We have MPS ansatz, now what we need to do is know how to manipulate MPS.
Actually, what we can do is recombining MPS periodically.

Different kinds of tensor networks: Canonical form

Computing expectation value

Finding ground state

A practical introduction to tensor networks: Matrix product states and projected entangled pair states

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Schmidt decomposition and Canonical form

Given a quantum state |ψ> in terms of an MPS with open boundary conditions, there is a choice of tensors called canonical form of the MPS which is extremely convenient.
This is defined as follows:
for a given MPS with open boundary conditions (either for finite for infinite system), we say that it is in its canonical form if, for each bond index α, the index corresponds to the labelling of Schmidt vectors in the Schmidt decomposition of |ψ> across that index, i.e.

$$\left|\psi\right\rangle = \sum_{i=1}^{D} \lambda_i \left|u_i^L\right\rangle \otimes \left|v_i^R\right\rangle$$

In the above equation, λ_i are Schmidt coefficients ordered into decreasing order ($\lambda_1 \geq \lambda_2 \ldots \geq 0$), and the Schmidt vectors form orthonormal sets, that is

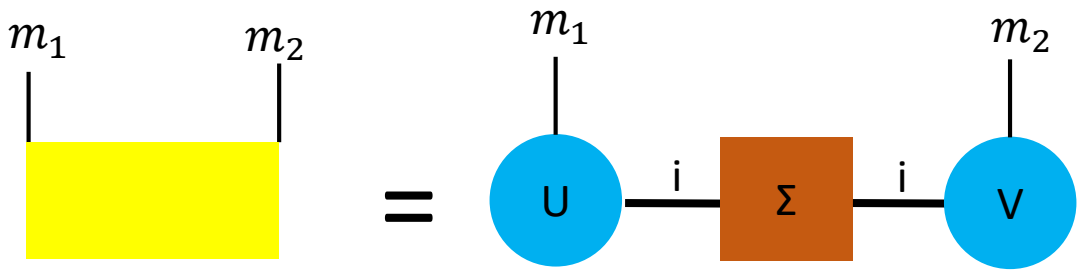
$$\left\langle u_i^L \middle| u_j^L \right\rangle = \left\langle v_i^R \middle| v_j^R \right\rangle = \delta_{ij}$$

If we expand in local physical basis

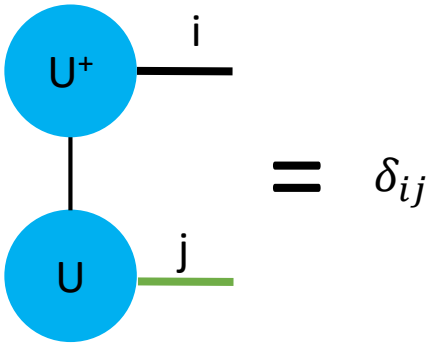
$$\left|u_k^L\right\rangle = \sum_i \left|m^L\right\rangle U_{ik}$$

$$\left|v_k^R\right\rangle = \sum_j (V^\dagger)_{kj} \left|m^R\right\rangle$$

Expressed in picture:

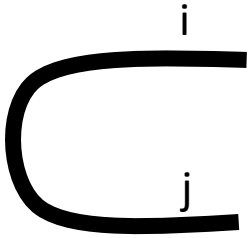


And the orthonormal condition written as:



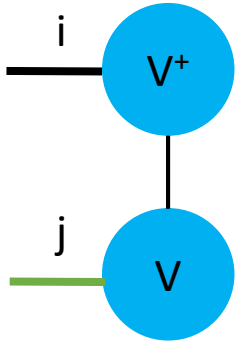
$= \delta_{ij}$

Or we can simplified as



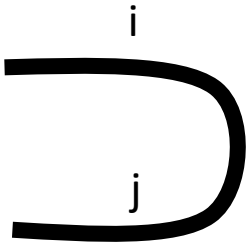
$= \delta_{ij}$

$\delta_{ij} =$

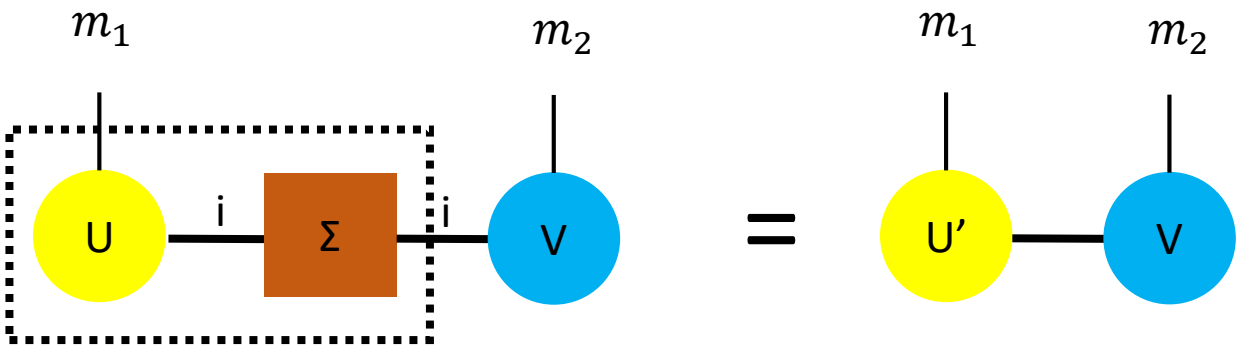


Or we can simplified as

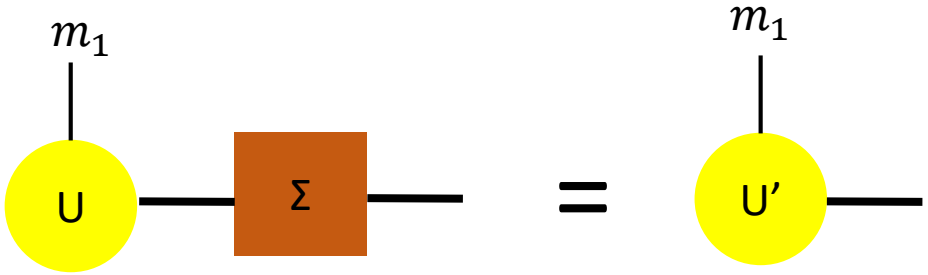
$\delta_{ij} =$



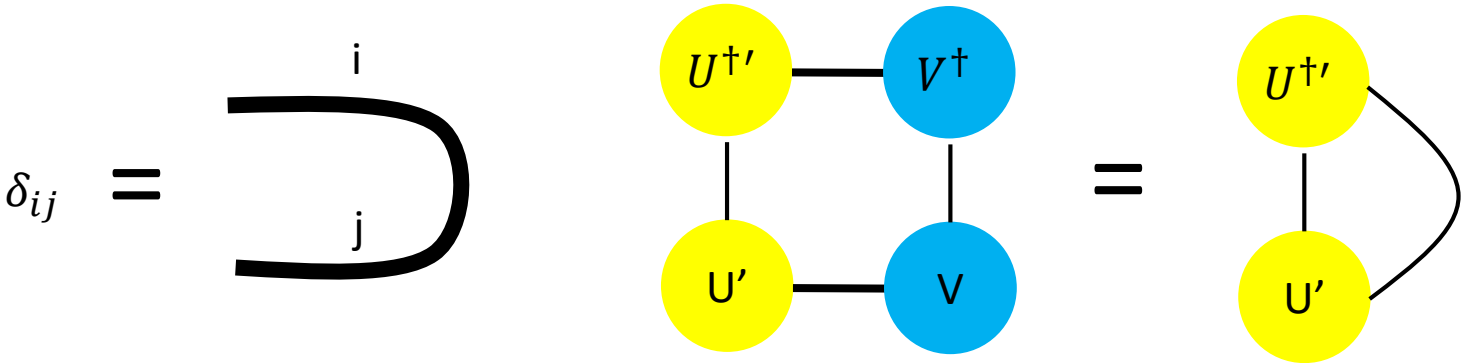
Right-canonical form: sweep from right to left



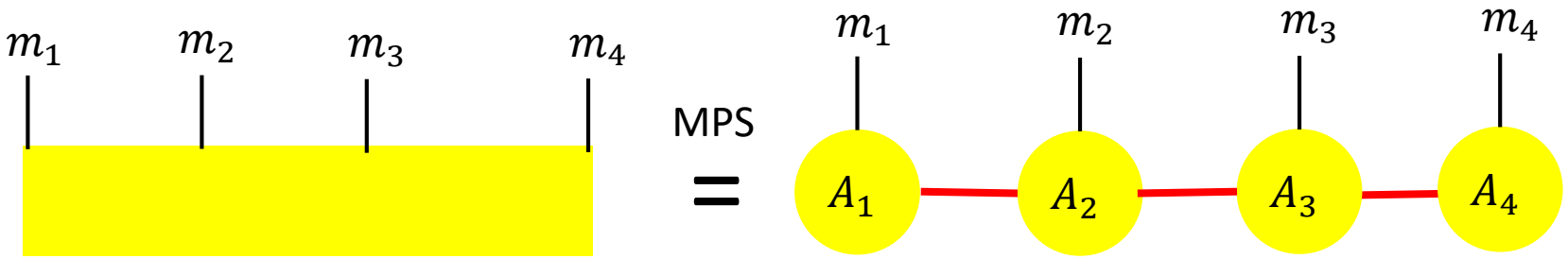
With



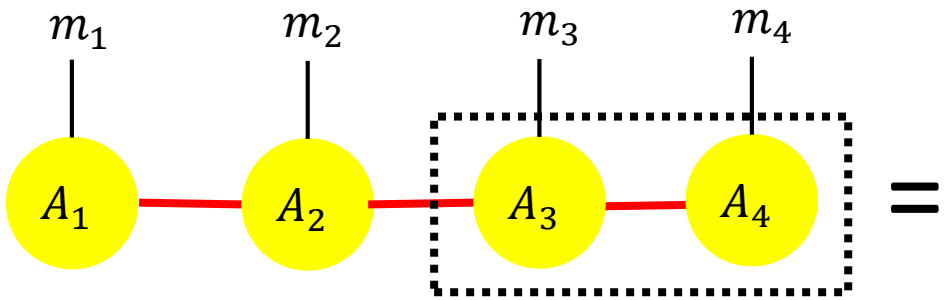
Since we sweep the gauge d.o.f. from right end to left end, we call it left-canonical form.

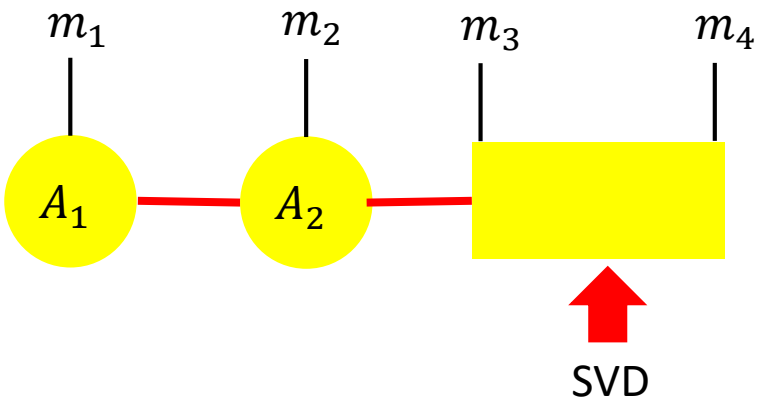


Now we consider 4 sites:



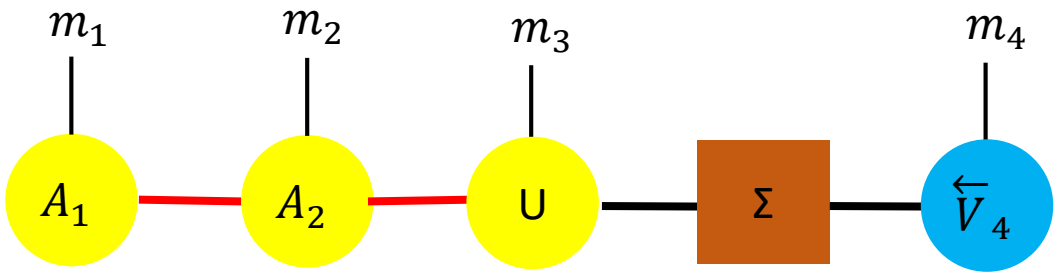
First we contract the last two sites:





Second we do SVD

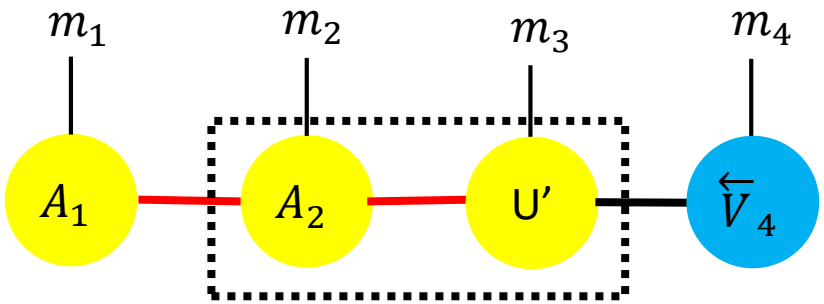
=



We write it to the right-canonical form

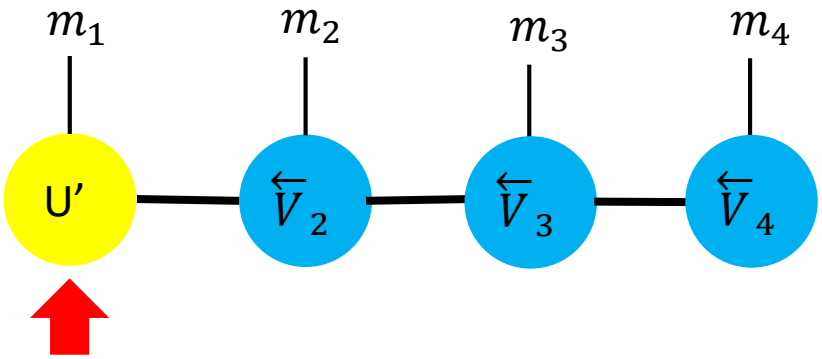
from now on, we use a arrow to mean the type of canonical form.

=



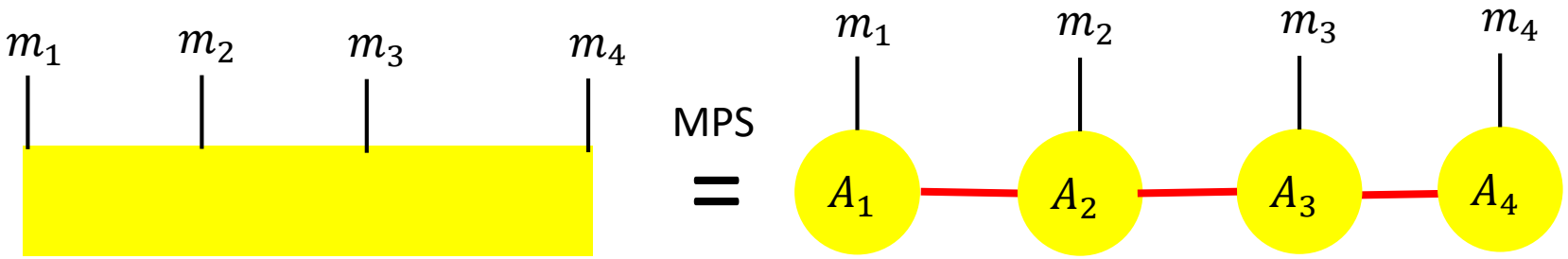
Contract, SVD, write into the right-canonical form

=

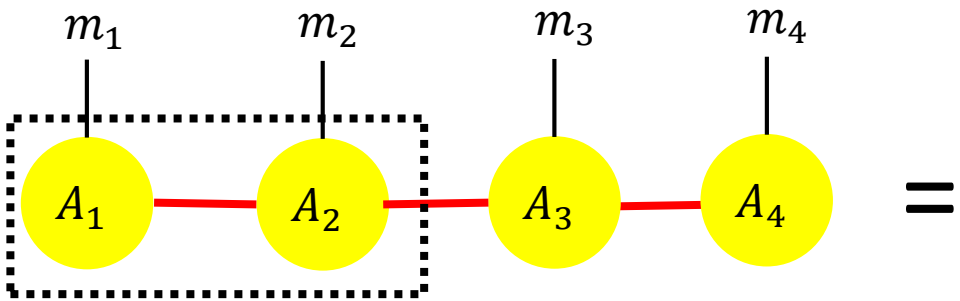


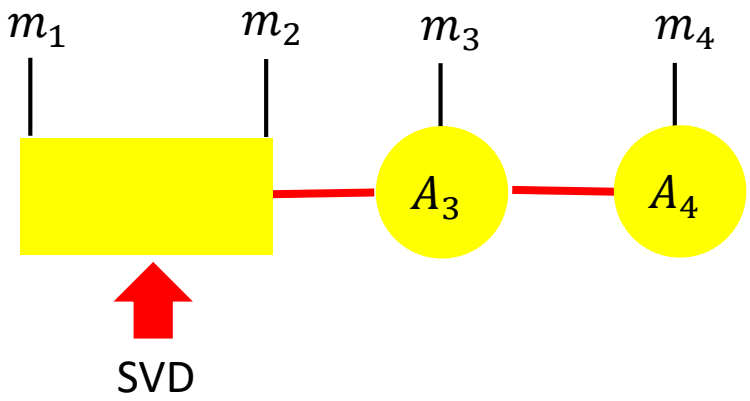
In a right-canonical form, only the left end site is not orthonormal.

