

ALGORITHMIC PERSPECTIVE ON STRONGLY CORRELATED SYSTEMS

Lecture: Introduction to Matrix Product States

Fall 2015

Professor: Bryan Clark

Last Time: Exact Diagonalization → Matrix Product States

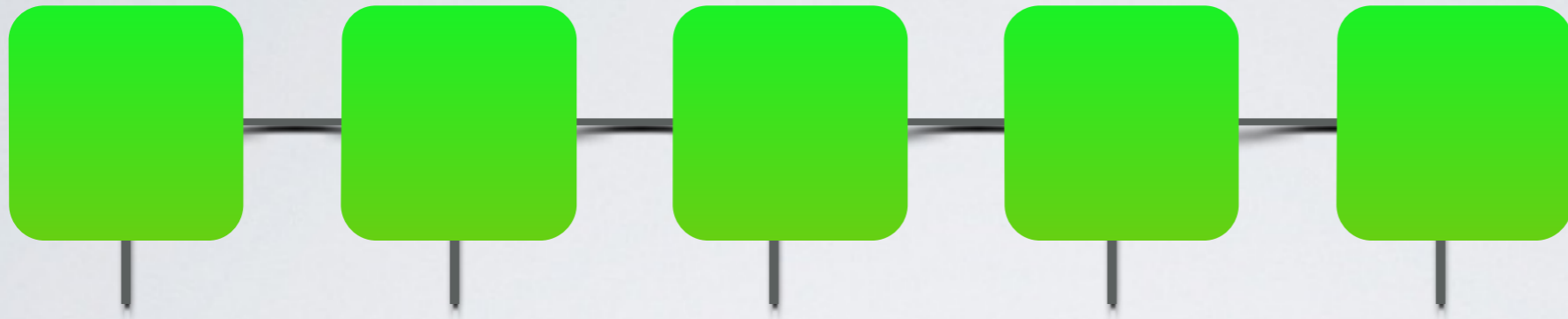
Today: More Matrix Product States

$$\langle \Psi | \sigma_1 \sigma_2 \sigma_3 \dots \sigma_n \rangle = M^{\sigma_1} M^{\sigma_2} M^{\sigma_3} \dots M^{\sigma_n}$$

