ALGORITHMIC PERSPECTIVE ON STRONGLY CORRELATED SYSTEMS

Lecture: Introduction to Matrix Product States

Fall 2015
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Last Time: Exact Diagonalization → Matrix Product States

Today: More Matrix Product States

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

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

$$\sum_{\sigma_1,\sigma_2,...\sigma_n}\langle\Psi|\sigma_1\sigma_2\sigma_3...\sigma_n\rangle\langle\sigma_1\sigma_2\sigma_3...\sigma_n|\Psi\rangle$$

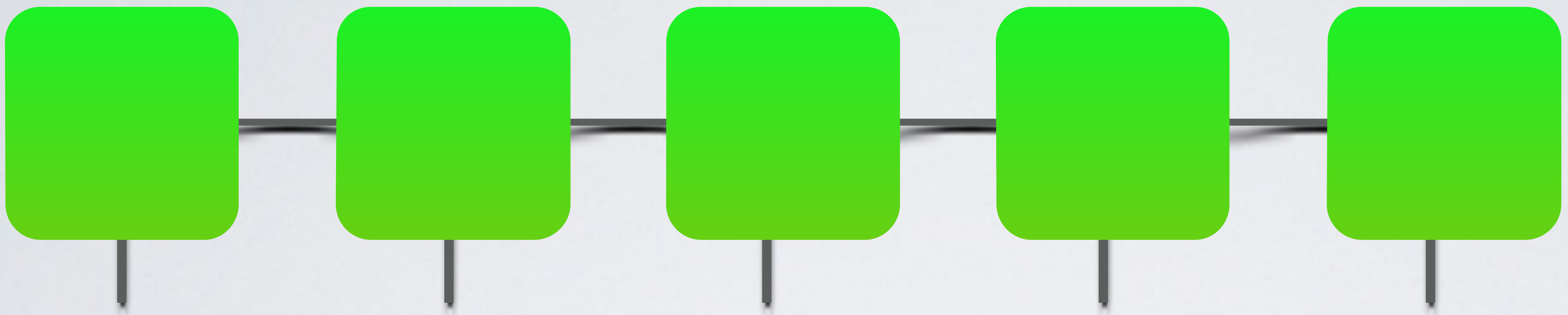
$$= \sum_{\sigma_1,\sigma_2...\sigma_n}(M^{\sigma_1}M^{\sigma_2}M^{\sigma_3}...M^{\sigma_n})(M^{\sigma_1}M^{\sigma_2}M^{\sigma_3}...M^{\sigma_n})^T$$

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

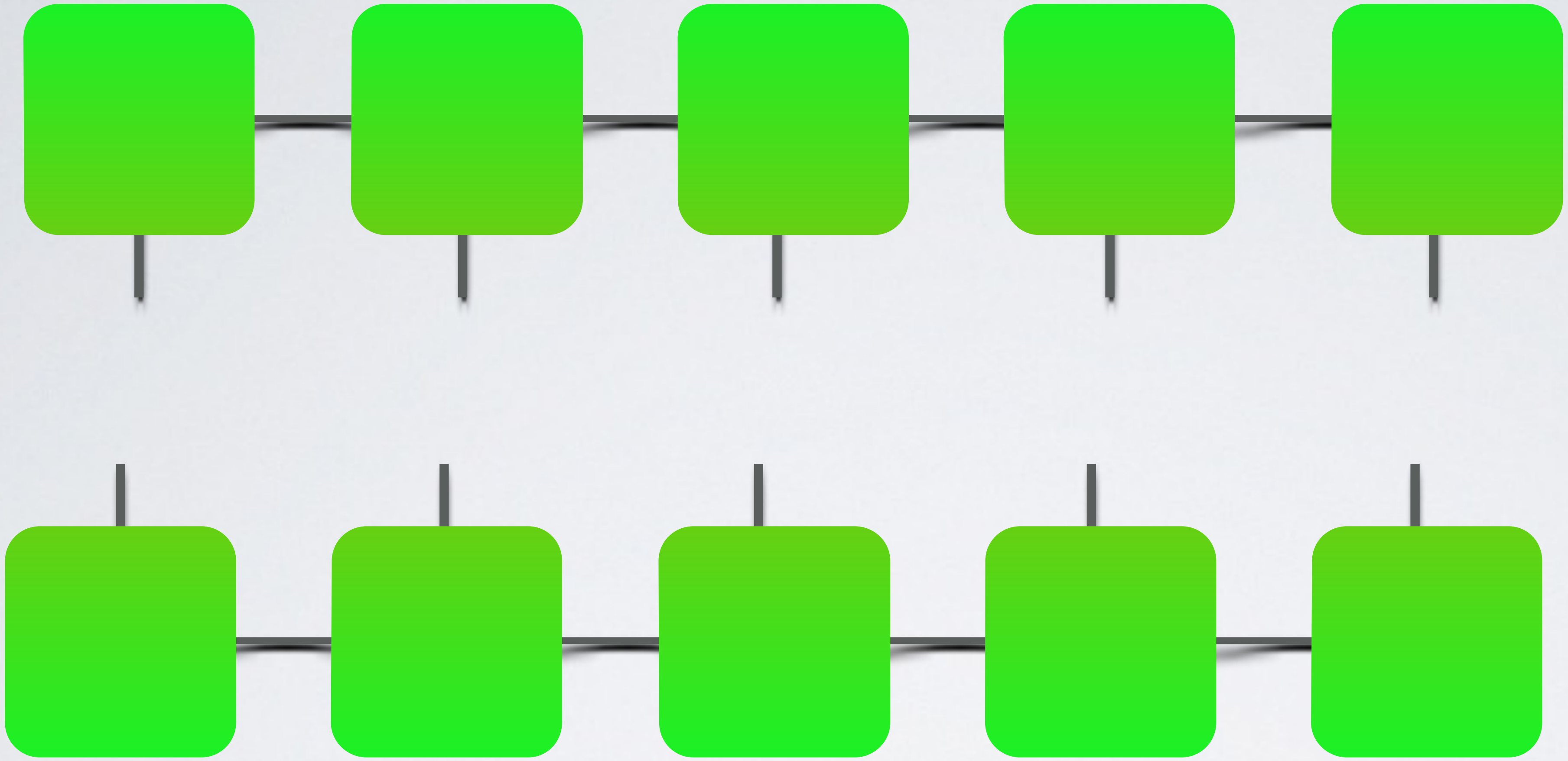
$$= \sum_{\sigma_1,\sigma_2...\sigma_{n-1}} M^{\sigma_1}M^{\sigma_2}M^{\sigma_3}...M^{\sigma_{n-1}}\underbrace{\sum_{\sigma_n}(M^{\sigma_n}M^{\sigma_n T})}_{A}M^{\sigma_{n-1} T}M^{\sigma_{n-2} T}...M^{\sigma_1 T}$$

