密度矩阵概念以及DMRG程序

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目录

- 密度矩阵背景知识简介
- 论文1008.3477 chapter 1-3
- DMRG程序

密度矩阵概念

- 密度算符：定义与量子态$|\psi\rangle$相应的投影算符$\rho = |\psi\rangle\langle\psi|$称为与量子态$|\psi\rangle$相应的密度算符。密度算符是量子态的另一种描述方式。对于纯态$|\psi\rangle$两种描述方式等价，对于不能用一个波函数$|\psi\rangle$来描述的混合态，需要用密度算符来描述。
- 密度矩阵：密度算符采用一个具体表象（离散），可表示成矩阵形式，称为密度矩阵。
- 混合态的密度算符定义：$\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k| = \sum_k p_k \rho_k$
- 力学量平均值可以用密度矩阵计算：$\langle G\rangle = \mathrm{Tr}(\rho G) = \mathrm{Tr}(G\rho)$
- 密度算符随时间演化方程：$\dfrac{d}{dt}\rho(t) = \dfrac{1}{i\hbar}[H, \rho(t)]$

Ref:量子力学 卷（II）曾谨言 著 第一章

约化密度矩阵

- 对于一个复合体系，若只对子体系的力学量进行观测，是一个不完全测量，为了描述子体系的量子态，需要引进约化密度矩阵。
- $Q = Q_A \otimes I_B \quad \langle Q \rangle = \mathrm{tr}_A(\rho_A Q_A)$
- 约化密度算符 $\rho_A = \mathrm{tr}_B(\rho_{AB}) = \sum_{j_B} \langle j_B | \psi_{AB} \rangle \langle \psi_{AB} | j_B \rangle = \psi \psi^\dagger$
- $|\psi_{AB}\rangle = \sum_{i_A j_B} \psi_{i_A j_B} |i_A\rangle |j_B\rangle$

Ref:量子力学 卷（II）曾谨言 著 第一章

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chapter 1 introduction

- DMRG是计算一维量子晶格最有力的数值方法。
- 当应用于二维系统，DMRG研究很小系统时可以获得很高精度，但是随着系统尺寸计算资源指数增加。DMRG在一维和二维不同的表现与多体态的量子纠缠的标度紧密联系。（面积律）
- MPS 起源于解析研究中一类有趣的量子态，一个例子是AKLT态的精确表示。MPS和DMRG的联系有两步：第一步是iDMRG过程可以表示为MPS的形式，第二步：finite-system DMRG 导出一个可变分优化的MPS的量子态

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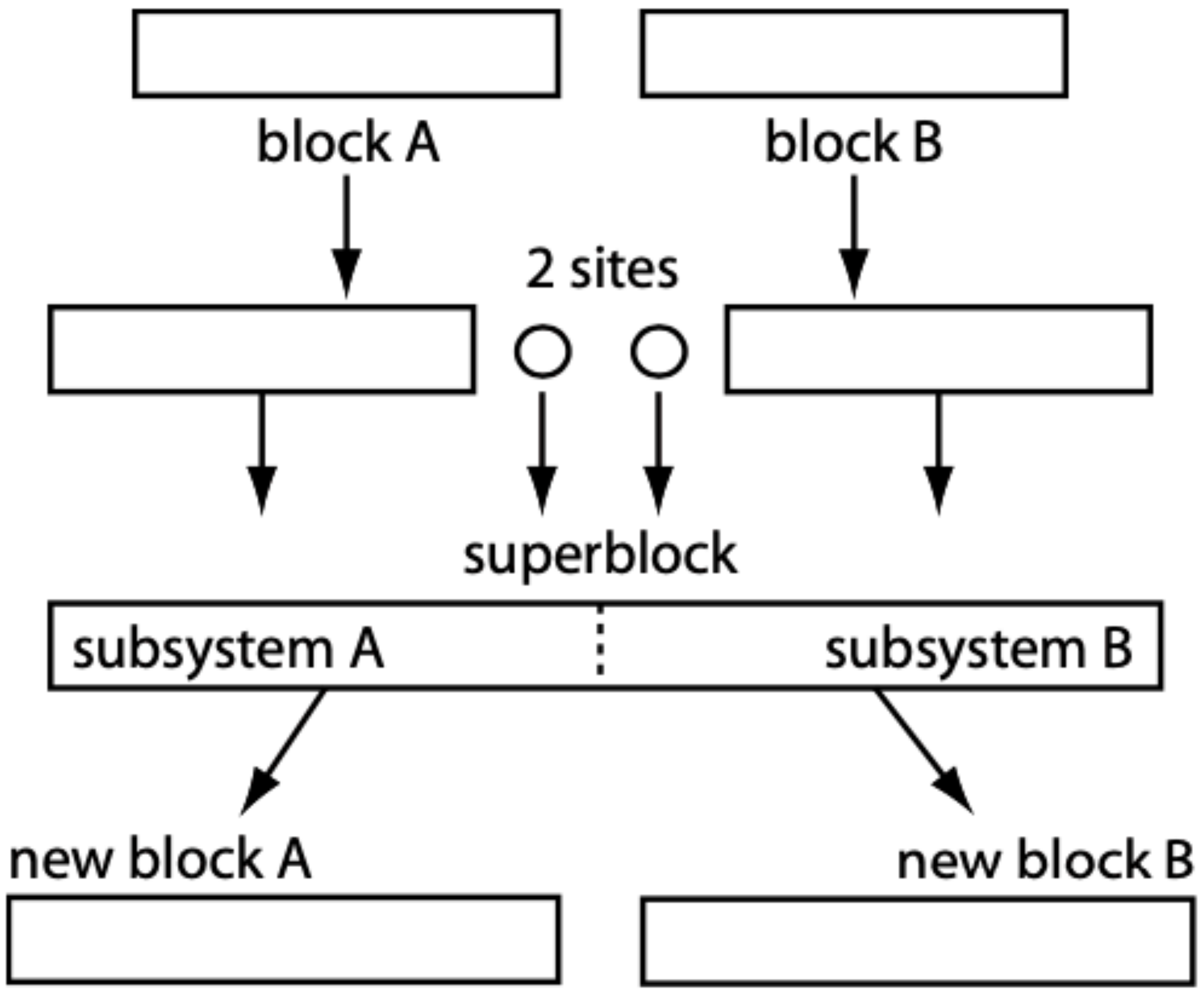
chapter 2 DMRG:infinite system DMRG



- $H_{A\cdot\cdot B} = H_A + H_{mid} + H_B$
- $E = \dfrac{\langle\psi|\hat{H}_{A\cdot\cdot B}|\psi\rangle}{\langle\psi|\psi\rangle}$
- $|\psi\rangle = \sum_{a_A\sigma_A\sigma_B a_B} \psi_{a_A\sigma_A\sigma_B a_B}|a\rangle_A|\sigma\rangle_A|\sigma\rangle_B|a\rangle_B \equiv \sum_{j_A j_B}\psi_{i_A j_B}|i\rangle_A|j\rangle_B$
- 证明reshape的形式问题
- $\hat{\rho}_{A\cdot} = \mathrm{Tr}_{\cdot B}|\psi\rangle\langle\psi| = \psi\psi^\dagger$
- $\hat{\rho}_{B\cdot} = (\psi^\dagger\psi)^T$
- $\langle a_{l+1}|\hat{F}|a'_{l+1}\rangle = \sum_{a_l,a'_l\sigma_{l+1}} \langle a_{l+1}|a_l\sigma_{l+1}\rangle\langle a_l|\hat{F}|a'_l\rangle\langle a'_l\sigma_{l+1}|a'_{l+1}\rangle = (O^\dagger F O)_{a_{l+1}a'_{l+1}}$

Matrix Product States

Content

1. SVD decomposition and Schmidt decomposition
2. QR decomposition
3. Decomposition of arbitrary quantum states into MPS
   Left canonical MPS
   Right canonical MPS
   Mixed canonical MPS
   Gauge degrees of freedom

SVD

- An arbitrary matrix M($N_A \times N_B$) can decompose as $M = USV^\dagger$
- U is of dimension $N_A \times \min(N_A, N_B)$ and has orthonormal columns i.e. $U^\dagger U = I$
- S is of dimension $\min(N_A, N_B) \times \min(N_A, N_B)$ diagonal with non-negative entries $S_{aa} \equiv s_a$
- $V^\dagger$ is of dimension $\min(N_A, N_B) \times N_B$ and has orthonormal rows I.e. $V^\dagger V = I$
- The optimal approximation of M (rank r) by a matrix M' (rank r' < r)
- $M' = US'V^\dagger \quad S' = \mathrm{diag}(s_1, s_2, \cdots, s_{r'}, 0, \cdots)$