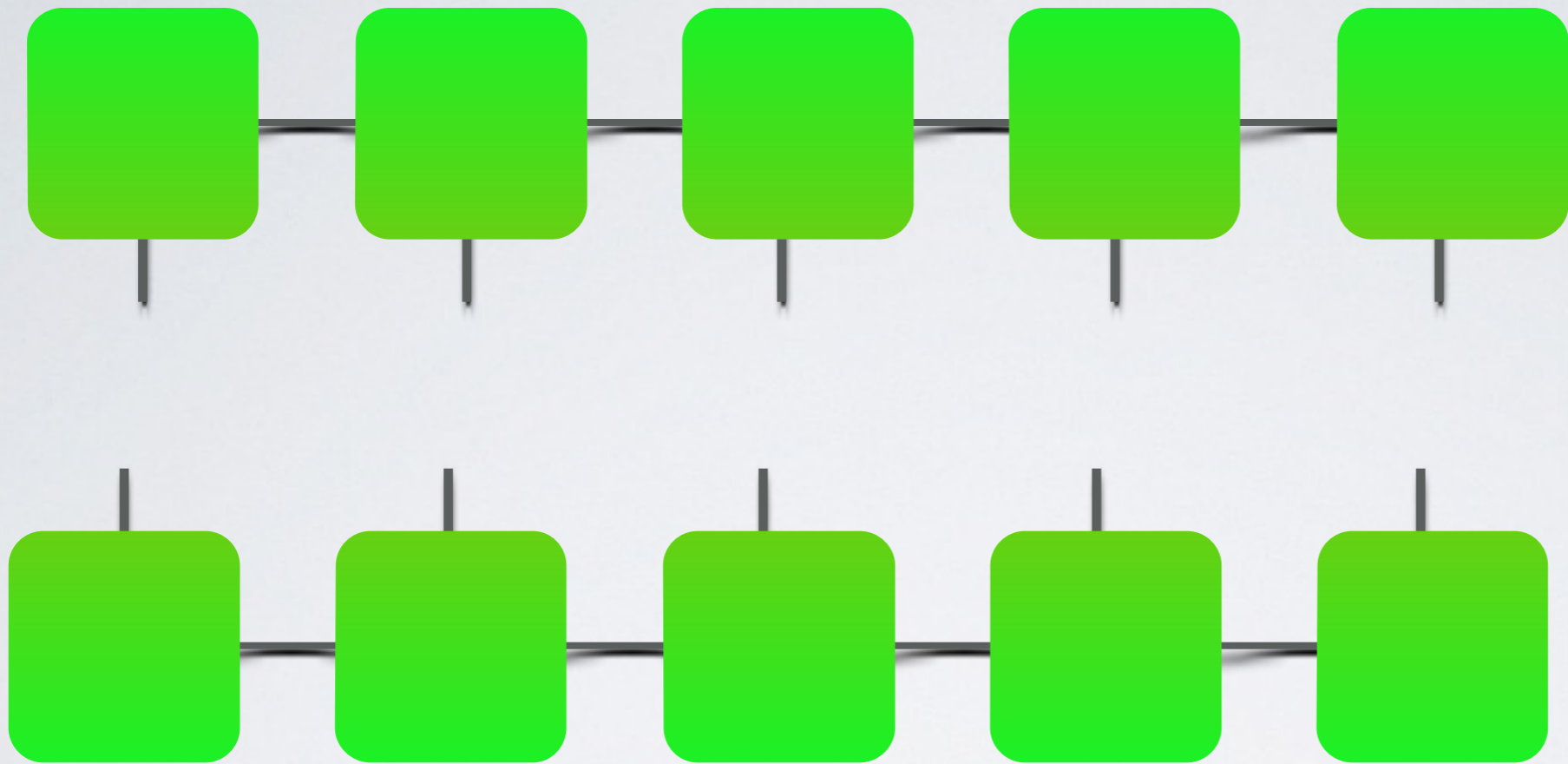
Overlap: $\langle \Psi | \Psi \rangle$

$$\begin{aligned} & \sum_{\sigma_1, \sigma_2, \dots, \sigma_n} \langle \Psi | \sigma_1 \sigma_2 \sigma_3 \dots \sigma_n \rangle \langle \sigma_1 \sigma_2 \sigma_3 \dots \sigma_n | \Psi \rangle \\ &= \sum_{\sigma_1, \sigma_2, \dots, \sigma_n} (M^{\sigma_1} M^{\sigma_2} M^{\sigma_3} \dots M^{\sigma_n}) (M^{\sigma_1} M^{\sigma_2} M^{\sigma_3} \dots M^{\sigma_n})^T \\ &= \sum_{\sigma_1, \sigma_2, \dots, \sigma_n} (M^{\sigma_1} M^{\sigma_2} M^{\sigma_3} \dots M^{\sigma_n}) (M^{\sigma_n T} M^{\sigma_{n-1} T} M^{\sigma_{n-2} T} \dots M^{\sigma_1 T}) \\ &= \sum_{\sigma_1, \sigma_2, \dots, \sigma_{n-1}} M^{\sigma_1} M^{\sigma_2} M^{\sigma_3} \dots M^{\sigma_{n-1}} \sum_{\sigma_n} (M^{\sigma_n} M^{\sigma_n T}) M^{\sigma_{n-1} T} M^{\sigma_{n-2} T} \dots M^{\sigma_1 T} \\ &= \sum_{\sigma_1, \sigma_2, \dots, \sigma_{n-2}} M^{\sigma_1} M^{\sigma_2} M^{\sigma_3} \dots \left(\sum_{\sigma_{n-1}} M^{\sigma_{n-1}} \mathbf{A} M^{\sigma_{n-1} T} \right) M^{\sigma_{n-2} T} \dots M^{\sigma_1 T} \end{aligned}$$

