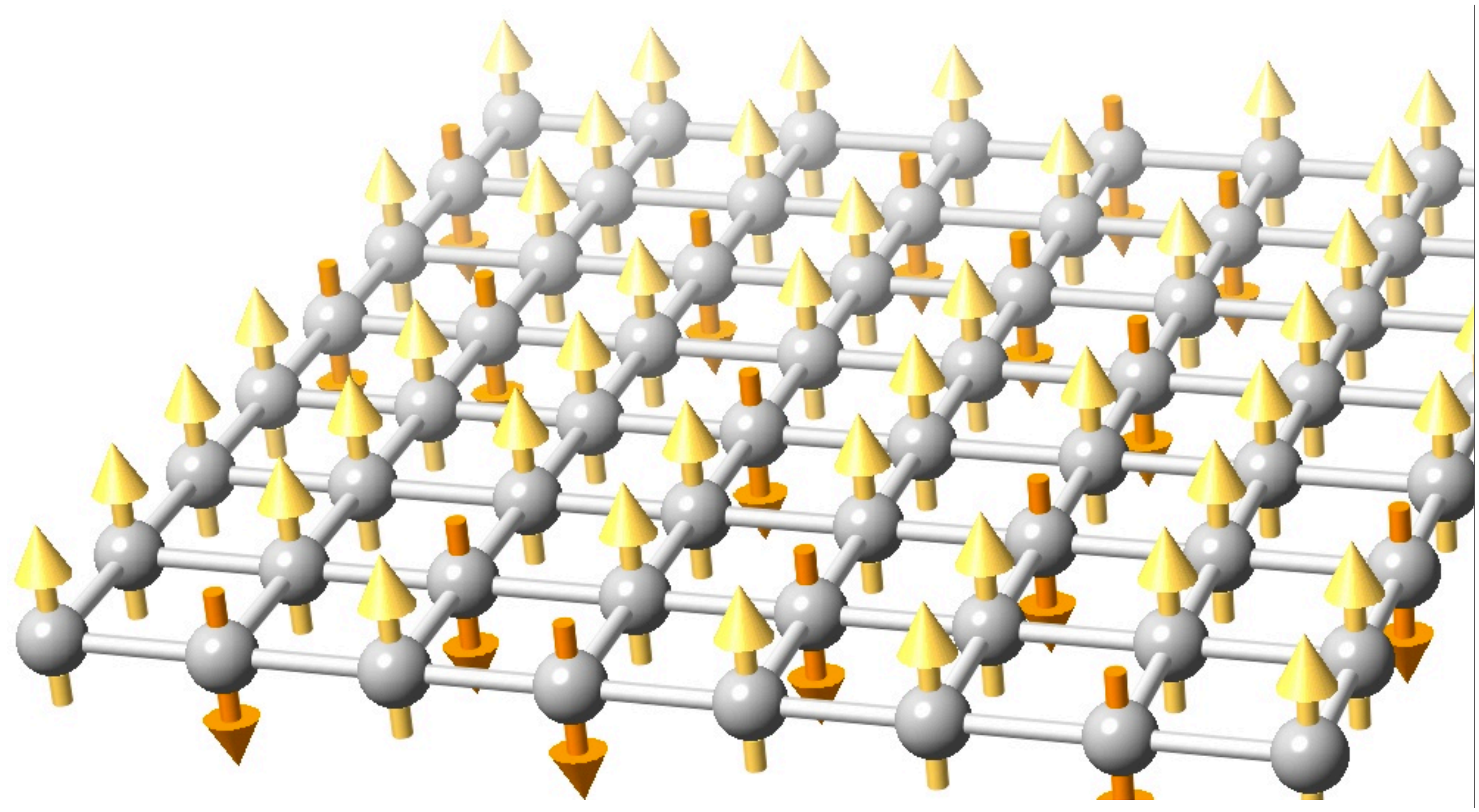
DMRG: Basics

Ying-Jer Kao
Department of Physics
National Taiwan University

Ministry of Science and Technology

Exponential Wall



- Size of the Hilbert space grows exponentially with system size $\sim d^N$

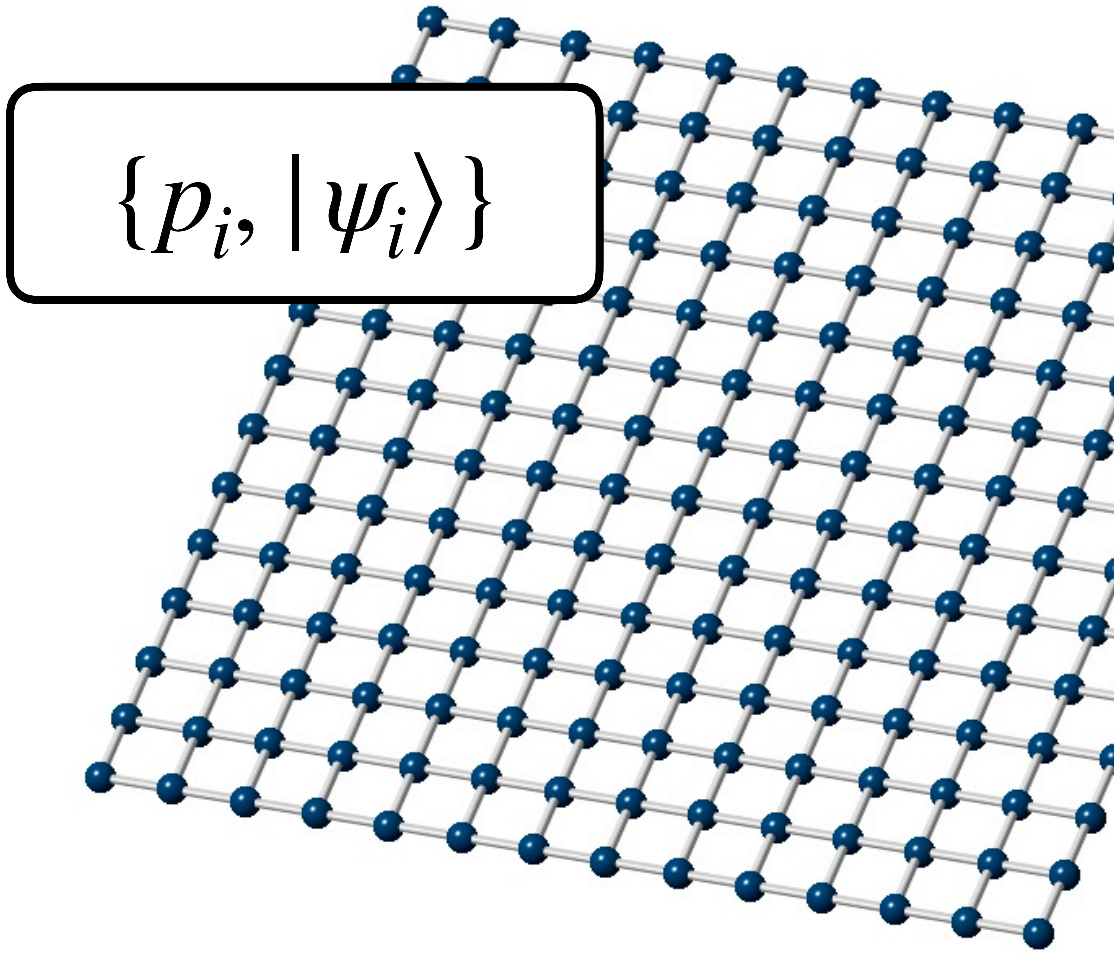
- Size of the Hilbert space occupied the ground state grows much slower $\sim dN$

Density Matrix

Probability p_i in the pure state $|\psi_i\rangle$

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

- $\operatorname{tr}\rho = 1$
- $\langle\psi|\rho|\psi\rangle \geq 0 \quad \forall\psi$



