(\alpha_1 s_2)$ and column index $(s_3 \dots s_L)$ and decompose it with a SVD:

$$\lambda_{\alpha_1} V^{\dagger}_{\alpha_1 (s_2 \dots s_L)} = \sum_{\alpha_2=1}^{4} \underbrace{U^{[2]}_{(\alpha_1 s_2)\alpha_2}}_{\text{4x4 matrix}} \lambda^{[2]}_{\alpha_2} V^{\dagger}_{\alpha_2 (s_3 \dots s_L)}$$

The summation index α_2 now goes up to 4, because of the possible combinations of $\alpha_1 = \{1, 2\}$ and $s_2 = \{\uparrow, \downarrow\}$.[1]
The 4×4 matrix $U^{[2]}$ is again unitary and a basis transformation from $\{\alpha_1 s_2\}$ to $\{\alpha_2\}$ which we split up into two 2×4 matrices $A^{[2]\uparrow}$ and $A^{[2]\downarrow}$ for the two spin indices s_2:

$$\boxed{U^{[2]}_{\alpha_1 s_2 \alpha_2}} \quad =: \quad \boxed{\begin{array}{c} A^{\uparrow}_{\alpha_2} \\ \hline A^{\downarrow}_{\alpha_2} \end{array}}$$

$\alpha_2 = 1 \ldots 4$ $\qquad$ $\alpha_2 = 1 \ldots 4$

• After iteration up to site j

After a sequence of j such steps we get the following representation of the state $|\Psi\rangle$:

$$|\Psi\rangle = \sum_{s_1 \ldots s_L} \sum_{\alpha_1}^{2} \sum_{\alpha_2}^{4} \sum_{\alpha_3}^{8} \cdots \; U^{[1]}_{s_1 \alpha_1} U^{[2]}_{(\alpha_1 s_2)\alpha_2} \ldots U^{[j]}_{(\alpha_{j-1} s_j)\alpha_j} \, \lambda^{[j]}_{\alpha_j} \, V^{\dagger}_{\alpha_j (s_{j+1} \ldots s_L)} \, |s_1 \ldots s_L\rangle \tag{4.2}$$

This is also a Schmidt decomposition of $|\Psi\rangle$, between sites j and $j+1$.
By splitting up each U-matrix into two distinct matrices for $\uparrow$ and $\downarrow$ spin indices, we can also write

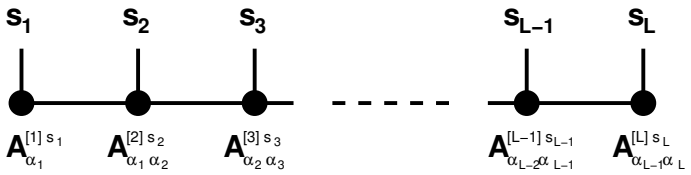
$$U^{[1]}_{s_1 \alpha_1} U^{[2]}_{(\alpha_1 s_2)\alpha_2} U^{[3]}_{(\alpha_2 s_3)\alpha_3} \cdots = A^{[1]s_1}_{\alpha_1} A^{[2]s_2}_{\alpha_1 \alpha_2} A^{[3]s_3}_{\alpha_2 \alpha_3} \ldots$$

• Exact MPS representation of $|\Psi\rangle$

Continuing until the last lattice site, we find that indeed an arbitrary state $|\Psi\rangle$ can be represented exactly by a Matrix Product State:

$$|\Psi\rangle \; = \; \sum_{s_1 \ldots s_L} \sum_{\{\alpha_i\}} A^{[1]s_1}_{\alpha_1} A^{[2]s_2}_{\alpha_1 \alpha_2} A^{[3]s_3}_{\alpha_2 \alpha_3} \ldots A^{[L-1]s_{L-1}}_{\alpha_{L-2} \alpha_{L-1}} A^{[L]s_L}_{\alpha_{L-1}} \; |s_1 \ldots s_L\rangle \tag{4.3}$$

Graphical representation:



The range of the intermediate indices α_i is equal to the rank of the corresponding SVD. Note that between sites $L-1$ and L, this rank is a most 2, and between sites $L-2$ and $L-1$, it is at most 4. Thus, an *exponentially large maximum rank of up to* $2^{L/2}$ is reached in the middle of the chain for a general state.