Overlap: $\langle \Psi | \Psi \rangle$

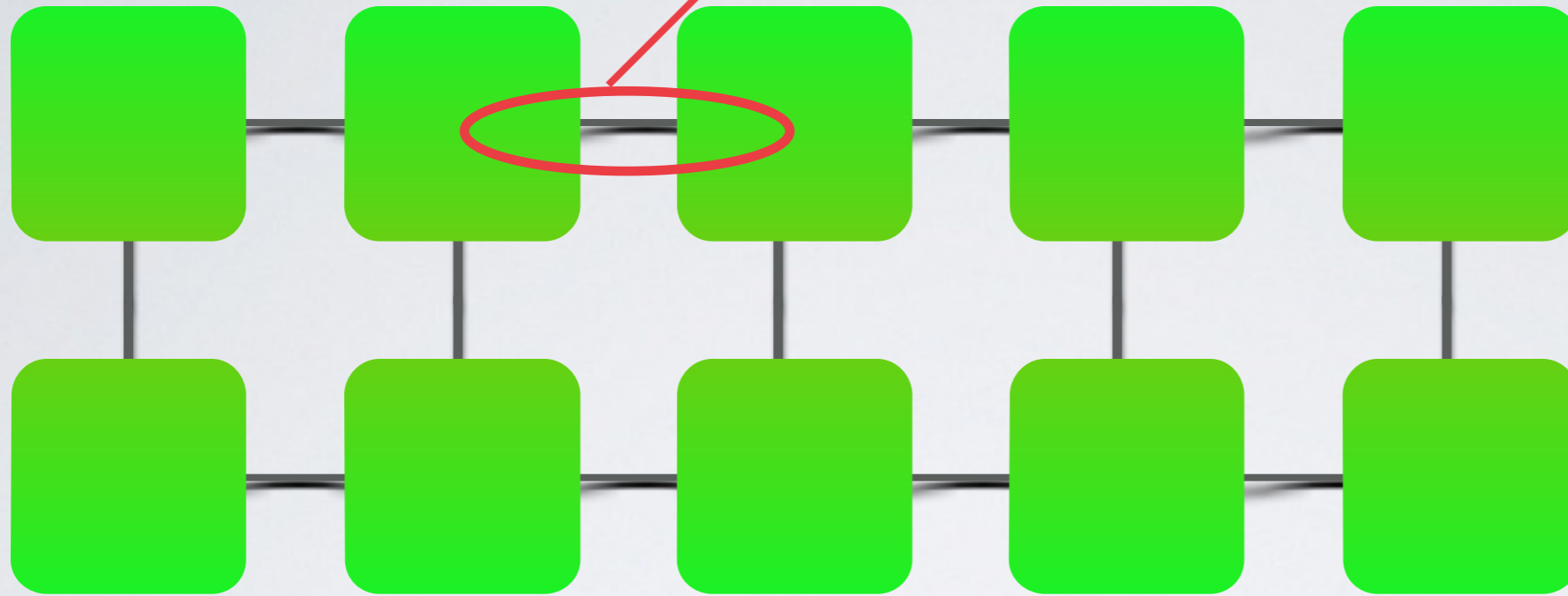


Overlap: $\langle \Psi | \Psi \rangle$

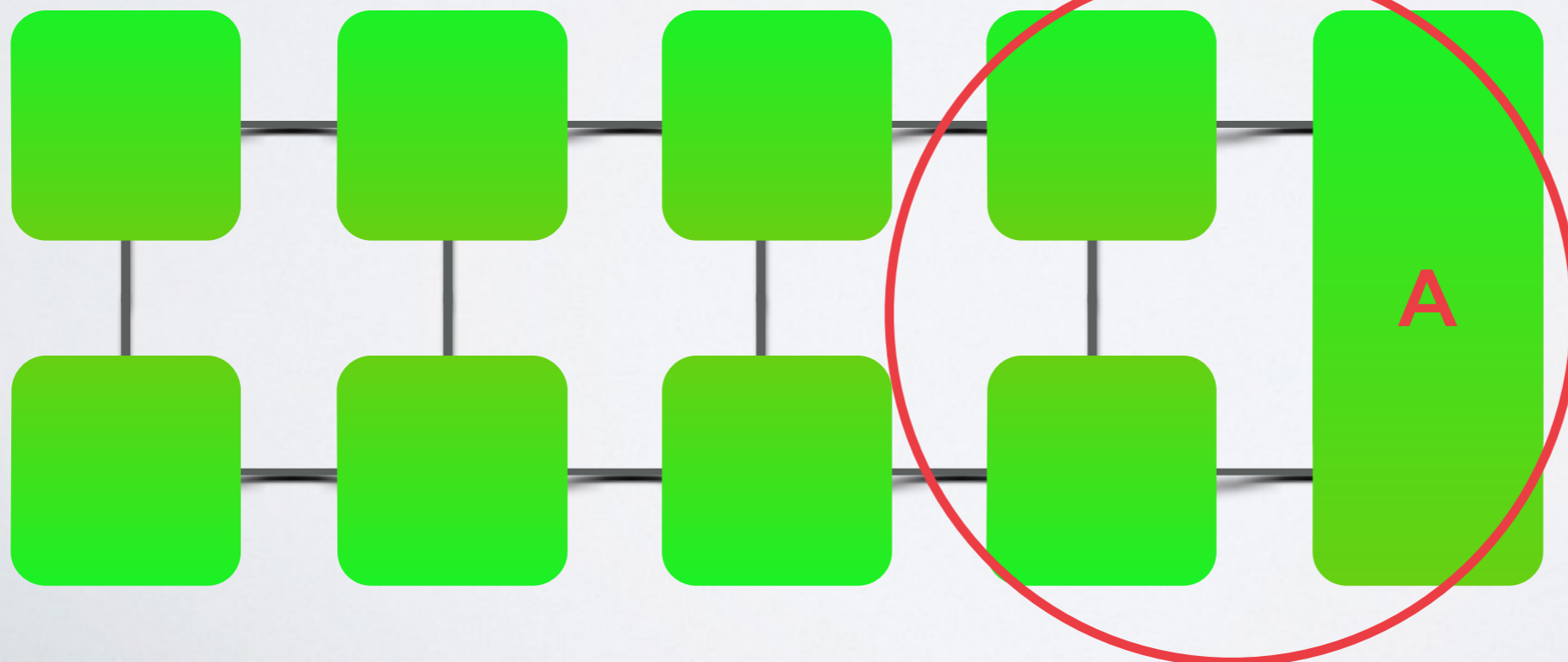
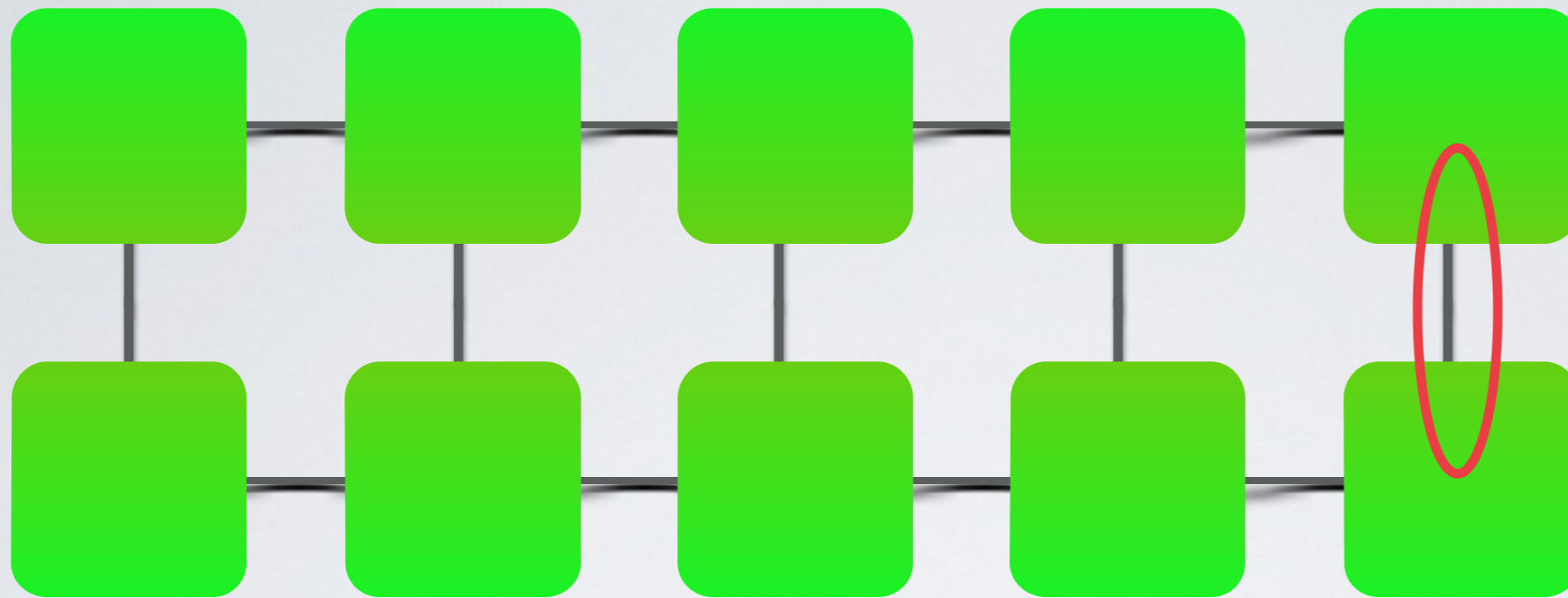