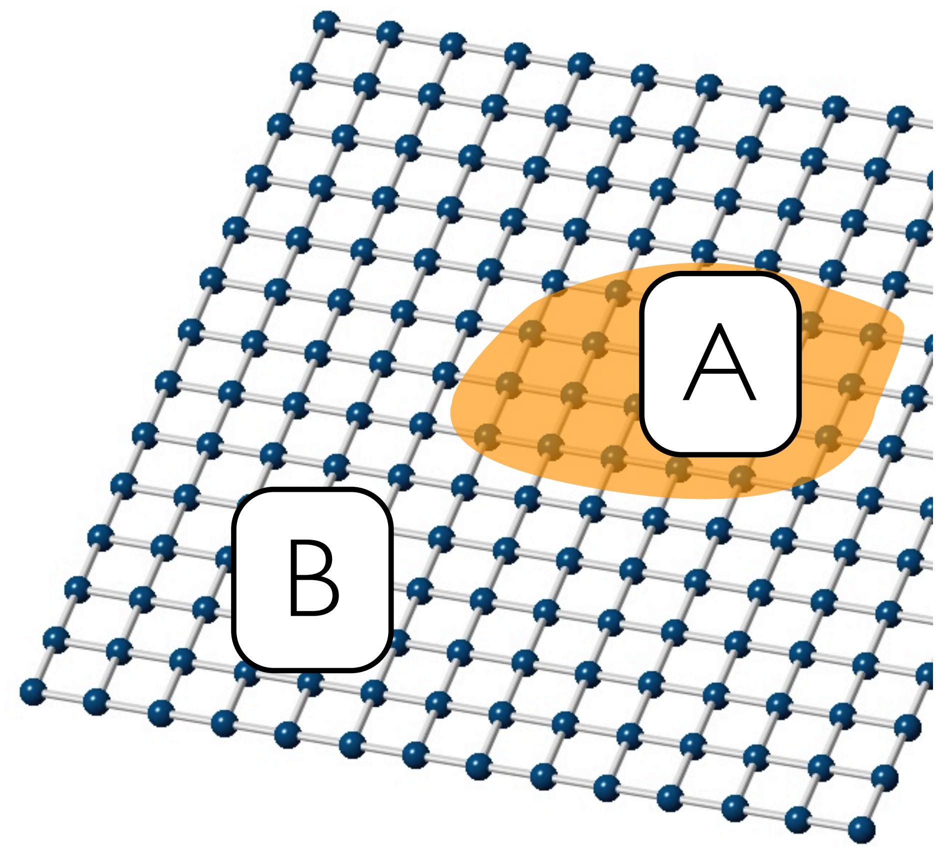
Observable

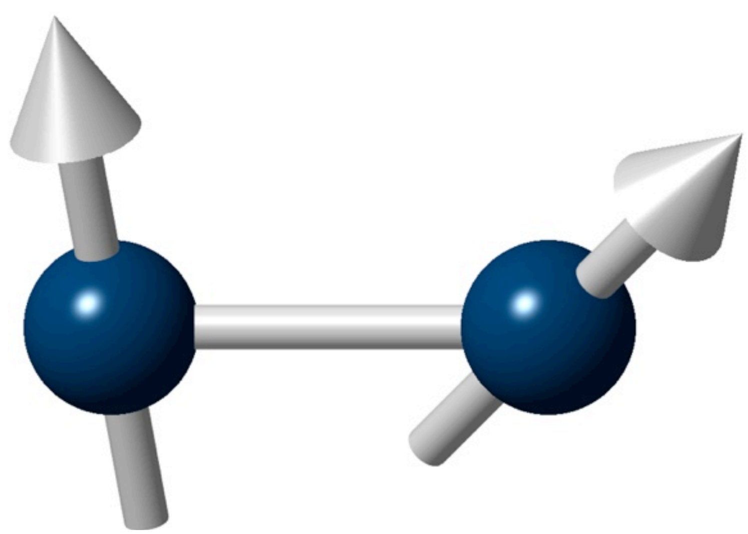
$$\langle\mathcal{O}\rangle = \operatorname{tr}(\rho\mathcal{O}) = \sum_i p_i \left\langle\psi_i\middle|\mathcal{O}\middle|\psi_i\right\rangle$$

