Waterloo
Density Matrix Renormalization Group
WINTER SCHOOL

# Introduction to the Density Matrix Renormalization Group


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Centro de Supercomputación de Galicia

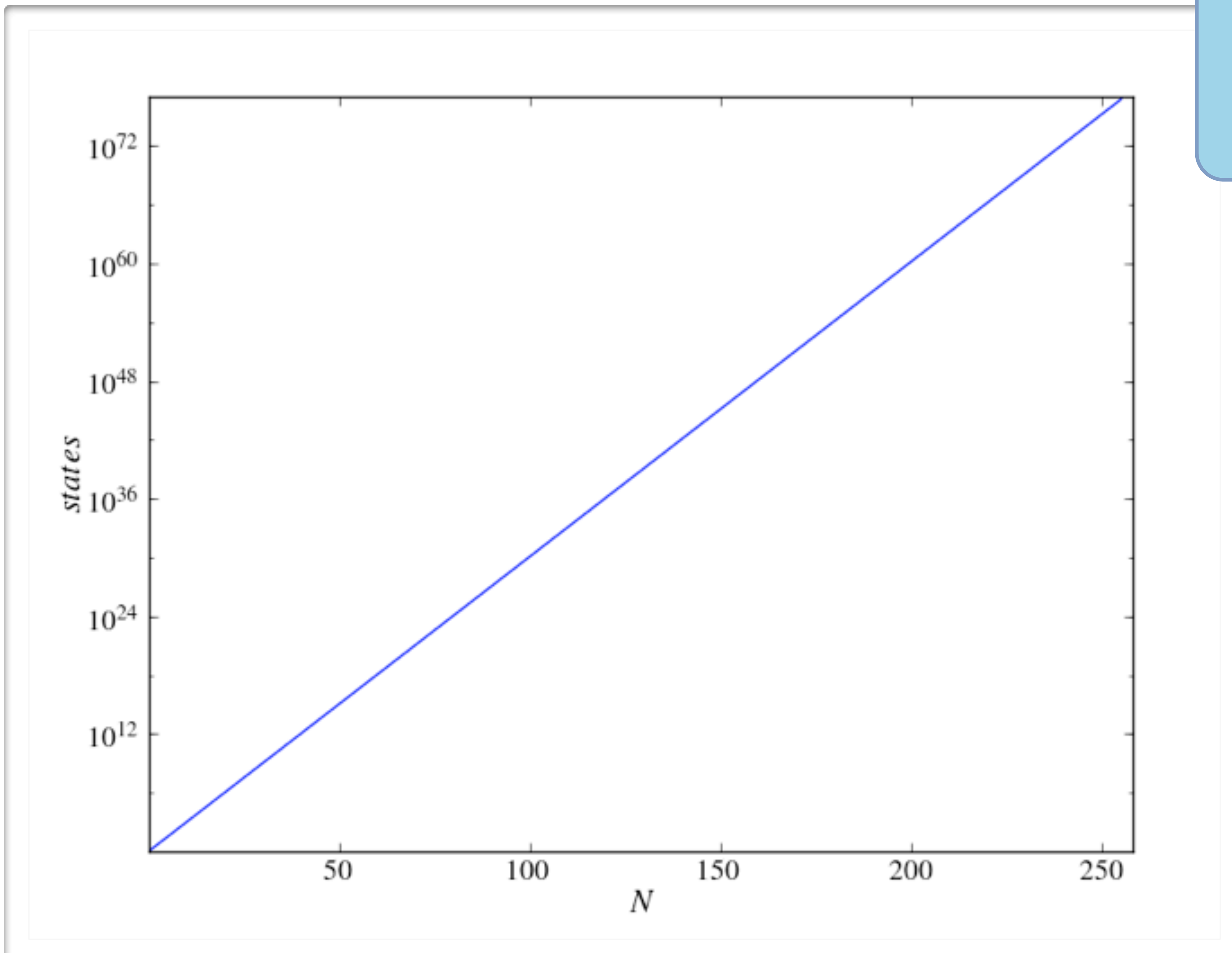

INDY
ULTRA


YDW
C-GNIH

# 1. The problem

# Hilbert space of spin systems

$$2^N$$



# Hilbert space of spin systems

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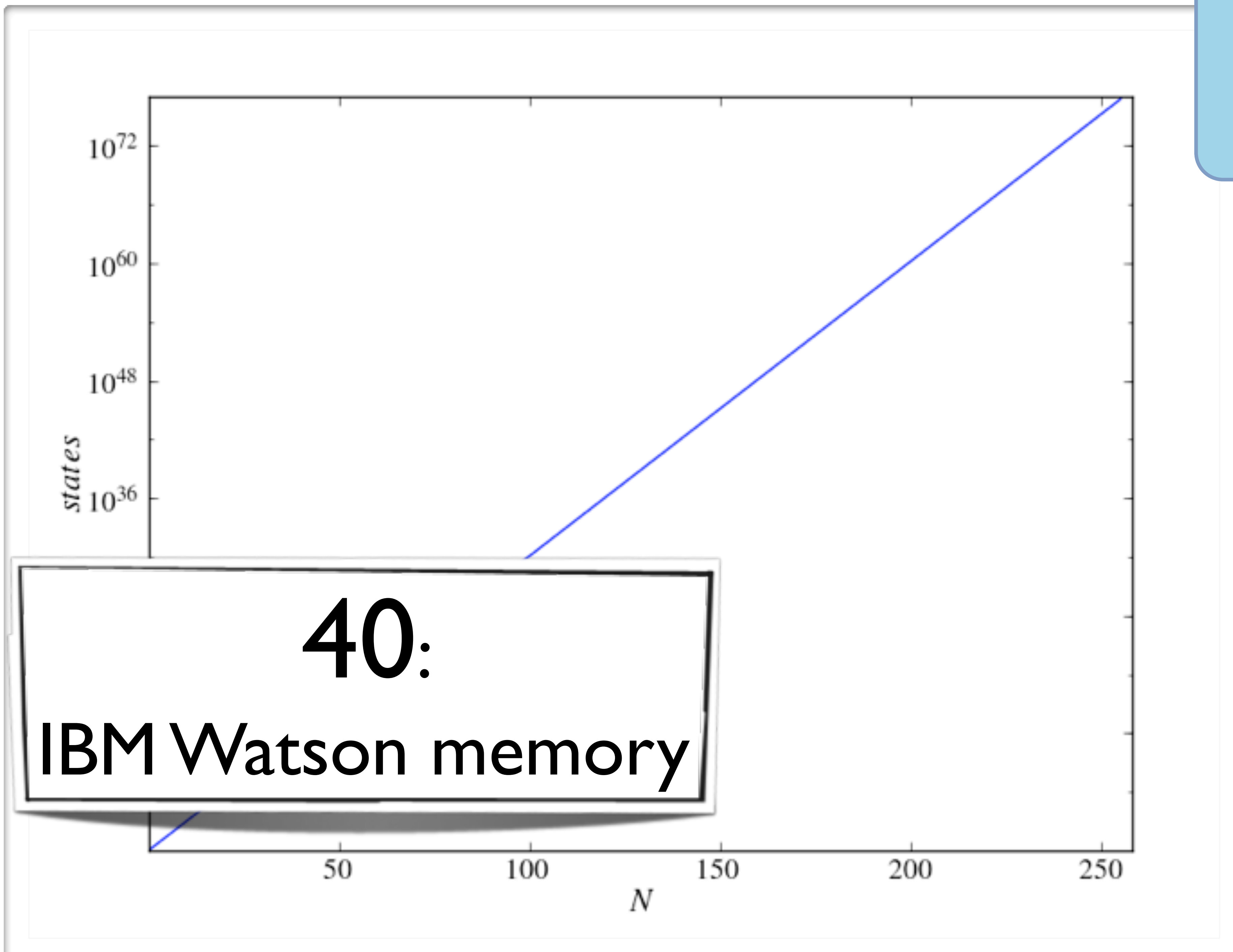
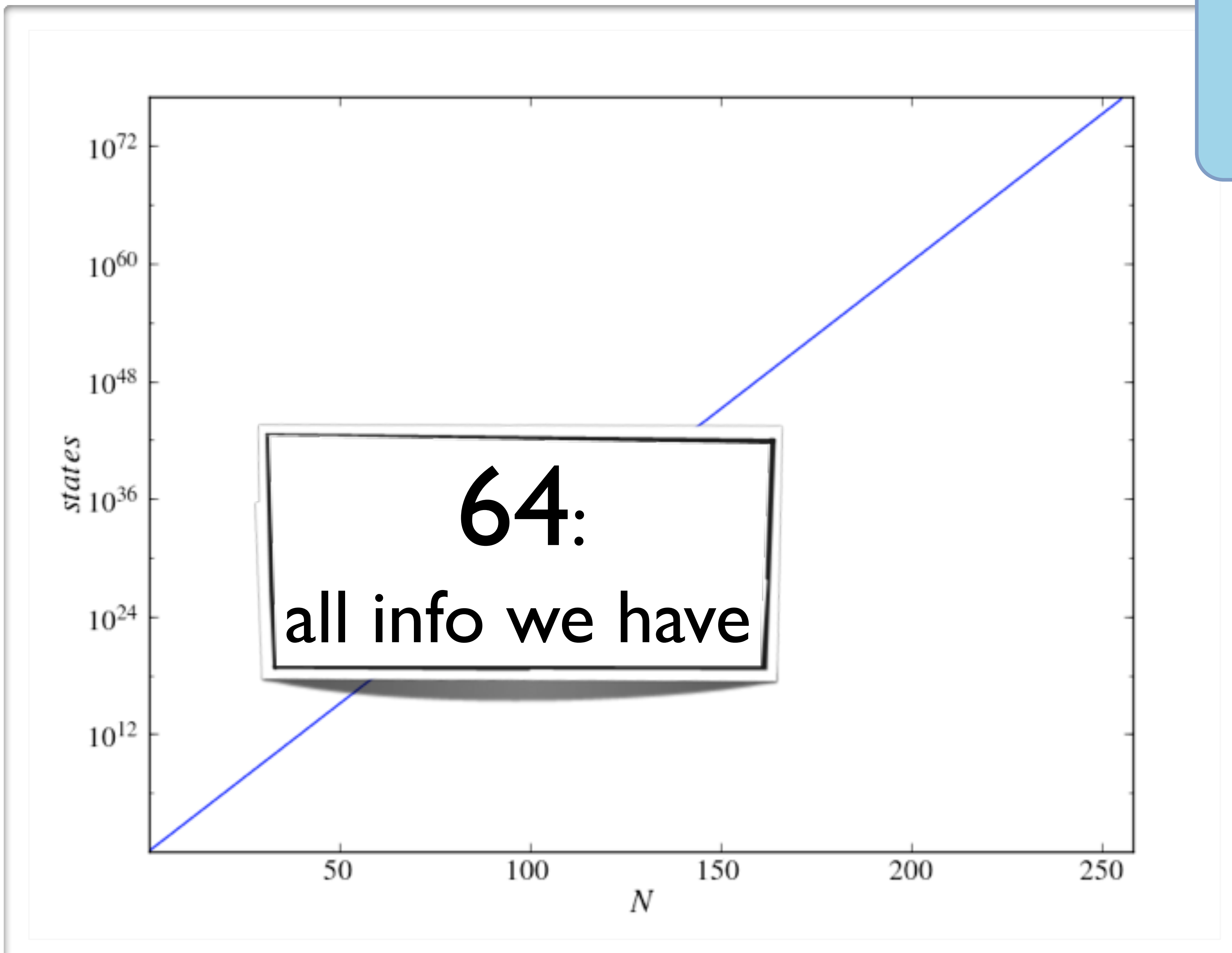



**40**:
IBM Watson memory

# Hilbert space of spin systems

$$2^N$$



# Hilbert space of spin systems

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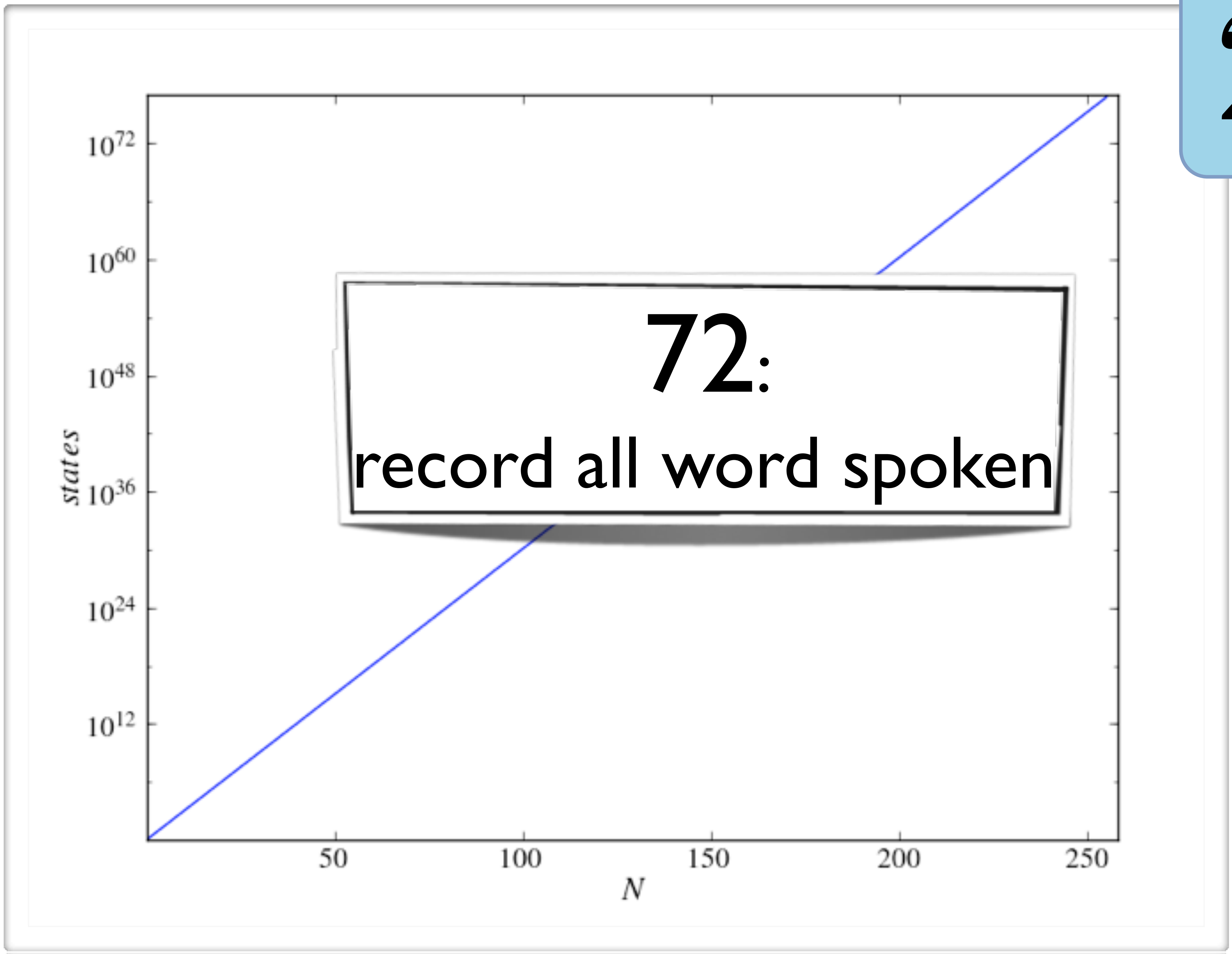


**72**:
record all word spoken

# Hilbert space of spin systems

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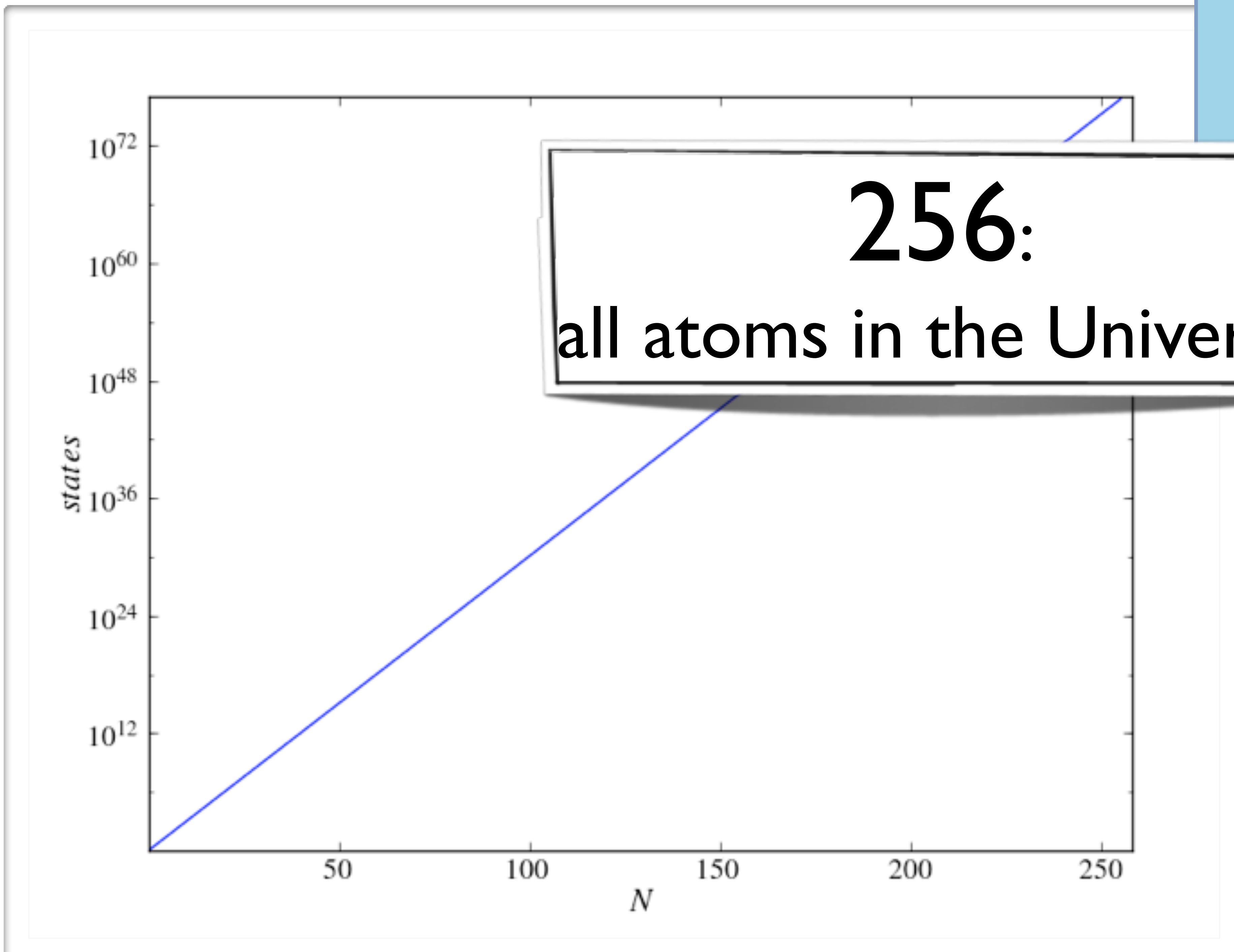


**256**:
all atoms in the Universe

# Dealing with huge Hilbert spaces

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- ED: Ignore and solve small

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- QMC: Importance sampling

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- ED: Ignore and solve small
- QMC: Importance sampling
- RG: Truncate

There are some states of some systems for which the relevant piece of the Hilbert space is small

ground states!

There are s[illegible]es of some systems for which the relevan[illegible] piece of the Hilbert space is small

ground states!

relevant

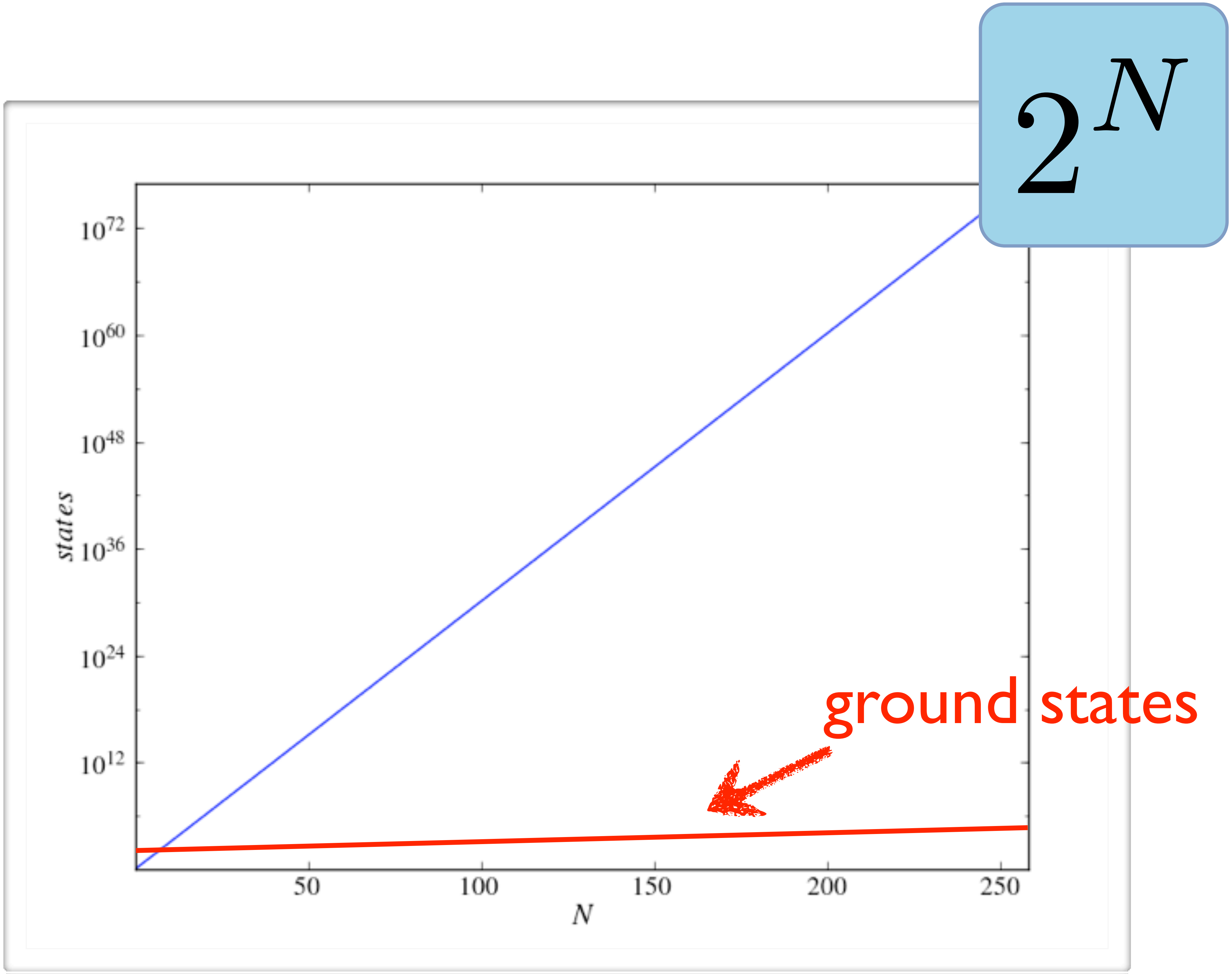
There are s[illegible]es of some systems for which the releva[illegible] piece of the Hilbert space is small

ground states!

relevant

There are s… es of some systems for which the relevant piece of the Hilbert space is ~~small~~

tiny!