Schmidt decomposition

Use SVD to derive Schmidt decomposition

- Any pure state on AB can be written as
  $|\psi\rangle = \sum_{ij} \Psi_{ij} |i\rangle_A |j\rangle_B$
- Reduced density operators
  $\hat{\rho}_A = \mathrm{Tr}_B |\psi\rangle\langle\psi| = \psi\psi^\dagger$
  $\hat{\rho}_B = (\psi^\dagger\psi)^T$
- Use SVD to derive the Schmidt decomposition of a general quantum state

$$
\begin{aligned}
|\psi\rangle &= \sum_{ij} \sum_{a=1}^{\min(N_A,N_B)} U_{ia} S_{aa} V^*_{ja} |i\rangle_A |j\rangle_B \\
&= \sum_{a=1}^{\min(N_A,N_B)} \left(\sum_i U_{ia} |i\rangle_A \right) s_a \left(\sum_j V^*_{ja} |j\rangle \right) \\
&= \sum_{a=1}^{\min(N_A,N_B)} s_a |a\rangle_A |a\rangle_B .
\end{aligned}
$$

Schmidt decomposition

- Restrict the sum over the $r \leq \min(N_A, N_B)$,we obtain the Schmidt decomposition
- $|\psi\rangle = \sum_{a=1}^{r} s_a |a\rangle_A |a\rangle_B$ r=1 corresponds to product states ,r>1 to entangled states
- Reduced density operators for A and B $\hat{\rho}_A = \sum_{a=1}^{r} s_a^2 |a\rangle_A \, {}_A\langle a| \qquad \hat{\rho}_B = \sum_{a=1}^{r} s_a^2 |a\rangle_B \, {}_B\langle a|,$
- approximate state $|\tilde{\psi}\rangle = \sum_{a=1}^{r'} s_a |a\rangle_A |a\rangle_B$
- Von Neumann entropy of entanglement

$$S_{A|B}(|\psi\rangle) = -\mathrm{Tr}\, \hat{\rho}_A \log_2 \hat{\rho}_A = -\sum_{a=1}^{r} s_a^2 \log_2 s_a^2.$$

QR decomposition

- An arbitrary matrix M of dimension $N_A \times N_B$ gives a decomposition $M = QR$
- Q is of dimension $N_A \times N_A$ and unitary ,$Q^\dagger Q = QQ^\dagger = I$
- R is of dimension $N_A \times N_B$ and upper triangular

Decomposition of arbitrary quantum states into MPS

Left-canonical matrix product state

- A pure quantum state on the lattice $|\psi\rangle = \sum_{\sigma_1,\cdots,\sigma_L} c_{\sigma_1\cdots\sigma_L}|\sigma_1,\cdots,\sigma_L\rangle$
- A notation gives a more local notion of the state while preserving the quantum non-locality of the state — MPS
- Reshape the state vector with d^L components into a matrix Ψ of dimension $d \times d^{L-1}$
- $\Psi_{\sigma_1,(\sigma_2\cdots\sigma_L)} = c_{\sigma_1\cdots\sigma_L}$

Decomposition of arbitrary quantum states into MPS

Left-canonical matrix product state

- An SVD of Ψ gives $$c_{\sigma_1\ldots\sigma_L} = \Psi_{\sigma_1,(\sigma_2\ldots\sigma_L)} = \sum_{a_1}^{r_1} U_{\sigma_1,a_1} S_{a_1,a_1} (V^\dagger)_{a_1,(\sigma_2\ldots\sigma_L)} \equiv \sum_{a_1}^{r_1} U_{\sigma_1,a_1} c_{a_1\sigma_2\ldots\sigma_L},$$
- Decompose U into a collection of d row vectors A^{σ_1} with entries $A^{\sigma_1}_{a_1} = U_{\sigma_1,a_1}$
- Reshape $c_{a_1\sigma_2\cdots\sigma_L}$ into a matrix $\Psi_{(a_1\sigma_2),(\sigma_3\cdots\sigma_L)}$ of dimension $r_1 d \times d^{L-2}$ to give

$$c_{\sigma_1\ldots\sigma_L} = \sum_{a_1}^{r_1} A^{\sigma_1}_{a_1} \Psi_{(a_1\sigma_2),(\sigma_3\ldots\sigma_L)}.$$

- Use SVD again we have

$$c_{\sigma_1\ldots\sigma_L} = \sum_{a_1}^{r_1}\sum_{a_2}^{r_2} A^{\sigma_1}_{a_1} U_{(a_1\sigma_2),a_2} S_{a_2,a_2} (V^\dagger)_{a_2,(\sigma_3\ldots\sigma_L)} = \sum_{a_1}^{r_1}\sum_{a_2}^{r_2} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \Psi_{(a_2\sigma_3),(\sigma_4\ldots\sigma_L)},$$

Decomposition of arbitrary quantum states into MPS

Left-canonical matrix product state

- Upon further SVDs we obtain $$c_{\sigma_1 \dots \sigma_L} = \sum_{a_1, \dots, a_{L-1}} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1, a_2} \dots A^{\sigma_{L_1}}_{a_{L-2}, a_{L-1}} A^{\sigma_L}_{a_{L-1}}$$

- The arbitrary quantum state is now represented exactly in the form of a MPS

$$|\psi\rangle = \sum_{\sigma_1, \dots, \sigma_L} A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_{L-1}} A^{\sigma_L} |\sigma_1, \dots, \sigma_L\rangle.$$

- At each SVD $U^\dagger U = I$, U replaced by a set of A^σ entails the following relationship
- Left-normalized condition $$\sum_{\sigma_\ell} A^{\sigma_\ell \dagger} A^{\sigma_\ell} = I.$$

Decomposition of arbitrary quantum states into MPS

Left-canonical matrix product state

- Split the lattice into parts A and B,A comprises sites 1 to l,and B l+1 to L

$$|a_\ell\rangle_A = \sum_{\sigma_1,\ldots,\sigma_\ell} (A^{\sigma_1}A^{\sigma_2}\ldots A^{\sigma_\ell})_{1,a_\ell}|\sigma_1,\ldots,\sigma_\ell\rangle$$
$$|a_\ell\rangle_B = \sum_{\sigma_{\ell+1},\ldots,\sigma_L} (A^{\sigma_{\ell+1}}A^{\sigma_{\ell+2}}\ldots A^{\sigma_L})_{a_\ell,1}|\sigma_{\ell+1},\ldots,\sigma_L\rangle$$

- The MPS can be written as $|\psi\rangle = \sum_{a_l} |a_l\rangle_A |a_l\rangle_B$

- This states look like Schmidt decomposition of $|\psi\rangle$ but this is not the case, the reason is that while the $\{|a_l\rangle_A\}$ form an orthonormal set ,the$\{|a_l\rangle_B\}$ in general not