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

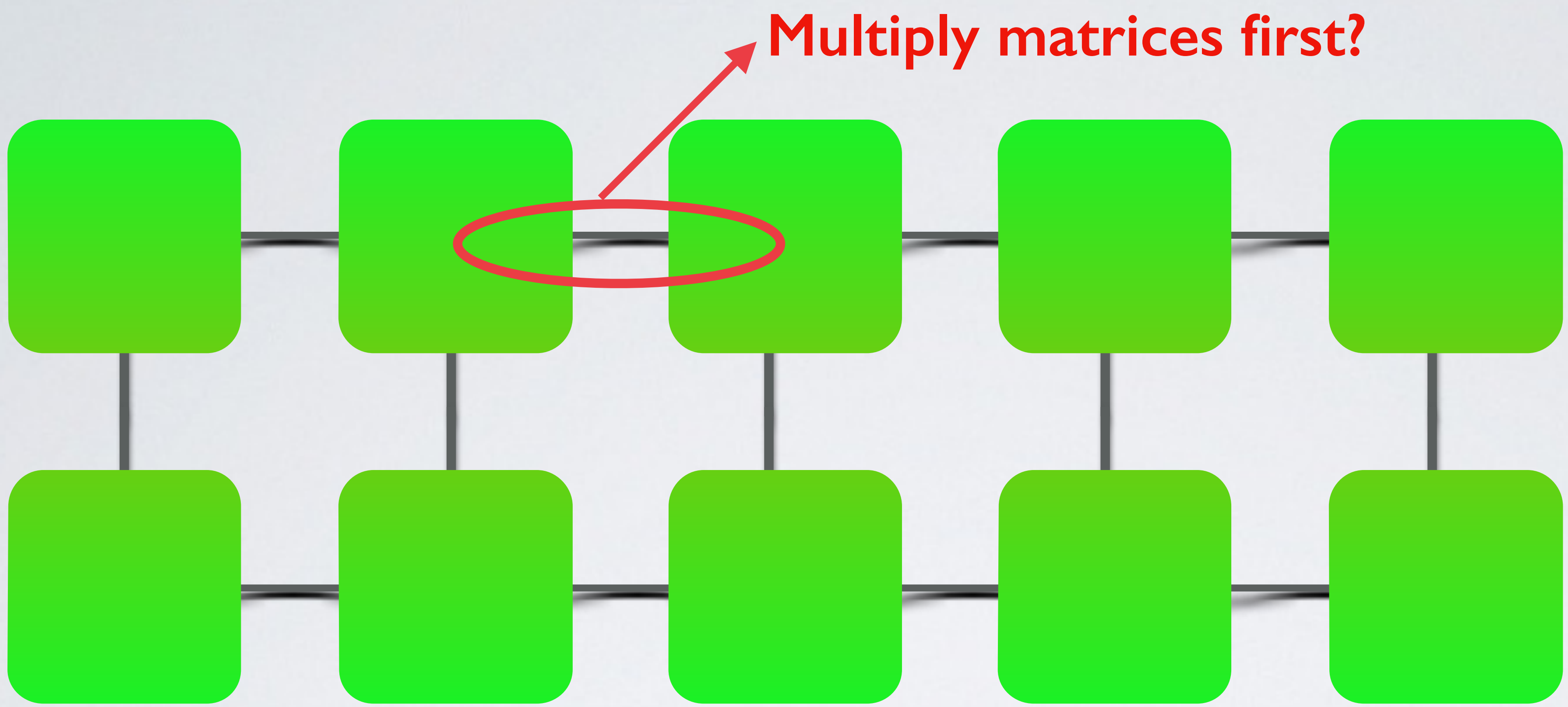
Overlap: $\langle \Psi | \Psi \rangle$



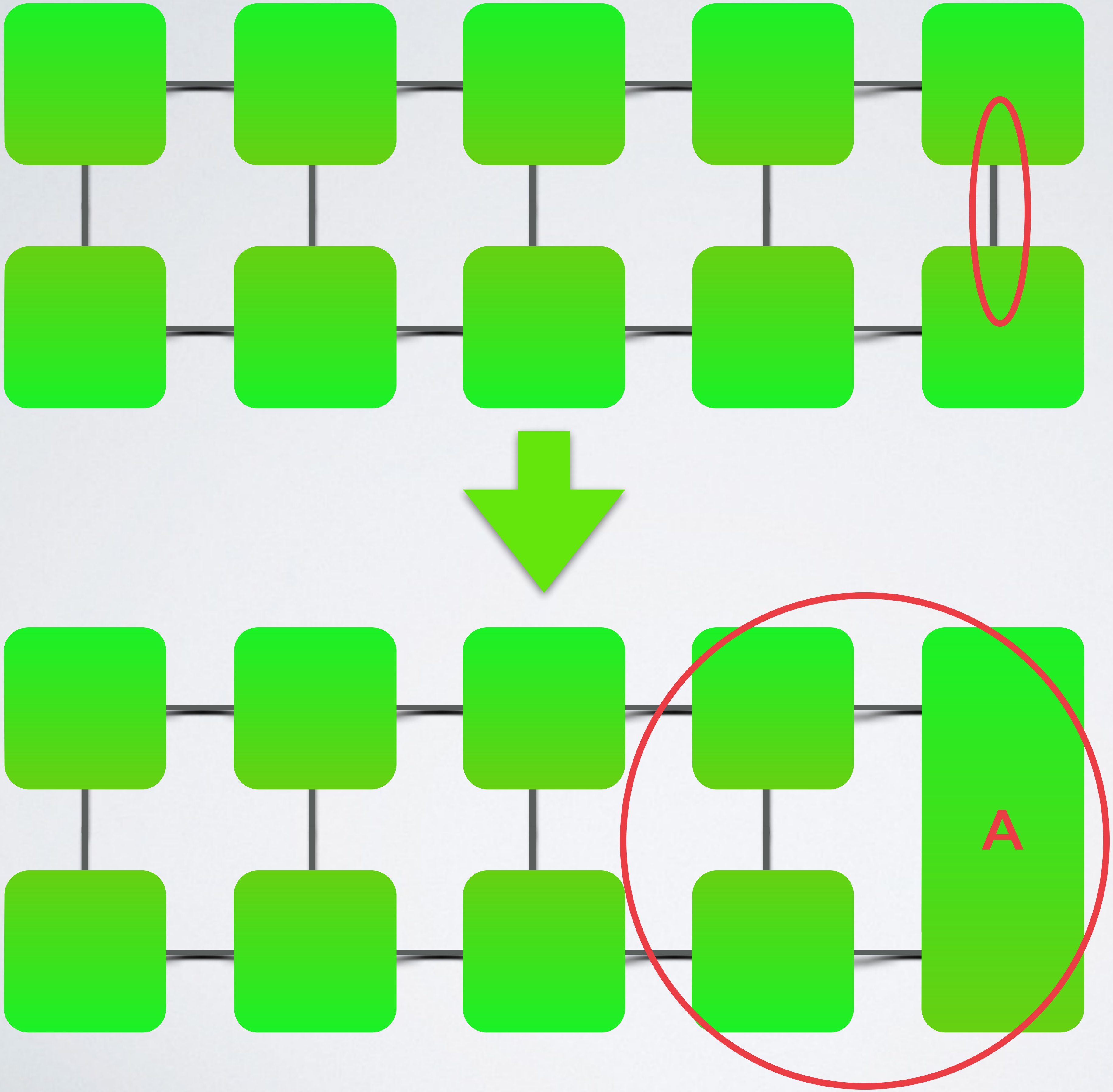