Reduced Density Matrix

$$\rho_A = \mathrm{tr}_B\left(\rho_{AB}\right)$$

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



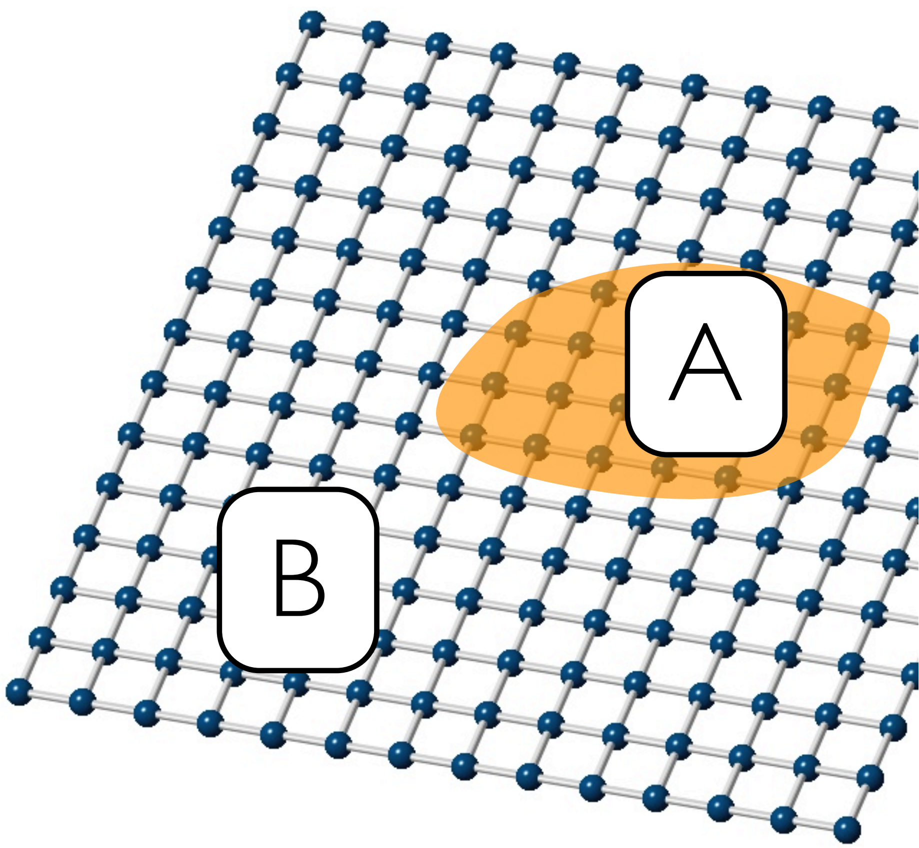


$$\rho_A = \mathrm{tr}_B(|\psi\rangle\langle\psi|) = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