Decomposition of arbitrary quantum states into MPS

Left-canonical matrix product state

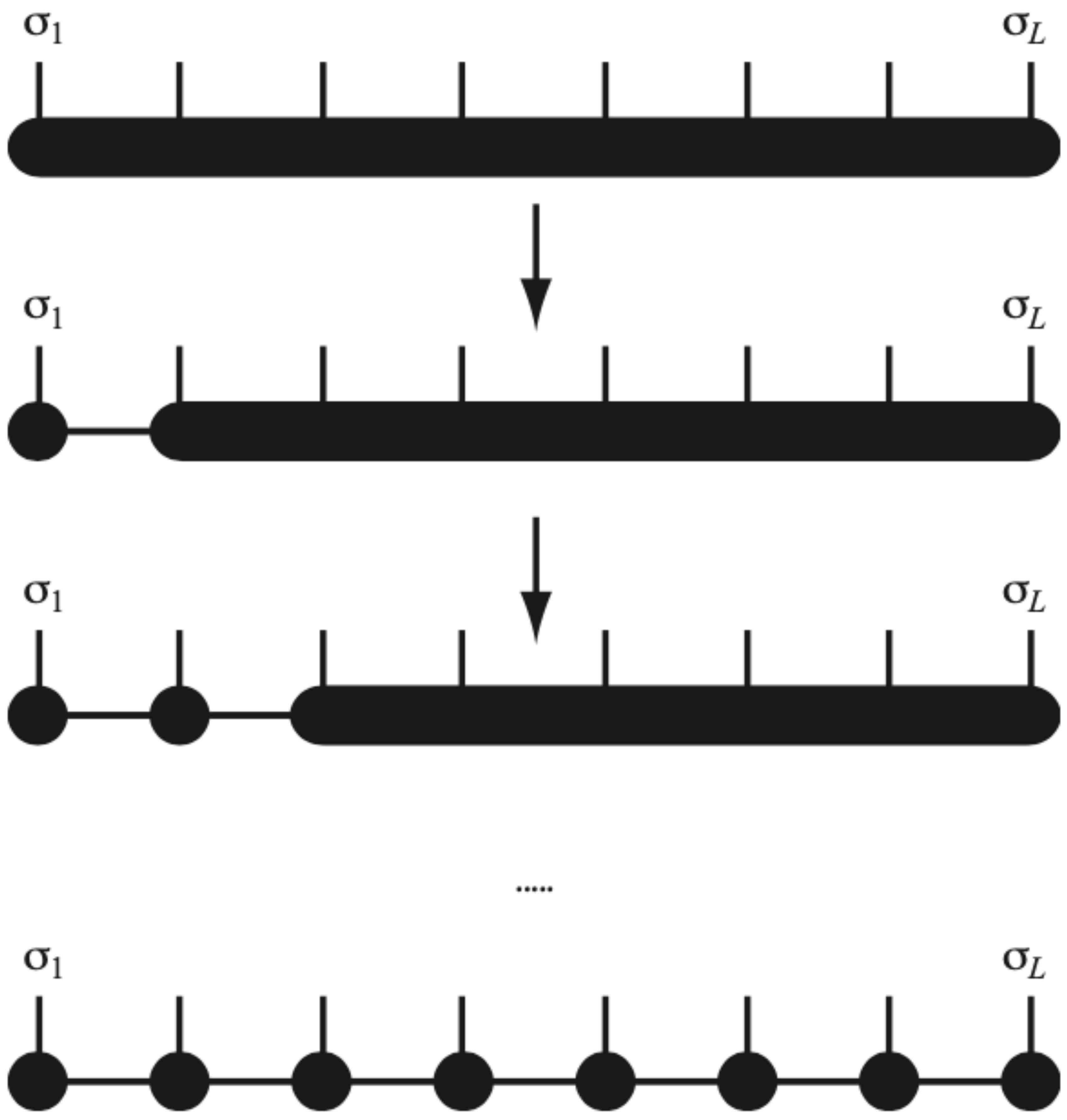
- Left normalized condition $\sum_{\sigma} A^{\sigma\dagger} A^{\sigma} = I$
- while ingeneral $\sum_{\sigma} A^{\sigma} A^{\sigma\dagger} \neq I$

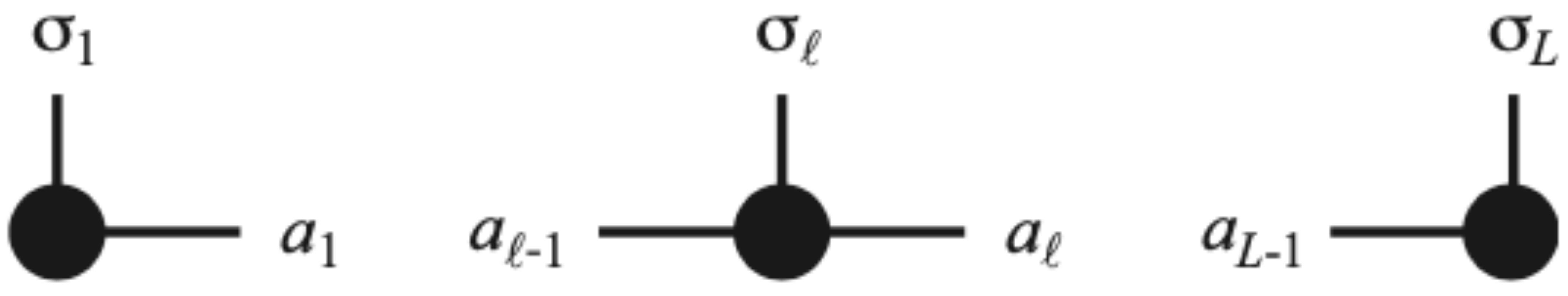
$$
\begin{aligned}
{}_A\langle a'_\ell | a_\ell \rangle_A &= \sum_{\sigma_1,\ldots,\sigma_\ell} (A^{\sigma_1} \ldots A^{\sigma_\ell})^*_{1,a'_\ell} (A^{\sigma_1} \ldots A^{\sigma_\ell})_{1,a_\ell} \\
&= \sum_{\sigma_1,\ldots,\sigma_\ell} (A^{\sigma_1} \ldots A^{\sigma_\ell})^\dagger_{a'_\ell,1} (A^{\sigma_1} \ldots A^{\sigma_\ell})_{1,a_\ell} \\
&= \sum_{\sigma_1,\ldots,\sigma_\ell} (A^{\sigma_\ell\dagger} \ldots A^{\sigma_1\dagger} A^{\sigma_1} \ldots A^{\sigma_\ell})_{a'_\ell,a_\ell} \\
&= \delta_{a'_\ell,a_\ell},
\end{aligned}
$$

$$
\begin{aligned}
{}_B\langle a'_\ell | a_\ell \rangle_B &= \sum_{\sigma_{\ell+1},\ldots,\sigma_L} (A^{\sigma_{\ell+1}} \ldots A^{\sigma_L})^*_{a'_\ell,1} (A^{\sigma_{\ell+1}} \ldots A^{\sigma_L})_{a_\ell,1} \\
&= \sum_{\sigma_{\ell+1},\ldots,\sigma_L} (A^{\sigma_L\dagger} \ldots A^{\sigma_{\ell+1}\dagger})_{1,a'_\ell} (A^{\sigma_{\ell+1}} \ldots A^{\sigma_L})_{a_\ell,1} \\
&= \sum_{\sigma_{\ell+1},\ldots,\sigma_L} (A^{\sigma_{\ell+1}} \ldots A^{\sigma_L} A^{\sigma_L\dagger} \ldots A^{\sigma_{\ell+1}\dagger})_{a'_\ell,a_\ell},
\end{aligned}
$$

Decomposition of arbitrary quantum states into MPS

Left-canonical matrix product state





$A^{\sigma_1}_{1,a_1}$ $\quad$ $A^{\sigma_l}_{a_{l-1},a_l}$ $\quad$ $A^{\sigma_L}_{a_L,1}$

- Graphical representation of A matrices

Decomposition of arbitrary quantum states into MPS

Use QR decomposition to derive MPS

$$c_{\sigma_1 \ldots \sigma_L} = \Psi_{\sigma_1,(\sigma_2 \ldots \sigma_L)} = \sum_{a_1} Q_{\sigma_1,a_1} R_{a_1,(\sigma_2 \ldots \sigma_L)} = \sum_{a_1} A^{\sigma_1}_{1,a_1} \Psi_{(a_1\sigma_2),(\sigma_3 \ldots \sigma_L)},$$

- Rehsape $Q \to A$ and $R \to \Psi$

$$c_{\sigma_1 \ldots \sigma_L} = \sum_{a_1,a_2} A^{\sigma_1}_{1,a_1} Q_{(a_1\sigma_2),a_2} R_{a_2,(\sigma_3 \ldots \sigma_L)} = \sum_{a_1,a_2} A^{\sigma_1}_{1,a_1} A^{\sigma_2}_{a_1,a_2} \Psi_{(a_2\sigma_3),(\sigma_4 \ldots \sigma_L)}$$