Overlap: $\langle \Psi | \Psi \rangle$

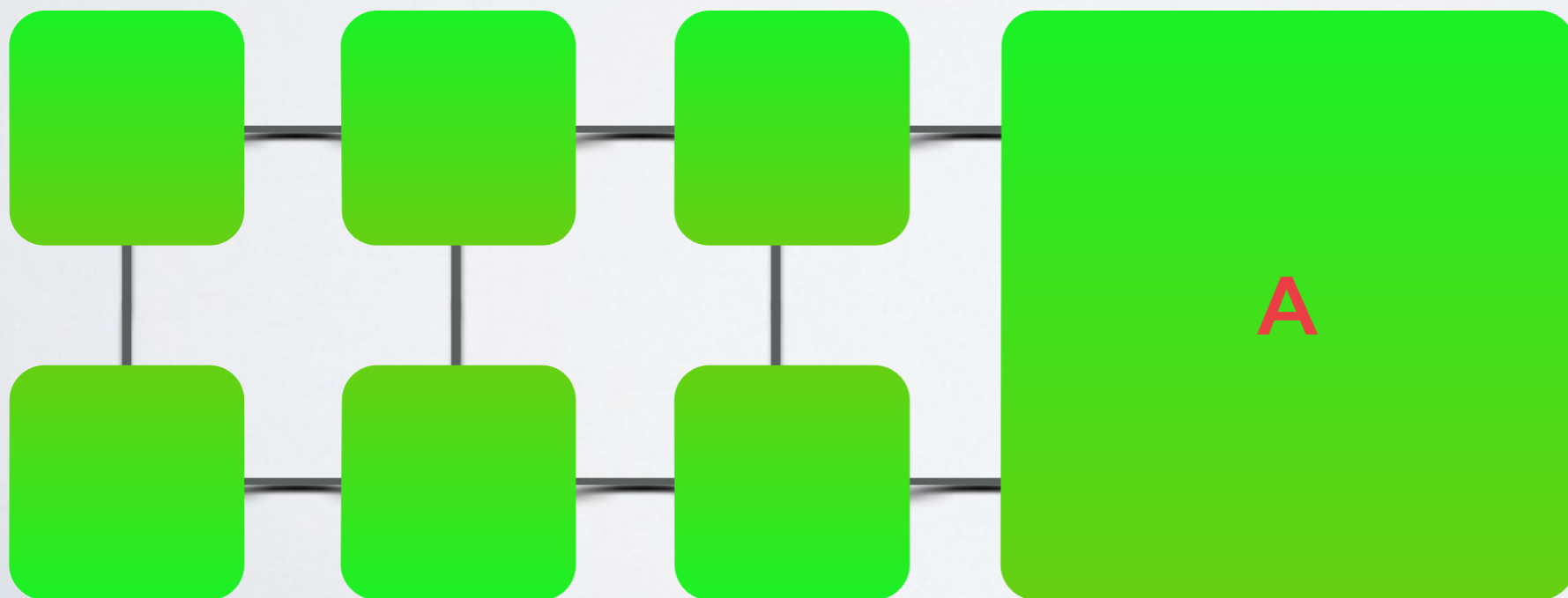
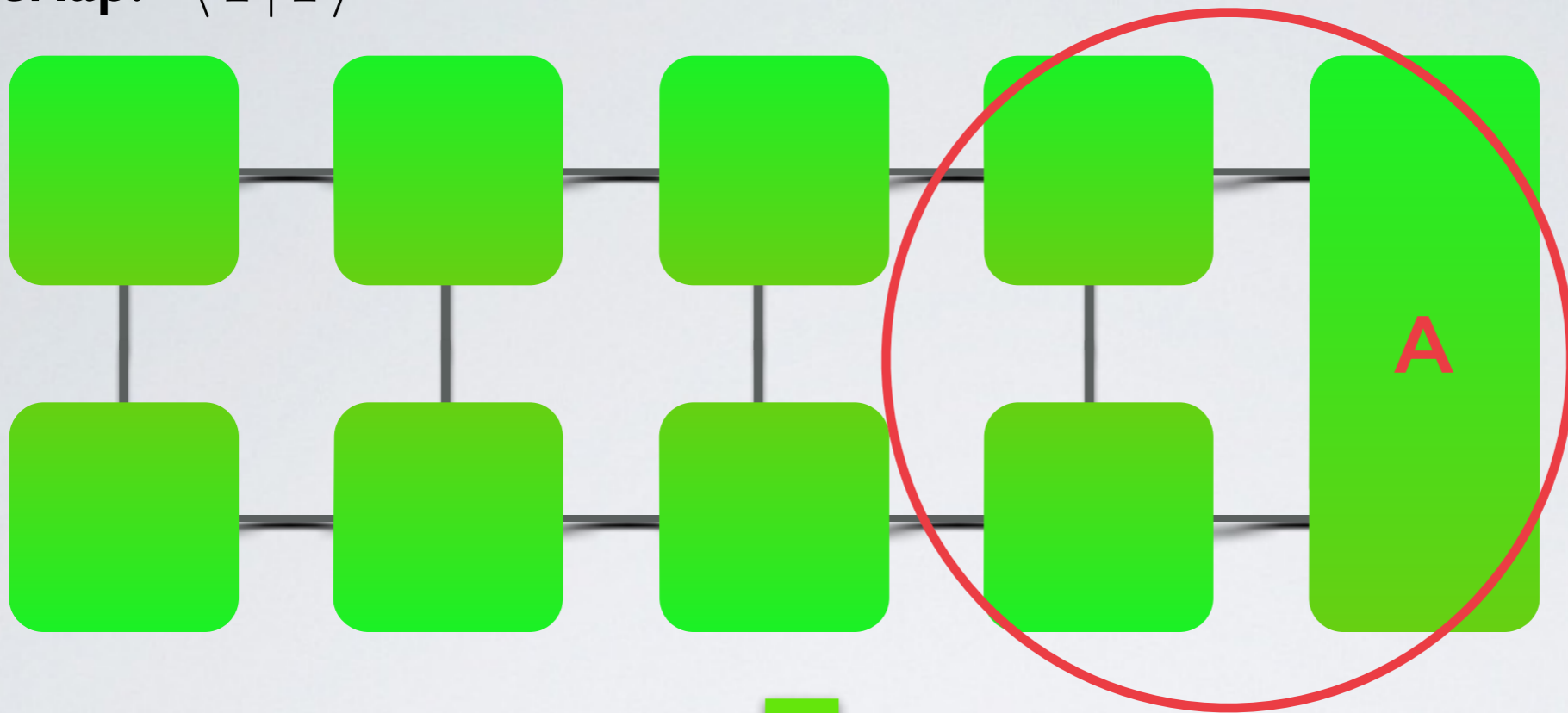
Multiply matrices first?