Overlap: $\langle \Psi | \Psi \rangle$



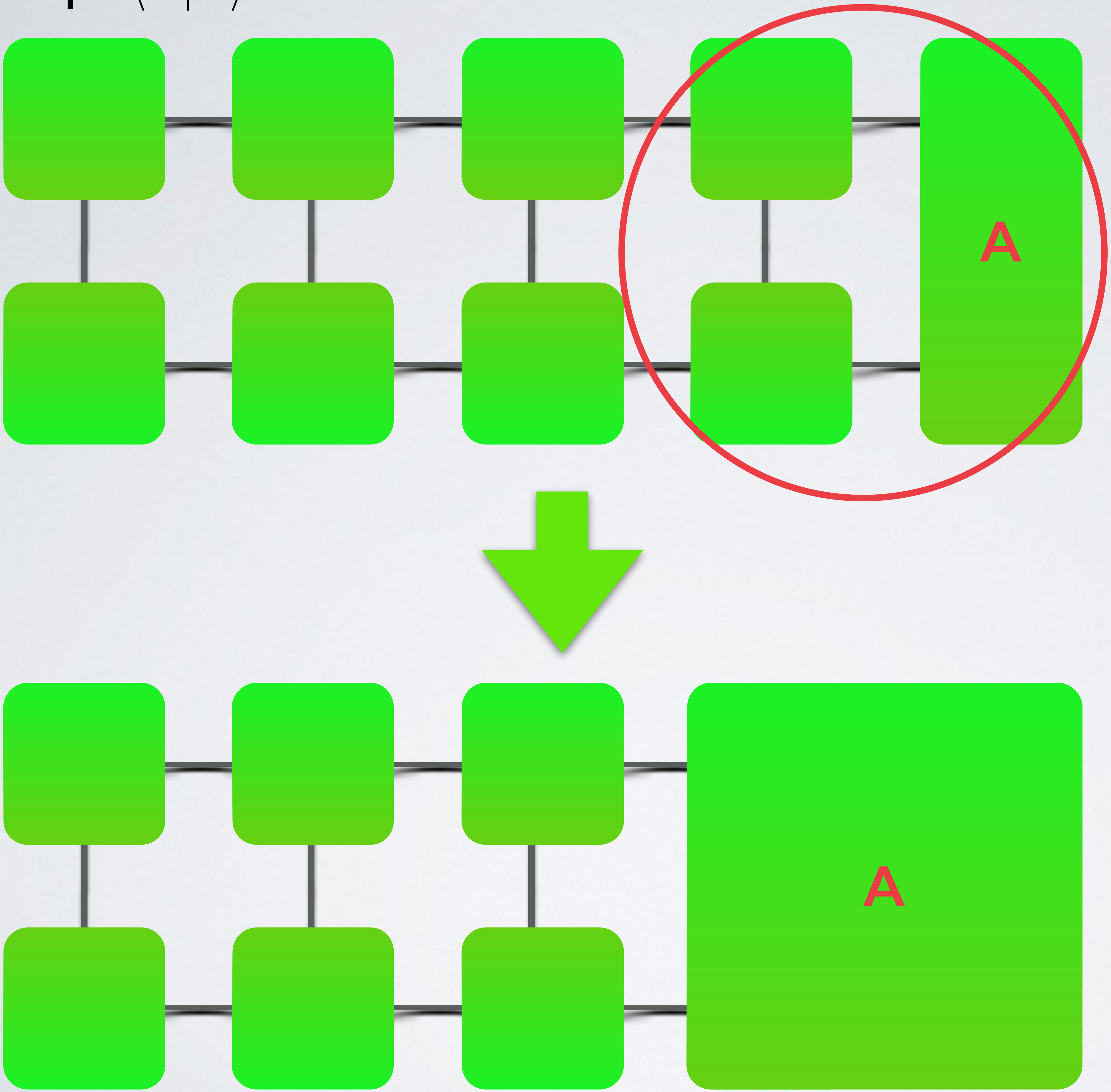
Overlap: $\langle\Psi|\Psi\rangle$



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