- $Q^\dagger Q = I$ implies the desired left-normalization of the A-matrices

Decomposition of arbitrary quantum states into MPS

Right-canonical matrix product state

$$
\begin{aligned}
c_{\sigma_1\ldots\sigma_L} &= \Psi_{(\sigma_1\ldots\sigma_{L-1}),\sigma_L} \\
&= \sum_{a_{L-1}} U_{(\sigma_1\ldots\sigma_{L-1}),a_{L-1}} S_{a_{L-1},a_{L-1}} (V^\dagger)_{a_{L-1},\sigma_L} \\
&= \sum_{a_{L-1}} \Psi_{(\sigma_1\ldots\sigma_{L-2}),(\sigma_{L-1}a_{L-1})} B^{\sigma_L}_{a_{L-1}} \\
&= \sum_{a_{L-2},a_{L-1}} U_{(\sigma_1\ldots\sigma_{L-2}),a_{L-2}} S_{a_{L-2},a_{L-2}} (V^\dagger)_{a_{L-2},(\sigma_{L-1}a_{L-1})} B^{\sigma_L}_{a_{L-1}} \\
&= \sum_{a_{L-2},a_{L-1}} \Psi_{(\sigma_1\ldots\sigma_{L-3}),(\sigma_{L-2}a_{L-2})} B^{\sigma_{L-1}}_{a_{L-2},a_{L-1}} B^{\sigma_L}_{a_{L-1}} = \ldots \\
&= \sum_{a_1,\ldots,a_{L-1}} B^{\sigma_1}_{a_1} B^{\sigma_2}_{a_1,a_2} \ldots B^{\sigma_{L-1}}_{a_{L-2},a_{L-1}} B^{\sigma_L}_{a_{L-1}}.
\end{aligned}
$$

- Right normalized condition

$$\sum_{\sigma_\ell} B^{\sigma_\ell} B^{\sigma_\ell \dagger} = I,$$

$$
\begin{aligned}
|a_\ell\rangle_A &= \sum_{\sigma_1,\ldots,\sigma_\ell} (B^{\sigma_1} B^{\sigma_2} \ldots B^{\sigma_\ell})_{1,a_\ell} |\sigma_1,\ldots,\sigma_\ell\rangle \\
|a_\ell\rangle_B &= \sum_{\sigma_{\ell+1},\ldots,\sigma_L} (B^{\sigma_{\ell+1}} B^{\sigma_{\ell+2}} \ldots B^{\sigma_L})_{a_\ell,1} |\sigma_{\ell+1},\ldots,\sigma_L\rangle
\end{aligned}
$$

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} B^{\sigma_1} B^{\sigma_2} \ldots B^{\sigma_{L-1}} B^{\sigma_L} |\sigma_1,\ldots,\sigma_L\rangle = \sum_{a_\ell} |a_\ell\rangle_A |a_\ell\rangle_B.$$

Decomposition of arbitrary quantum states into MPS

Mixed-canonical matrix product state

- We did a decomposition from the left up to site l

$$c_{\sigma_1\ldots\sigma_L} = \sum_{a_\ell}(A^{\sigma_1}\ldots A^{\sigma_\ell})_{a_\ell}S_{a_\ell,a_\ell}(V^\dagger)_{a_\ell,(\sigma_{\ell+1}\ldots\sigma_L)}.$$

- We reshape $V^\dagger$ as $\Psi_{(a_l\sigma_{l+1}\cdots a_{L-1}),\sigma_L}$ and carry out successive SVDs from the right up to and including site σ_{l+2}

$$(V^\dagger)_{a_\ell,(\sigma_{\ell+1}\ldots\sigma_L)} = \sum_{a_{\ell+1},\ldots,a_{L-1}} B^{\sigma_{\ell+1}}_{a_\ell,a_{\ell+1}}\ldots B^{\sigma_L}_{a_{L-1}}.$$

- End up with a decomposition
- $$c_{\sigma_1\ldots\sigma_L} = A^{\sigma_1}\ldots A^{\sigma_\ell}S\,B^{\sigma_{\ell+1}}\ldots B^{\sigma_L},$$

Decomposition of arbitrary quantum states into MPS

Mixed-canonical matrix product state

- Introduce vectors

$$
\begin{aligned}
|a_\ell\rangle_A &= \sum_{\sigma_1,\ldots,\sigma_\ell} (A^{\sigma_1}\ldots A^{\sigma_\ell})_{1,a_\ell}|\sigma_1,\ldots,\sigma_\ell\rangle \\
|a_\ell\rangle_B &= \sum_{\sigma_{\ell+1},\ldots,\sigma_L} (B^{\sigma_{\ell+1}}\ldots B^{\sigma_L})_{a_\ell,1}|\sigma_{\ell+1},\ldots,\sigma_L\rangle
\end{aligned}
$$

- The state have Schmidt decomposition

$$
|\psi\rangle = \sum_{a_\ell} s_a |a_\ell\rangle_A |a_\ell\rangle_B,
$$

Decomposition of arbitrary quantum states into MPS

Gauge degree of freedom

$$M^{\sigma_i} \to M^{\sigma_i} X, \qquad M^{\sigma_{i+1}} \to X^{-1} M^{\sigma_{i+1}}.$$

MPS II

Contents

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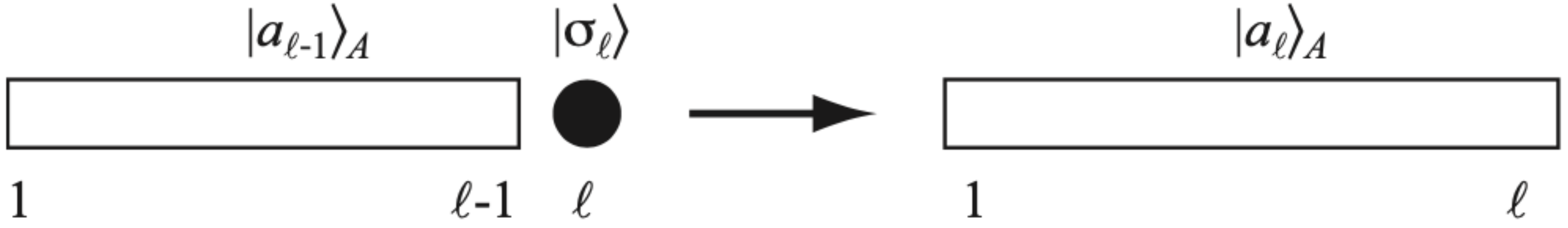
MPS and single-site decimation in one dimension

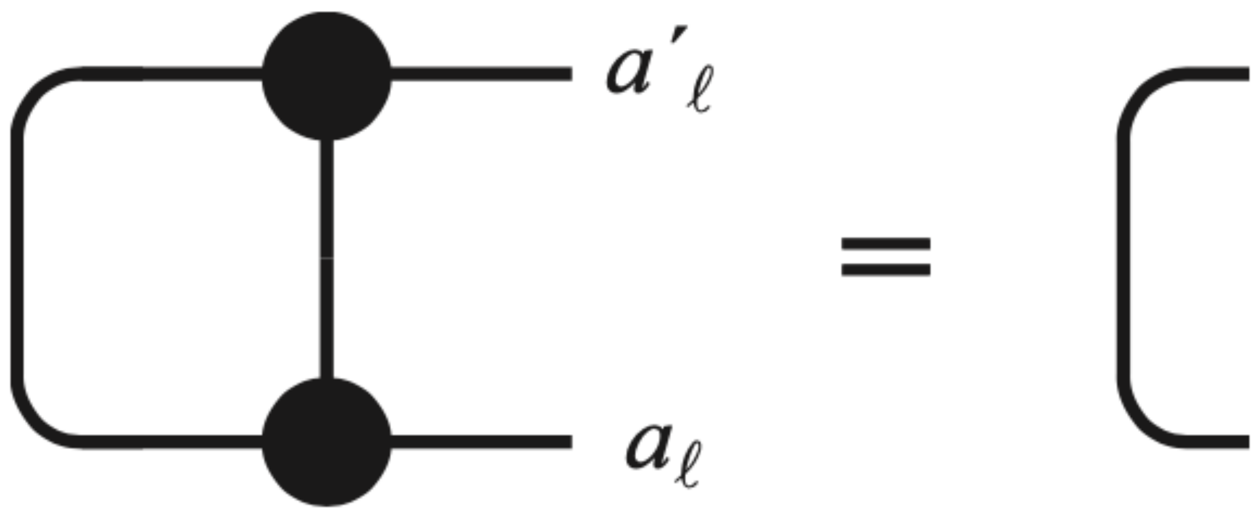
- Set up an iterative growth procedure for spin chain: $l \to l+1$