Overlap: $\langle \Psi | \Psi \rangle$



Overlap: $\langle \Psi | \Psi \rangle$



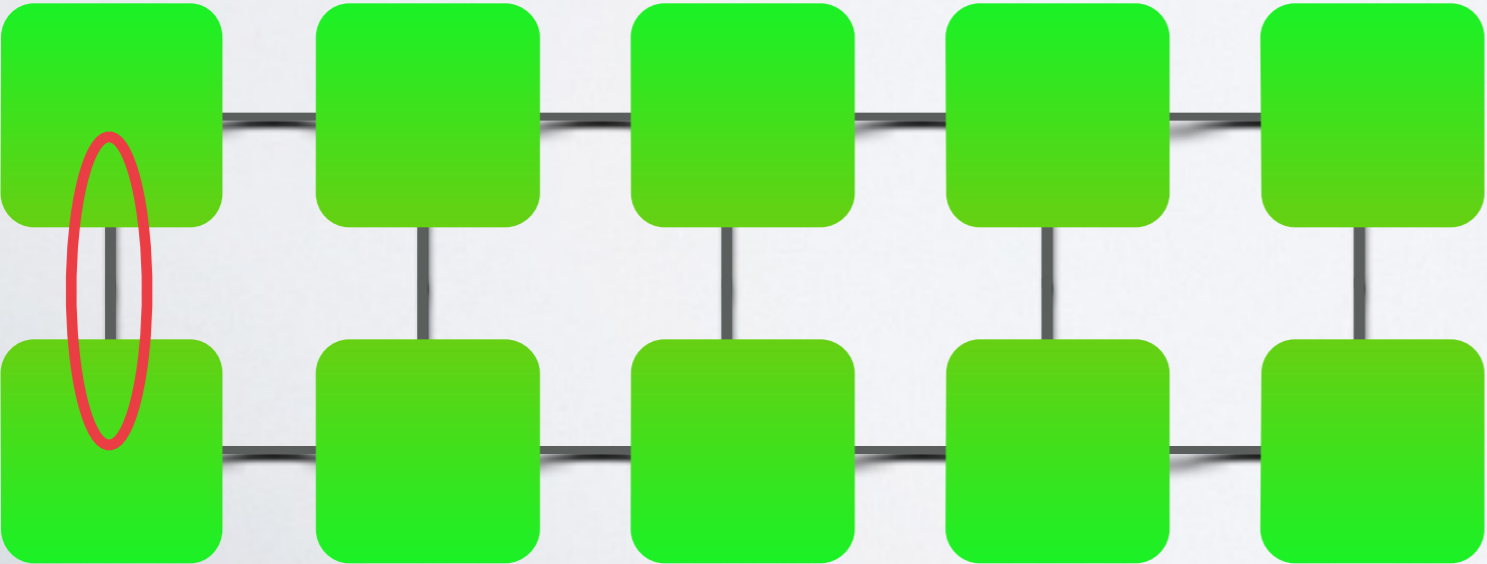
Suppose I want to start in the other direction?