Left-canonical form: sweep from left to right

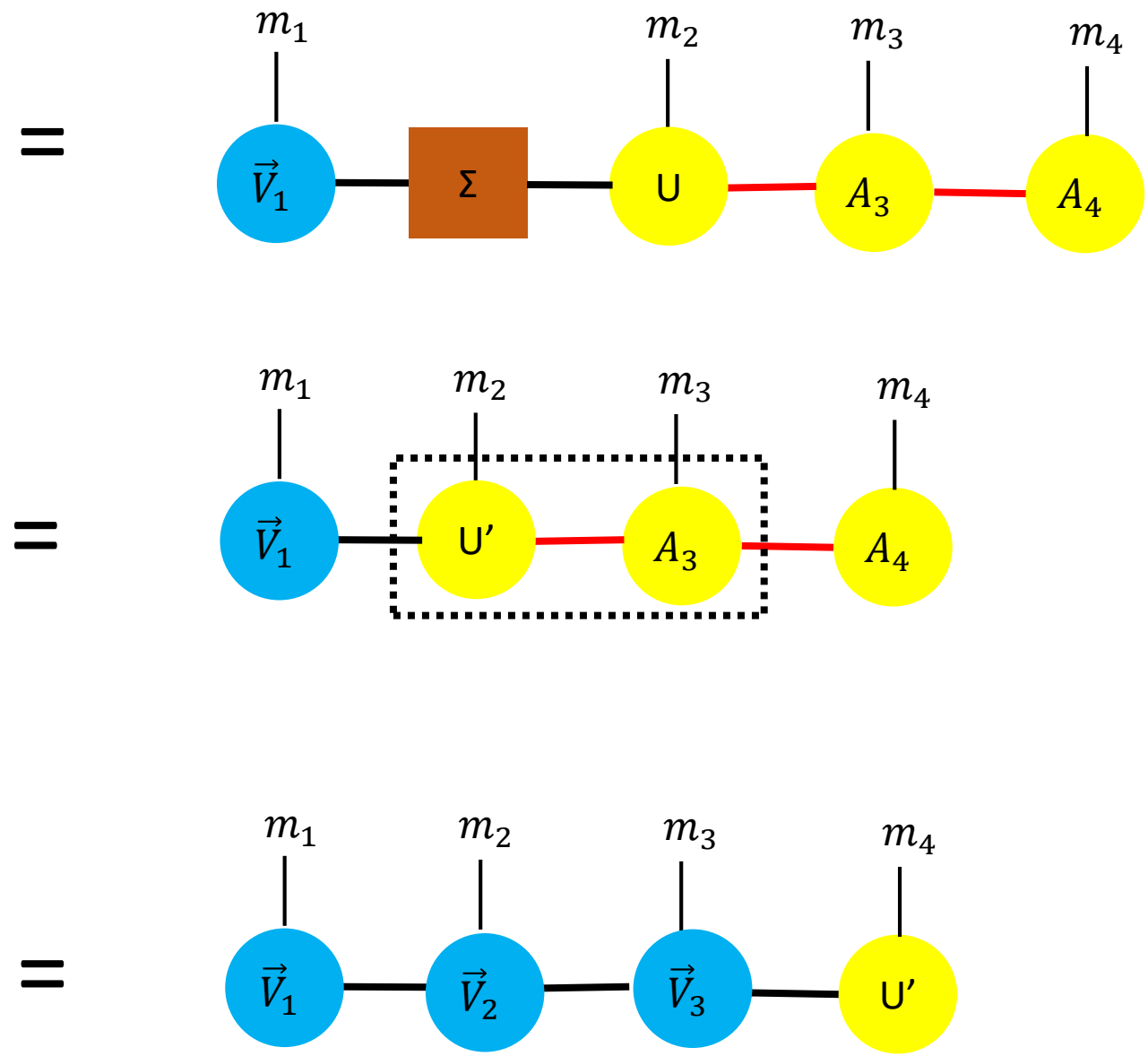


First we contract the last two sites:

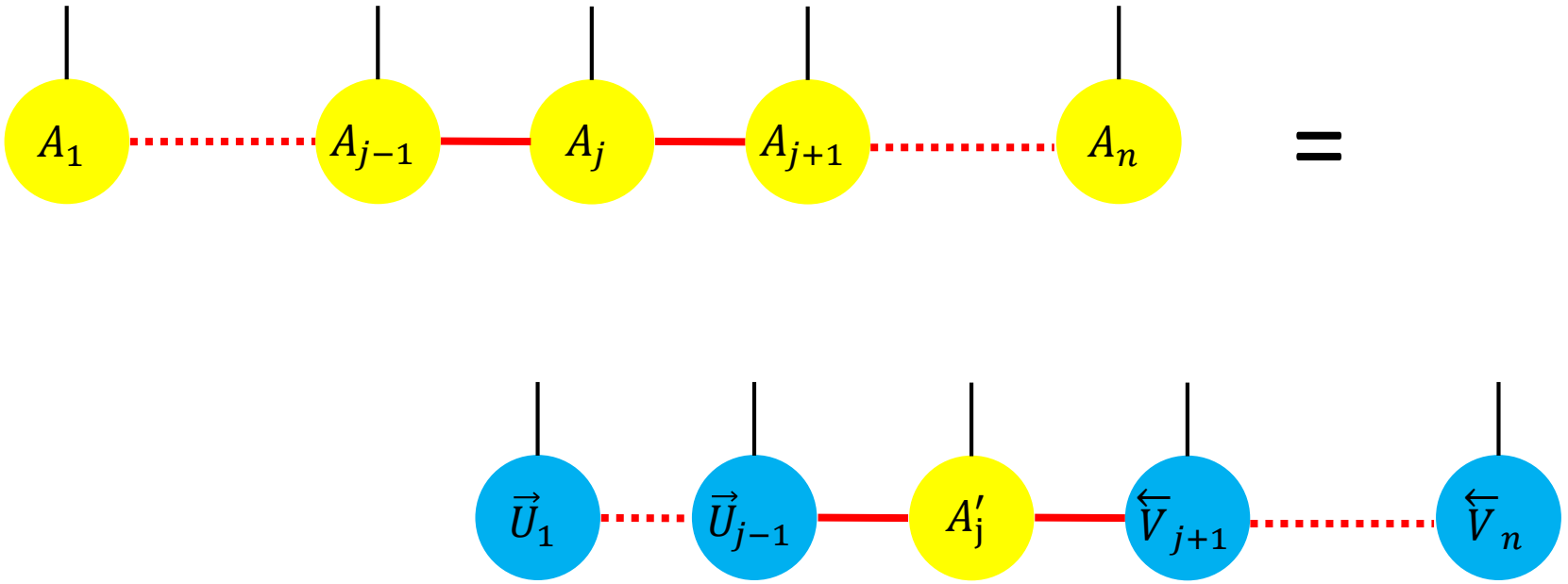




Second we do SVD

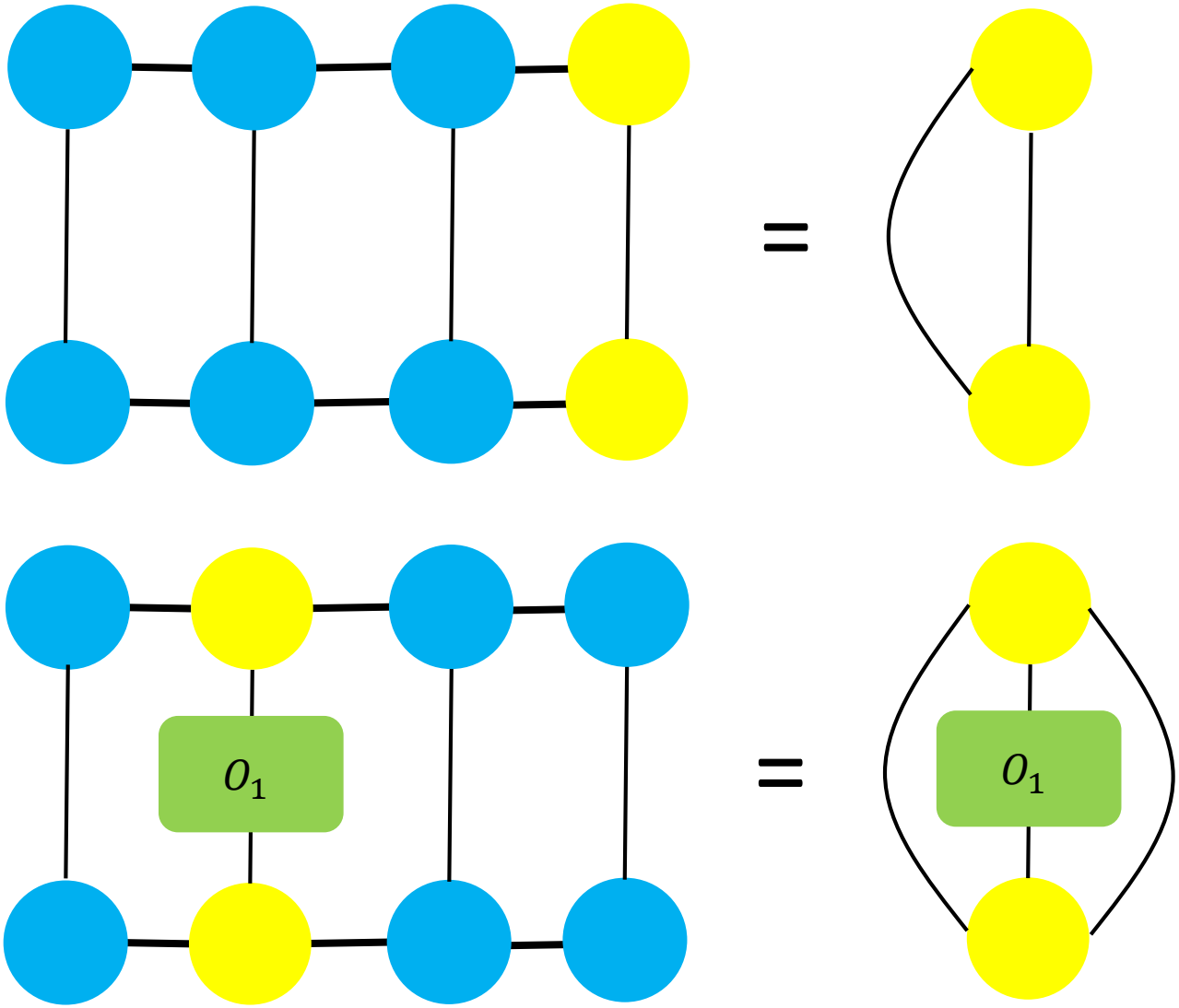

=
m_1
m_2
m_3
m_4
$\vec{V}_1$
Σ
U
A_3
A_4
=
m_1
m_2
m_3
m_4
$\vec{V}_1$
U'
A_3
A_4
=
m_1
m_2
m_3
m_4
$\vec{V}_1$
$\vec{V}_2$
$\vec{V}_3$
U'

Mixed-canonical form: sweeping from two ends to a middle site:



Why would we need a canonical form?