$2^N$
$10^{72}$
$10^{60}$
$10^{48}$
$10^{36}$
$10^{24}$
$10^{12}$
states
ground states
50
100
150
200
250
N

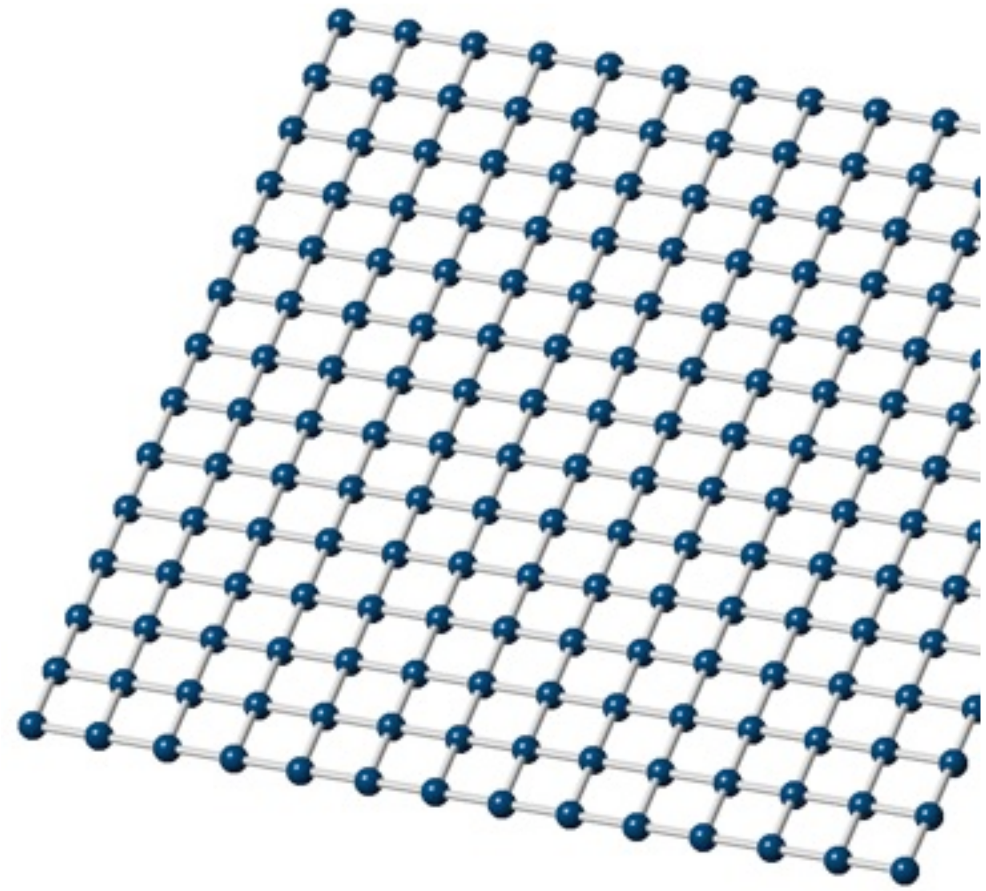
DMRG finds this small piece of the Hilbert space

DMRG finds this small piece of the Hilbert space

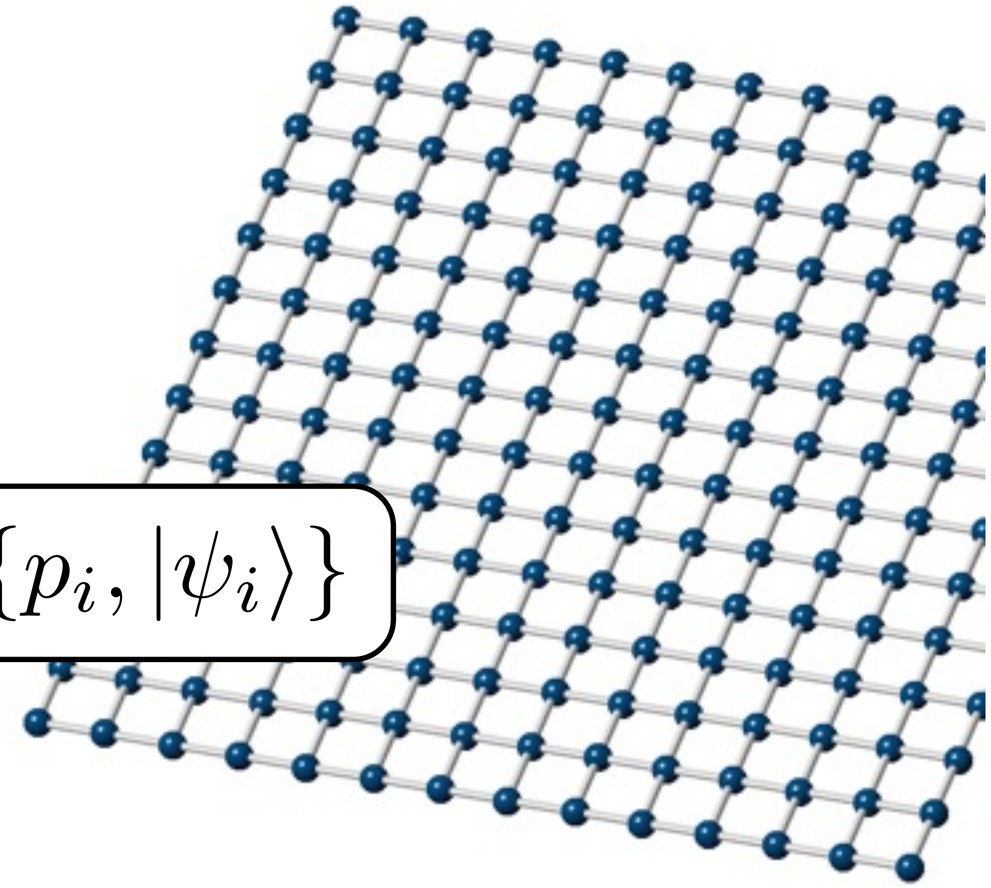
(so you can use ED to solve the problem)

# II. The Basics

# Density Matrix operator



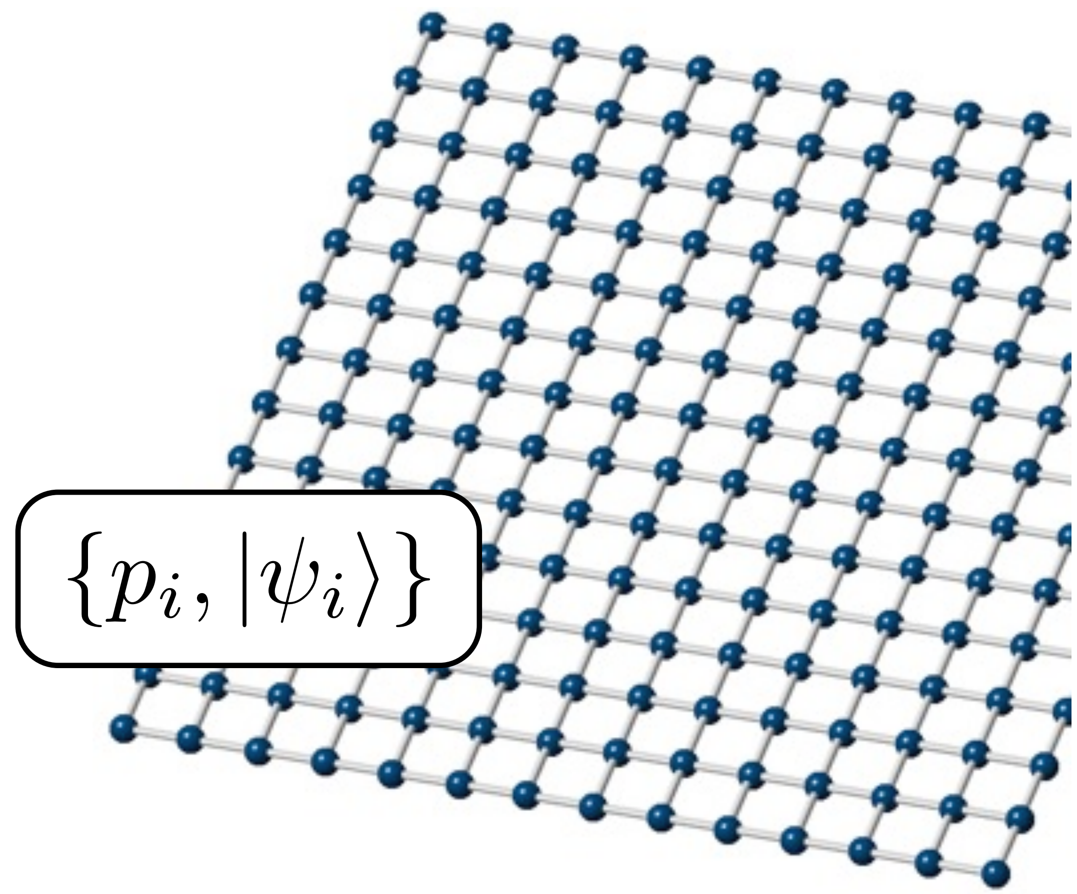
# Density Matrix operator



$$\{p_i, |\psi_i\rangle\}$$

# Density Matrix operator

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$



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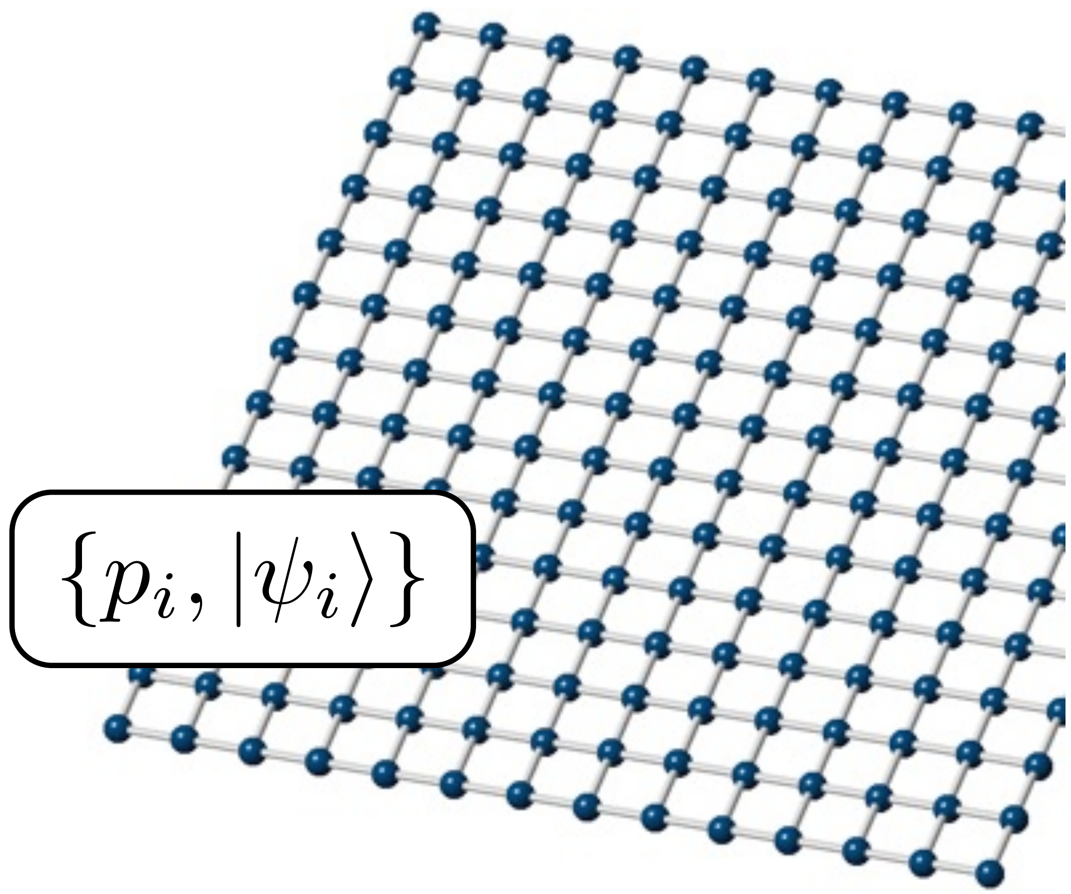


Observables:

$$\langle\mathcal{O}\rangle = tr(\rho\mathcal{O}) = \sum_i p_i \langle\psi_i|\mathcal{O}|\psi_i\rangle$$

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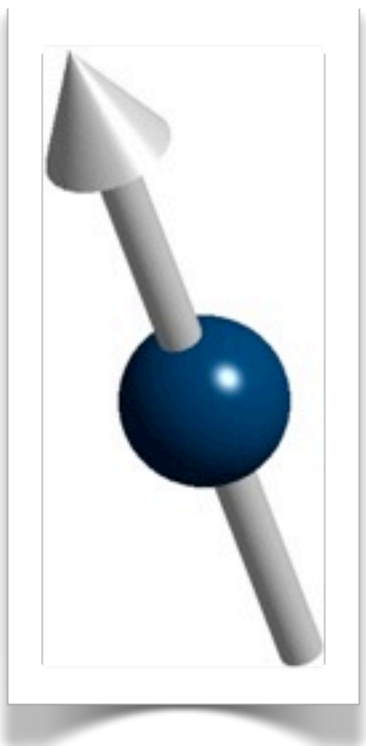

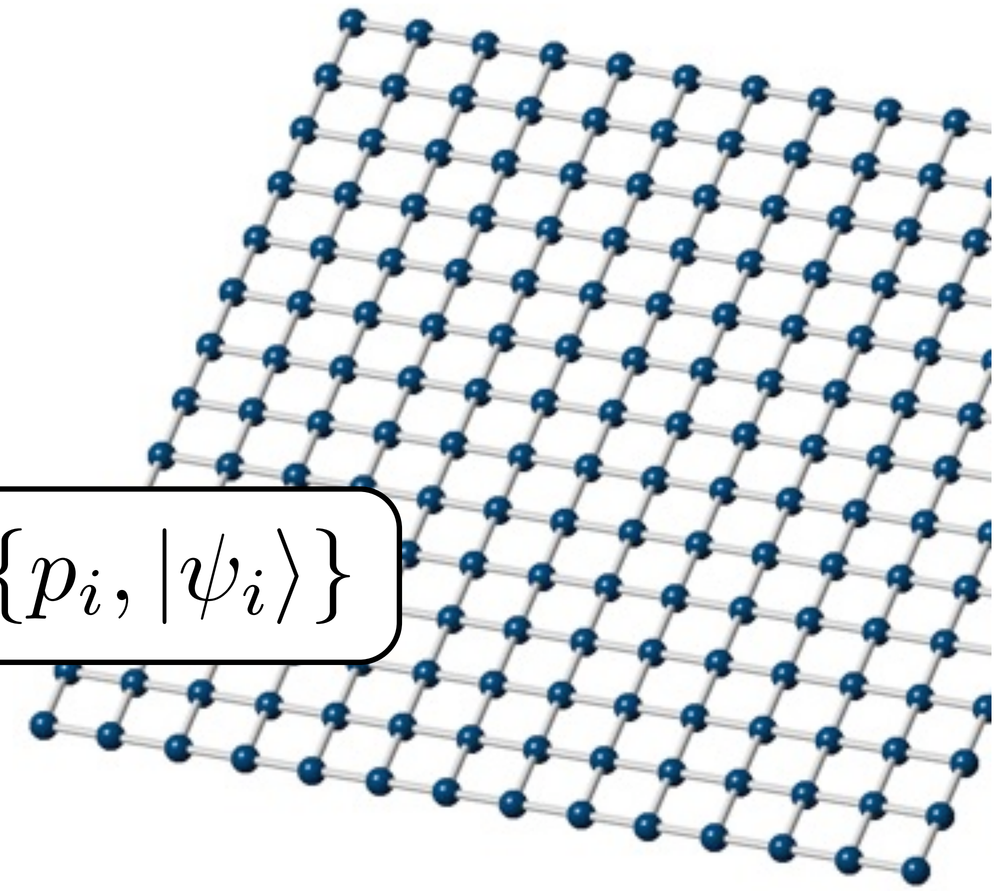

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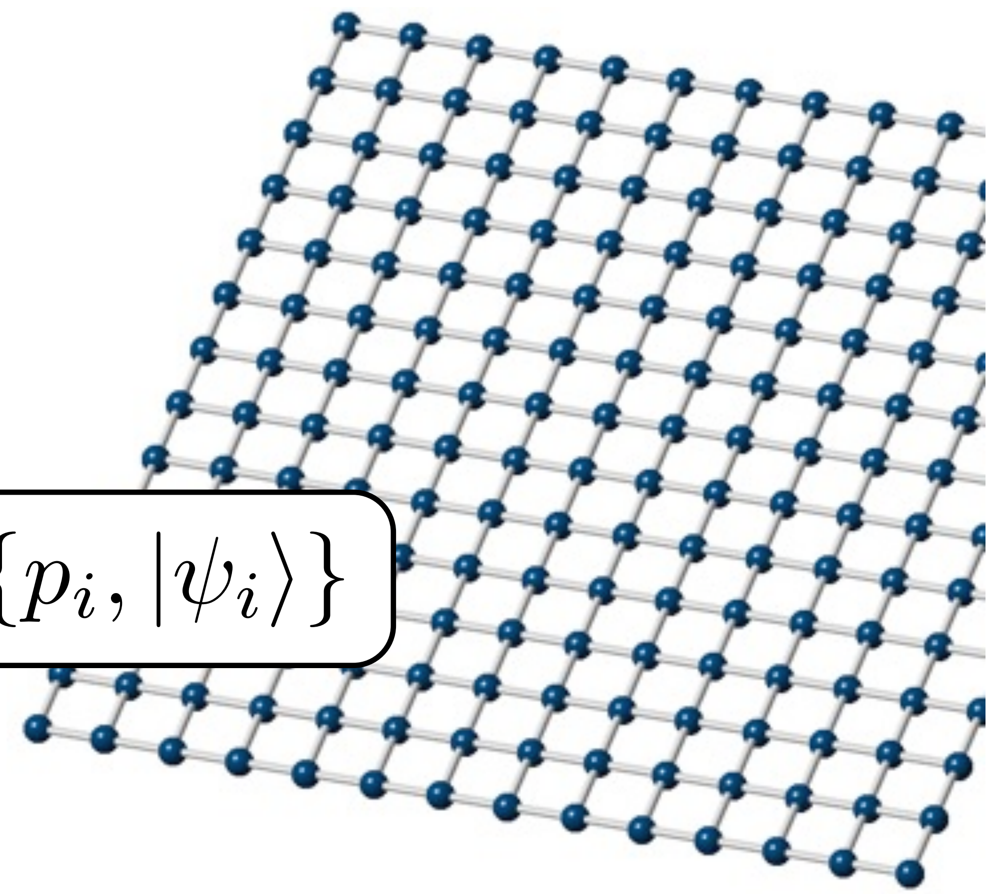

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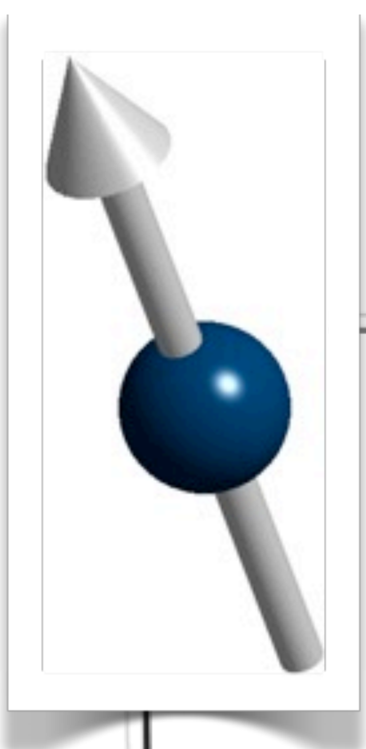

$$|\psi\rangle = \frac{1}{2}\left(|\downarrow\rangle - \sqrt{3}|\uparrow\rangle\right)$$