$$\sum_{\sigma_1, \sigma_2 \dots \sigma_n} (M^{\sigma_1} M^{\sigma_2} M^{\sigma_3} \dots M^{\sigma_n}) (M^{\sigma_n T} M^{\sigma_{n-1} T} M^{\sigma_{n-2} T} \dots M^{\sigma_1 T})$$

$$\text{Tr} \left[\sum_{\sigma_1, \sigma_2 \dots \sigma_n} (M^{\sigma_1} M^{\sigma_2} M^{\sigma_3} \dots M^{\sigma_n}) (M^{\sigma_n T} M^{\sigma_{n-1} T} M^{\sigma_{n-2} T} \dots M^{\sigma_1 T}) \right]$$

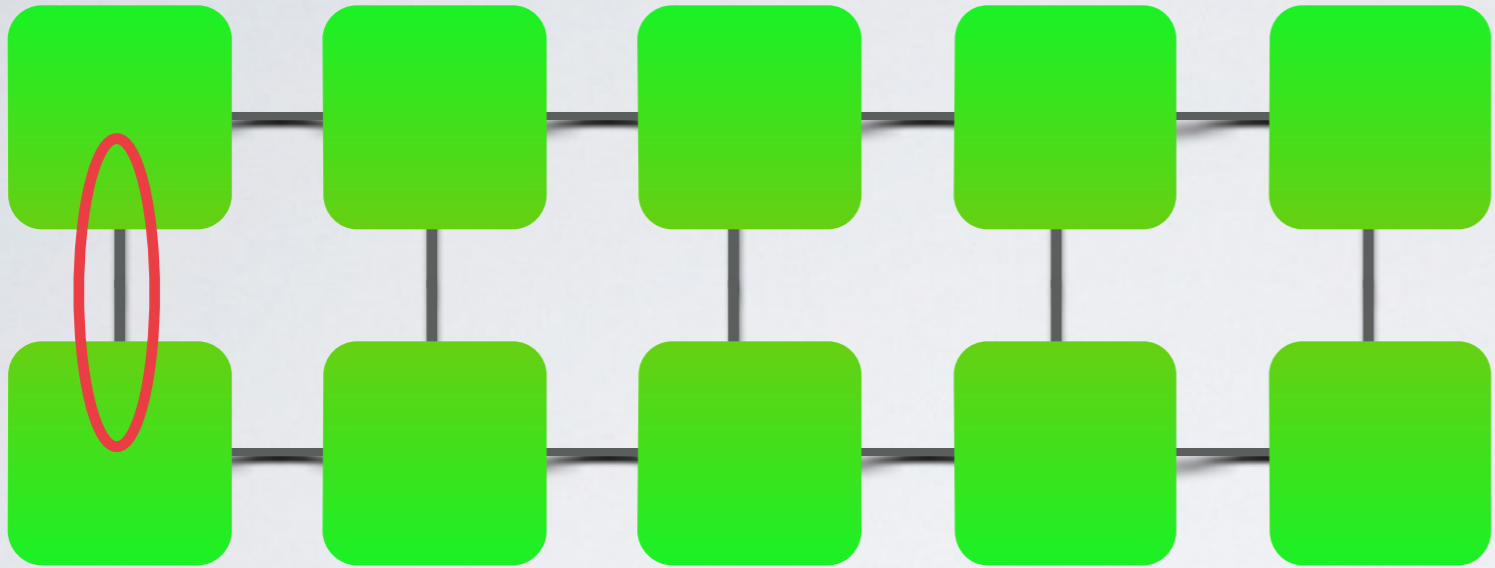
$$\text{Tr} \left[\sum_{\sigma_1, \sigma_2 \dots \sigma_n} (M^{\sigma_n T} M^{\sigma_{n-1} T} M^{\sigma_{n-2} T} \dots M^{\sigma_1 T}) (M^{\sigma_1} M^{\sigma_2} M^{\sigma_3} \dots M^{\sigma_n}) \right]$$