1. the calculation of expectation value is very easy



2. makes the truncation process very simple

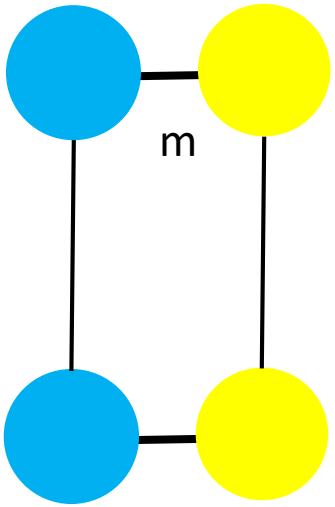
In the above picture, we haven't use the idea of compression.

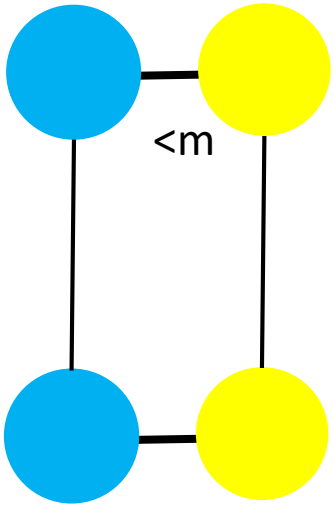
$$A_{m\times n} = U_{m\times m}\Sigma_{m\times n}(V^{\dagger})_{n\times n} \approx U_{m\times k}\Sigma_{k\times k}(V^{\dagger})_{k\times n}$$

Actually, we can use it.

So we can always choose a smaller number (m) of singular values in each SVD.

Therefore, the truncation process is just the compression in SVD.





Calculating expectation values

Expectation values of local operators can be computed exactly for an MPS without the need for further approximations. In the case of open boundary conditions, this is achieved for finite and infinite systems using the canonical form. The trick for infinite systems is to contract from the left and from the right assuming some boundary condition placed at infinity.

If the MPS has periodic boundary conditions, we can't define canonical form:

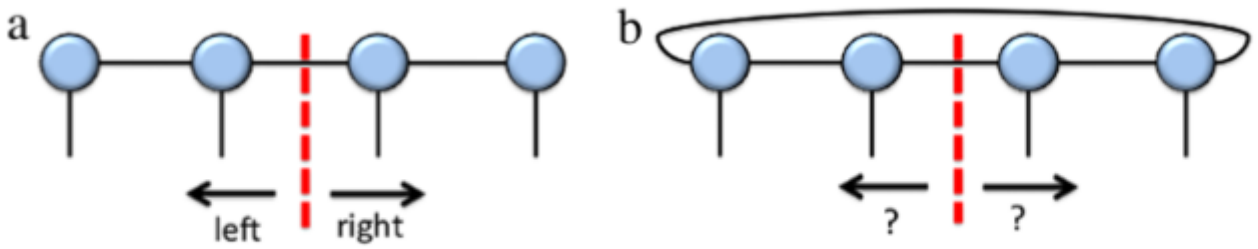


Fig. 28. (Color online) By "cutting" a link in a TN, one can define left and right pieces if there are no other connecting indices between the two pieces (a), whereas this is not possible if other connecting indices exist (b).

then the tensor network contractions for expectation values are similar to the following figure:

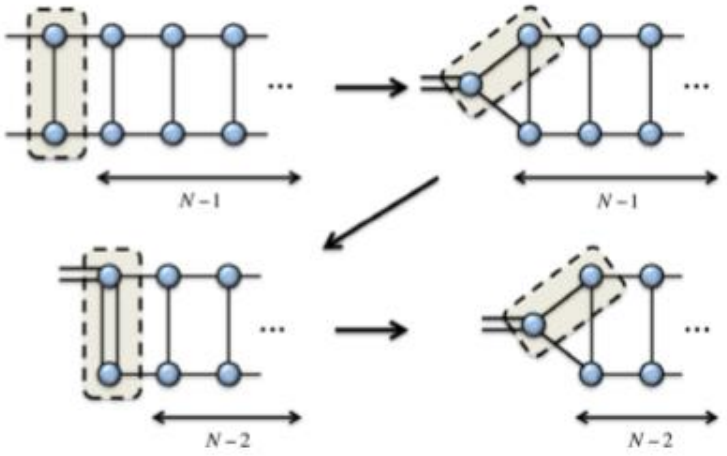


Fig. 33. (Color online) Order of contractions for an MPS with periodic boundary conditions.

Finding ground state

Finding the ground state is equivalent to the following question:
how do we fill in the coefficients of the tensors of MPS?

- Variational optimization;
- Imaginary time evolution;

Variational optimization

Given a Hamiltonian H, the variational principle states that for a given quantum state |ψ> it will always be the case that

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_0$$

where Eo the lowest eigenvalue of H. Therefore, if |ψ> is a tensor network belonging to some family of states like MPS with a fixed bond dimension D, we can always approach the G.S. energy from above by minimizing this expectation value over the relevant family:

$$\min_{|\psi\rangle \in MPS} (\langle\psi|H|\psi\rangle - \lambda\langle\psi|\psi\rangle)$$

where λ is a Lagrange multiplier that introduces the constraint that |ψ> must have norm one.