[1] The actual range of α can be smaller, when the coefficients of $|\Psi\rangle$ are such that the SVD has a lower rank, e.g. for a product state (rank 1).

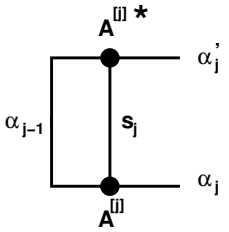
4.2 Normalization

Each of the matrices $U^{[i]}$ comes from an SVD and therefore satisfies $U^{[j]\dagger}U^{[j]} = \mathbb{1}$, which also provides for normalized basis transformations. In terms of the matrices $A^{[j]}$ this becomes

$$\boxed{\sum_{s_j} A^{[j]s_j\dagger} A^{[j]s_j} = \mathbb{1}} \tag{4.4}$$

Written in matrix components, this equation reads

$$\sum_{s_j, a_{j-1}} A^{*[j]s_j}_{\alpha_{j-1}\alpha'} \, A^{[j]s_j}_{a_{j-1}\alpha} = \delta_{\alpha_j\alpha'_j} \quad \text{or graphically:}$$



(4.5)

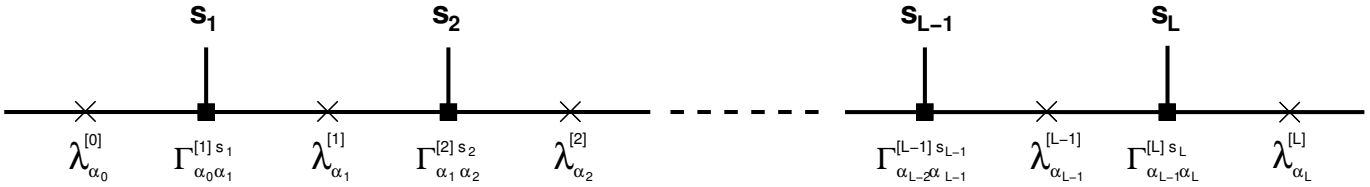
In the graphical representation, closed lines imply a summation.
The normalization of the whole MPS. $\langle\Psi|\Psi\rangle = 1$, can now be deduced in a simple way, by applying the graphical form of eq. 4.5 site by site.

4.3 Canonical form of an MPS

Each Schmidt decomposition in the derivation of the MPS also gave us the singular values λ_α, i.e. information about the reduced density matrix at that step. We now write this information explicitely in the MPS. We take the singular values λ_α out of the A-matrices; this defines new matrices "Γ":

$$A^{[j]s_j}_{\alpha_{j-1}\,\alpha_j} =: \lambda^{[j-1]}_{\alpha_{j-1}} \, \Gamma^{[j]s_j}_{\alpha_{j-1}\,\alpha_j} \tag{4.6}$$

When the A-matrices are given, one can obtain the Γ matrices by multiplying A with the *pseudoinverse* of λ.
Graphically, the "MPS state" (actually the coefficient $c_{s_1 s_2 \ldots s_L}$) now becomes