# Density Matrix operator

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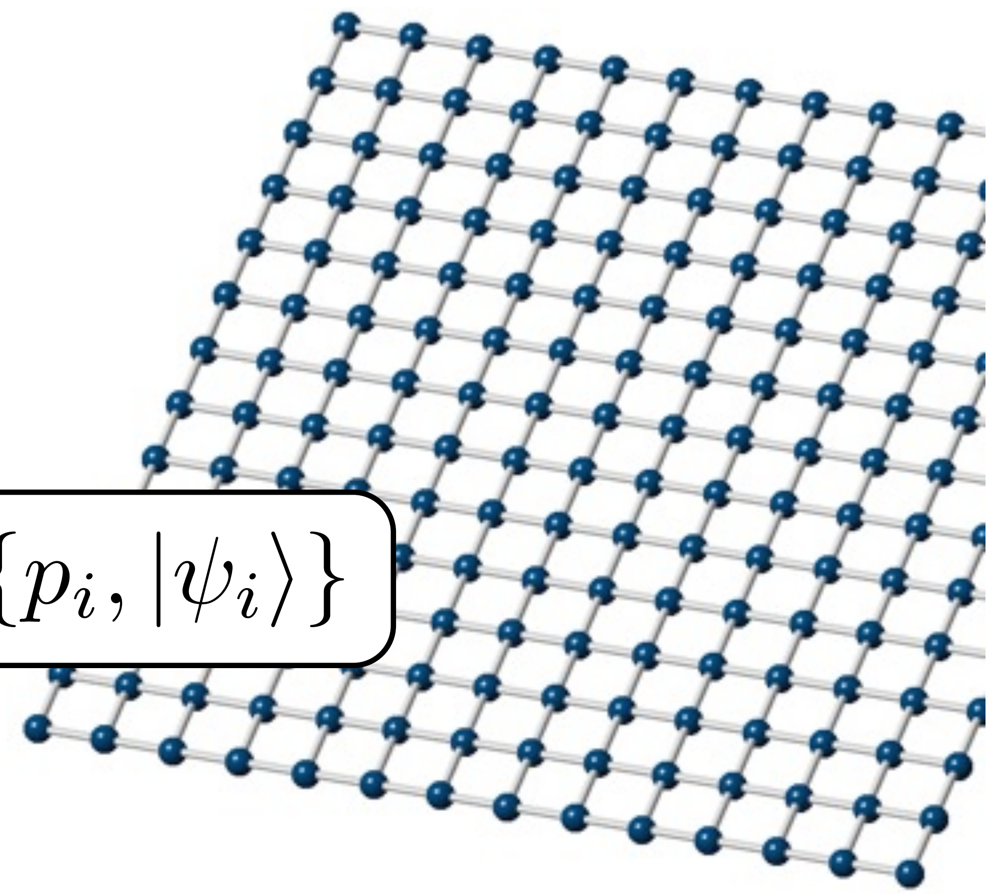
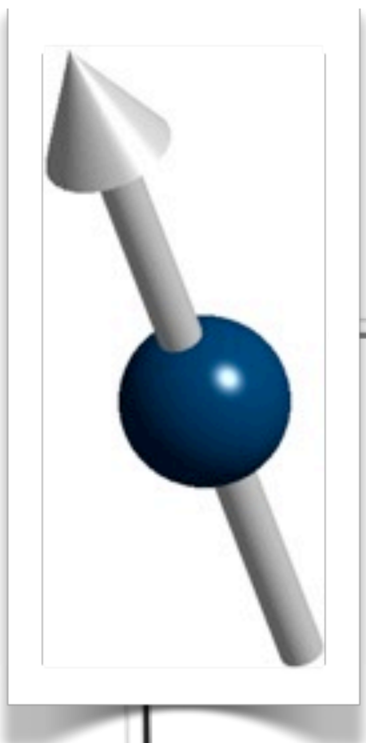


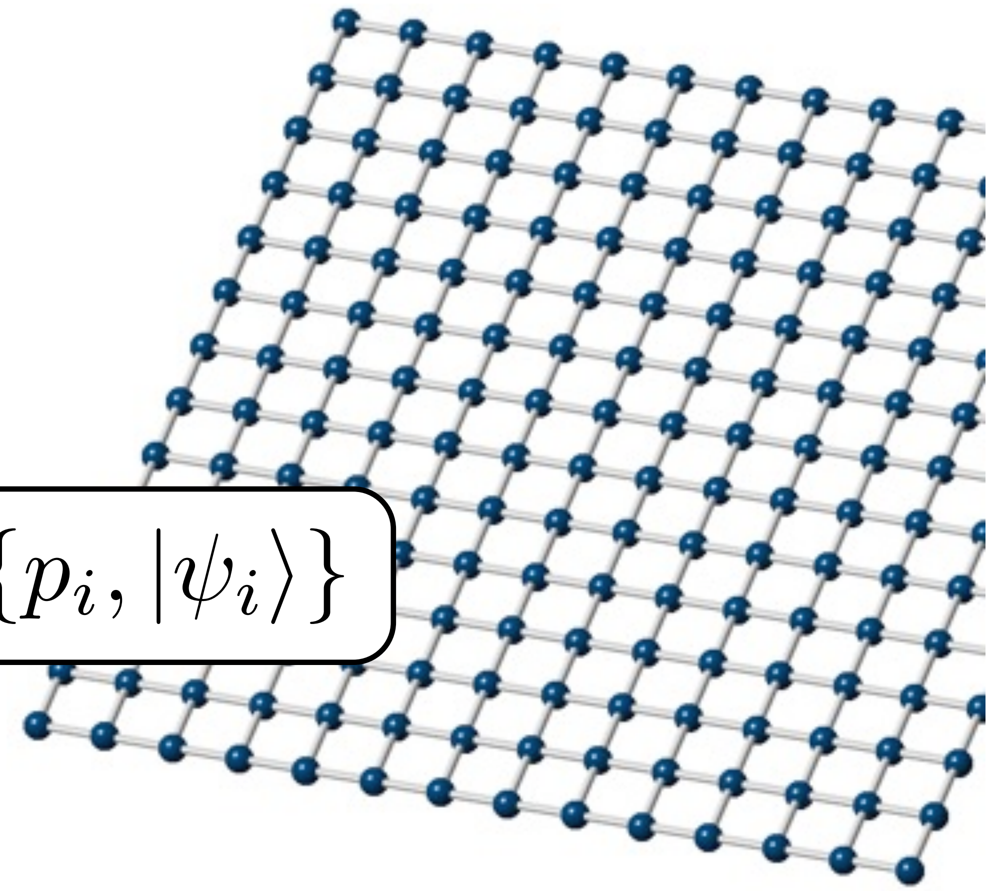
$\{p_i, |\psi_i\rangle\}$



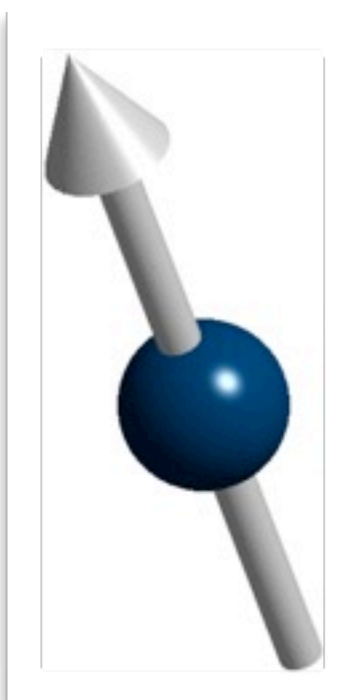
$$\rho = |\psi\rangle\langle\psi| = \frac{1}{4}\left(|\downarrow\rangle - \sqrt{3}|\uparrow\rangle\right)\left(\langle\downarrow| - \sqrt{3}\langle\uparrow|\right)$$

# Density Matrix operator

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$



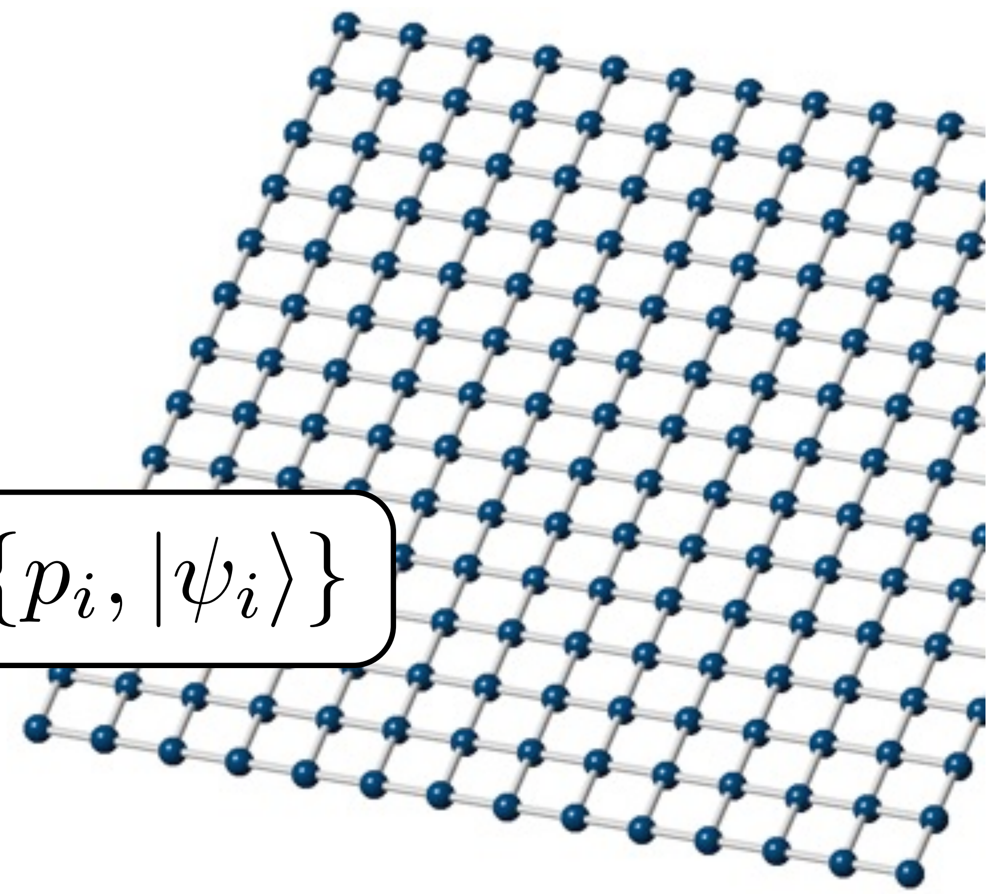
$$\{p_i, |\psi_i\rangle\}$$



$$= \frac{1}{4}\Big(|\downarrow\rangle\langle\downarrow| - \sqrt{3}|\downarrow\rangle\langle\uparrow| - \sqrt{3}|\uparrow\rangle\langle\downarrow| + 3|\uparrow\rangle\langle\uparrow|\Big)$$

# Density Matrix operator

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$



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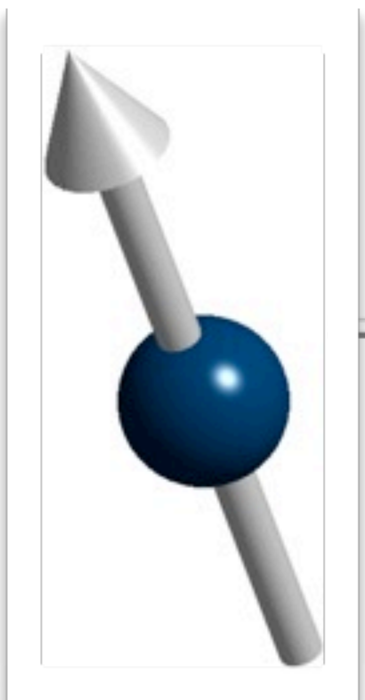

$$\rho = \frac{1}{4}\begin{pmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & 3 \end{pmatrix}$$

# Density Matrix characterization

$\rho$ is a DM iff:

- $tr\rho = 1$
- $\langle\psi|\rho|\psi\rangle \geq 0 \ \forall\psi$

Nielsen & Chuang p. 101

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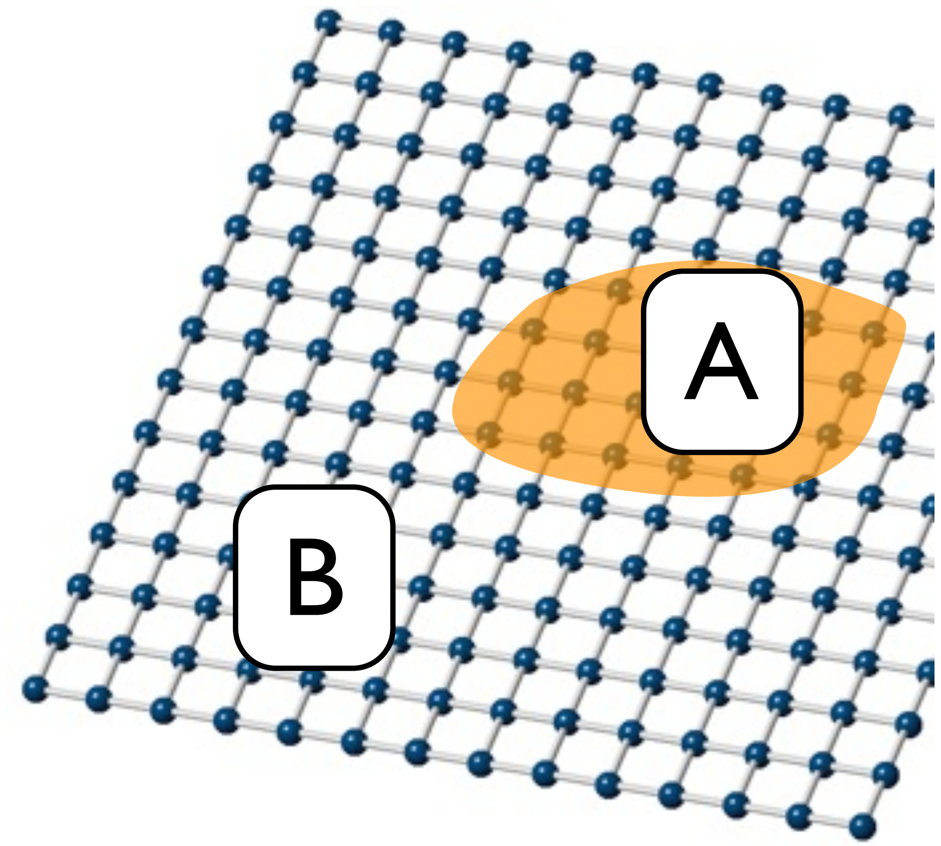
Nielsen & Chuang p. 101

# Reduced density matrix

$$\rho_A = tr_B(\rho_{AB})$$



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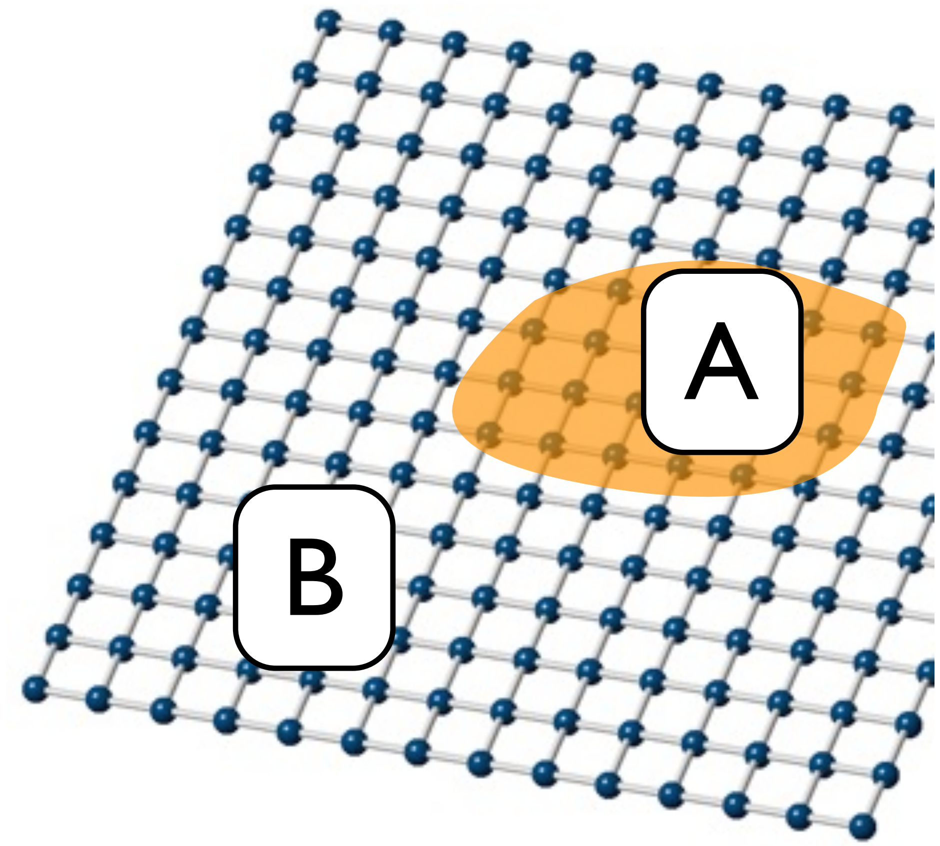
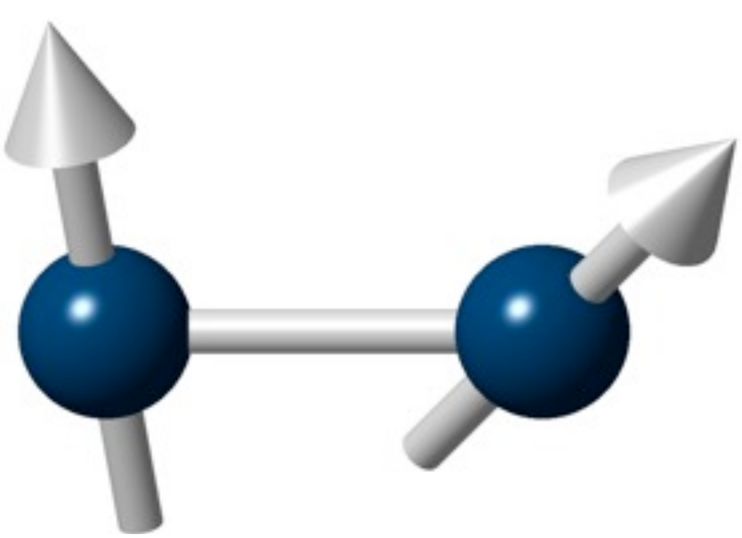



$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$$



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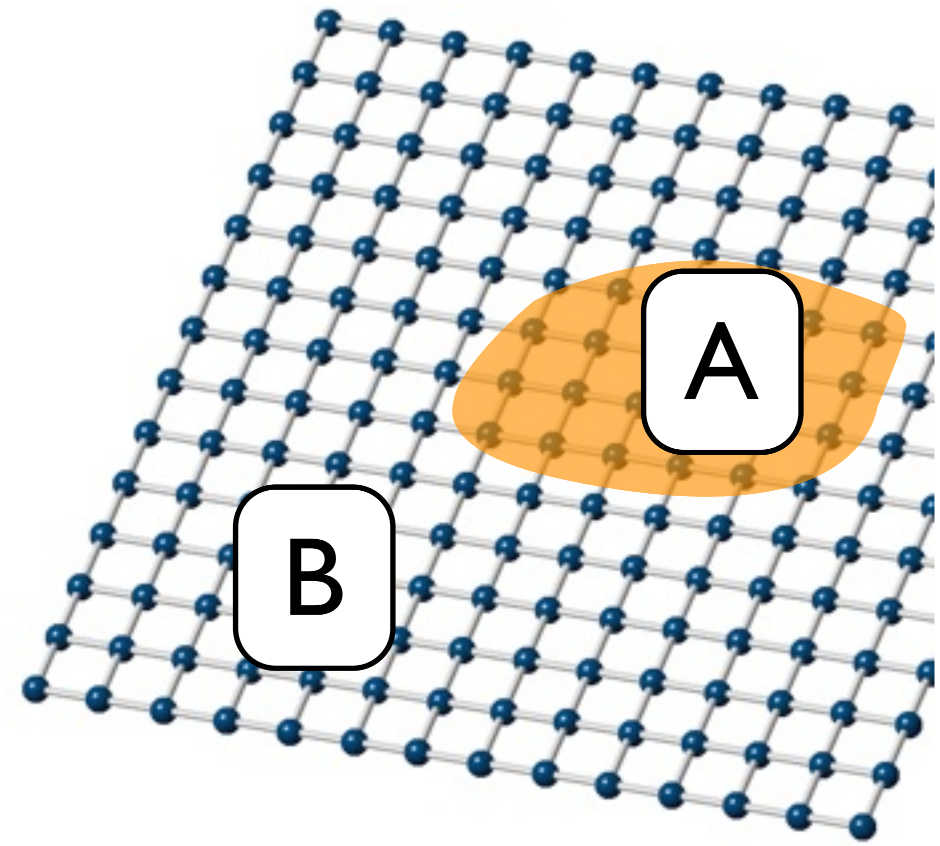