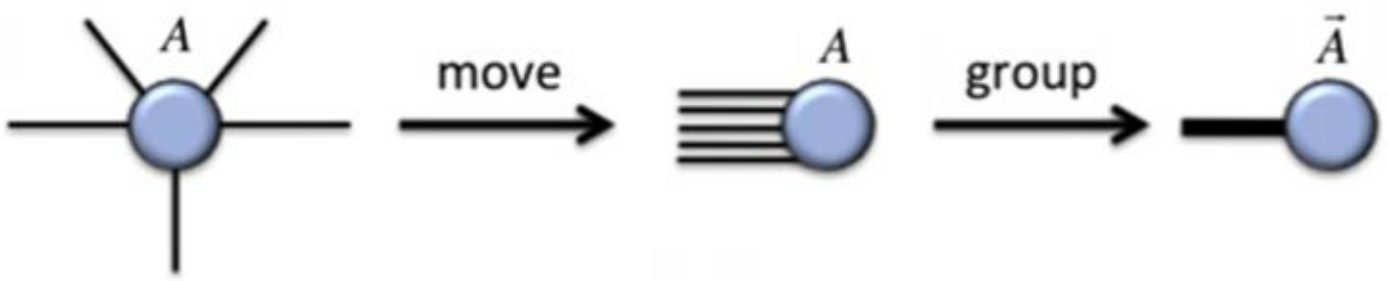
Recall tensor network differentiation and eigenvalue problem. What we need to do is minimize simultaneously over all the free parameters of the MPS, hence over all the coefficients of all the tensors for all sites.

However, this is normally quite difficult to implement and not particular efficient. Instead of this, the strategy is to proceed tensor by tensor.
This is, to minimize with respect to one tensor while keeping the other fixed, then move to another tensor and repeat the minimization, and so on. In practice one sweeps over all the tensors several times until the desired convergence in expectation values is attained.

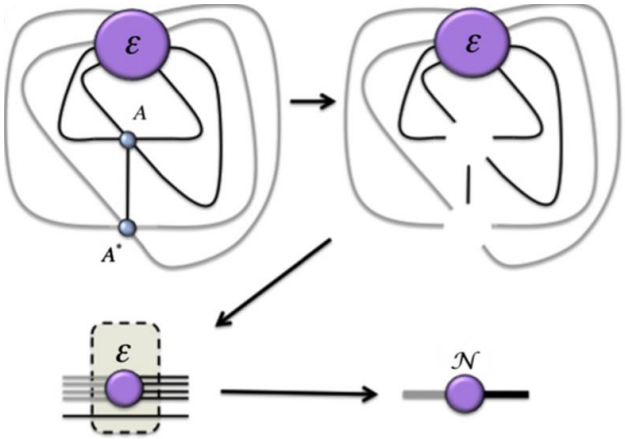
The way to minimize with respect to one tensor works as follows:
Imagine that we fix all the tensors in the tensor network except one of them which we call A. The coefficients of A are now our variational parameters. The minimization is thus written as:

$$\min_A(\langle\psi|H|\psi\rangle - \lambda\langle\psi|\psi\rangle) = \min_A(\vec{A}^\dagger H_{eff}\vec{A} - \lambda\vec{A}^\dagger N\vec{A})$$

In the above equation, $\vec{A}$ is just the tensor A but with all its coefficients arranged as a vector (fusion).



H_{eff} is an effective Hamiltonian and N is a normalization matrix, which are the tensor networks without tensors A and A*. For example, for N, we have



Now this minimization can be done as

$$\frac{\partial(\vec{A}^{\dagger} H_{eff} \vec{A} - \lambda \vec{A}^{\dagger} N \vec{A})}{\partial \vec{A}^{\dagger}} = 0$$

which leads to the generalized eigenvalue problem

$$H_{eff} \vec{A} = \lambda N \vec{A}$$

Once H_{eff} and N are known, this generalized eigenvalue problem can be solved numerically by using standard linear algebra packages. And to calculate both H_{eff} and N, one must use the tools explained in previous section to compute expectation values of physical observables and effective environments in a tensor network.

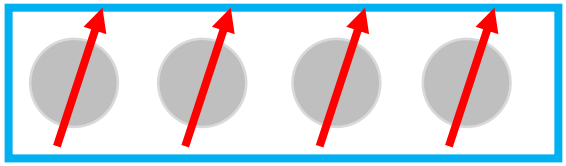
DMRG=variational optimization + MPS

Here we show a miracle thing, DMRG is developed before MPS, but since MPS is wider than DMRG, therefore, DMRG should find it's place in MPS.

Here we show this point:
if we perform variational optimization for an MPS with open boundary conditions, then what we recover is nothing but the famous DMRG algorithm in the language of MPS.