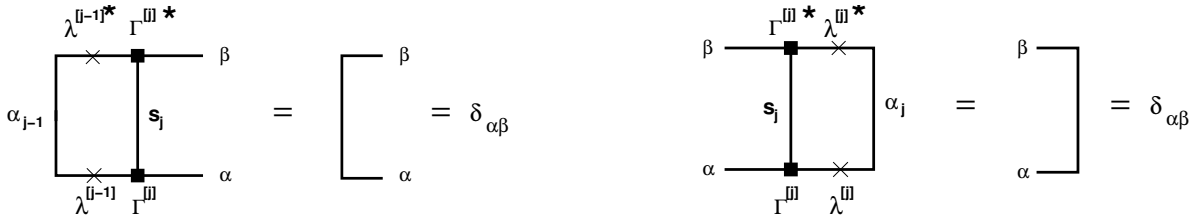


We denote A-matrices by circles, and Γ matrices by squares. The $\lambda^{[j]}$ are located between sites j and $j+1$. They are the singular values of the Schmidt decomposition at that bond, $c_{s_1 s_2 \ldots s_L} = U\lambda V^\dagger$. In a product state, all $\Gamma^{[i]}$ are numbers 0 or 1, and all $\lambda^{[i]} = 1$.
Since the first „matrix" $A^{[1]s_1}_{\alpha_1}$ is just a vector, the first index α_0 on $\Gamma^{[1]s_1}_{\alpha_0\alpha_1}$ is superfluous. We still write $\Gamma^{[1]s_1}_{\alpha_0\alpha_1}$ as a matrix, for easier notation later on, by letting the index α_0 only have one value $\alpha_0 = 1$ and $\lambda^{[0]}_{\alpha_0} \equiv 1$. Similarly, α_L has only the one value $\alpha_L \equiv 1$ and $\Gamma^{[1]s_1}_{\alpha_{L-1}\alpha_L}$ is actually a vector. At the right hand side we have introduced a final $\lambda^{[L]}_{\alpha_L} \equiv 1$.

Normalization The normalization eq. 4.5 now becomes an equation for Γ and λ, shown below on the left hand side:

(4.7)

$$\sum_{s_j} \left(\Gamma^{[j]s_j}\right)^\dagger \left(\lambda^{[j-1]}\right)^2 \Gamma^{[j]s_j} = \mathbb{1} \qquad \sum_{s_j} \Gamma^{[j]s_j} \left(\lambda^{[j]}\right)^2 \left(\Gamma^{[j]s_j}\right)^\dagger = \mathbb{1}$$



A similar normalization can also be shown to hold when summing over the second matrix index of $\Gamma^{[j]}$. This normalization is displayed on the right side of the equation above.

5 Operations on MPS

5.1 Truncation

In order to achieve an efficient representation of a state, with relatively small matrices, we can approximate the state by discarding small singular values λ_α. This is done most easily in the canonical representation. When all $\lambda^{[j]}_{\alpha>\alpha_0}$ are discarded, the matrices $\Gamma^{[j]}$ and $\Gamma^{[j+1]}$ can be *truncated* correspondingly beyond matrix index α_0. One can either discard values below a certain threshold ϵ (e.g. 10^{-10}), which results in a varying matrix dimension, or one can set a maximum matrix dimension χ_{max} beyond which all singular values are discarded.
The quality of the approximation is related to how much of the reduced density matrix $\rho = \mathrm{diag}(\lambda_1^2, \lambda_2^2, \dots)$ ist discarded. This can be quantified by the so-called *discarded weight* (which should stay below a small threshold $\ll 10^{-6}$).

$$w = 1 - \sum_{\alpha=1}^{\chi_{max}} \lambda_\alpha^2 \tag{5.1}$$

In order to keep the state normalized, we have to re-normalize the remaining λ_α:

$$\lambda_\alpha \;\to\; \lambda_\alpha/\sqrt{1-w}\,, \quad \text{so that} \quad \sum_\alpha \lambda_\alpha^2 = 1\,. \tag{5.2}$$

The normalizations of the A-matrices and the Γ matrices are unaffected by the truncation, except that the matrix $\mathbb{1}$ in eq. 4.4 is also truncated.

5.2 How large do the matrices need to be ?

The discarded weight w is small when the singular values λ_α decay quickly. This is the case when the entanglement entropy eq. 3.11, $S_A = -\sum_{\gamma=1}^{\chi} \lambda_\gamma^2 \ln \lambda_\gamma^2$ is small. We saw earlier that the maximum entanglement entropy of a reduced density matrix of size χ is $\ln \chi$. Thus one can estimate that one needs matrices of size about

$$\chi_{max} \sim e^{S_A} \tag{5.3}$$

for a good representation of a state.

• 1D

In 1D, the border of two subsystem A and B is just a point. All entanglement between A and B must go through this point. It is related to the spin correlations between A and B. When the Hamiltonian contains only local couplings, these correlations are limited in spatial extent. One can show that for the ground state of Hamiltonians with local couplings one needs only

$$\chi_{max} \sim \ln \xi \tag{5.4}$$

where ξ is the spatial correlation length of the system. When ξ is finite, a finite value of χ_{max} is therefore sufficient, even on very large systems. Even when the system is "critical", $\xi = \infty$, $\chi_{max} \sim \ln L$ is sufficient. This is the **reason why Matrix Product States work so well in one-dimensional physical systems**.
Note that for large systems, this χ_{max} is many orders of magnitude smaller than the generic $2^{L/2}$ behavior found earlier for an arbitrary state.