A



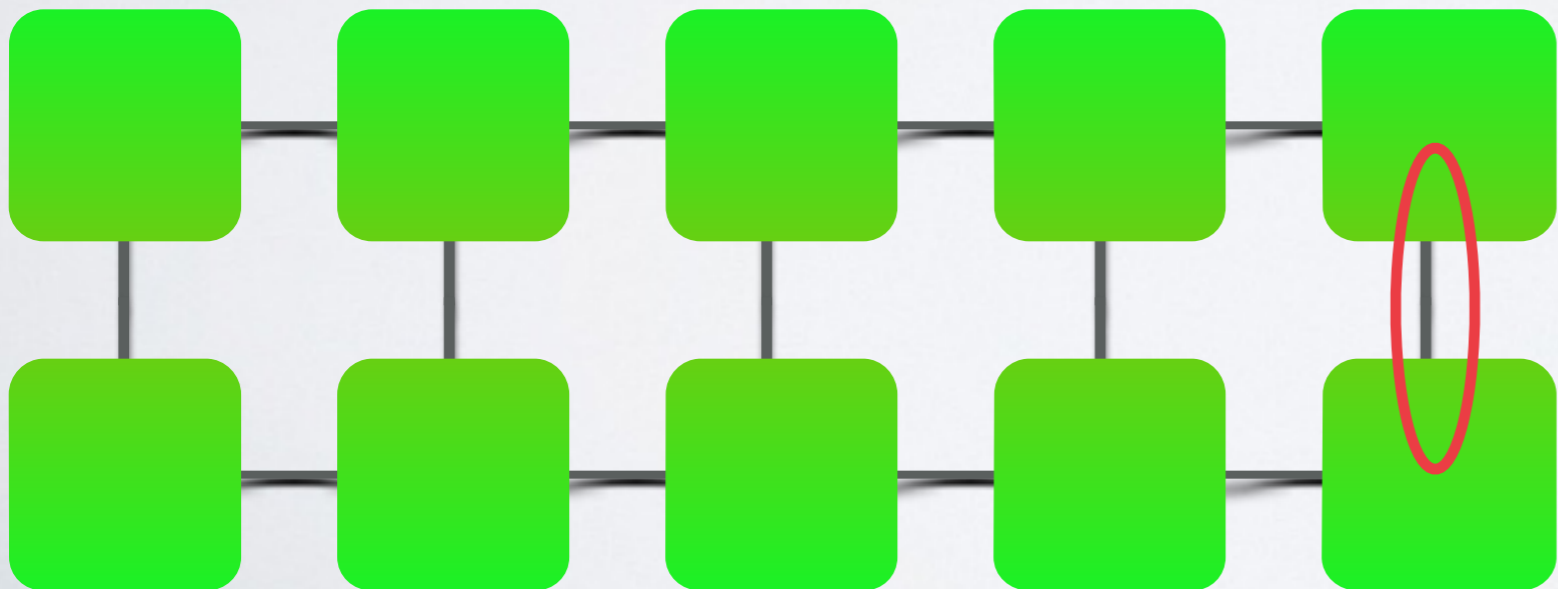
$$\text{Tr} \left[\sum_{\sigma_1, \sigma_2, \dots, \sigma_n} (M^{\sigma_n T} M^{\sigma_{n-1} T} M^{\sigma_{n-2} T} \dots M^{\sigma_1 T}) (M^{\sigma_1} M^{\sigma_2} M^{\sigma_3} \dots M^{\sigma_n}) \right]$$

A



$$= \sum_{\sigma_1, \sigma_2, \dots, \sigma_{n-1}} M^{\sigma_1} M^{\sigma_2} M^{\sigma_3} \dots M^{\sigma_{n-1}} \sum_{\sigma_n} (M^{\sigma_n} M^{\sigma_n T}) M^{\sigma_{n-1} T} M^{\sigma_{n-2} T} \dots M^{\sigma_1 T}$$

A



Canonization $\langle \Psi | \sigma_1 \sigma_2 \sigma_3 \dots \sigma_n \rangle = M^{\sigma_1} M^{\sigma_2} M^{\sigma_3} \dots M^{\sigma_n}$

Gauge Freedom: $\underline{M^{\sigma_1}} \underline{U U^\dagger} M^{\sigma_2} M^{\sigma_3} \dots M^{\sigma_n}$

Q: How should we use our gauge freedom?

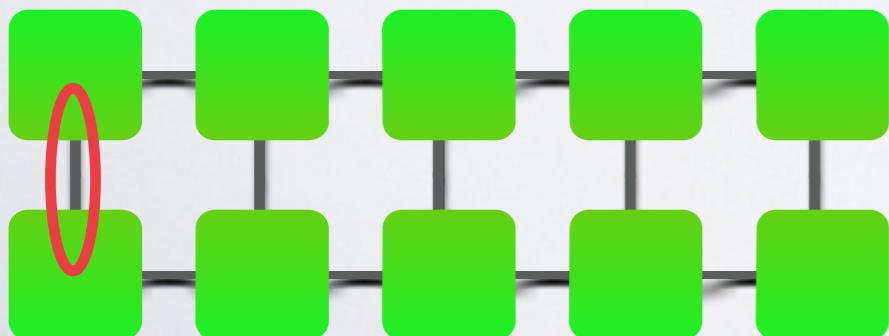
$$\begin{array}{c}
 8 \times 4 \\
 \boxed{M^\downarrow} \\
 4 \times 4 \\
 \boxed{M^\uparrow} \\
 4 \times 4
 \end{array}
 =
 \begin{array}{c}
 \boxed{U^\downarrow} \\
 \boxed{U^\uparrow} \\
 U \quad D \quad V \\
 (8 \times 4) \quad (4 \times 4) \quad (4 \times 4)
 \end{array}$$