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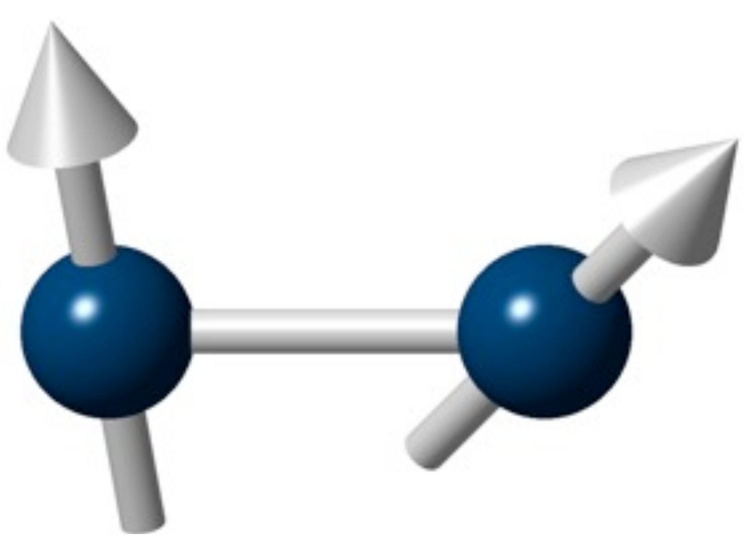

$$\rho_A = tr_B(|\psi\rangle\langle\psi|) = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Best description of part A

# Reduced density matrix

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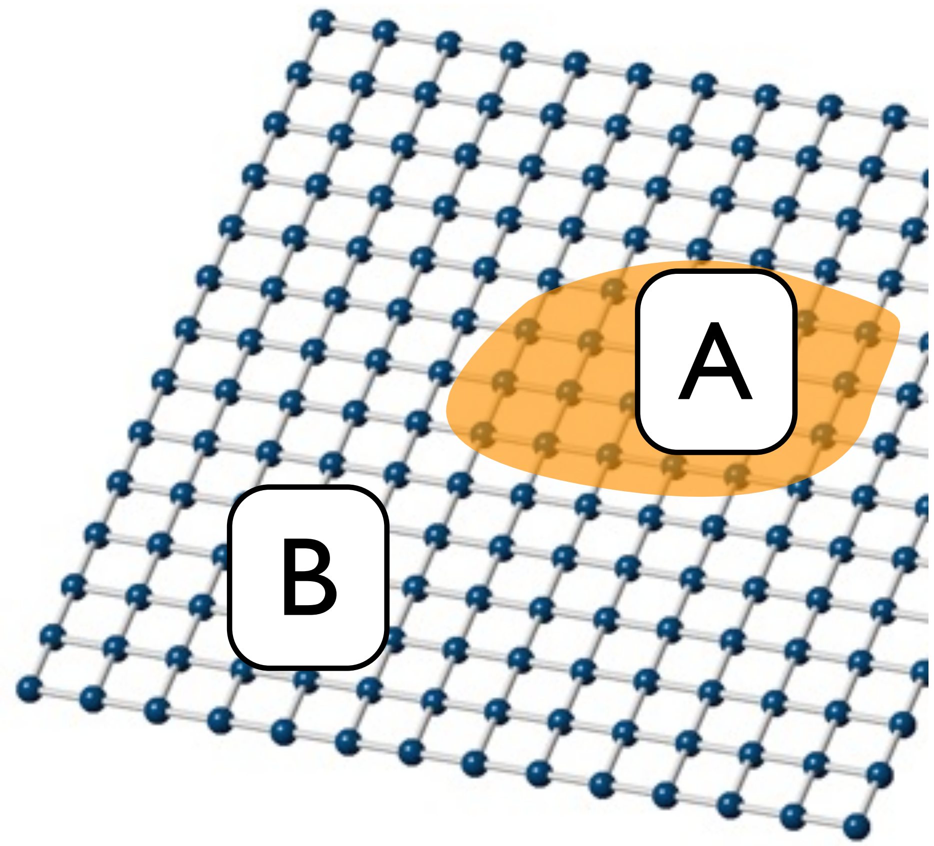


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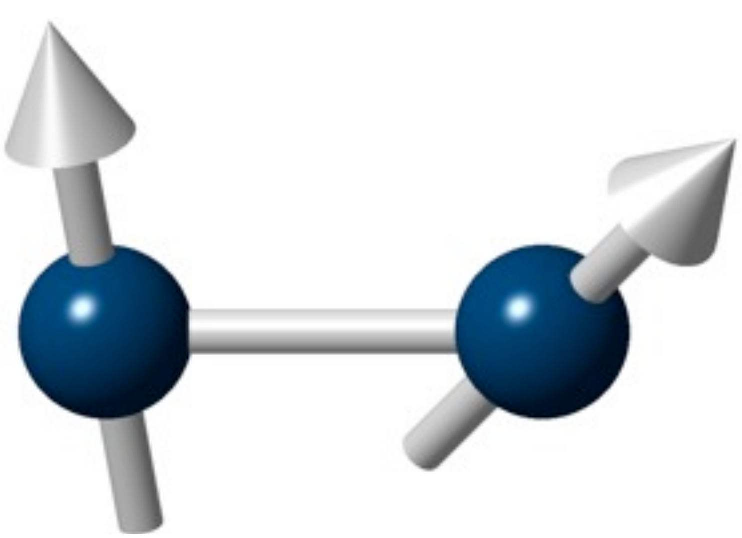


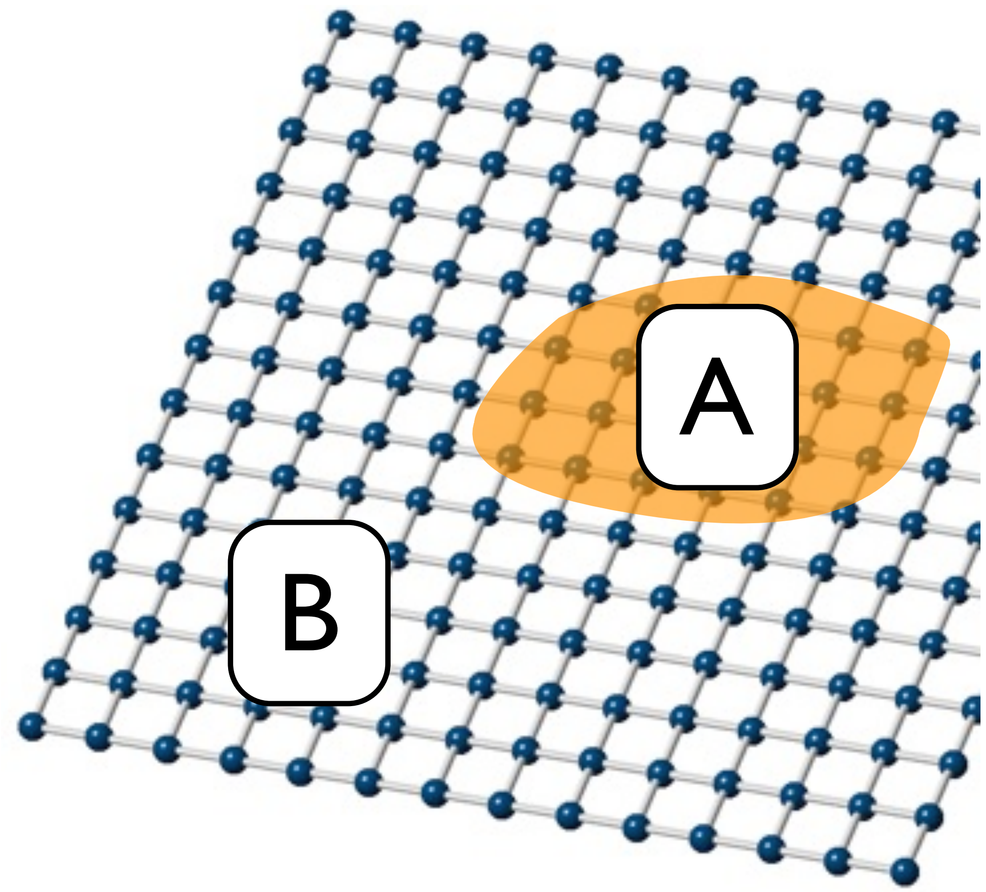
$$\rho_B = tr_A(|\psi\rangle\langle\psi|) = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Best description of part B

# Schmidt decomposition

If $|\psi\rangle$ is a pure state:

$$|\psi\rangle = \sum_{i}^{N_{Sch}} \lambda_i |i_A\rangle |i_B\rangle$$




$/\lambda_i \geq 0;\ \{|i_A\rangle\},\ \{|i_B\rangle\}$ orthonormal basis A, B

Nielsen & Chuang p. 109

# Putting all together

$|\psi\rangle$

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$$|\psi\rangle$$

$$\rho_A = tr_B(|\psi\rangle\langle\psi|)$$

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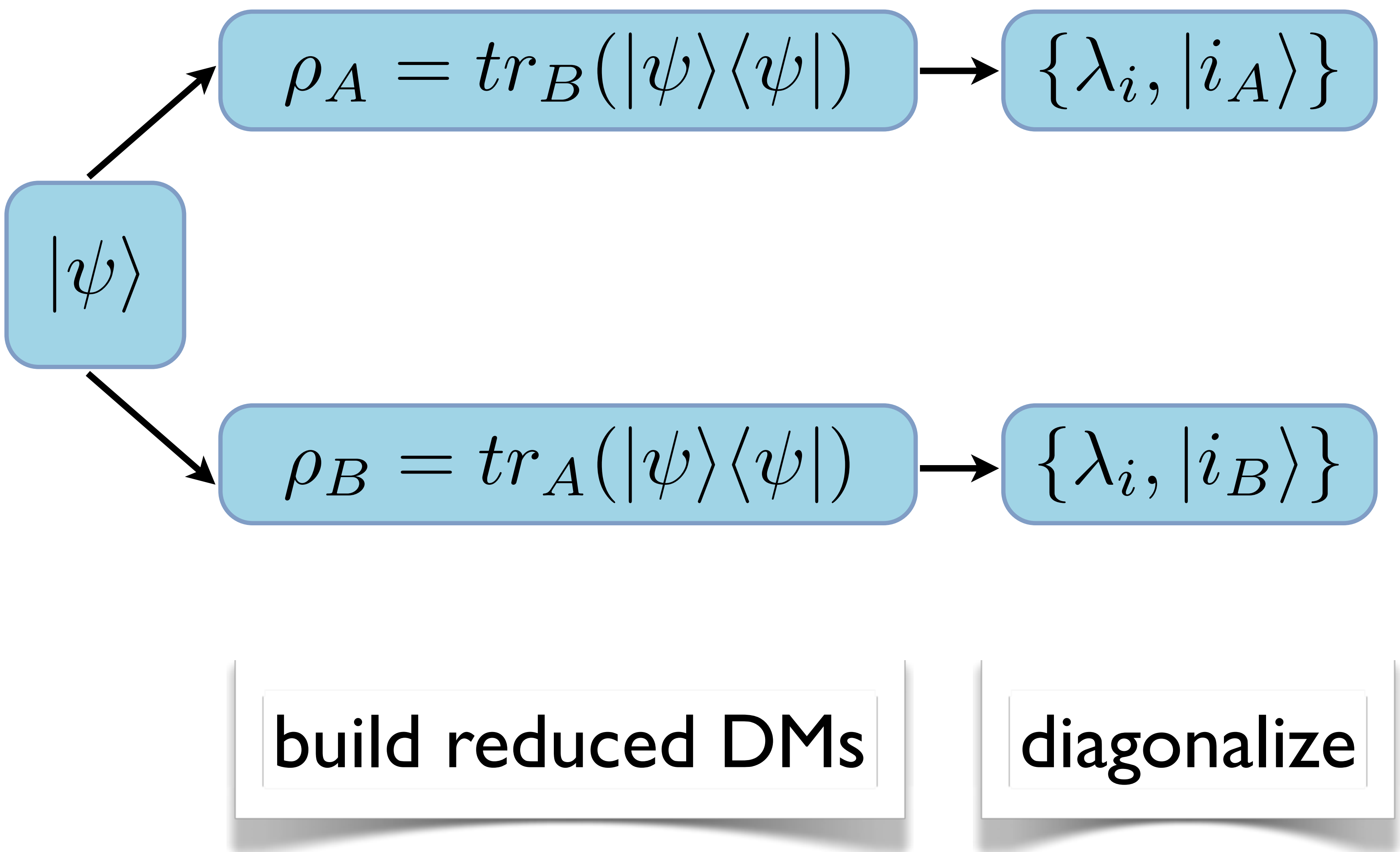
build reduced DMs

# Putting all together



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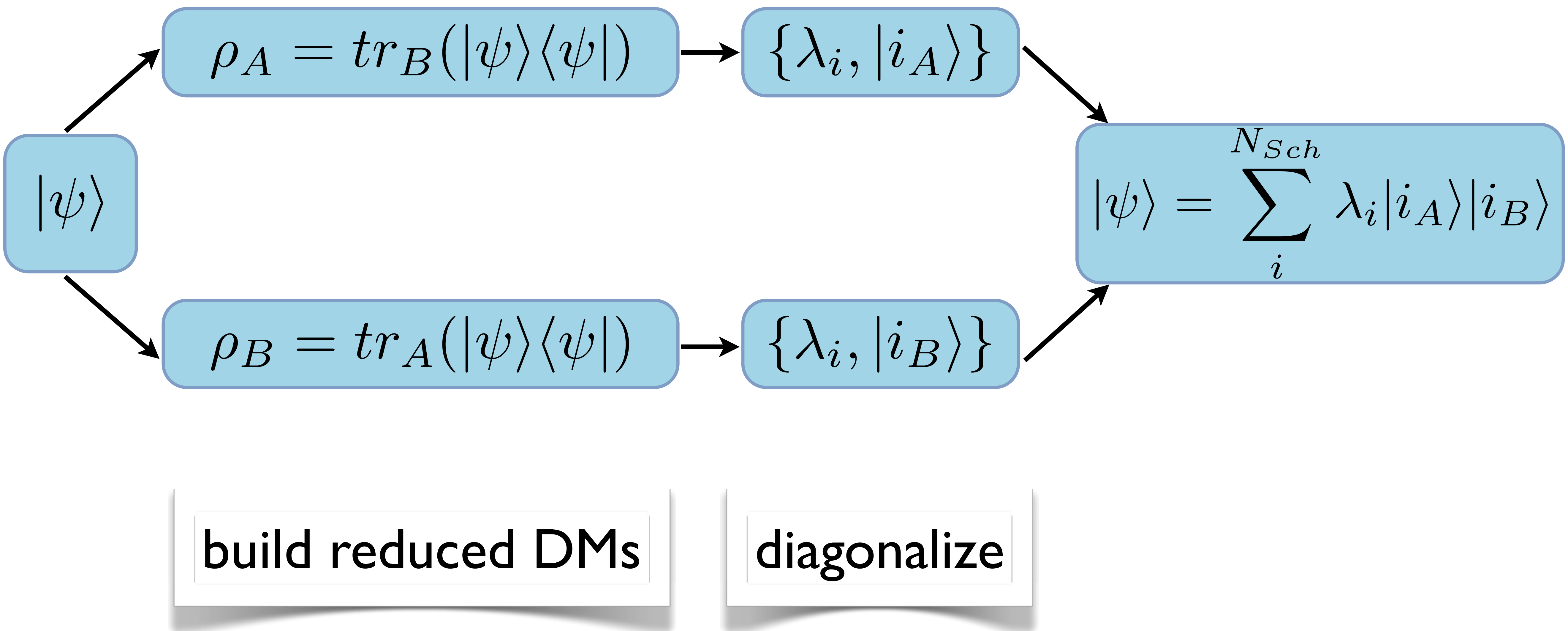
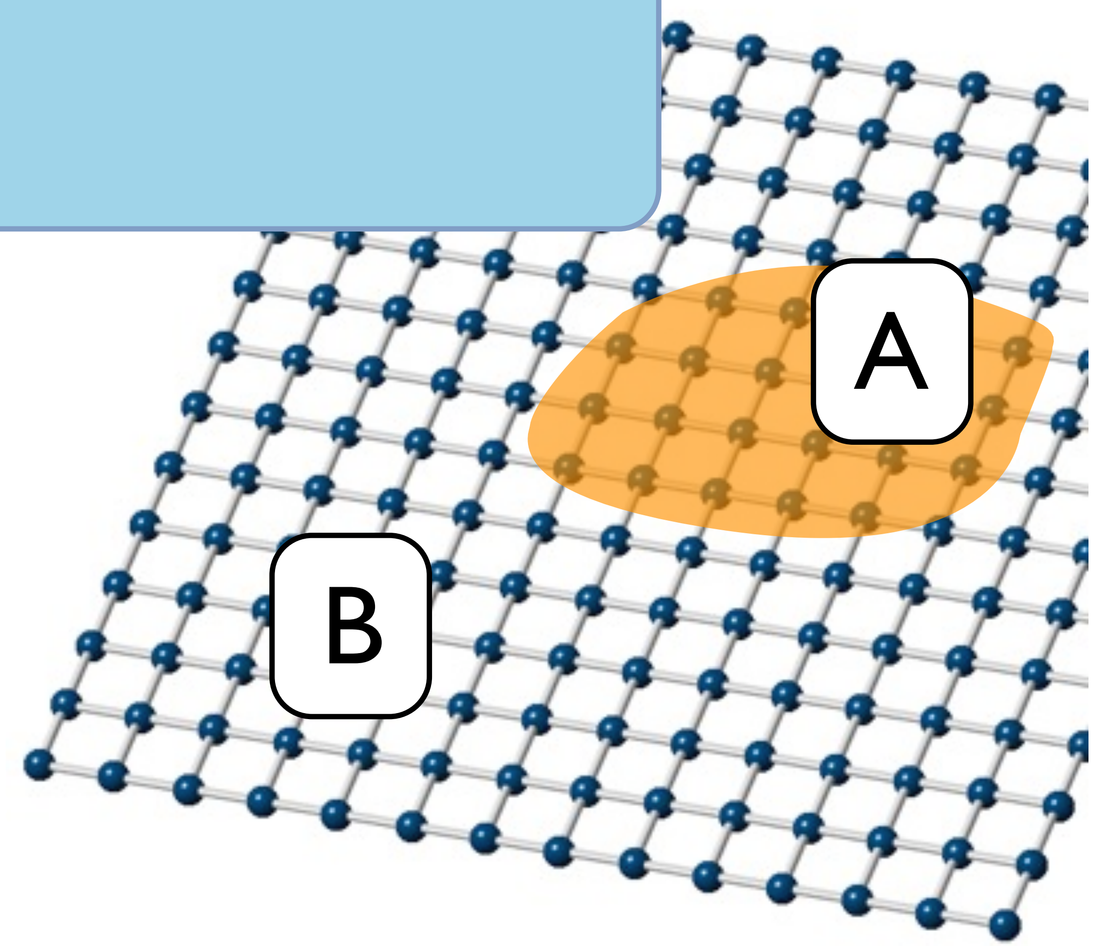


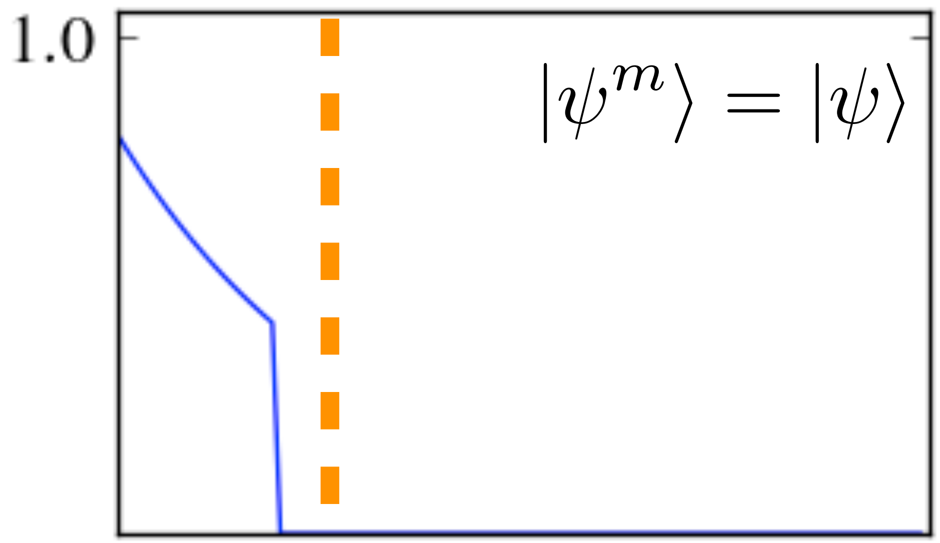
# Controlled approximation

$$|\psi\rangle \approx |\psi^m_{AB}\rangle \equiv \sum_i^m \lambda_i |i_A\rangle |i_B\rangle, \quad m < N_{Sch}$$

$$\epsilon = 1 - \sum_{i=m+1}^{N_{Sch}} \lambda_i^2$$



# Approximating wavefunctions $m \ll N_{Sch}$




m-dimensional MPS

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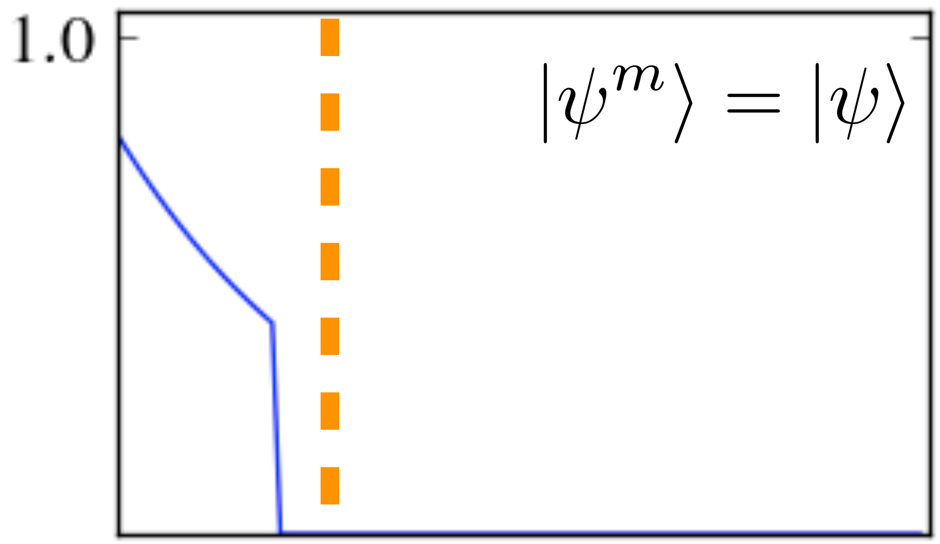
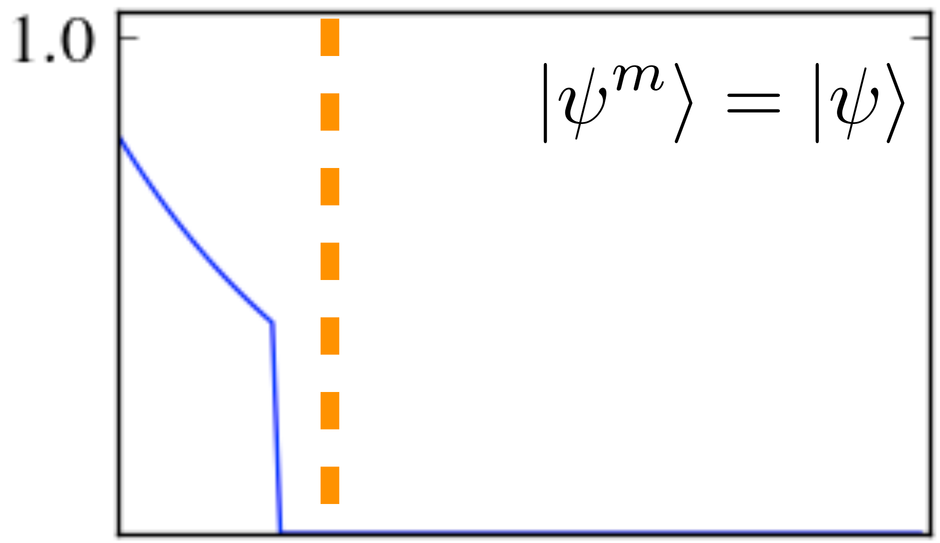



$$H = \sum_i \left[ \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3} \left( \vec{S}_i \cdot \vec{S}_{i+1} \right)^2 \right]$$