• 2D

In two dimensions, the border between subsystems A and B is a line. Correlations and entanglement can go accross any point of this line. Since the length of the border in 2D is proportional to subsystem size L, the von-Neumann entropy S_A is also proportional to L and thus χ_{max} has to grow exponentially:

$$S_A \sim L \quad \rightarrow \quad \chi_{max} \sim e^L \tag{5.5}$$

This is the reason why the MPS-Ansatz fails for dimensions $D > 1$,[1] where an exponentially growing computational effort is required to accurately represent $|\Psi\rangle$ by an MPS.

A special case occurs when 1D chains are coupled. The required matrix dimension then grows exponentially in the number of coupled chains, but when this number remains small (e.g. 2 or 3 or 4), the resulting matrix dimension remains within reach.

[1] In D=3, the boundary is an area, and the general relation $\chi_{max} \sim L^{D-1}$ is therefore called the *area law*, even though it actually refers to a boundary.

5.3 Expectation values of one-site operators

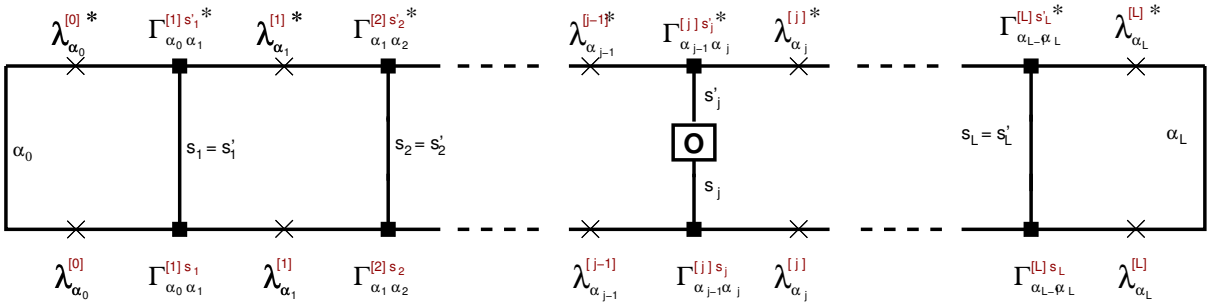
A very big advantage of the MPS representation of states is that **only a few local matrices are needed to calculate the effect of a local operator** on the state (see below), or its expectation value. We will here look at the expectation value of a one-site operator $\hat{O}^{[j]}$ that acts only on the spin at site j. Example: the operator $\hat{S}_z^{[j]}$, with matrix elements (in z-basis)

$$(S_z) \;=\; \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{5.6}$$

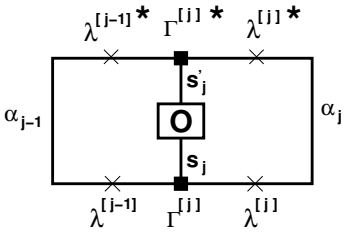
The expectation value is

$$\langle\Psi|\hat{O}^{[j]}|\Psi\rangle = \sum_{\{s\},\{s'\}} \langle s'_1 \dots s'_L| \dots \lambda^{*[j]}\Gamma^{*[j]s'_j}\lambda^{*[j-1]} \dots \; O^{[j]}_{s_j s'_j} \; \dots \lambda^{[j-1]}\Gamma^{[j]s_j}\lambda^{[j]} \dots |s_1 \dots s_L\rangle \tag{5.7}$$

In graphical representation, this becomes



At the interior vertical lines, the spins $s_i{}'$ from the bra vector $\langle\psi|$ and s_i from the ket vector $|\psi\rangle$ meet. Since $\langle s'_i|s_i\rangle = \delta_{s_i s'_i}$, they have to be equal, except at the location j of the operator $\hat{O}^{[j]}$. Note that all lambda values are actually real, since they are singular values.
This expression can now be simplified by using the normalization eqs. 4.7, which iteratively cause all matrices from both ends of the chain up to site j to just contribute Kronecker deltas. The remaining contribution is, in graphical representation and as an equation



$$\langle\Psi|\hat{O}^{[j]}|\Psi\rangle = \sum_{s_j,s'_j} \langle s'_j| \; \lambda^{[j]}\Gamma^{*[j]s'_j}\lambda^{[j-1]} \; O^{[j]}_{s_j s'_j} \; \lambda^{[j-1]}\Gamma^{[j]s_j}\lambda^{[j]} \; |s_j\rangle \;\; . \tag{5.8}$$