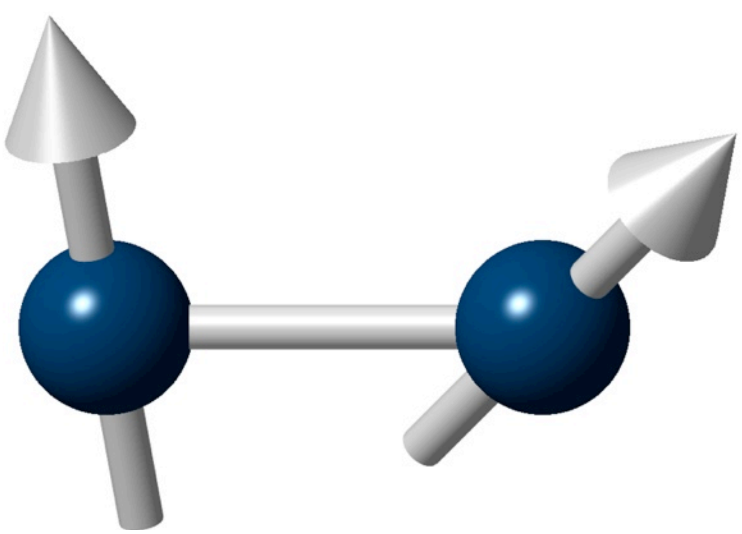
Best description of region A

Reduced Density Matrix

$$\rho_A = \mathrm{tr}_B\left(\rho_{AB}\right)$$



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



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

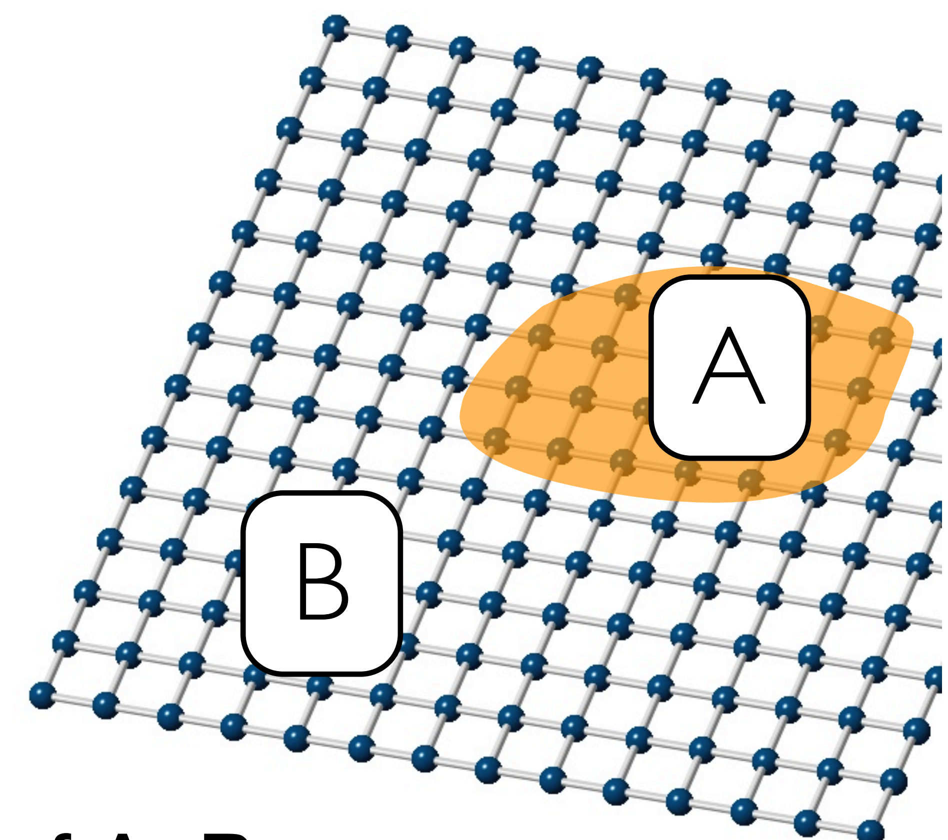
Best description of region B

Schmidt Decomposition

- If $|\psi\rangle$ is a pure state, it can always be decomposed into

$$|\psi\rangle = \sum_{i}^{N_\lambda} \lambda_i \left|i_A\right\rangle \left|i_B\right\rangle$$

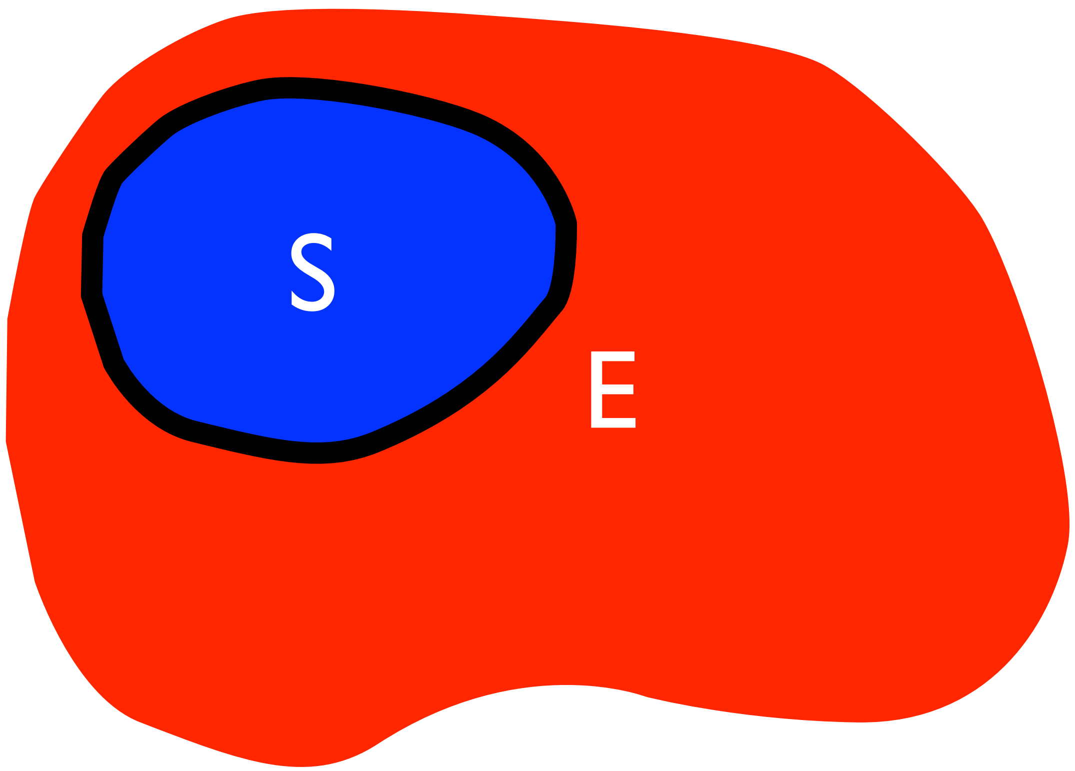
where
$\lambda_i \geq 0$ and
$\{|i_A\rangle\}, \{|i_B\rangle\}$ are orthonormal basis of A, B