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

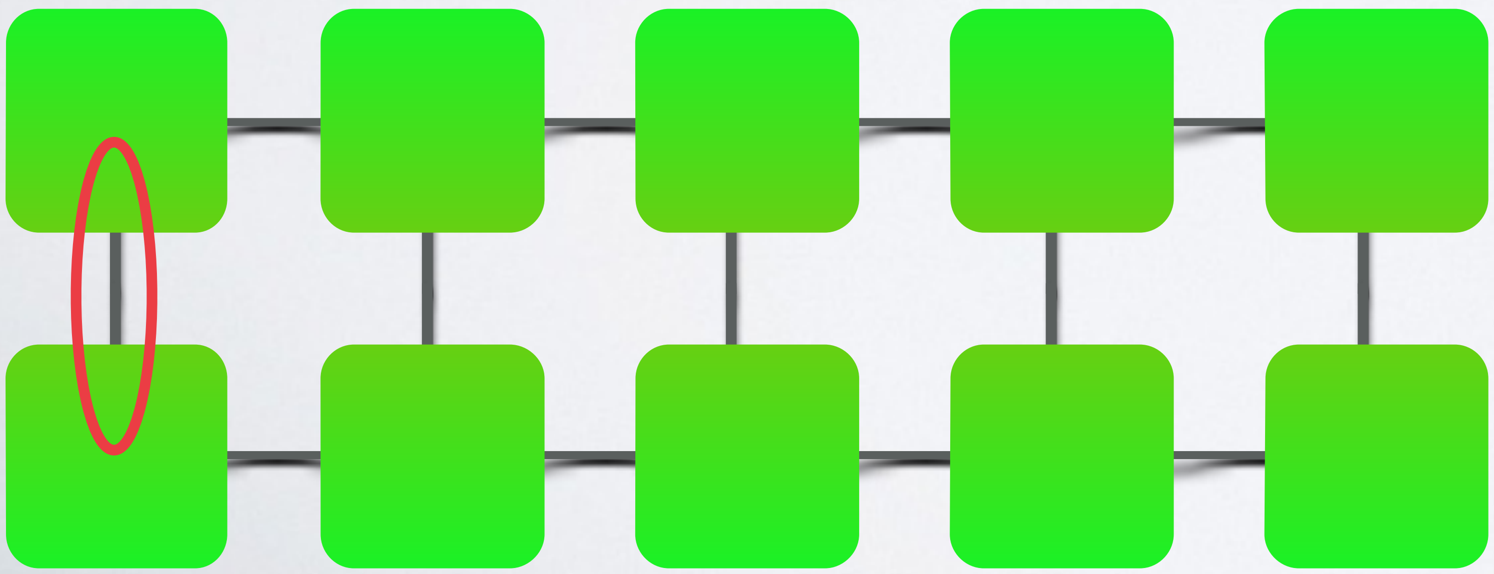


Suppose I want to start in the other direction?