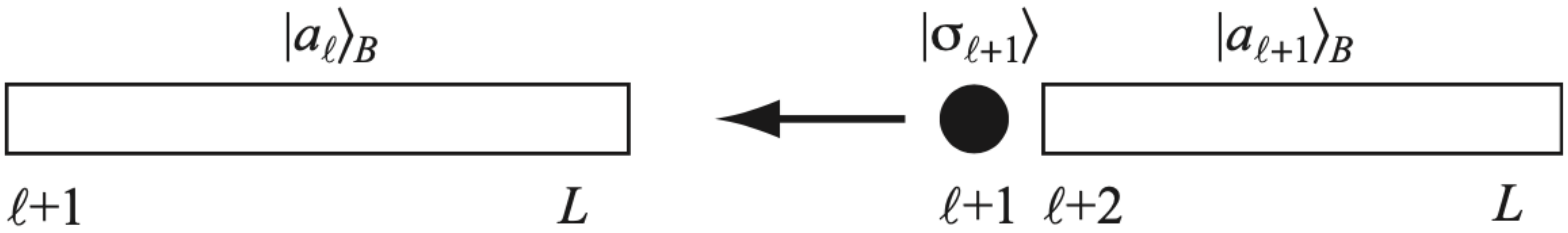
$$|a_\ell\rangle_A = \sum_{a_{\ell-1}\sigma_\ell} {}_A\langle a_{\ell-1}\sigma_\ell|a_\ell\rangle_A \; |a_{\ell-1}\rangle_A|\sigma_\ell\rangle \; = \sum_{a_{\ell-1}\sigma_\ell} A^{[\ell]\sigma_\ell}_{a_{\ell-1},a_\ell}|a_{\ell-1}\rangle_A|\sigma_\ell\rangle$$

$$A^{[\ell]\sigma_\ell}_{a_{\ell-1},a_\ell} \equiv {}_A\langle a_{\ell-1}\sigma_\ell|a_\ell\rangle_A .$$

$$\begin{aligned}
|a_\ell\rangle_A &= \sum_{a_{\ell-1}}\sum_{\sigma_\ell} A^{\sigma_\ell}_{a_{\ell-1},a_\ell}|a_{\ell-1}\rangle_A|\sigma_\ell\rangle \\
&= \sum_{a_{\ell-1},a_{\ell-2}}\;\sum_{\sigma_{\ell-1},\sigma_\ell} A^{\sigma_{\ell-1}}_{a_{\ell-2},a_{\ell-1}}A^{\sigma_\ell}_{a_{\ell-1},a_\ell}|a_{\ell-2}\rangle_A|\sigma_{\ell-1}\rangle|\sigma_\ell\rangle = \ldots \\
&= \sum_{a_1,a_2,\ldots,a_{\ell-1}}\;\sum_{\sigma_1,\sigma_2,\ldots,\sigma_\ell} A^{\sigma_1}_{1,a_1}A^{\sigma_2}_{a_1,a_2}\ldots A^{\sigma_\ell}_{a_{\ell-1},a_\ell}|\sigma_1\rangle|\sigma_2\rangle\ldots|\sigma_\ell\rangle \\
&= \sum_{\sigma_i\in\mathrm{A}}(A^{\sigma_1}A^{\sigma_2}\ldots A^{\sigma_\ell})_{1,a_\ell}|\sigma_1\rangle|\sigma_2\rangle\ldots|\sigma_\ell\rangle,
\end{aligned}$$



$$\begin{aligned}
\delta_{a'_\ell,a_\ell} = {}_A\langle a'_\ell|a_\ell\rangle_A &= \sum_{\sigma'_\ell,\sigma_\ell}\;\sum_{a'_{\ell-1},a_{\ell-1}} A^{\sigma'^{*}_\ell}_{a'_{\ell-1},a'_\ell}A^{\sigma_\ell}_{a_{\ell-1},a_\ell}\;{}_A\langle a'_{\ell-1}\sigma'_\ell|a_{\ell-1}\sigma_\ell\rangle_A \\
&= \sum_{\sigma_\ell}\sum_{a_{\ell-1}} A^{\sigma_\ell\dagger}_{a'_\ell,a_{\ell-1}}A^{\sigma_\ell}_{a_{\ell-1},a_\ell} = \sum_{\sigma_\ell}(A^{\sigma_\ell\dagger}A^{\sigma_\ell})_{a'_\ell,a_\ell}.
\end{aligned}$$



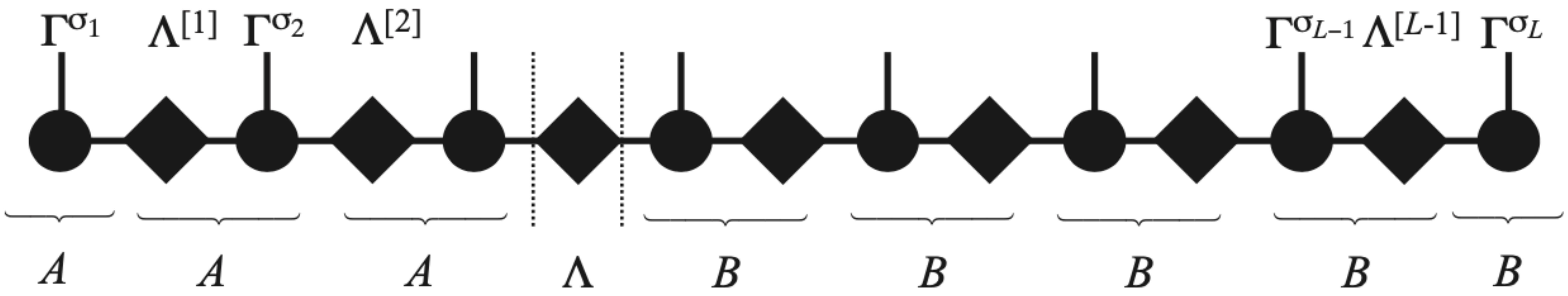
$$|a_\ell\rangle_B = \sum_{a_{\ell+1}\sigma_{\ell+1}} {}_B\langle a_{\ell+1}\sigma_{\ell+1}|a_\ell\rangle_B \; |a_{\ell+1}\rangle_B|\sigma_{\ell+1}\rangle$$

$$|a_\ell\rangle_B = \sum_{a_{\ell+1}\sigma_{\ell+1}} B^{[\ell+1]\sigma_{\ell+1}}_{a_\ell,a_{\ell+1}}|a_{\ell+1}\rangle_B|\sigma_{\ell+1}\rangle$$

$$B^{[\ell+1]\sigma_{\ell+1}}_{a_\ell,a_{\ell+1}} = {}_B\langle a_{\ell+1}\sigma_{\ell+1}|a_\ell\rangle_B.$$

$$|a_\ell\rangle_B = \sum_{\sigma_i \in \mathrm{B}} (B^{\sigma_{\ell+1}}B^{\sigma_{\ell+2}}\dots B^{\sigma_L})_{a_{\ell+1},1}|\sigma_{\ell+1}\rangle|\sigma_{\ell+2}\rangle\dots|\sigma_L\rangle,$$

- The advantage of the matrix notation is that
- 1:it allows for a simple recursion from a block of length l to the smallest
- 2:we can hide summations in matrix multiplications.



$$
\begin{aligned}
c_{\sigma_1\ldots\sigma_L} &= \Psi_{\sigma_1,(\sigma_2\ldots\sigma_L)} \\
&= \sum_{a_1} A^{\sigma_1}_{a_1} \underbrace{\Lambda^{[1]}_{a_1,a_1}(V^\dagger)_{a_1,(\sigma_2\ldots\sigma_L)}} \\
&= \sum_{a_1} \Gamma^{\sigma_1}_{a_1} \Psi_{(a_1\sigma_2),(\sigma_3\ldots\sigma_L)} \\
&= \sum_{a_1,a_2} \Gamma^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \underbrace{\Lambda^{[2]}_{a_2,a_2}(V^\dagger)_{a_2,(\sigma_3\ldots\sigma_L)}} \\
&= \sum_{a_1,a_2} \Gamma^{\sigma_1}_{a_1} \overbrace{\Lambda^{[1]}_{a_1,a_1}\Gamma^{\sigma_2}_{a_1,a_2}} \Psi_{(a_2\sigma_3),(\sigma_4\ldots\sigma_L)} \\
&= \sum_{a_1,a_2,a_3} \Gamma^{\sigma_1}_{a_1}\Lambda^{[1]}_{a_1,a_1}\Gamma^{\sigma_2}_{a_1,a_2} A^{\sigma_3}_{a_2,a_3} \underbrace{\Lambda^{[3]}_{a_3,a_3}(V^\dagger)_{a_3,(\sigma_4\ldots\sigma_L)}} \\
&= \sum_{a_1,a_2,a_3} \Gamma^{\sigma_1}_{a_1}\Lambda^{[1]}_{a_1,a_1}\Gamma^{\sigma_2}_{a_1,a_2} \overbrace{\Lambda^{[2]}_{a_2,a_2}\Gamma^{\sigma_3}_{a_2,a_3}} \Psi_{(a_3\sigma_4),(\sigma_5\ldots\sigma_L)}
\end{aligned}
$$

$$
A^{\sigma_\ell}_{a_{\ell-1},a_\ell} = \Lambda^{[\ell-1]}_{a_{\ell-1},a_{\ell-1}}\Gamma^{\sigma_\ell}_{a_{\ell-1},a_\ell}, \qquad B^{\sigma_\ell}_{a_{\ell-1},a_\ell} = \Gamma^{\sigma_\ell}_{a_{\ell-1},a_\ell}\Lambda^{[\ell]}_{a_\ell,a_\ell},
$$