$$\rho_A = \mathrm{tr}_B(|\psi\rangle\langle\psi|) = \sum_{i}^{N_\lambda} \lambda_i^2 \left|i_A\right\rangle \left\langle i_A\right|$$

Subsystem states

- What are the most important subsystem states ?



Hamiltonian

$$H = H_S + H_E + H_{SE}$$

Wavefunction

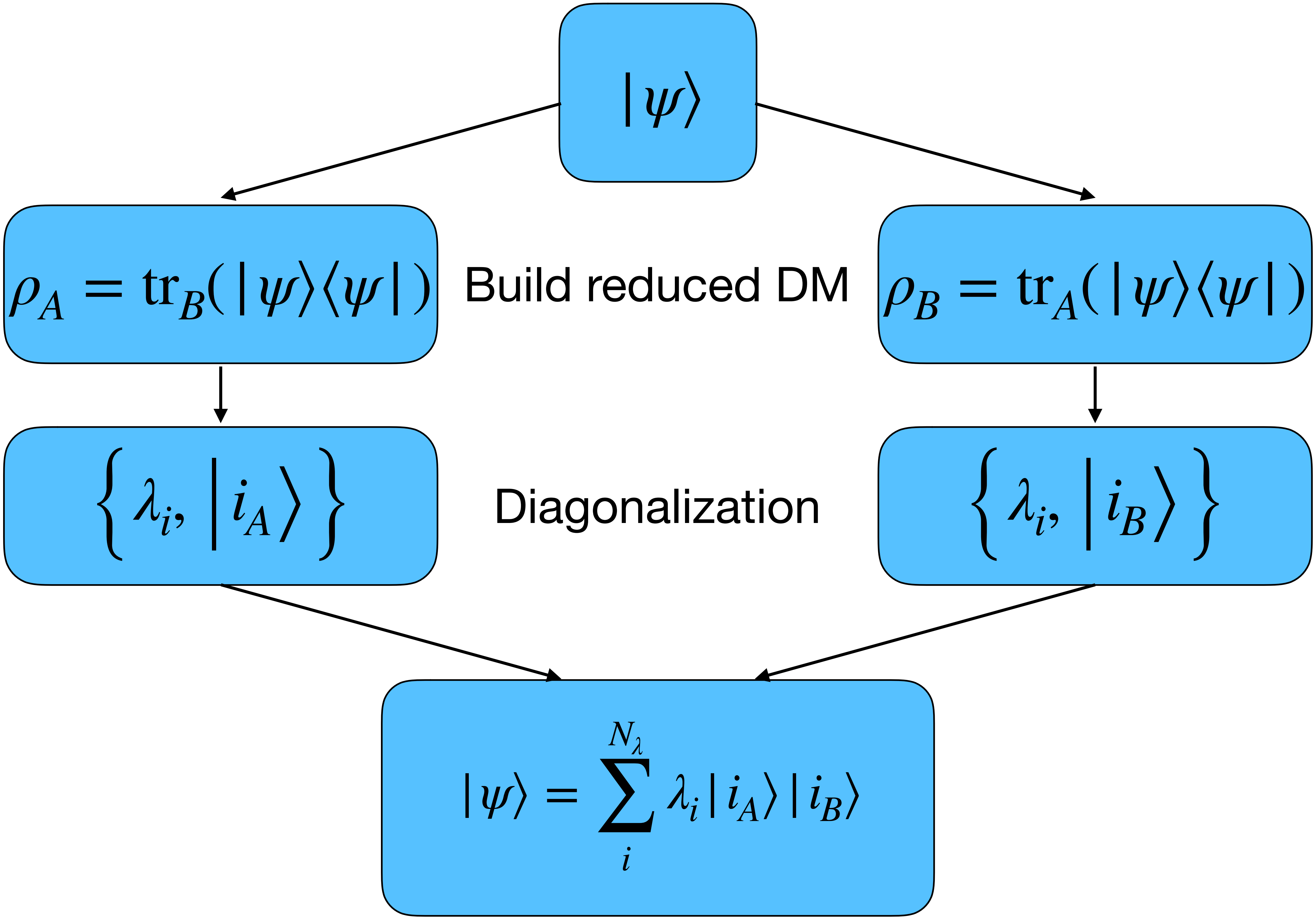
$$|\psi\rangle = \sum_{i,\alpha} \psi_{i,\alpha} \, |i\rangle_S \, |\alpha\rangle_E$$