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

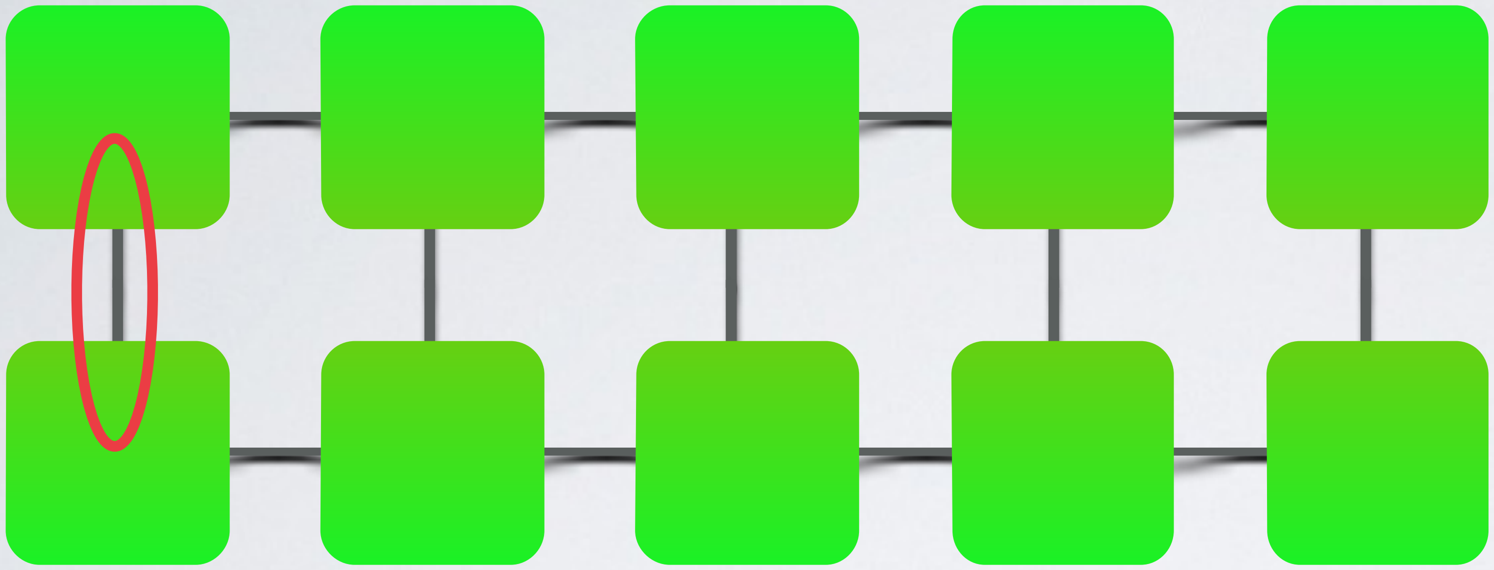
$$Tr\left[\sum_{\sigma_1,\sigma_2\ldots\sigma_n} (M^{\sigma_1} M^{\sigma_2} M^{\sigma_3} \ldots M^{\sigma_n})(M^{\sigma_n T} M^{\sigma_{n-1} T} M^{\sigma_{n-2} T} \ldots M^{\sigma_1 T})\right]$$