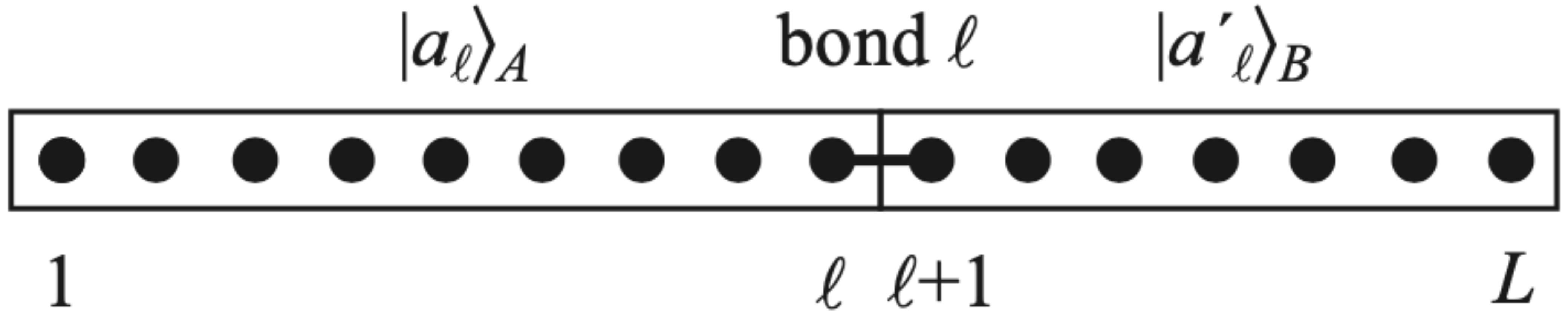
$$
I = \sum_{\sigma_i} A^{\sigma_i\dagger}A^{\sigma_i} = \sum_{\sigma_i} \Gamma^{\sigma_i\dagger}\Lambda^{[i-1]\dagger}\Lambda^{[i-1]}\Gamma^{\sigma_i}
$$

$$
\sum_{\sigma_i} \Gamma^{\sigma_i}\rho_A^{[i]}\Gamma^{\sigma_i\dagger} = I. \qquad \sum_{\sigma_i} \Gamma^{\sigma_i\dagger}\rho_B^{[i-1]}\Gamma^{\sigma_i} = I.
$$

$$
\rho_A^{[\ell]} = \rho_B^{[\ell]} = (\Lambda^{[\ell]})^2,
$$

$$
|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} \Gamma^{\sigma_1}\Lambda^{[1]}\Gamma^{\sigma_2}\Lambda^{[2]}\Gamma^{\sigma_3}\Lambda^{[3]}\ldots\Gamma^{\sigma_{L-1}}\Lambda^{[L-1]}\Gamma^{\sigma_L}|\sigma_1,\ldots,\sigma_L\rangle,
$$

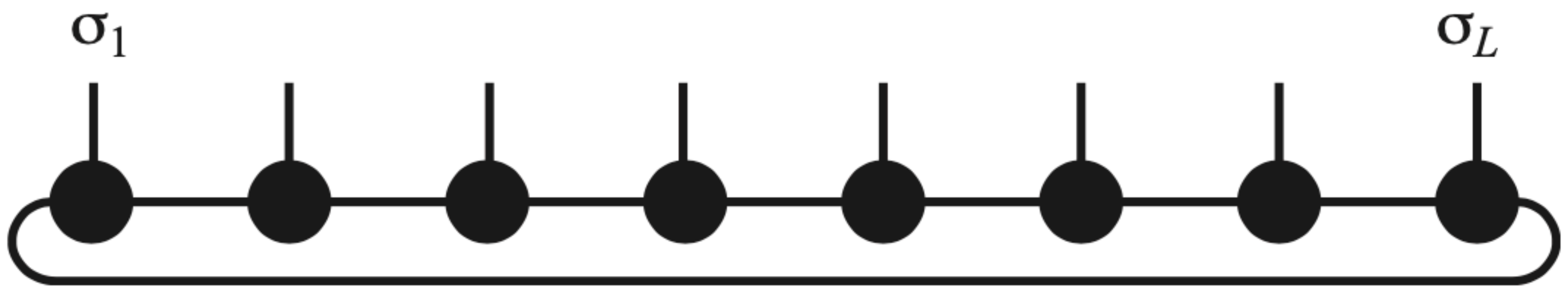
MPS for OBC and PBC



$$|\psi\rangle = \sum_{a_\ell, a'_\ell} \Psi_{a_\ell, a'_\ell} |a_\ell\rangle_A |a'_\ell\rangle_B.$$

$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} A^{\sigma_1} \dots A^{\sigma_\ell} \Psi B^{\sigma_{\ell+1}} \dots B^{\sigma_L} |\boldsymbol{\sigma}\rangle.$$

$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} M^{\sigma_1} \dots M^{\sigma_L} |\boldsymbol{\sigma}\rangle \quad \text{(MPS for OBC)},$$

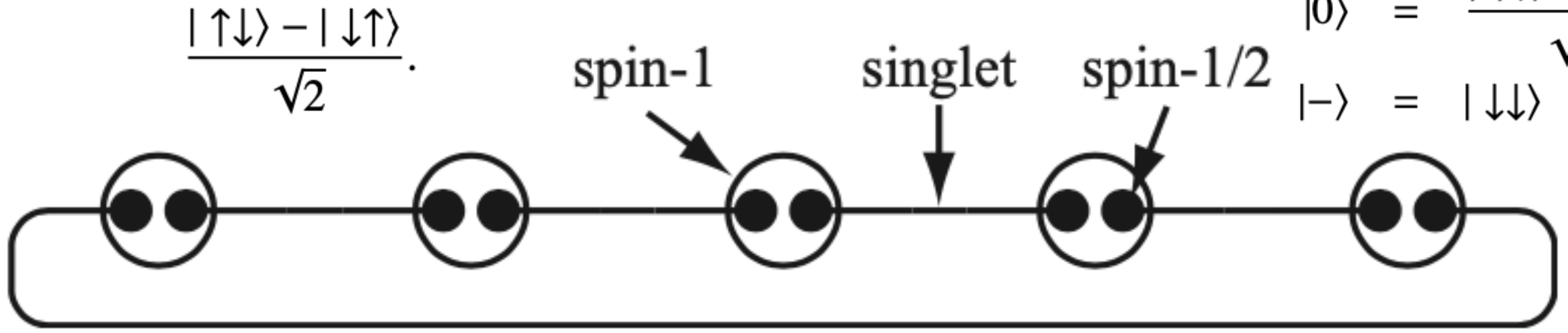


$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} \mathrm{Tr}(M^{\sigma_1} \dots M^{\sigma_L}) |\boldsymbol{\sigma}\rangle \quad \text{(MPS for PBC)}.$$

$$\sum_{\sigma} A^{\sigma\dagger} A^{\sigma} = I. \quad \sum_{\sigma} B^{\sigma} B^{\sigma\dagger} = I$$