This is the same as

$$\langle\Psi|\hat{O}|\Psi\rangle = \sum_{\alpha_{j-1}\alpha_j} \sum_{s,s'} \left(\lambda^{[j-1]}_{\alpha_{j-1}}\lambda^{[j]}_{\alpha_j}\right)^2 \left(\Gamma^{[k]s'}_{\alpha_{j-1}\alpha_j}\right)^* \Gamma^{[j]s}_{\alpha_{j-1}\alpha_j} \langle s'|\hat{O}|s\rangle \tag{5.9}$$

or by defining the (spatially local) matrix M:

$$M^{s_j}_{\alpha_{j-1}\alpha_j} \;:=\; \lambda^{[j-1]}_{\alpha} \; \Gamma^{[j]\,s_j}_{\alpha_{j-1}\alpha_j} \; \lambda^{[j]}_{\alpha_j} \;. \tag{5.10}$$

the expectation value of $\hat{O}$ can be calculated as:

$$\langle\psi|\hat{O}^{[j]}|\psi\rangle \;\; = \;\; \sum_{s,s'} \langle s'|\,\hat{O}\,|s\rangle \;\; \mathrm{tr}\left(M^{s'}\right)^\dagger \; M^s \;. \tag{5.11}$$

6 Time evolution

The time evolution of a state in the Schrödinger picture for a time-independent hamiltonian is given by

$$|\Psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\Psi(0)\rangle$$

6.1 Trotter Suzuki decomposition

For the Heisenberg-model the Hamilton operator $\hat{H}$ can be expressed as:

$$\hat{H} = \sum_i \hat{H}_i \quad \text{with} \quad \hat{H}_i = \frac{J_{xy}}{2}\left[\hat{S}_i^+\hat{S}_{i+1}^- + \hat{S}_i^-\hat{S}_{i+1}^+\right] + J_z\hat{S}_i^z\hat{S}_{i+1}^z$$

The problem now is that the Hamiltonians of to adjacent sites do not commute, $[\hat{H}_i, \hat{H}_{i+1}] \neq 0$ and as a consequence the exponential $e^{-i\hat{H}t}$ is not expressible as a product of local operators:

$$e^{-i\hat{H}t} \neq \prod_j e^{-i\hat{H}_j t}$$

But the Hamiltonians of next nearest neighbor sites do commute: $[\hat{H}_i, \hat{H}_{i+2}] = 0$.
It is therefore helpful to decompose $\hat{H}$ into a sum of even and odd site Hamiltonians:

$$\hat{H} = \hat{H}_{even} + \hat{H}_{odd} = \sum_{j,odd}\hat{H}_j + \sum_{j,even}\hat{H}_j \tag{6.1}$$

such that

$$e^{-i\hat{H}_{even}t} = \prod_{j,even} e^{-i\hat{H}_j t} \quad \text{and} \quad e^{-i\hat{H}_{odd}t} = \prod_{j,odd} e^{-i\hat{H}_j t}\,. \tag{6.2}$$

Within $\hat{H}_{even}$, all terms commute, and also within H_{odd}, but $[\hat{H}_{even}, \hat{H}_{odd}] \neq 0$.
Next we subdivide the time t into small "time slices" of length Δt

$$e^{-i\hat{H}t} = \left(e^{-i\hat{H}\Delta t}\right)^{\frac{t}{\Delta t}} = \left(e^{-i(\hat{H}_{even}+\hat{H}_{odd})\Delta t}\right)^{\frac{t}{\Delta t}}$$

Now we use the Baker-Hausdorff formula to get

$$e^{-i\hat{H}t} = \left\{e^{-i\hat{H}_{even}\Delta t}e^{-i\hat{H}_{odd}\Delta t}\ \left(1 + \mathcal{O}\left((\Delta t)^2[\hat{H}_{even}, \hat{H}_{odd}]\right)\right)\ \right\}^{\frac{t}{\Delta t}}$$

Writing this product of $t/\Delta t$ terms explicitely yields

$$e^{-i\hat{H}t} = \left(e^{-i\hat{H}_{even}\Delta t}e^{-i\hat{H}_{odd}\Delta t}e^{-i\hat{H}_{even}\Delta t}\ldots e^{-i\hat{H}_{even}\Delta t}\right)(1 + \mathcal{O}(\Delta t)). \tag{6.3}$$

We lost one order of Δt because of the $(t/\Delta t)$ many factors.