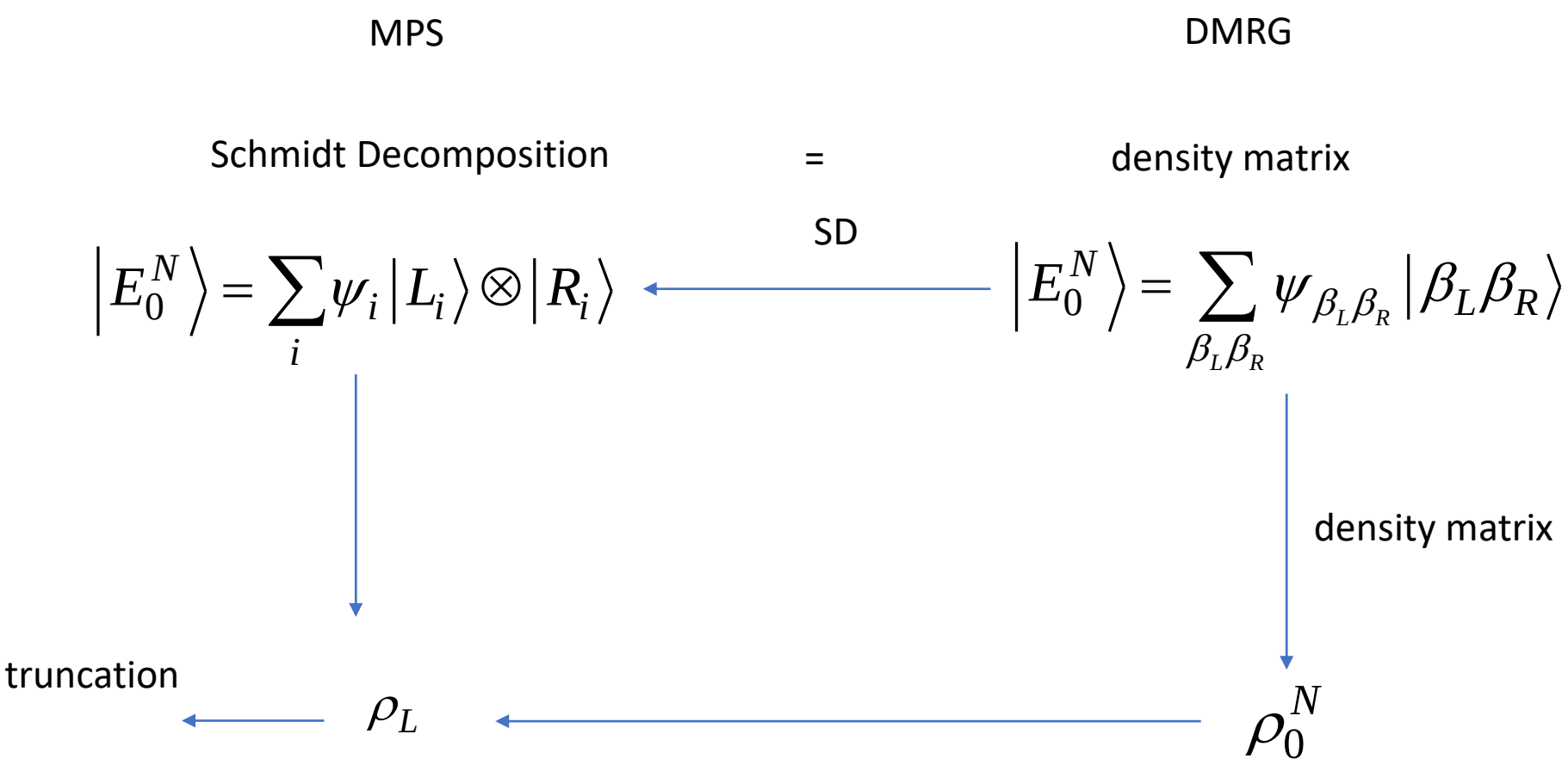
Here we show this in three points:

First we have MPS (or the start many-body state for 2M+2 sites before sweep)



MPS many-body state for 2M+2 sites

Second we have the equivalence between reduced density matrix and Schmidt decomposition:



This is the reason why DMRG works so well, since entanglement has been encoded.

Third, variational optimization in MPS is equivalent to sweep in DMRG

The following equivalence

DMRG=variational optimization + MPS

is quite appealing, since

1, using this MPS picture is now quite clear how to extend to periodic boundary conditions;

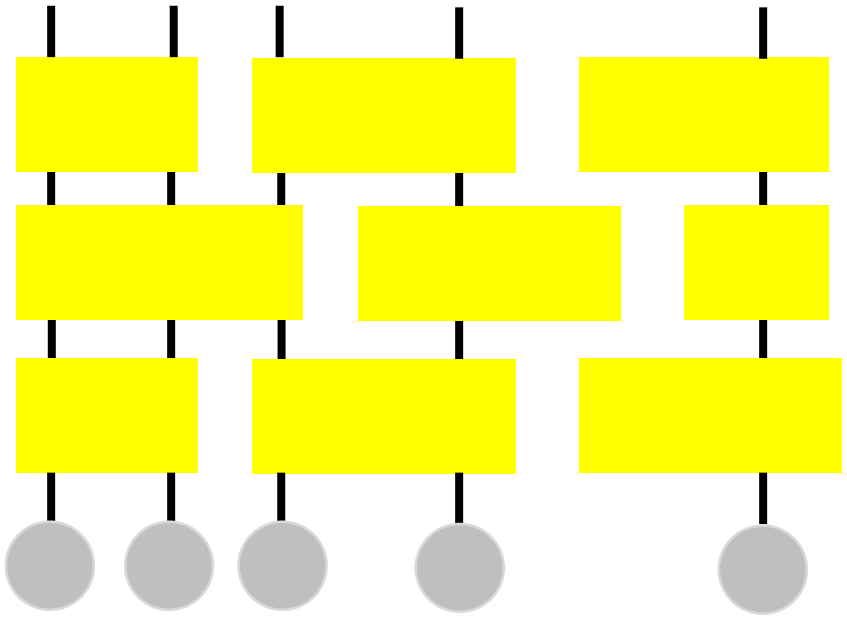
2, this variational technique has also been applied successfully for infinite MPS;

Imaginary time evolution

Consider a state is composed of linear combination of all basis state, after long enough time, the lowest energy state should be picked out, therefore, for very long times the quantum state tends to be in the ground state $|E_0\rangle$, namely

$$\left|E_0\right\rangle = \lim_{\tau\to 0} \frac{e^{-\tau H}\left|\psi(0)\right\rangle}{\sqrt{\left\langle\psi(\tau)\middle|\psi(\tau)\right\rangle}}, \left|\psi(\tau)\right\rangle = e^{-\tau H}\left|\psi(0)\right\rangle$$

So we can use the language of quantum circuits with thermal temperature-imaginary time equivalence.



$$\exp[-\mathrm{i}H\delta t]$$