Affleck et al, PRL 59 (1987) 799

# Approximating wavefunctions $m \ll N_{Sch}$

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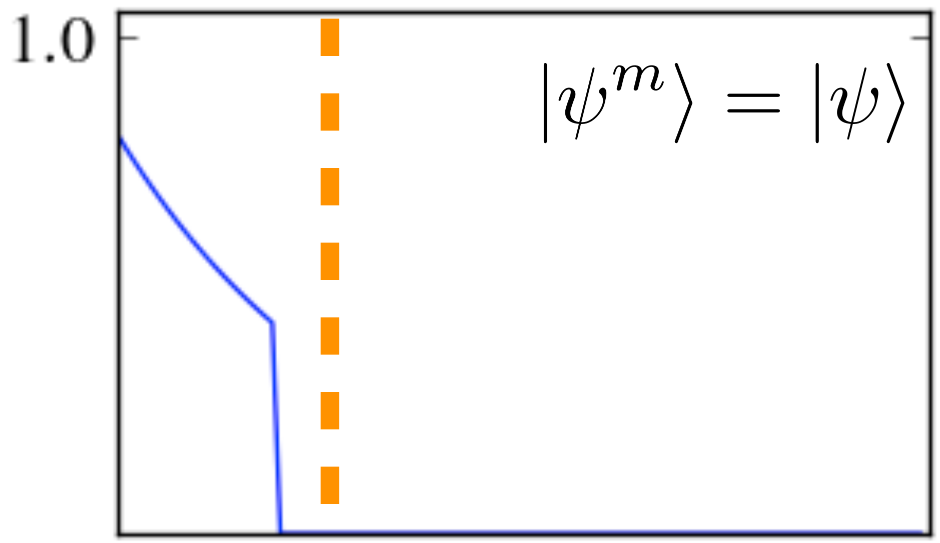
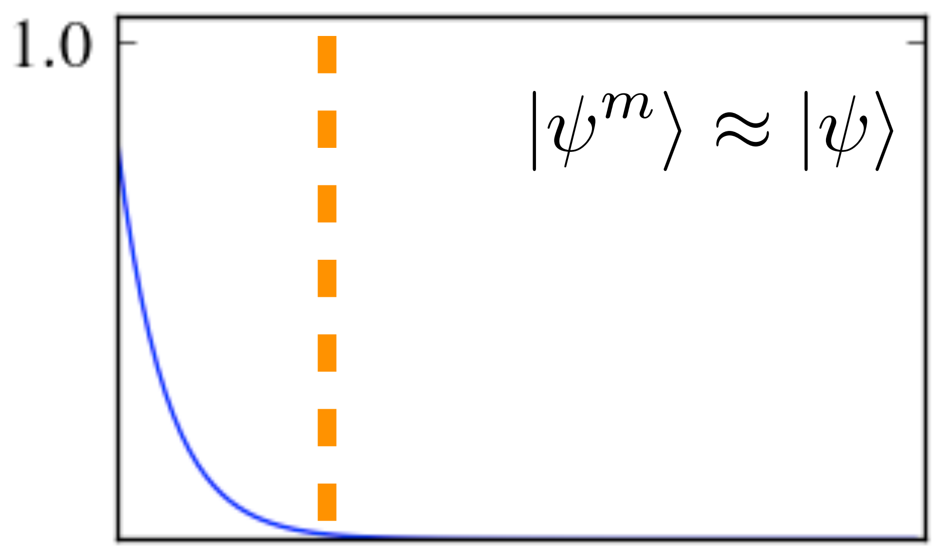
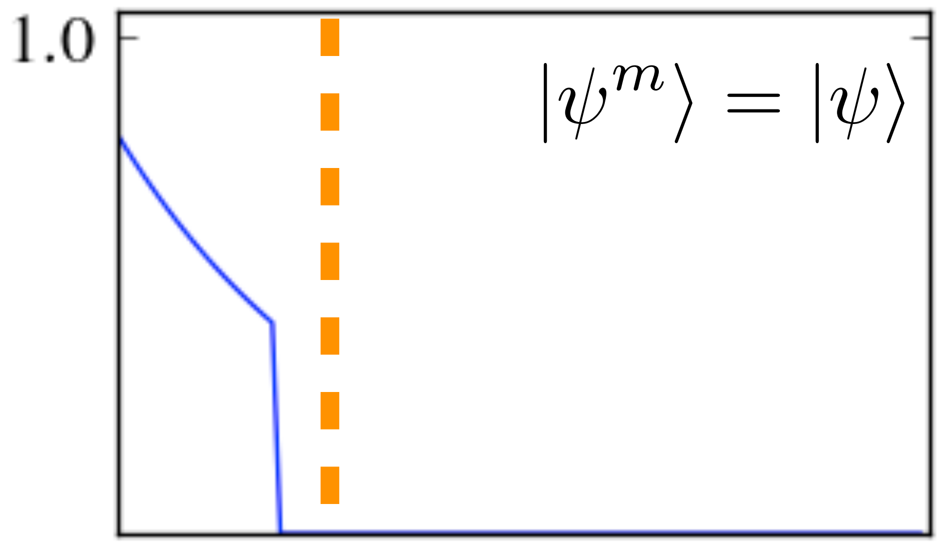



m-dimensional MPS

1D ground states

# Approximating wavefunctions $m \ll N_{Sch}$

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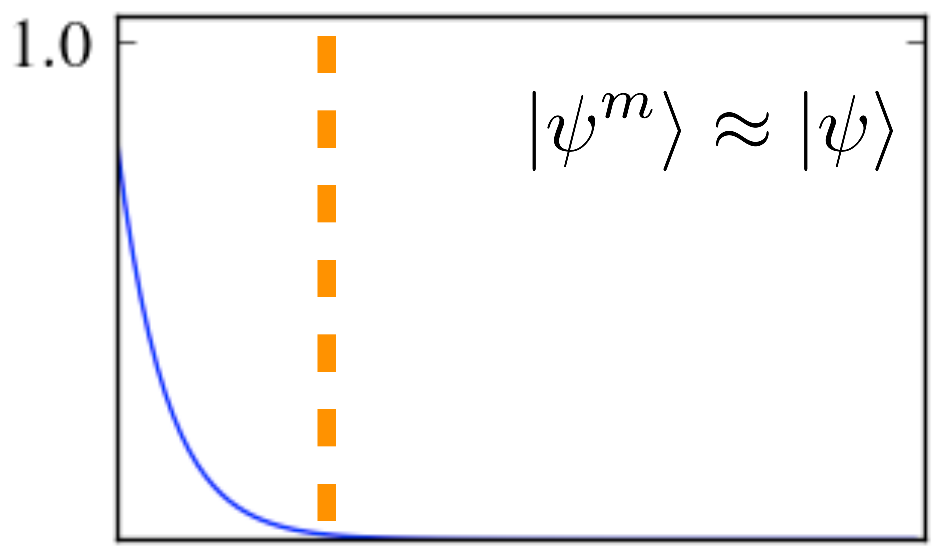
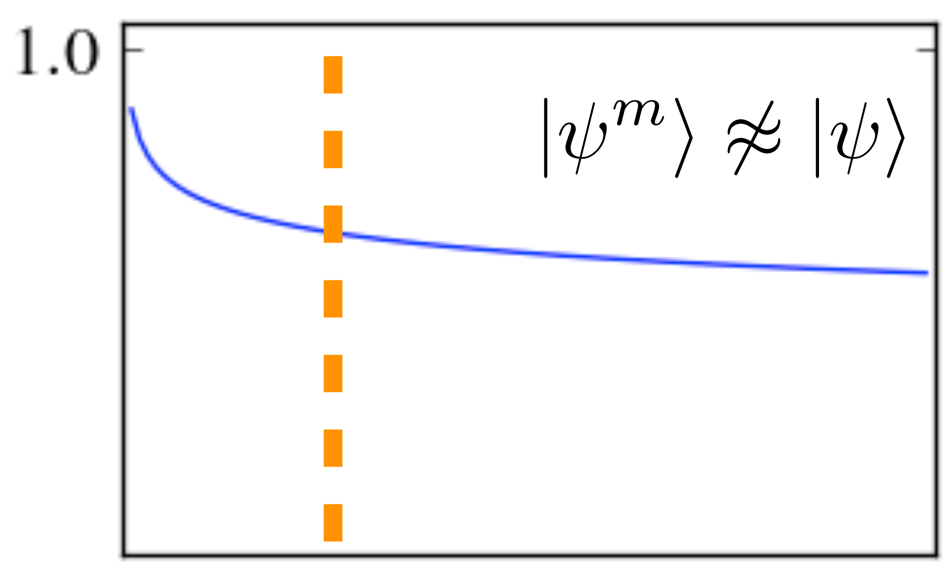
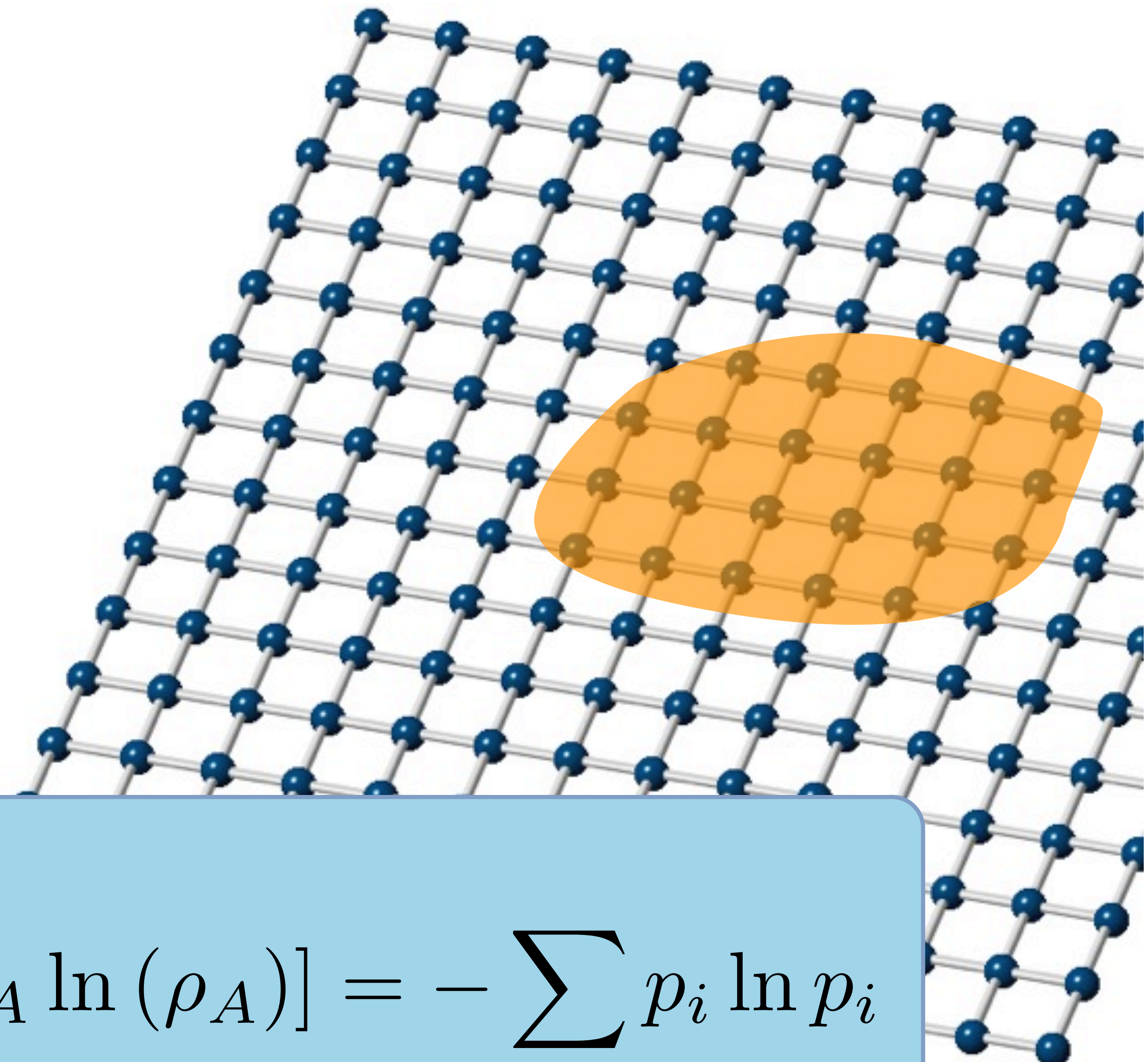



1D ground states



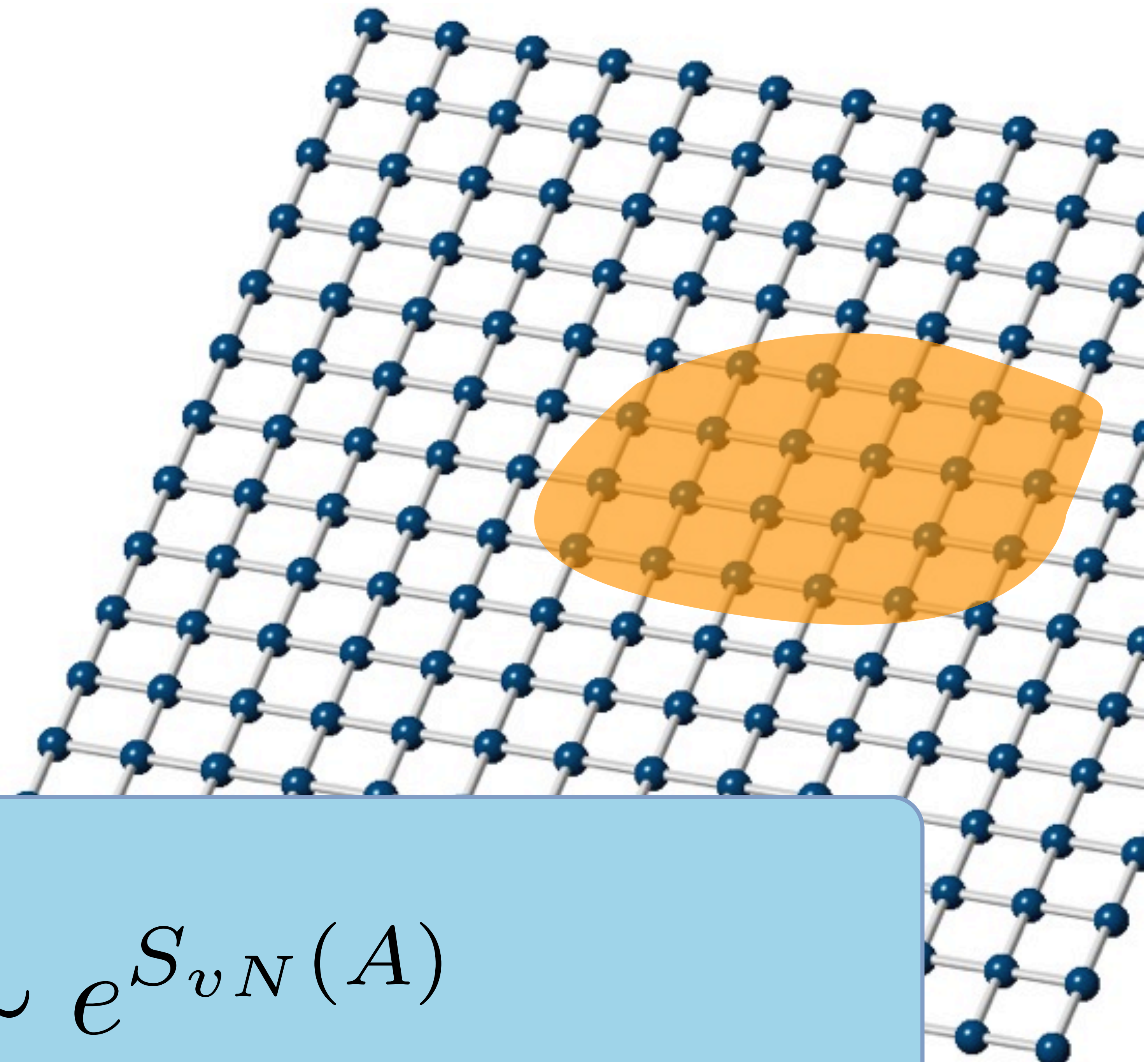

General, incl. 2D

# Von Neumann Entropy



$$S_{vN}(A) = -tr\left[\rho_A \ln\left(\rho_A\right)\right] = -\sum_i p_i \ln p_i$$

# Von Neumann Entropy



$$m \sim e^{S_{vN}(A)}$$

# Scaling of the entanglement entropy

1D gapped: $S_{vN}(L) \sim \log(\xi) \Rightarrow \lim_{L\to\infty} m \sim const$

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OK for DMRG!

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2D gapped:

Area law?

2D gapless: $S_{vN}(L) \sim L^{d-1} \Rightarrow \lim_{L \to \infty} m \sim e^{L^{d-1}}$

# Scaling of the entanglement entropy

1D gapped: $S_{vN}(L) \sim \log(\xi) \Rightarrow \lim m \sim const$

OK for DMRG!

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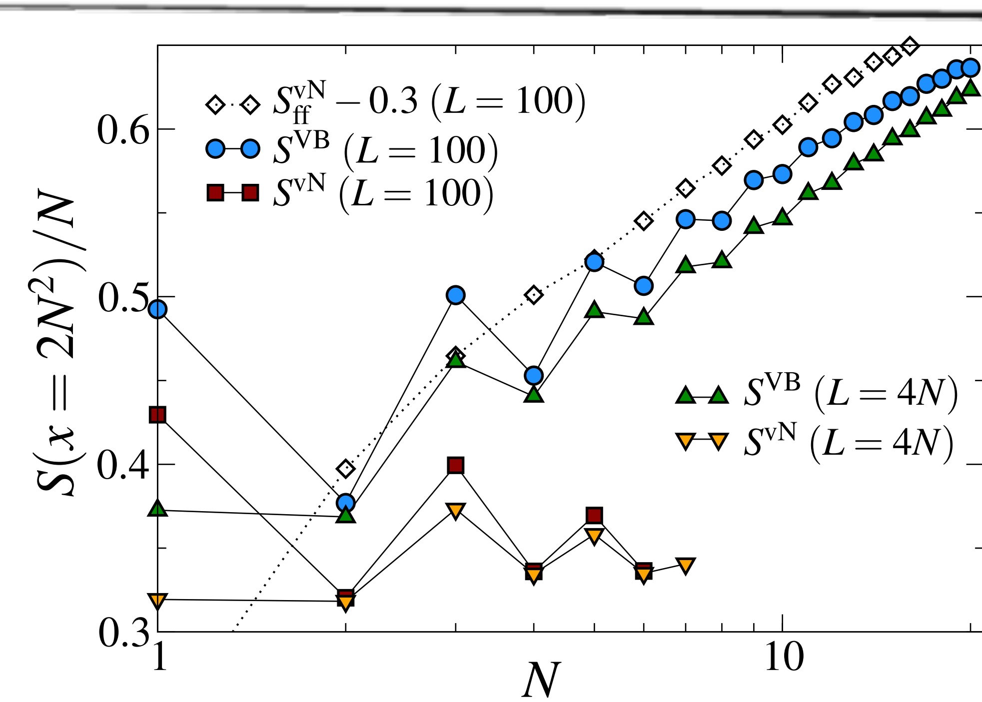
2D gapped:

2D gapless: $S_{v}$ ... $^{d-1}$




Ann B. Kallin et al, PRL177203

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OK for DMRG!