The Trotter-Suzuki decomposition leads to a series of operators $e^{-i\hat{H}_j t}$ which only act on two adjacent sites at once. The time evolution of the system is traced back to application of these 2-site operators.

The smaller the time step Δt, the smaller the error in the method. One can gain another order of Δt with almost no effort by the so-called 2nd order Trotter Suzuki approximation:

$$\mathrm{e}^{-i\hat{H}\Delta t} \;=\; \mathrm{e}^{-i\hat{H}_{even}\frac{\Delta t}{2}}\;\mathrm{e}^{-i\hat{H}_{odd}\Delta t}\;\mathrm{e}^{-i\hat{H}_{even}\frac{\Delta t}{2}} \quad + \quad O((\Delta t)^3\,, \tag{6.4}$$

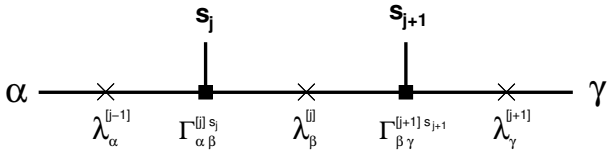
For the time evolution of the state $|\Psi\rangle$ this is the *same* as the first order approximation, because $\mathrm{e}^{-i\hat{H}_{even}\frac{\Delta t}{2}}\mathrm{e}^{-i\hat{H}_{even}\frac{\Delta t}{2}} = \mathrm{e}^{-i\hat{H}_{even}\Delta t}$ The only difference occurs when measurements are performed: for the 2nd order approximation, measurements have to be performed after *half*-time-steps $\mathrm{e}^{-i\hat{H}_{even}\frac{\Delta t}{2}}$.

6.2 Application of 2-site operators

In order to calculate the time evolution, we need to apply the 2-site operators $\hat{H}_i$ to $|\Psi\rangle$. For a general 2-site operator, we want to calculate

$$|\Psi'\rangle \;=\; \hat{O}^{[j,j+1]}\,|\Psi\rangle\,. \tag{6.5}$$

The structure of MPS as products of matrices located on individual sites is again very helpful. Since $\hat{O}^{[j,j+1]}$ acts on sites j and $j+1$, only the Γ matrices at these sites and the λ matrix in between are affected ! Let χ be the dimension of these matrices. The calulations turn out to be easier when one also includes the two λ matrices to the left and the right. We therefore look at the following part of the MPS:



This object has spin indices s_j, s_{j+1} on which the operator will act, and free matrix indices α and γ. It is the graphical representation of

$$\Theta^{s_j\,s_{j+1}}_{\alpha\gamma} \;:=\; \sum_{\beta} \lambda^{[j-1]}_{\alpha}\,\Gamma^{[j]\,s_j}_{\alpha\beta}\,\lambda^{[j]}_{\beta}\,\Gamma^{[j+1]\,s_{j+1}}_{\beta\gamma}\,\lambda^{[j+1]}_{\gamma} \tag{6.6}$$

The application of $\hat{O}$ on Θ yields

$$\tilde{\Theta}^{s'_j\,s'_{j+1}}_{\alpha\gamma} \;:=\; \sum_{s_j,s_{j+1}} \langle s'_j\,s'_{j+1}|\,\hat{O}\,|s_j\,s_{j+1}\rangle\,\Theta^{s_j\,s_{j+1}}_{\alpha\gamma} \tag{6.7}$$