AKLT state as a matrix product state

$$|+\rangle = |\uparrow\uparrow\rangle$$
$$|0\rangle = \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}}$$
$$|-\rangle = |\downarrow\downarrow\rangle$$



$$\hat{H} = \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2,$$

$$\begin{aligned} |\psi\rangle &= \prod_i (|{+1/2}\rangle_{r_i}, |{-1/2}\rangle_{r_i}) \begin{pmatrix} 0 & 1/\sqrt{2} \\ -1/\sqrt{2} & 0 \end{pmatrix} \begin{pmatrix} |{+1/2}\rangle_{l_{i+1}} \\ |{-1/2}\rangle_{l_{i+1}} \end{pmatrix} \\ &= \sum_{\vec{a},\vec{b}} S_{b_1 a_2} S_{b_2 a_3} \cdots S_{b_N a_1} |\vec{a}, \vec{b}\rangle, \end{aligned}$$

$$H = 2J \sum_j P^{(S=2)}_{j,j+1} \,.$$

$$\begin{aligned} |\psi_{\mathrm{AKLT}}\rangle \propto \left(\prod_i P_i\right) |\psi\rangle &= \sum_{\vec{m}=\vec{a}+\vec{b}} P^{m_1}_{a_1 b_1} S_{b_1 a_2} P^{m_2}_{a_2 b_2} S_{b_2 a_3} \cdots P^{m_N}_{a_N b_N} S_{b_N a_1} |\vec{a}, \vec{b}\rangle \\ &= \sum_{\vec{m}} \mathrm{Tr}(P^{m_1} S P^{m_2} S \cdots P^{m_N} S) |\vec{m}\rangle \\ &= \sum_{\vec{m}} \mathrm{Tr}(A^{m_1} A^{m_2} \cdots A^{m_N}) |\vec{m}\rangle, \end{aligned}$$

$$S = \begin{pmatrix} 0 & 1/\sqrt{2} \\ -1/\sqrt{2} & 0 \end{pmatrix}. \quad P = \sum_{m=-1}^{1} P^m,$$

$$P^{+1} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad P^{-1} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad P^0 = \begin{pmatrix} 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 \end{pmatrix}.$$

Notations and conversions

- MPS notation based on one set of matrices per site
- Special normalization roperties for these matrices
- In the view of DMRG,it would be useful to be able to access easily all L-1 possible bipartitionings of the system
- Such a notation has been introduced by Vidal

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} \Gamma^{\sigma_1}\Lambda^{[1]}\Gamma^{\sigma_2}\Lambda^{[2]}\Gamma^{\sigma_3}\Lambda^{[3]}\ldots\Gamma^{\sigma_{L-1}}\Lambda^{[L-1]}\Gamma^{\sigma_L}|\sigma_1,\ldots,\sigma_L\rangle,$$

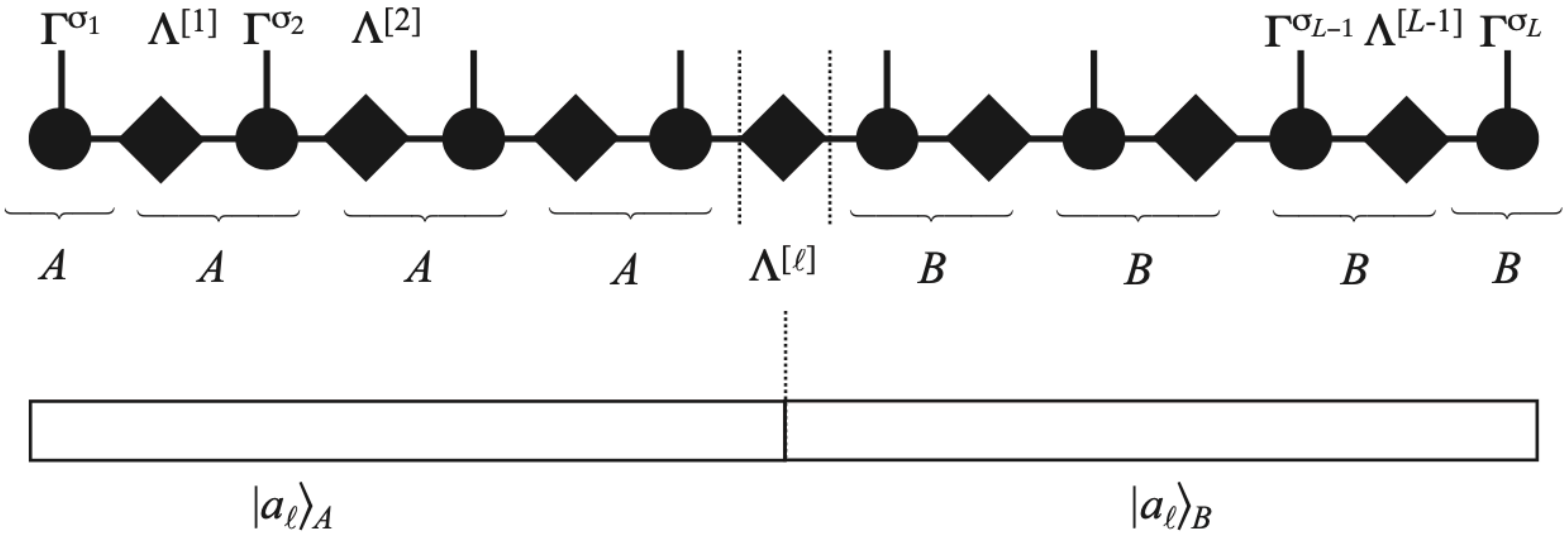


Figure 31: Vidal's MPS notation, A, B-matrix MPS notation, and DMRG block notation. The A-matrices generate the left block states, the B matrices generate the right block states. The matrix $\Lambda^{[\ell]}$ connects them via singular values.

$$|\psi\rangle = \sum_{a_\ell} |a_\ell\rangle_A s_{a_\ell} |a_\ell\rangle_B.$$

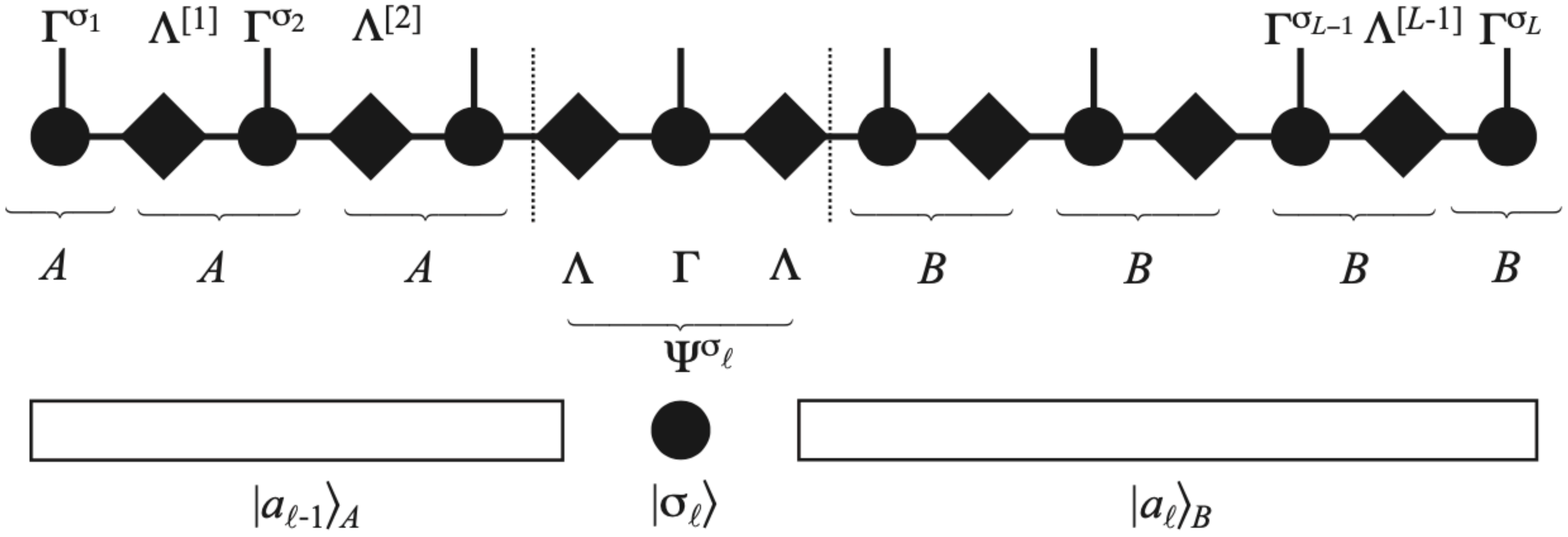


Figure 32: Representation of a state in single-site DMRG: translating Vidal's MPS notation and A, B-matrix MPS notation into DMRG block notation. The A-matrices generate the left block states, the B matrices generate the right block states. The matrix elements of Ψ^{σ_ℓ} are just the coefficients of the DMRG state.