SVD

$$\begin{array}{c}
 \boxed{U^\downarrow} \quad \boxed{U^\uparrow} \\
 4 \times 8 \\
 \boxed{U^\downarrow} \\
 \boxed{U^\uparrow} \\
 8 \times 4
 \end{array}
 = I_{4 \times 4}$$

$$U^{\uparrow T} U^\uparrow + U^{\downarrow T} U^\downarrow = I$$

(left canonical)



Canonization $\langle \Psi | \sigma_1 \sigma_2 \sigma_3 \dots \sigma_n \rangle = M^{\sigma_1} M^{\sigma_2} M^{\sigma_3} \dots M^{\sigma_n}$

Gauge Freedom: $\underline{M^{\sigma_1}} \underline{U U^\dagger} M^{\sigma_2} M^{\sigma_3} \dots M^{\sigma_n}$

Q: How should we use our gauge freedom?

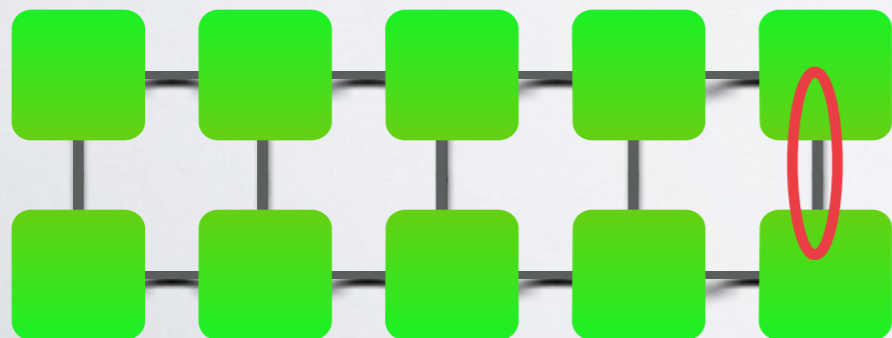
$$\begin{array}{c}
 \begin{array}{|c|c|}
 \hline
 \begin{array}{c} 4 \times 4 \\ M^\uparrow \end{array} & \begin{array}{c} 4 \times 4 \\ M^\downarrow \end{array} \\
 \hline
 \end{array} \\
 \begin{array}{c} 4 \times 8 \end{array}
 \end{array}
 =
 \begin{array}{c}
 U \quad D \quad V \\
 \begin{array}{c} (4 \times 4) \quad (4 \times 4) \quad (4 \times 8) \end{array}
 \end{array}$$

SVD

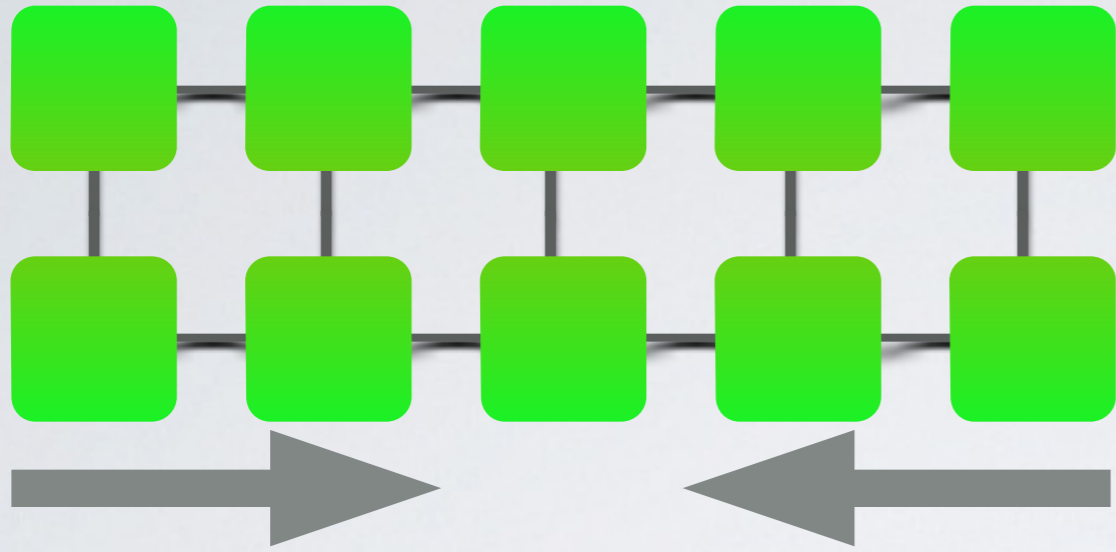
$$\begin{array}{|c|c|}
 \hline
 V^\uparrow & V^\downarrow \\
 \hline
 \end{array}
 \begin{array}{|c|}
 \hline
 V^\downarrow \\
 \hline
 V^\uparrow \\
 \hline
 \end{array}
 = I$$

$$V^\uparrow V^{\uparrow T} + V^\downarrow V^{\downarrow T} = I$$

(right canonical)



Mixed canonical



Matrix Product Operator



$$\langle \sigma_1 \sigma_2 \sigma_3 \sigma_4 \sigma_5 | H | \sigma'_1 \sigma'_2 \sigma'_3 \sigma'_4 \sigma'_5 \rangle$$