Best approximation with m subsystem states:

$$|\tilde{\psi}\rangle = \sum_{n=1}^{m} \sum_{\alpha} \tilde{\psi}_{n,\alpha} \, |\phi_n\rangle_S \, |\alpha\rangle_E$$

Minimize the distance between states: $S = \left| |\tilde{\psi}\rangle - |\psi\rangle \right|^2$

Eigenstates of reduced DM

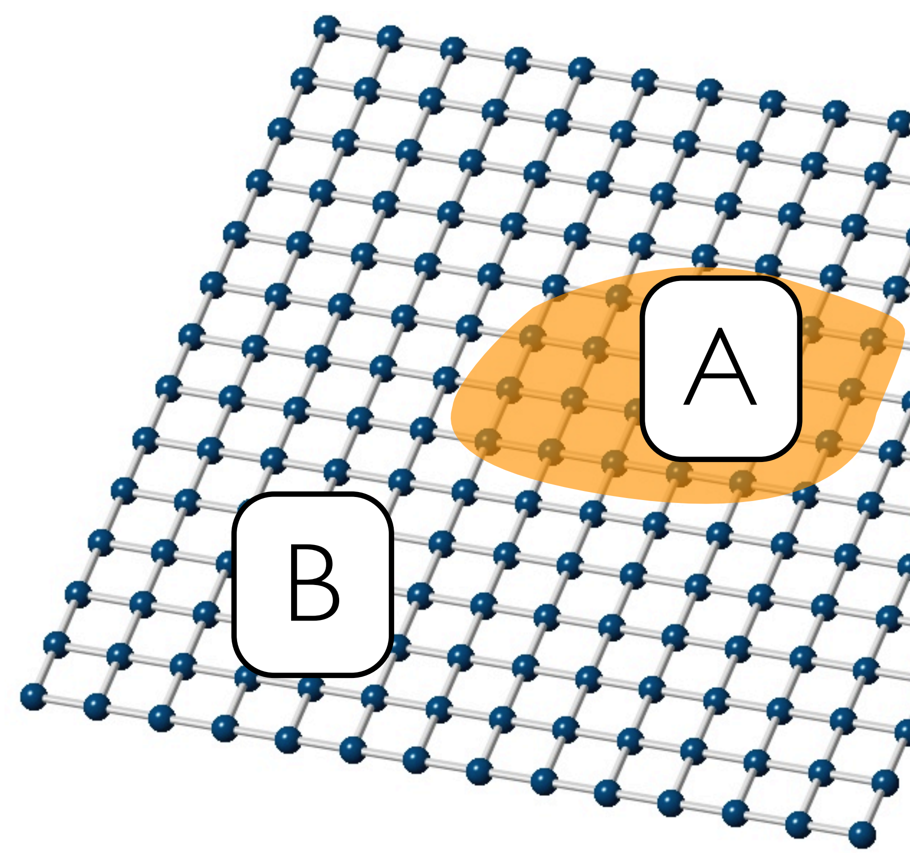


Controlled Approximation

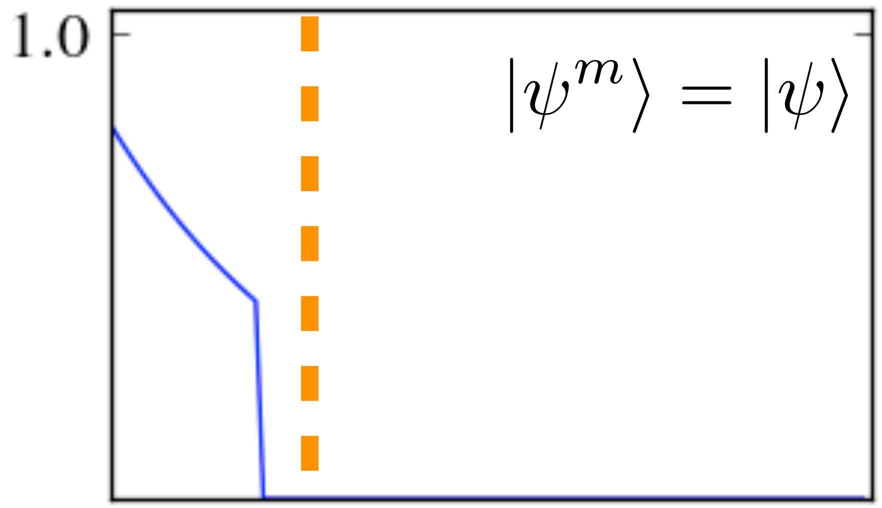