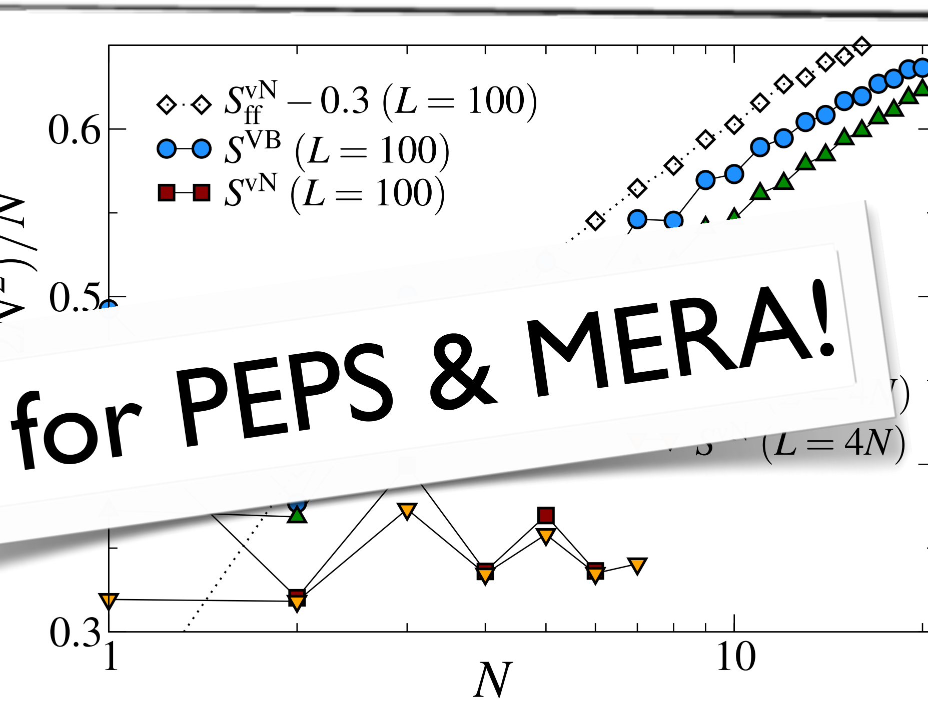
1D gapless: $S_{vN}(L) \sim \frac{c}{3}\log(L) \Rightarrow \lim_{L\to\infty} m \sim L^{c/3}$

2D gapped:

OK for PEPS & MERA!

2D gapless:

$d-1$




Ann B. Kallin et al, PRL177203

# Truncating matrices

$$\rho_A^{diag} = U \rho_A U^{-1}$$

$$U = \begin{pmatrix} u_{00} & u_{01} & \cdots & u_{0N_{Sch}} \\ u_{10} & u_{11} & \cdots & u_{1N_{Sch}} \\ \vdots & \vdots & \ddots & \vdots \\ u_{N_{Sch}0} & u_{N_{sch}1} & \cdots & u_{N_{Sch}N_{Sch}} \end{pmatrix}$$

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$$|0_A\rangle \qquad |1_A\rangle$$

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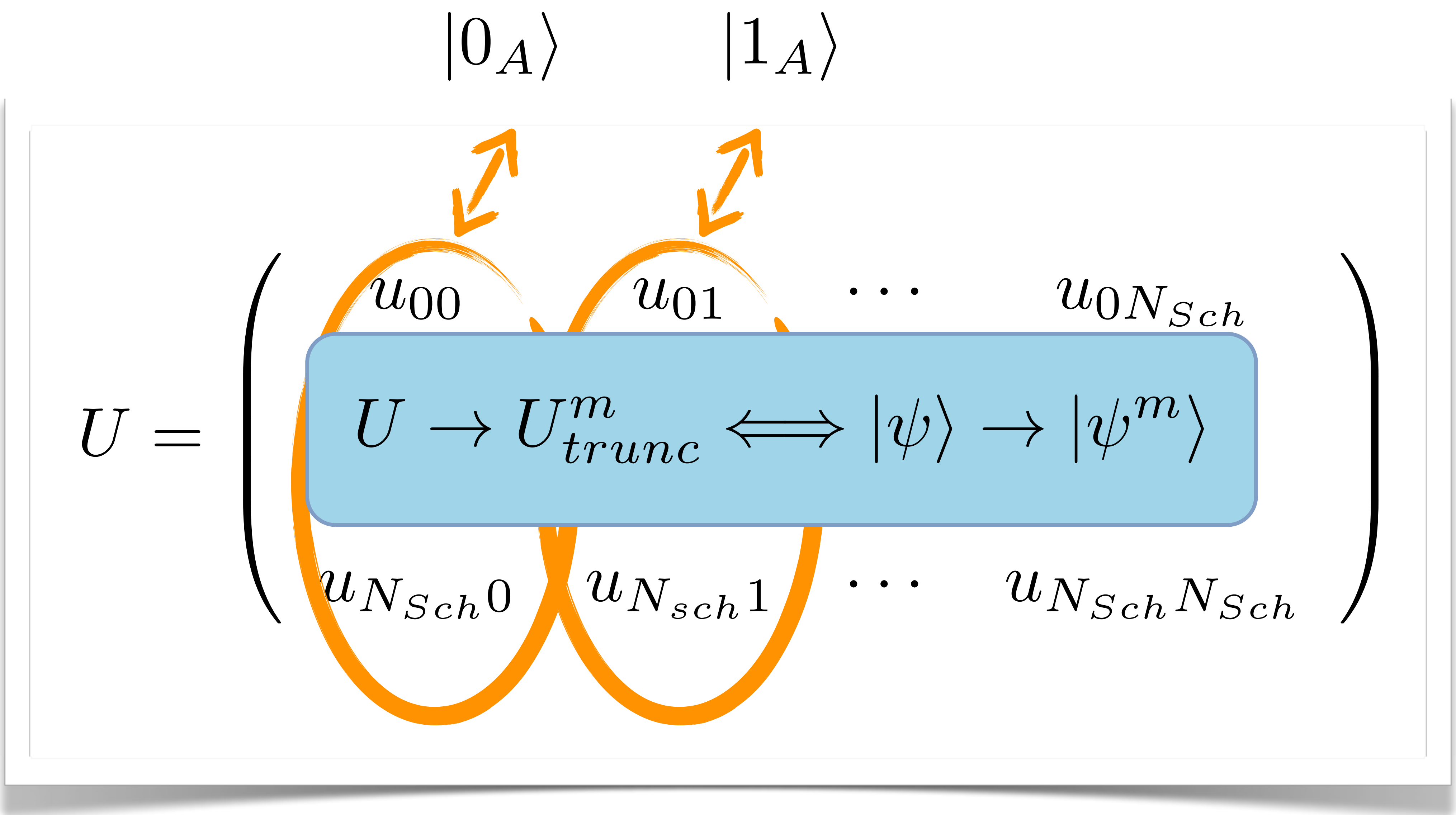
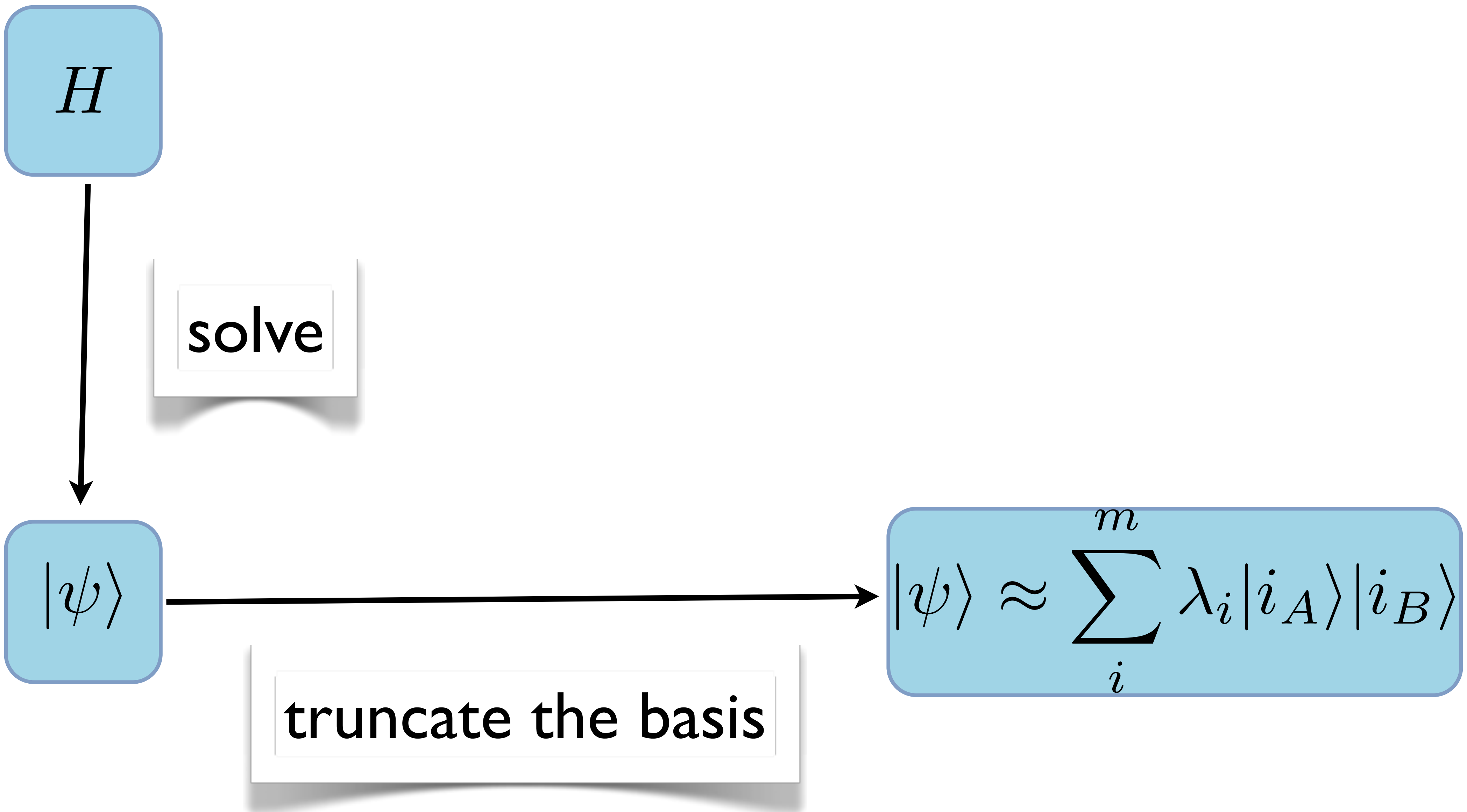


# A renormalization transformation



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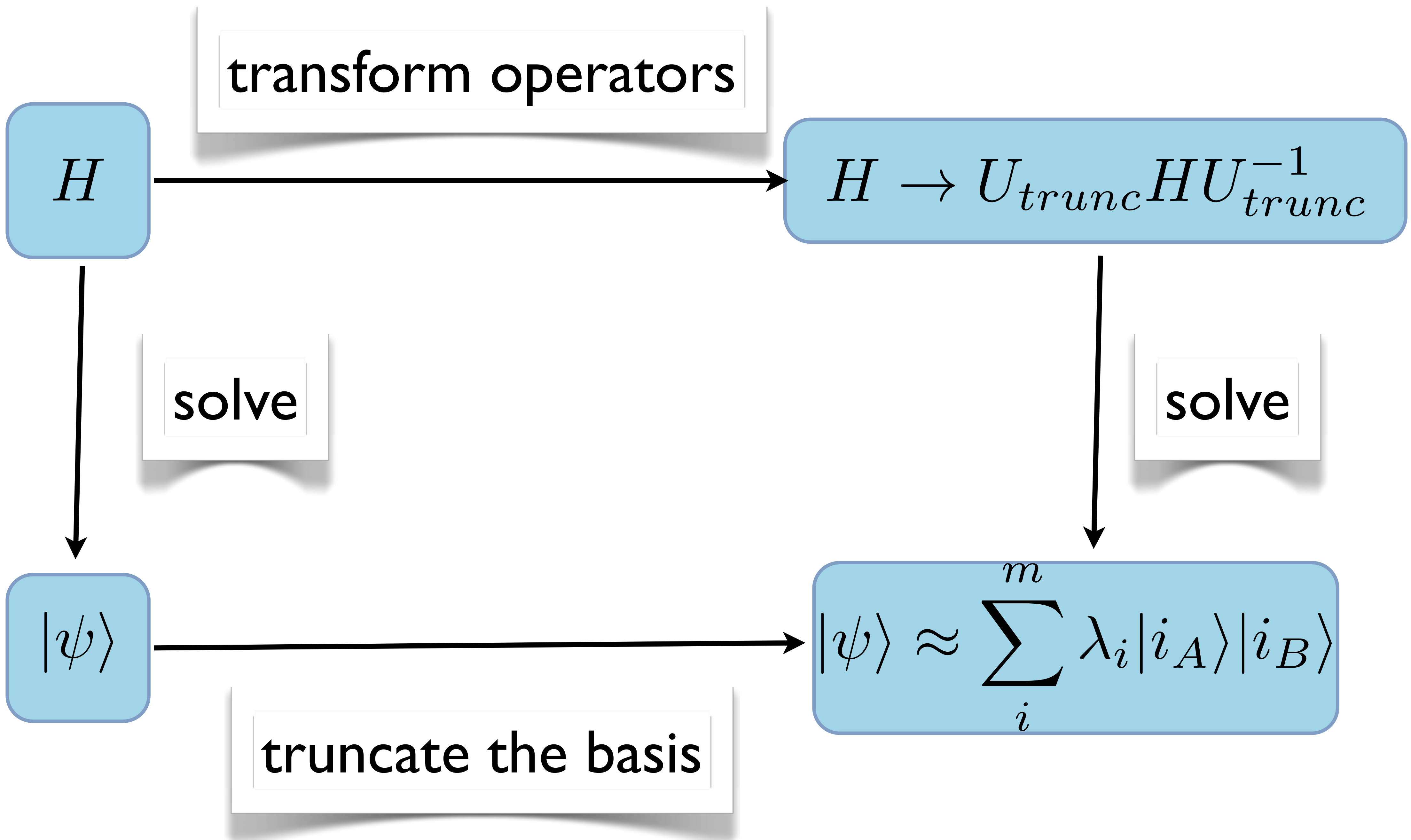

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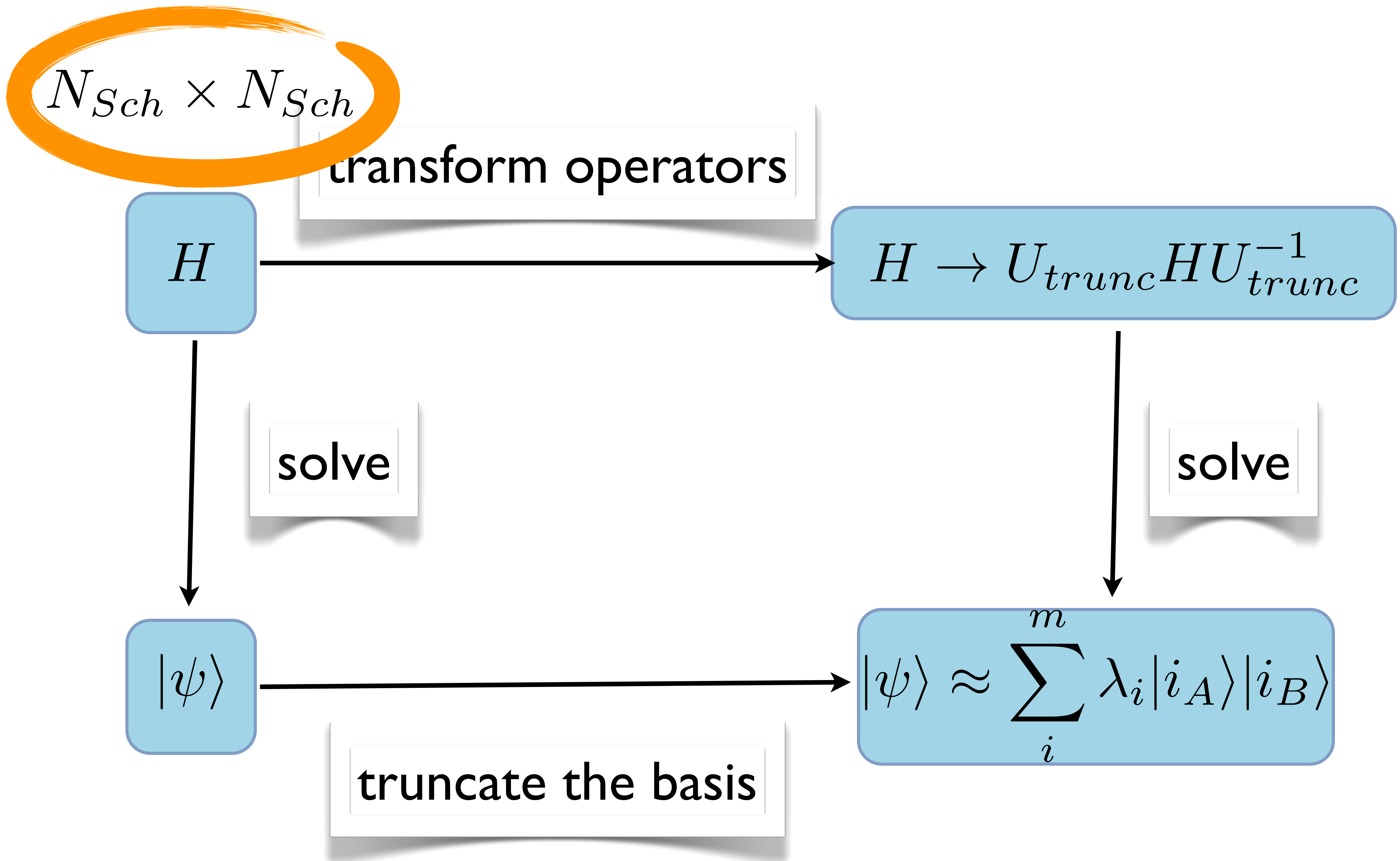

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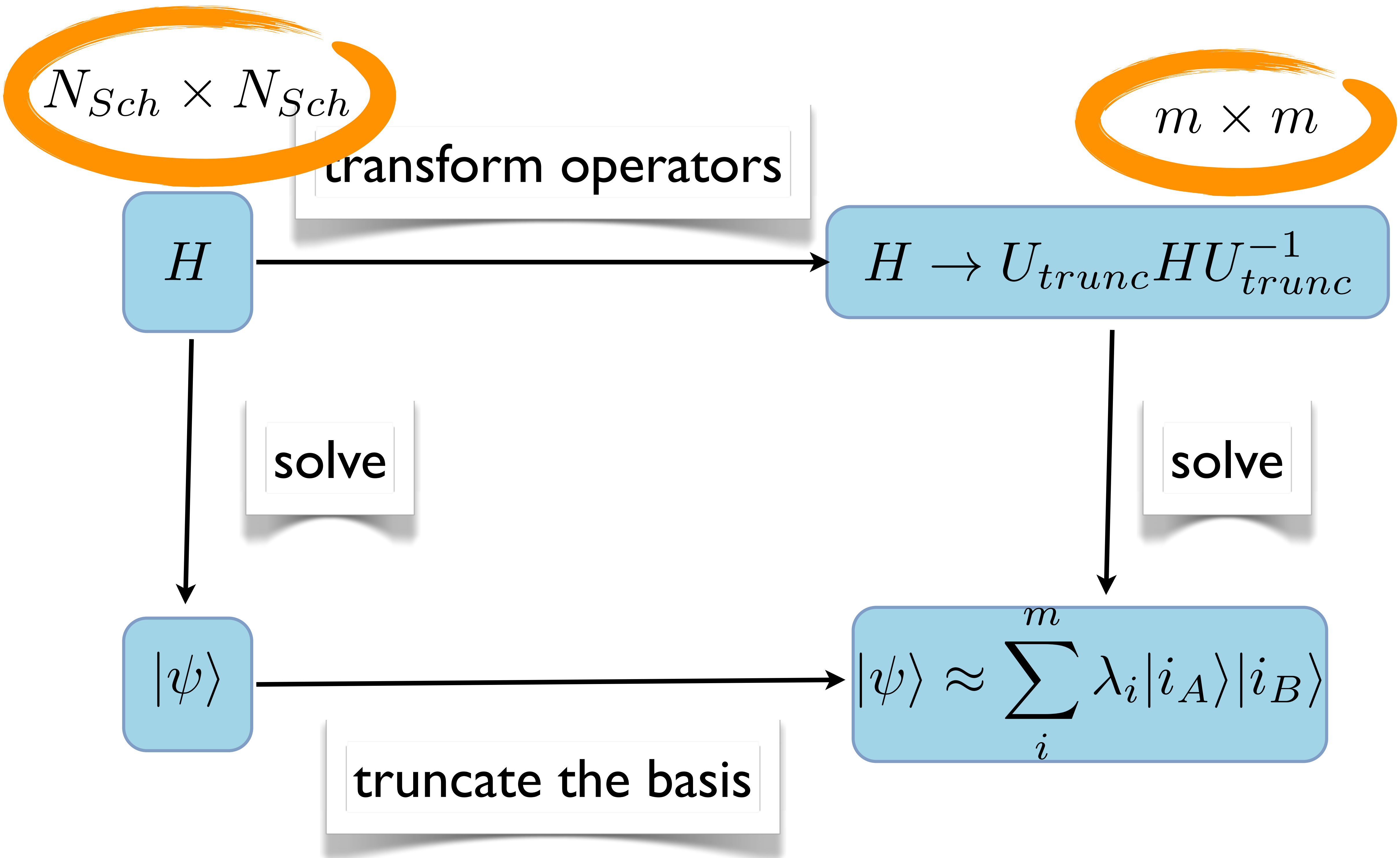
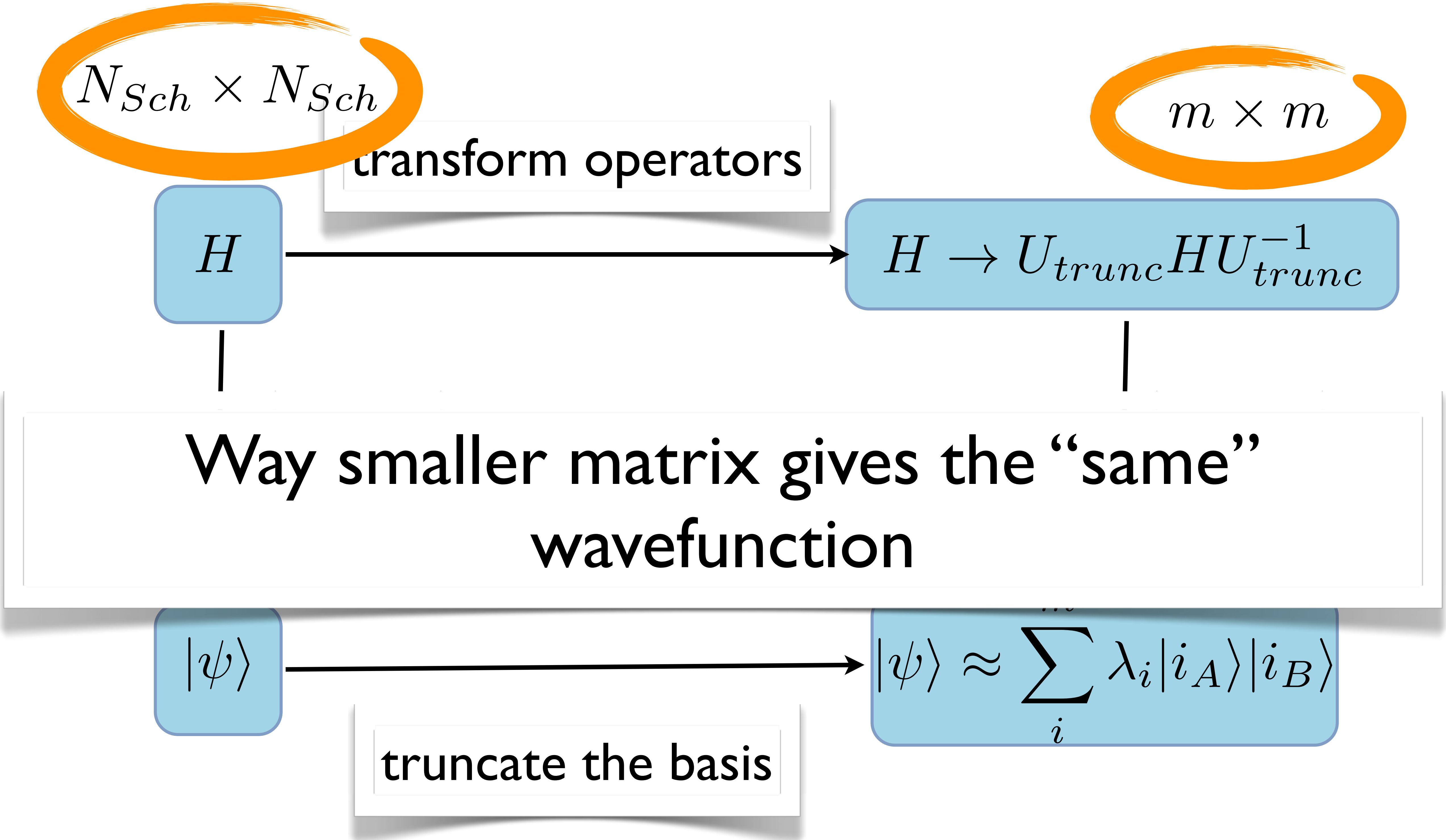