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



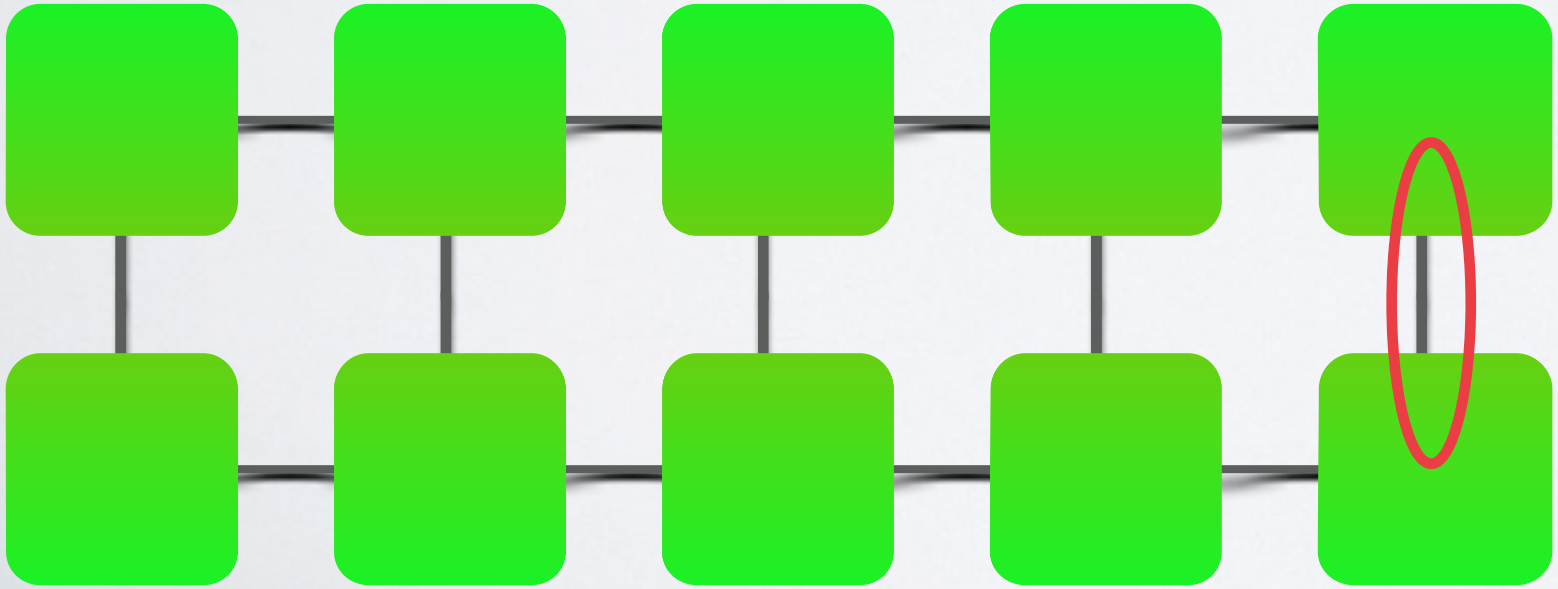
$$Tr\left[\sum_{\sigma_1,\sigma_2\ldots\sigma_n}(M^{\sigma_n T}M^{\sigma_{n-1} T}M^{\sigma_{n-2} T}\ldots M^{\sigma_1 T})(M^{\sigma_1}M^{\sigma_2}M^{\sigma_3}\ldots M^{\sigma_n})\right]$$