We want to express $|\Psi'\rangle$ as a normalized MPS, similar to $|\Psi\rangle$. We therefore need to write $\tilde{\Theta}$ in the same form as the original Θ, with new normalized matrices $\tilde{\Gamma}^{[j]s'_j}_{\alpha\beta}$, $\tilde{\lambda}_\beta$, and $\tilde{\Gamma}^{[j+1]s'_{j+1}}_{\beta\gamma}$.
In order to get there, we first interpret $\tilde{\Theta}$ as a matrix with two indices, a row index $(\alpha s'_j)$ and a column index $(\gamma s'_{j+1})$

$$\bar{\Theta}_{(\alpha s'_j),(\gamma s'_{j+1})} \;:=\; \tilde{\Theta}^{s'_j\,s'_{j+1}}_{\alpha\gamma} \tag{6.8}$$

Next we perform an SVD on $\bar{\Theta}$:

$$\bar{\Theta}_{(\alpha s'_j),(\gamma s'_{j+1})} \;=\; \sum_{\beta=1}^{2\chi} U_{(\alpha s'_j)\,\beta}\,\tilde{\lambda}_\beta\,V^{\dagger}_{\beta\,(\gamma s'_{j+1})} \tag{6.9}$$

Because of the presence of s'_j and s'_{j+1} in the indices (with 2 values $\uparrow, \downarrow$), this SVD has a Schmidt rank up to *twice the rank* of the original matrices Γ, λ. If we kept this increased rank, then the matrix dimensions would explode exponentially during the time evolution.

We therefore need to *truncate* the matrix dimensions, for example back to the original χ (or a smaller value), by discarding the smallest singular values in $\tilde{\lambda}$. We then need to calculate the discarded weight w and re-normalize $\tilde{\lambda}_\beta \to \tilde{\lambda}_\beta \,/\, \sqrt{1-w}$. The matrices U and $V^\dagger$ are also truncated at the new size.

Finally, we extract new Γ matrices, by splitting the *unchanged* outer matrices $\lambda^{[j-1]}$ and $\lambda^{[j]}$ off U and $V^\dagger$, by means of applying the pseudoinverse:

$$\tilde{\Gamma}^{[j]s'_j}_{\alpha\beta} \;=\; (\lambda^{[j-1]}_\alpha)^{\text{inv}}\, U_{(\alpha s'_j)\,\beta} \quad , \qquad \tilde{\Gamma}^{[j+1]s'_{j+1}}_{\beta\gamma} \;=\; V^\dagger_{\beta\,(\gamma s'_{j+1})}\, (\lambda^{[j+1]}_\gamma)^{\text{inv}} \tag{6.10}$$

As desired, this results in updated $\chi \times \chi$ matrices $\tilde{\Gamma}^{[j]s'_j}_{\alpha\beta}$, $\tilde{\lambda}_\beta$, and $\tilde{\Gamma}^{[j+1]s'_{j+1}}_{\beta\gamma}$.

6.3 Recipe for calculating the time evolution of a 1D many body state

1. Write the initial state as a canonical MPS.
   For a product state, this is very simple: the "matrices" $\Gamma^{[j]s_j}$ are just numbers, e.g. when $s_j = \uparrow$, then $\Gamma^{[j]\uparrow} = 1$ and $\Gamma^{[j]\downarrow} = 0$. The "matrices" $\lambda^{[j]}$ are all just the number 1.

2. Calculate the matrix elements $\langle s'_j s'_{j+1} | \mathrm{e}^{-i\hat{H}_{j,j+1}\Delta t} | s_j s_{j+1} \rangle$ (and also for $\Delta t/2$).

3. One time step (2nd order Trotter Suzuki):

   - Apply $\mathrm{e}^{-i\hat{H}_{even}\Delta t/2}$ to the matrix product state, by applying all of the two-site operators H_i for even i to the MPS. This can be done in any sequence since these operators commute.
   - Apply $\mathrm{e}^{-i\hat{H}_{odd}\Delta t}$.
   - Apply $\mathrm{e}^{-i\hat{H}_{even}\Delta t/2}$.

4. After one or several time steps, perform measurements, e.g. of $\langle S^{[j]}_z \rangle$.

This algorithm, the so-called *Time Evolved Block Decimation (TEBD)*, was invented in 2004 by G. Vidal and in a closely related form (*tDMRG*) at the same time by White and Feiguin. These methods have provided a great leap forward in the investigation of large 1D many-body quantum systems, including strongly correlated ones, by finally permitting the precise and rather fast calculation of their time evolution from arbitrary initial states.