# A renormalization transformation



# Recap

- 1D ground states are slightly entangled
- controlled approximation to wavefunction
- reduced DM diagonalization gives RG transformation

# III. Implementation of the (two-site) DMRG algorithm

# Tutorial code: Heisenberg model

$$H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}, \qquad S = 1/2$$

# Tutorial code: Heisenberg model

$$H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}, \qquad S = 1/2$$

$$S_{vN}(l) = \frac{1}{6} \ln \left[ \frac{2L}{\pi} \sin\left( \frac{\pi l}{L} \right) \right] + \frac{1}{2} c'_{vN} + \ln g$$

$$m \sim e^{S_{vN}(L/2)} \approx L^{1/6}$$

Calabrese & Cardy JPhysA (2009)

# The DMRG plan

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1. Find the small part of the Hilbert space spanning the ground state wavefunction

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2. Diagonalize exactly the Hamiltonian in this subspace

# Splitting the chain in blocks

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$$H = H_{e_{i-1}} + \vec{S}_{i-1} \cdot \vec{S}_i + \vec{S}_i \cdot \vec{S}_{i+1} + \vec{S}_i \cdot \vec{S}_{i+2} + H_{b_{i+2}}$$

blockHamiltonian blockHamiltonian

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$$H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}, \qquad S = 1/2$$

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blockHamiltonian blockHamiltonian

system environment

$$|\psi\rangle = \sum_{\substack{e_{i-1},\sigma_i,\\ \sigma_{i+1},b_{i+2}}} c_{e_{i-1},\sigma_i,\sigma_{i+1},b_{i+2}} |e_{i-1}\rangle \otimes |\sigma_i\rangle \otimes |\sigma_{i+1}\rangle \otimes |b_{i+2}\rangle$$

# Building the Hamiltonian

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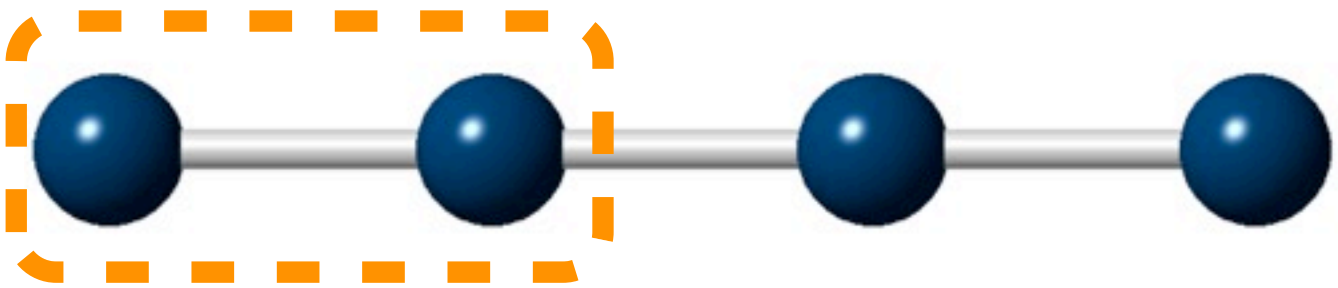

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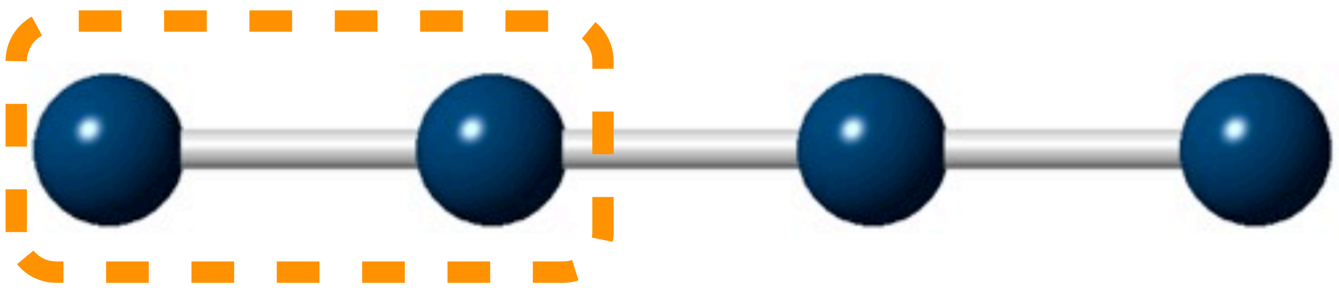
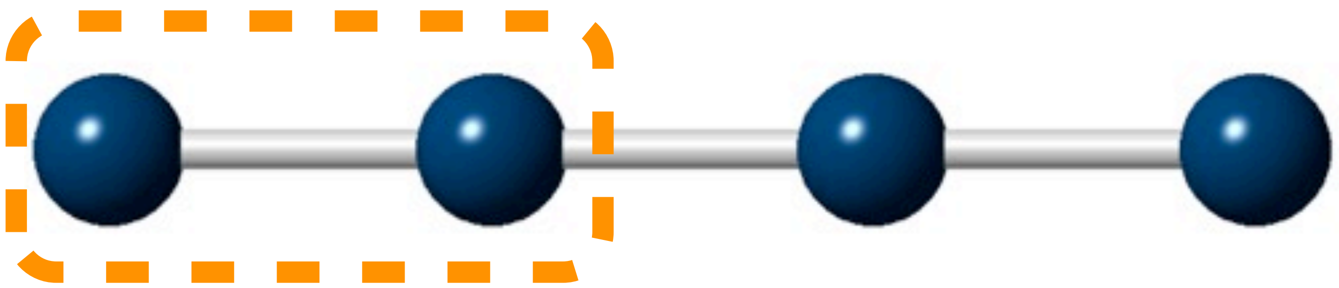


$\texttt{system.blockH=}(\sigma^x \otimes \sigma^x + \sigma^y_s \otimes \sigma^y_s + \sigma^z_s \otimes \sigma^z_s)_{ijkl}$

# Building the Hamiltonian



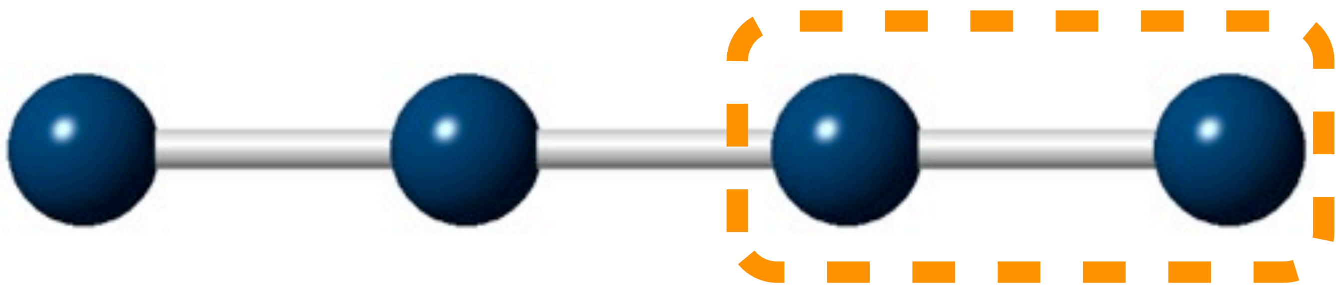
system.blockH=$(\sigma^x \otimes \sigma^x + \sigma_s^y \otimes \sigma_s^y + \sigma_s^z \otimes \sigma_s^z)_{ijkl}$

Sx=$(\mathbb{I} \otimes \sigma_x)_{ijkl}$

Sy=$(\mathbb{I} \otimes \sigma_y)_{ijkl}$

Sz=$(\mathbb{I} \otimes \sigma_z)_{ijkl}$

# Building the Hamiltonian



```
environ.blockH=system.blockH
```

Sx=$(\mathbb{I}\otimes\sigma_x)_{ijkl}$

Sy=$(\mathbb{I}\otimes\sigma_y)_{ijkl}$

Sz=$(\mathbb{I}\otimes\sigma_z)_{ijkl}$

# Building the Hamiltonian

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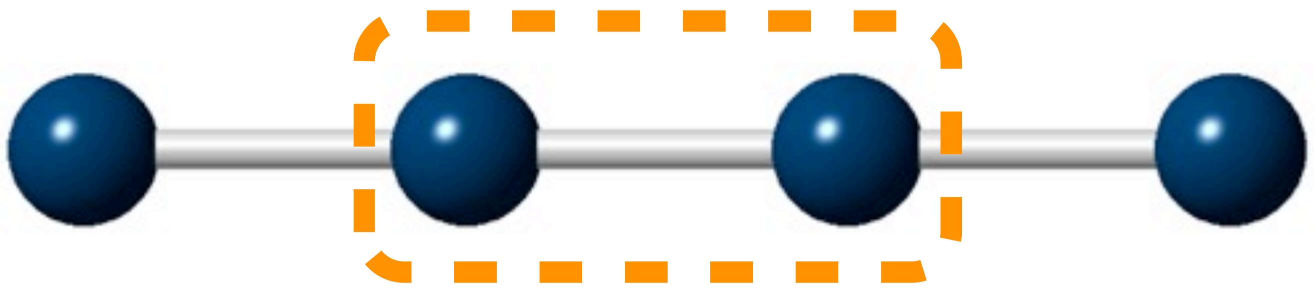
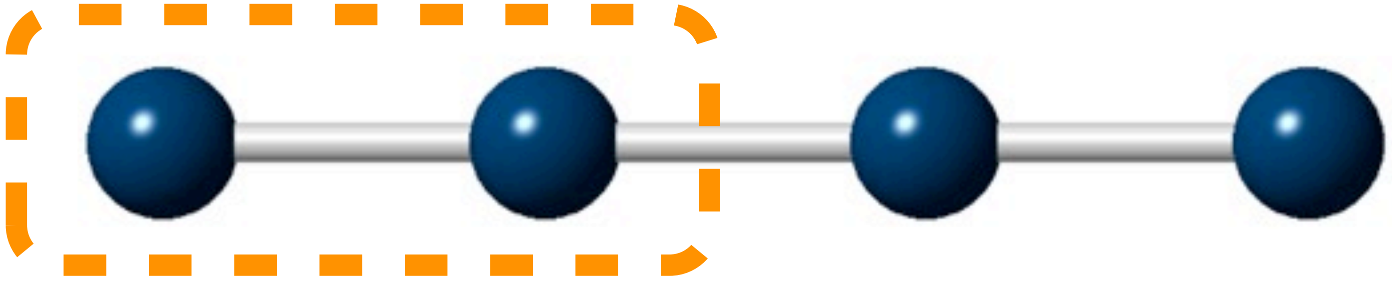


$$\text{Hse}=(\text{Sx} \otimes \text{Sx} + \text{Sy} \otimes \text{Sy} + \text{Sz} \otimes \text{Sz})$$

# Building the Hamiltonian

$$\texttt{Habcd=system.blockH} \otimes \mathbb{I} + \mathbb{I} \otimes \texttt{environ.blockH} + (\texttt{Sx} \otimes \texttt{Sx} + \texttt{Sy} \otimes \texttt{Sy} + \texttt{Sz} \otimes \texttt{Sz})$$

# Implementing the RG transformation



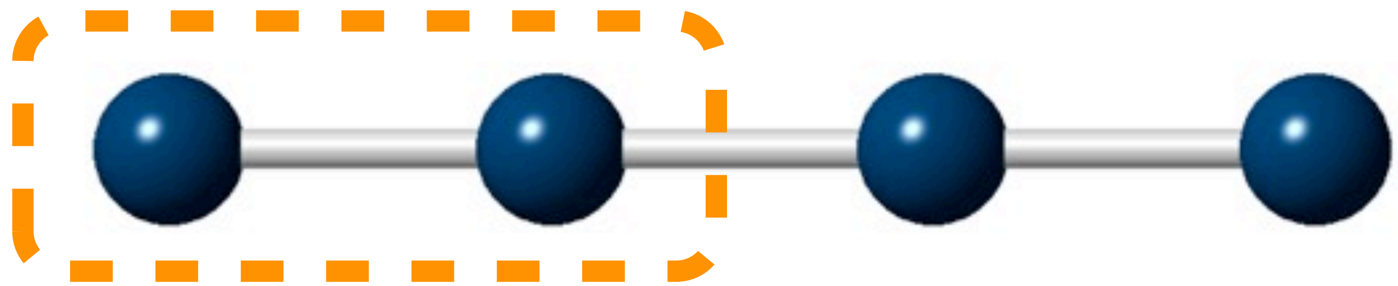
# Implementing the RG transformation

$$\texttt{blockH'} = U_{trunc} * \texttt{system.blockH} * U_{trunc}^T$$
$$\texttt{Sx'} = U_{trunc} * \texttt{Sx} * U_{trunc}^T$$
$$\texttt{Sy'} = U_{trunc} * \texttt{Sy} * U_{trunc}^T$$
$$\texttt{Sz'} = U_{trunc} * \texttt{Sz} * U_{trunc}^T$$

# Implementing the RG transformation

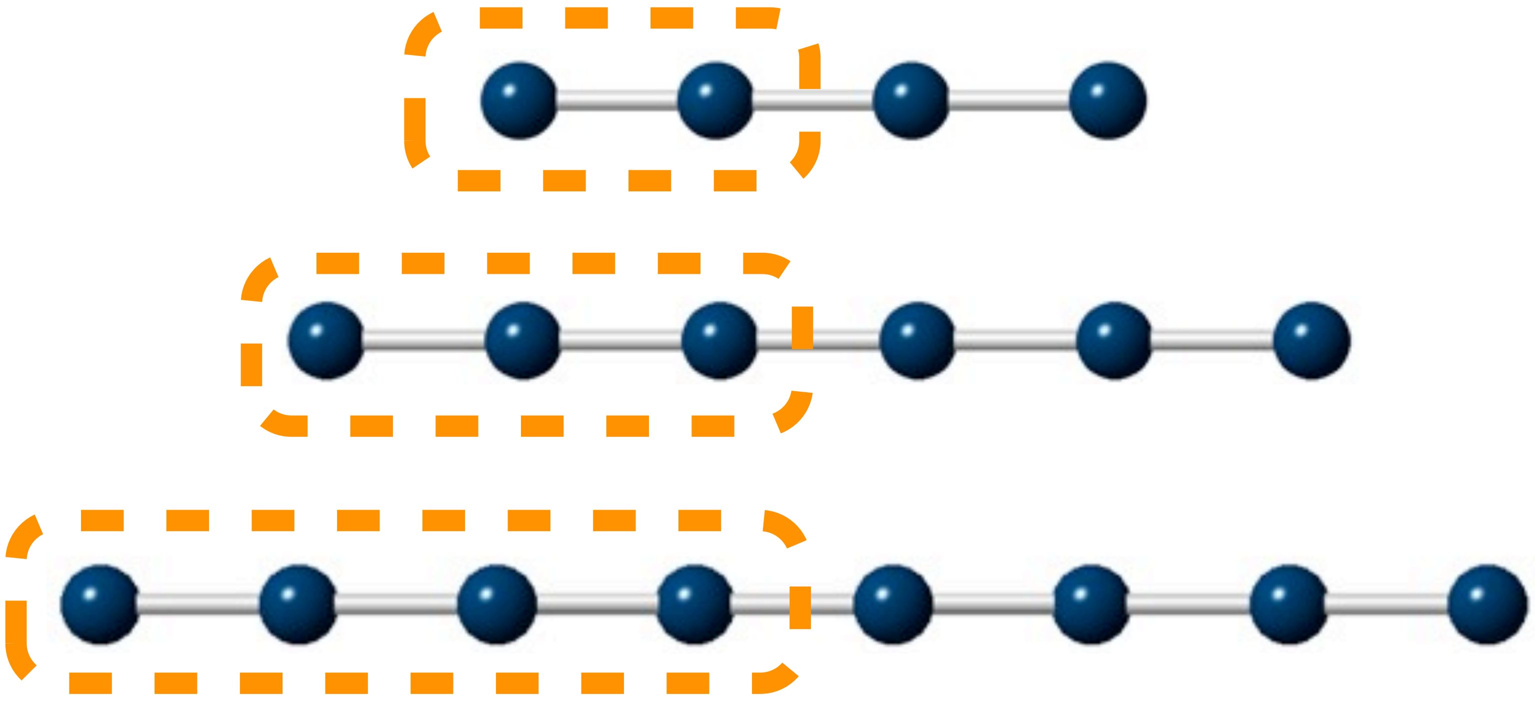
$$\texttt{system.blockH} = \texttt{blockH'} + \texttt{Sx'} \otimes \sigma^x + \texttt{Sy'} \otimes \sigma^y + \texttt{Sz'} \otimes \sigma^z$$