A



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

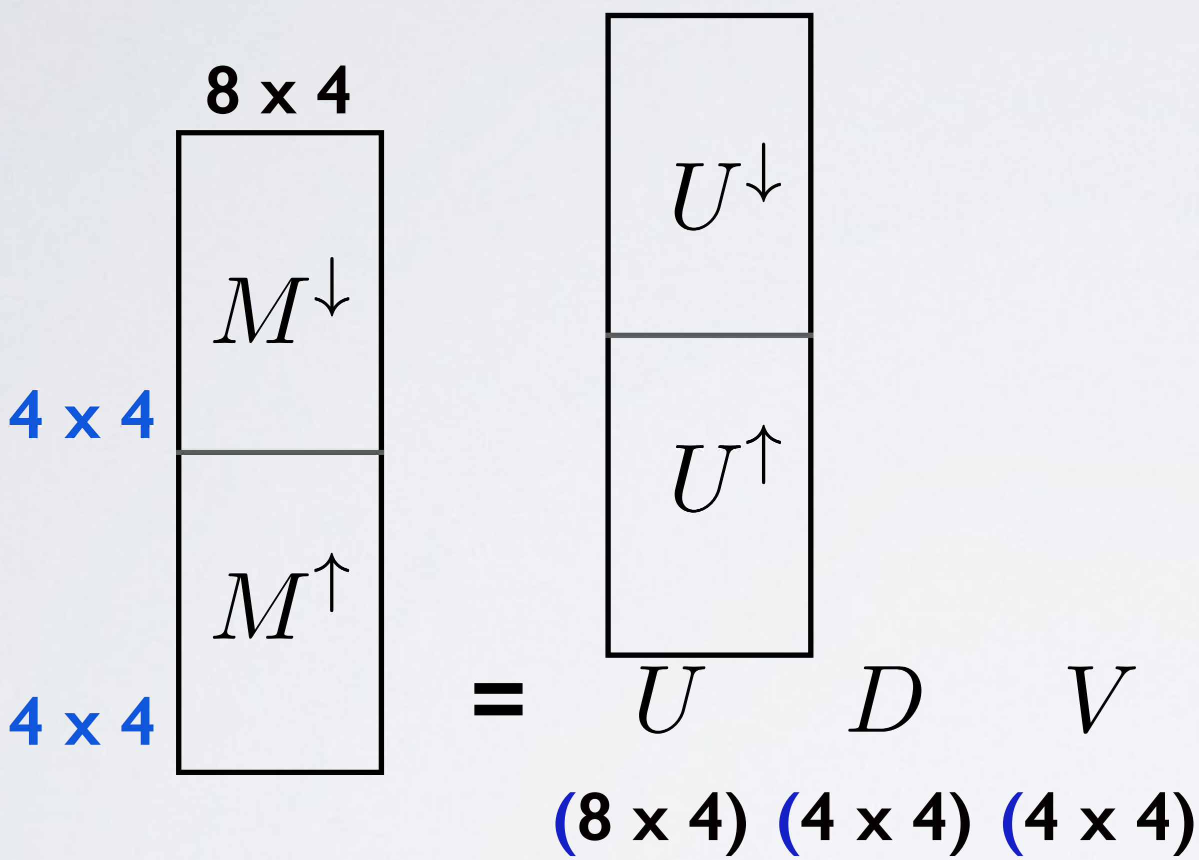
A



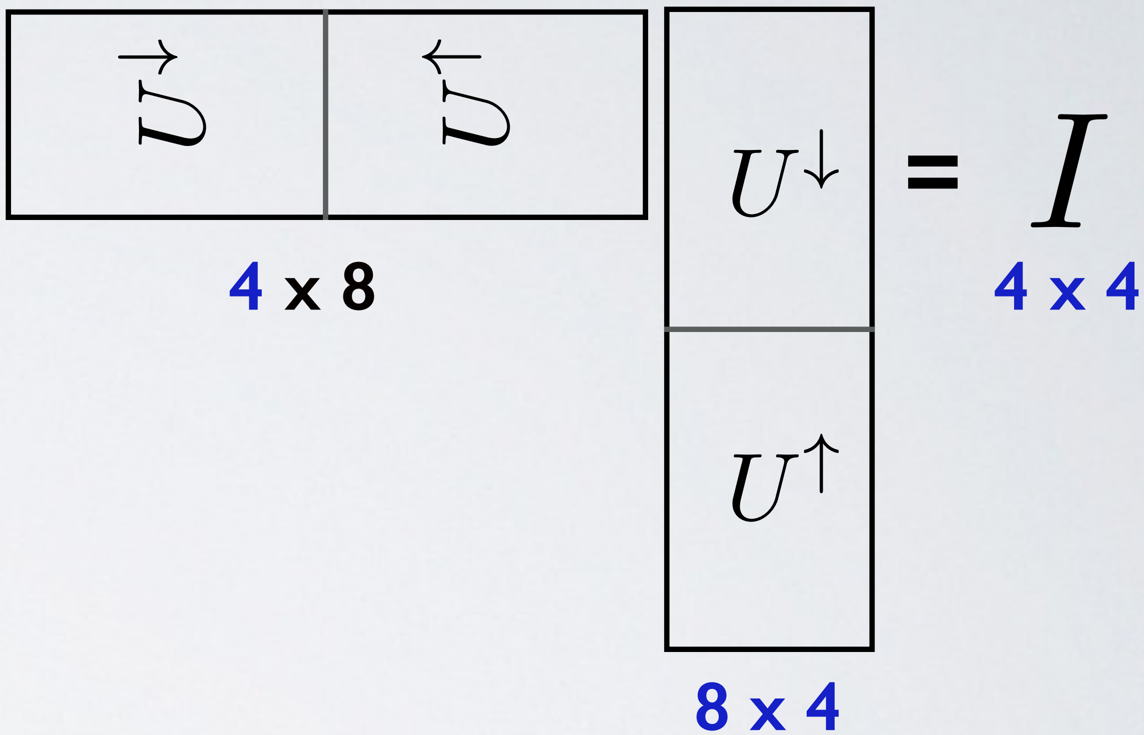
Canonization $\langle\Psi|\sigma_1\sigma_2\sigma_3...\sigma_n\rangle = M^{\sigma_1}M^{\sigma_2}M^{\sigma_3}...M^{\sigma_n}$

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

Q: How should we use our gauge freedom?

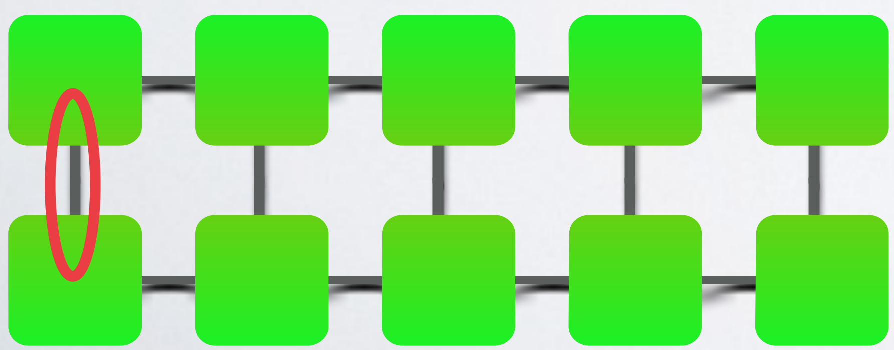


SVD



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

(left canonical)