$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} A^{\sigma_1} \ldots A^{\sigma_{\ell-1}} \Psi^{\sigma_\ell} B^{\sigma_{\ell+1}} \ldots B^{\sigma_L} |\boldsymbol{\sigma}\rangle \qquad |\psi\rangle = \sum_{a_{\ell-1}, a_\ell, \sigma_\ell} |a_{\ell-1}\rangle_A \Psi^{\sigma_\ell}_{a_{\ell-1} a_\ell} |a_\ell\rangle_B.$$

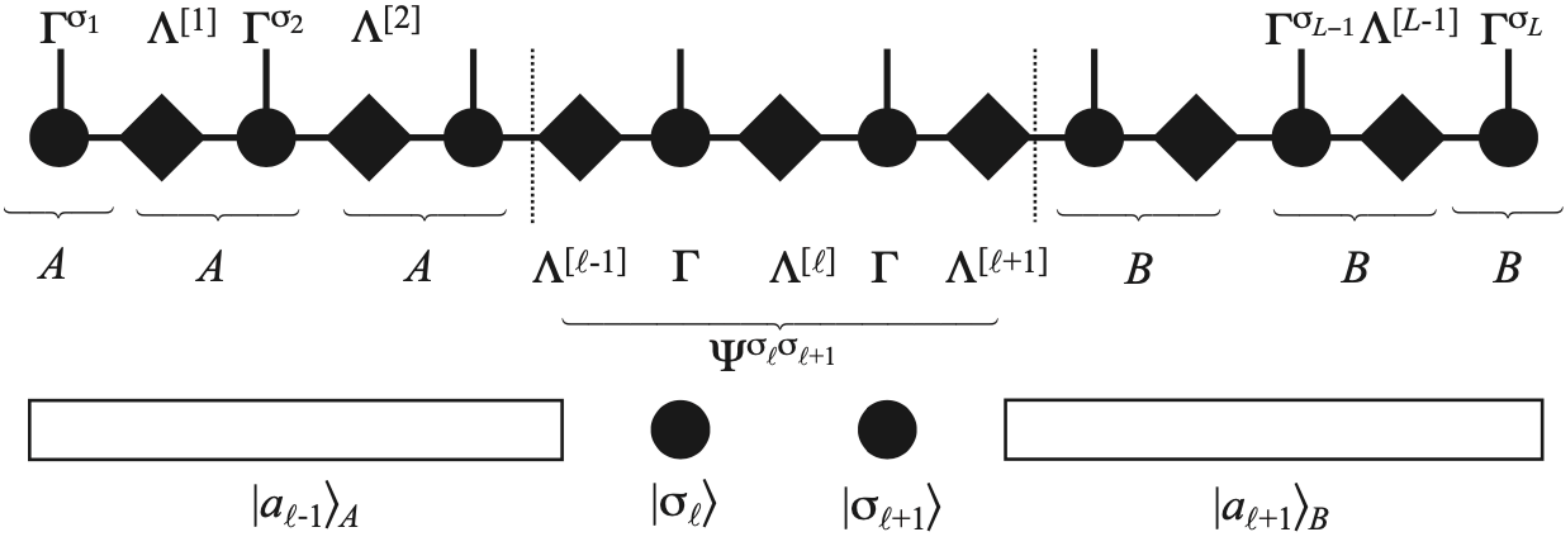


Figure 33: Representation of a state in two-site DMRG: translating Vidal's MPS notation and A, B-matrix MPS notation into DMRG block notation. The A-matrices generate the left block states, the B matrices generate the right block states. The elements of matrix $\Psi^{\sigma_\ell \sigma_{\ell+1}}$ are just the coefficients of the DMRG state.

$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} A^{\sigma_1} \dots A^{\sigma_{\ell-1}} \Psi^{\sigma_\ell \sigma_{\ell+1}} B^{\sigma_{\ell+2}} \dots B^{\sigma_L} |\boldsymbol{\sigma}\rangle \qquad |\psi\rangle = \sum_{a_{\ell-1}, a_{\ell+1}, \sigma_\ell, \sigma_{\ell+1}} |a_{\ell-1}\rangle_A \Psi^{\sigma_\ell \sigma_{\ell+1}}_{a_{\ell-1} a_{\ell+1}} |a_{\ell+1}\rangle_B.$$

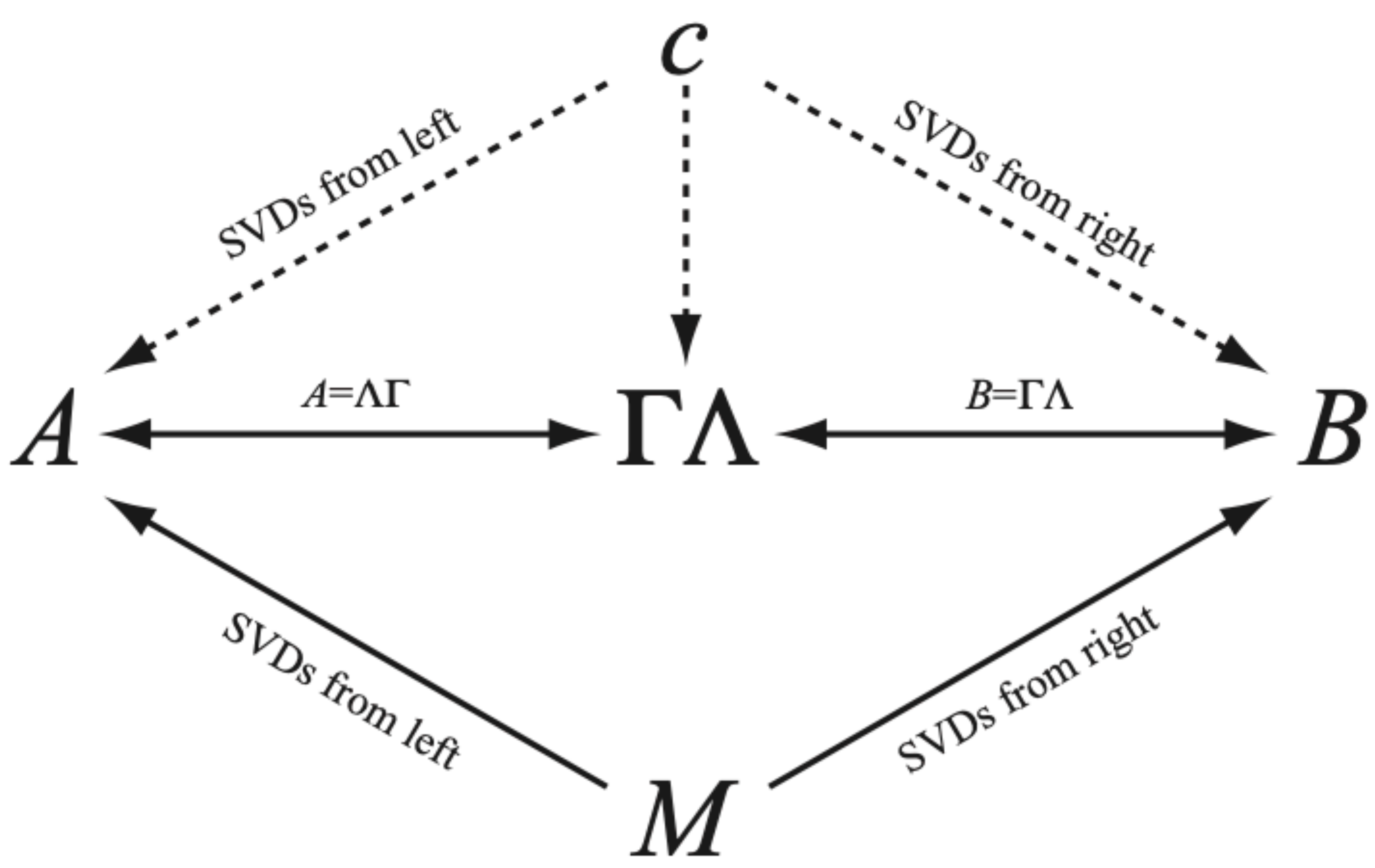


Figure 34: Conversions of representations: c is the explicit representation by the exponentially large number of state coefficients; A, B and $\Gamma\Lambda$ stand for left-canonical, right-canonical and canonical MPS; M stands for an arbitrary MPS. Solid lines indicate computationally feasible conversions, dashed lines more hypothetical ones.