# Implementing the RG transformation



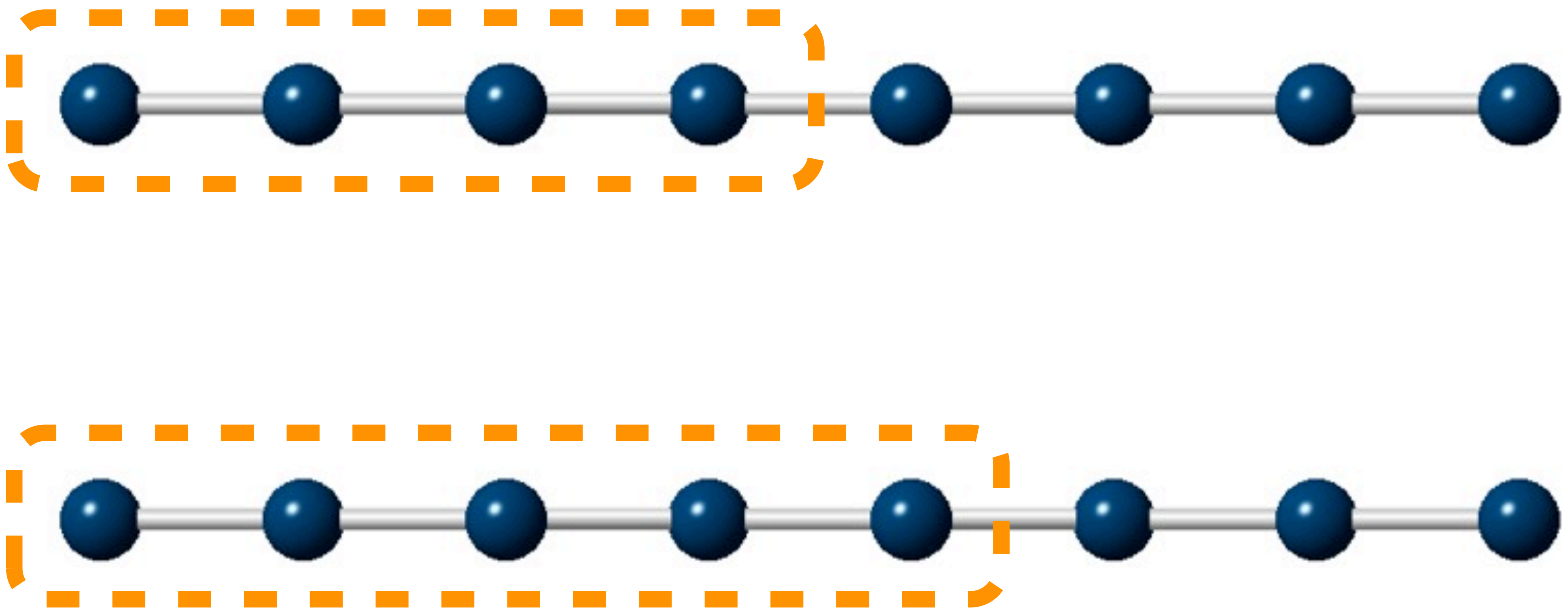
$$\texttt{system.blockH} = \texttt{blockH'} + \texttt{Sx'} \otimes \sigma^x + \texttt{Sy'} \otimes \sigma^y + \texttt{Sz'} \otimes \sigma^z$$

# Growing the system

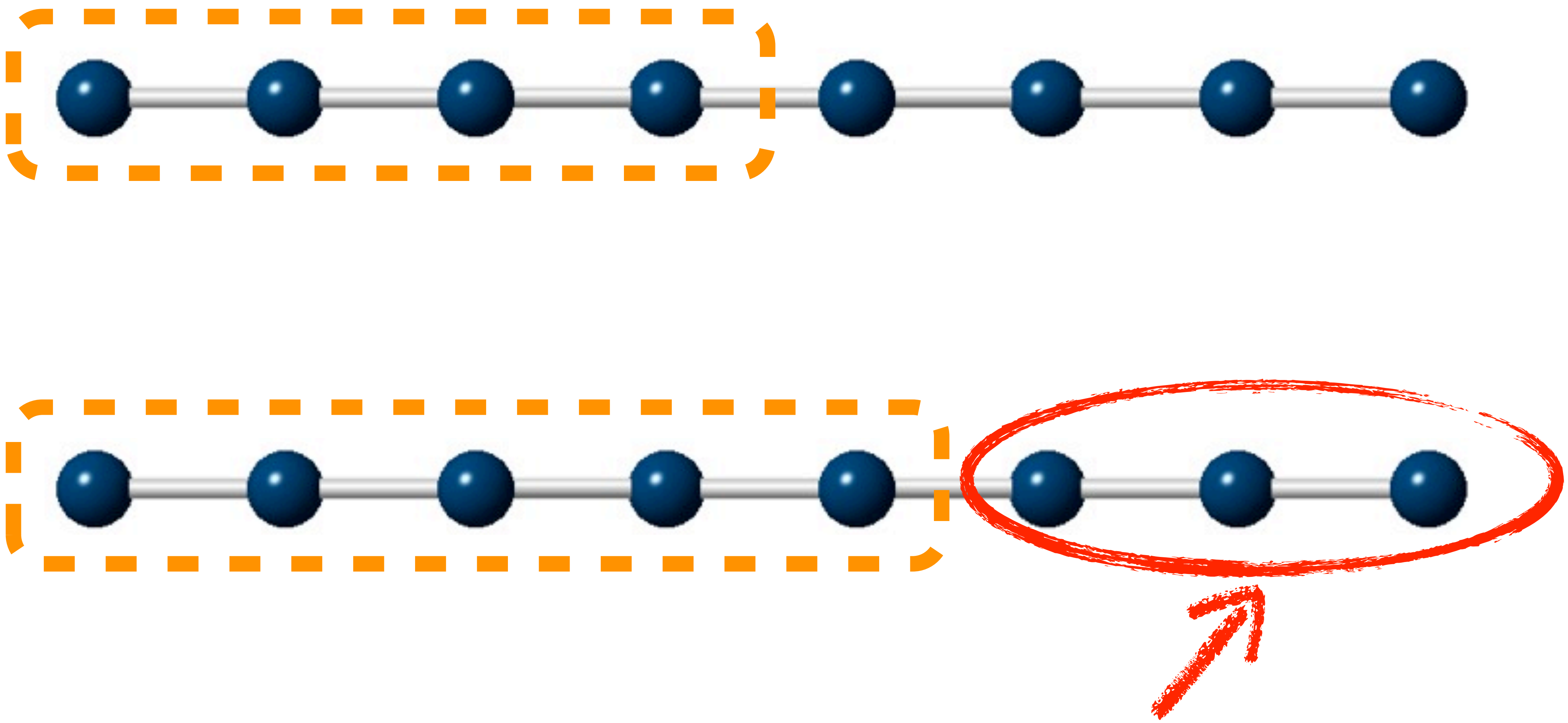


aka. infinite-size algorithm

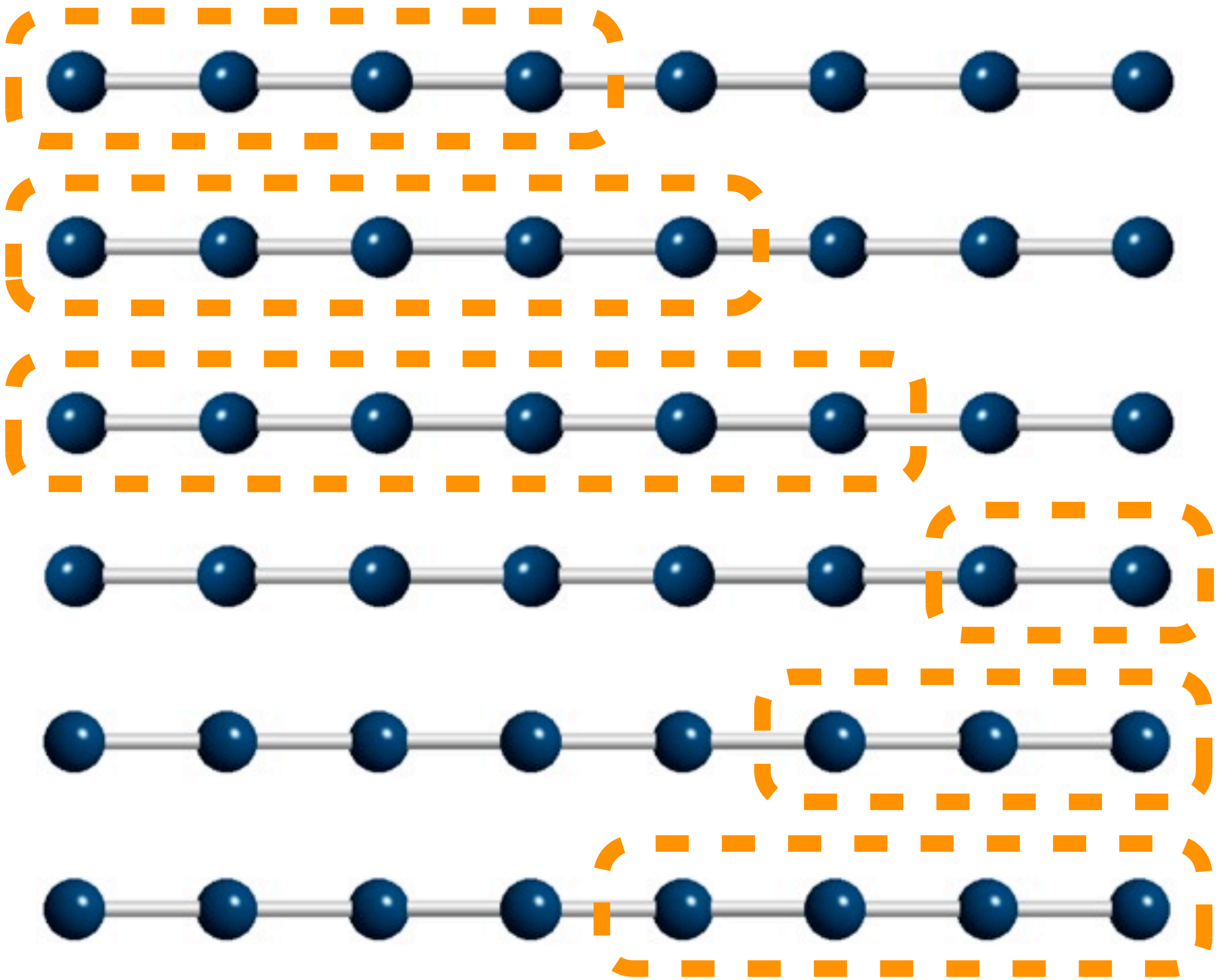
# Now what?



# Now what?

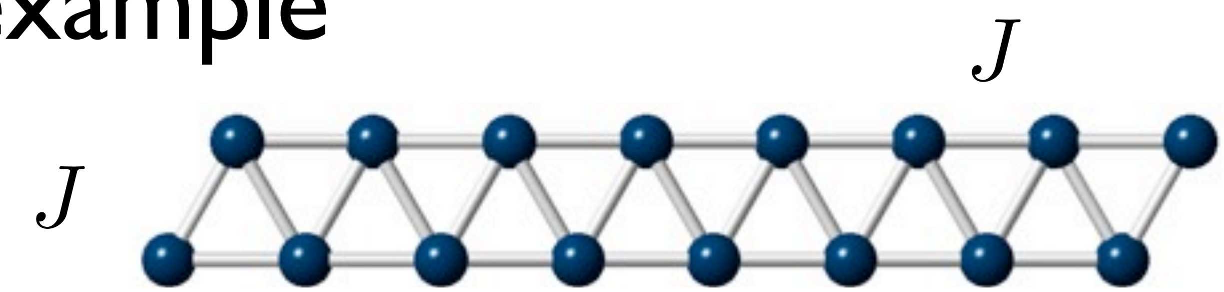


# First sweep to the left, then sweep to the right

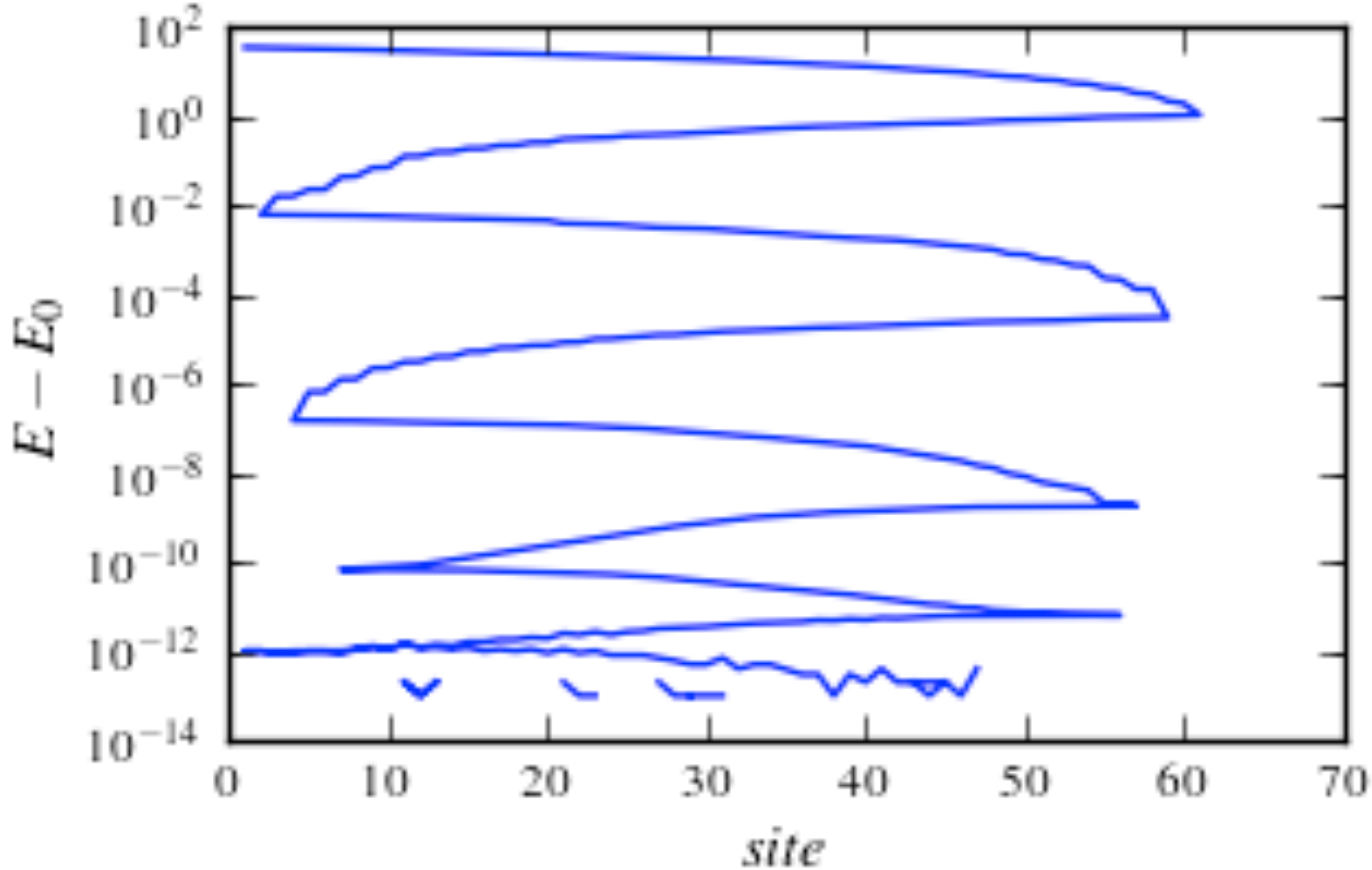


aka. finite-size algorithm

# A real-life example




$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$



# Summary

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- reduced DM diagonalization gives a RG transformation
- DMRG iterative algorithm implementing that RG

# IV. Becoming a pro

# Optimizations

http://boulder.research.yale.edu/Boulder-2010/Lectures/White/

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- Use symmetries

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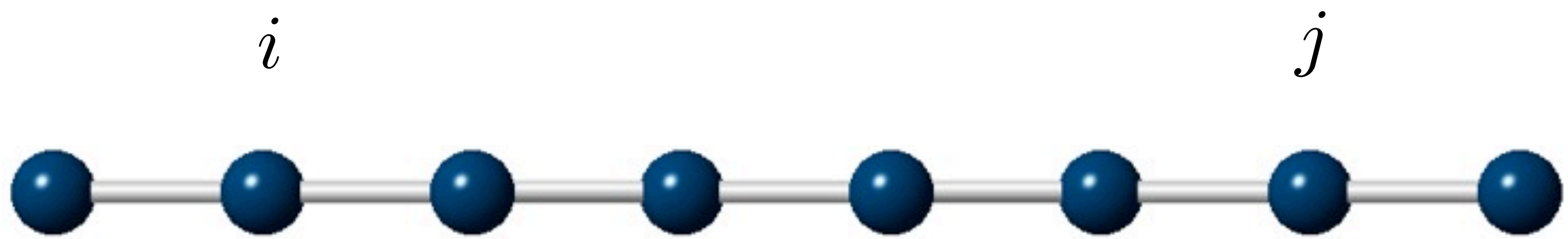
# Optimizations

- Use symmetries
- Guess for Lanczos (aka wf transformation)
- Everything under $m^3$
- Aim for 95% in dgemm

http://boulder.research.yale.edu/Boulder-2010/Lectures/White/

# Measurements

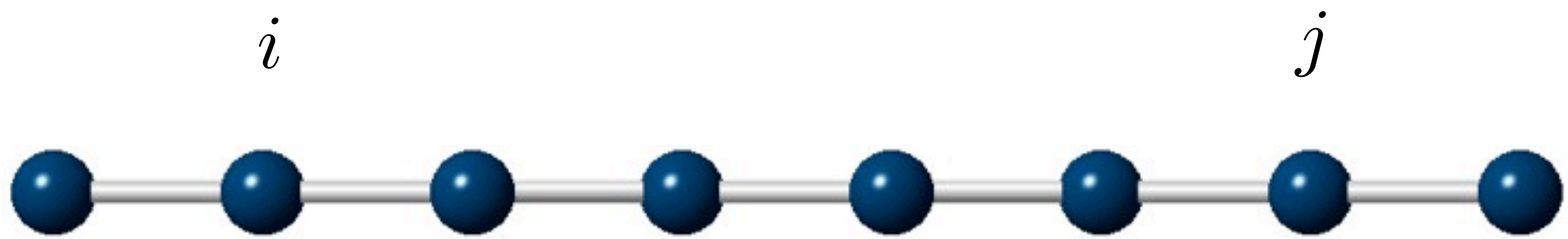



$$\langle\psi|S_i^z S_j^z|\psi\rangle \approx \langle\psi_{L/2}^m|\tilde{S}_i^z \tilde{S}_j^z|\psi_{L/2}^m\rangle$$

$$\tilde{S}_i^z = O(i, L/2) S_i^z O^t(i, L/2),$$

$$O(i, L/2) = U_{trunc}(i) U_{trunc}(i+1) \cdots U_{trunc}(L/2)$$

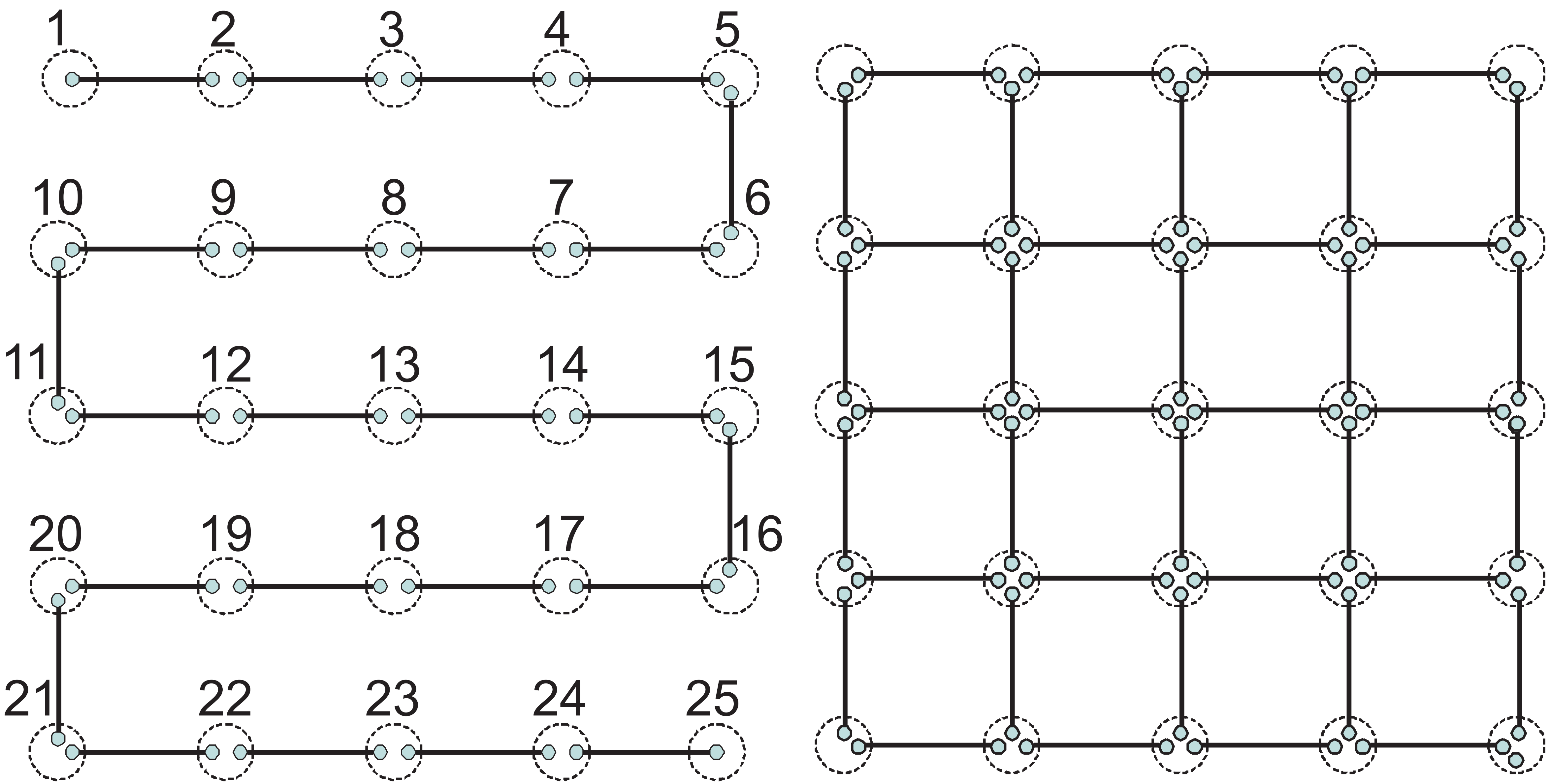
# Fermionic sign




$$c_i^\dagger c_j = \tilde{c}_i^\dagger s_{i+1} \cdots s_{j-1} \tilde{c}_j, \qquad s_i = e^{i\pi n_i}$$

Jordan-Wigner transformation

# MPS, PEPS & stuff



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