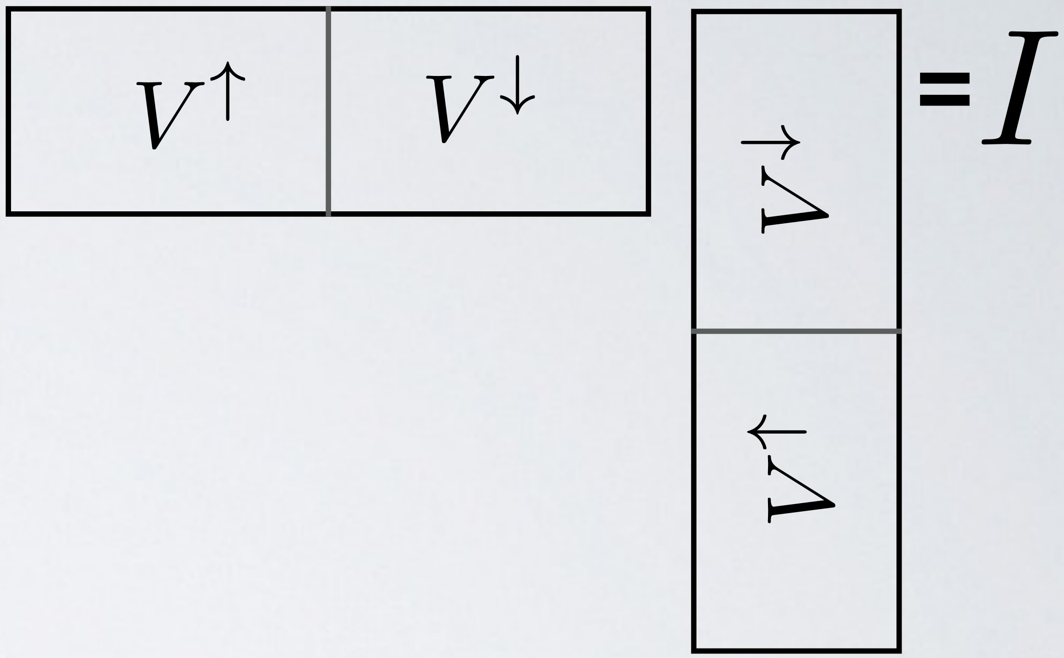
Canonization $\langle \Psi | \sigma_1 \sigma_2 \sigma_3 ... \sigma_n \rangle = M^{\sigma_1} M^{\sigma_2} M^{\sigma_3} ... M^{\sigma_n}$

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

Q: How should we use our gauge freedom?

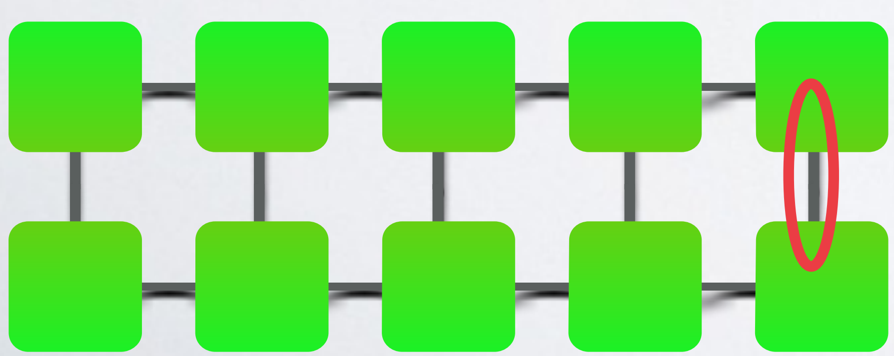
4 x 4	4 x 4				
$M^\uparrow$	$M^\downarrow$	=	U	D	V
4 x 8			(4 x 4)	(4 x 4)	(4 x 8)

SVD

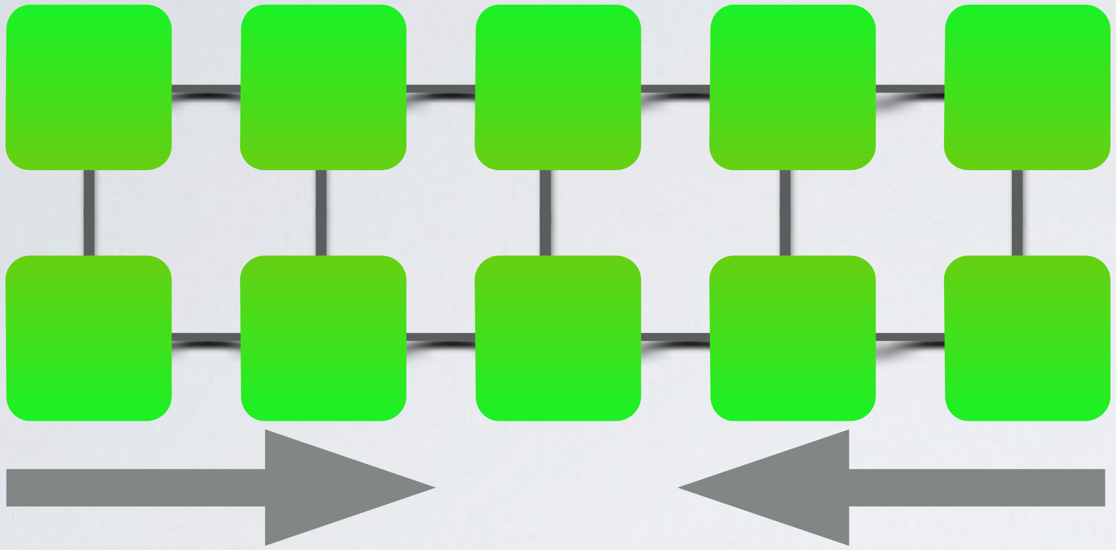


$$V^\uparrow V^{\uparrow T} + V^\downarrow V^{\downarrow T} = I$$

(right canonical)



Mixed canonical



Matrix Product Operator

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