$$|\psi\rangle \approx \left|\psi_{AB}^{m}\right\rangle \equiv \sum_{i}^{m} \lambda_i \left|i_A\right\rangle \left|i_B\right\rangle, \quad m < N_\lambda$$

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

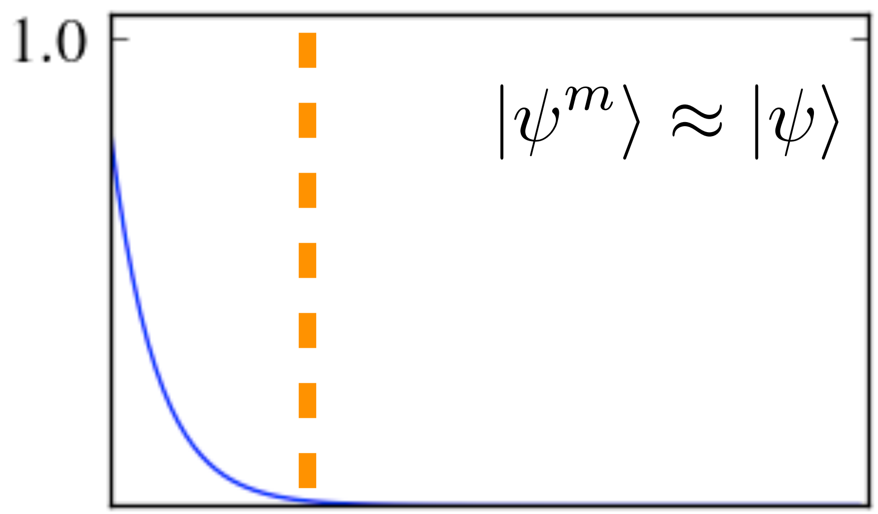
- The accuracy of the approximation depends on how fast λ_i decays.



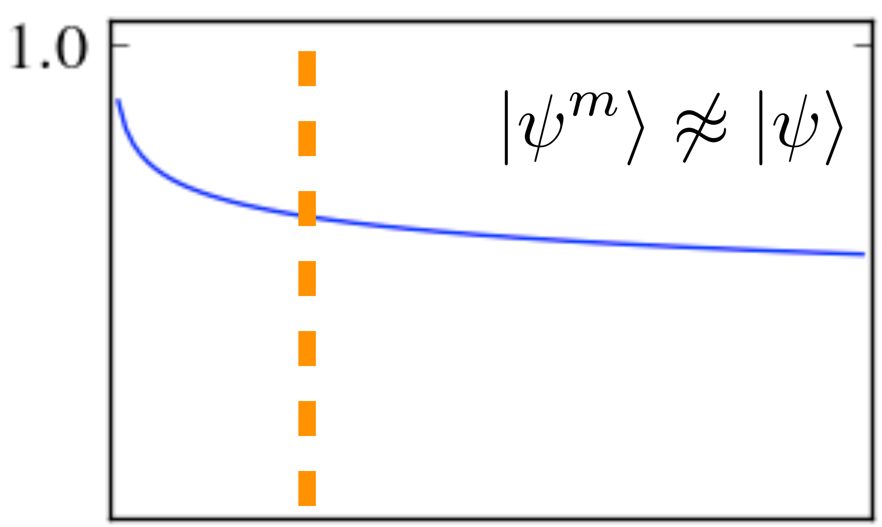
Approximate Wavefunctions



m-dimensional MPS



1D ground state



General, including 2D

Entanglement Entropy

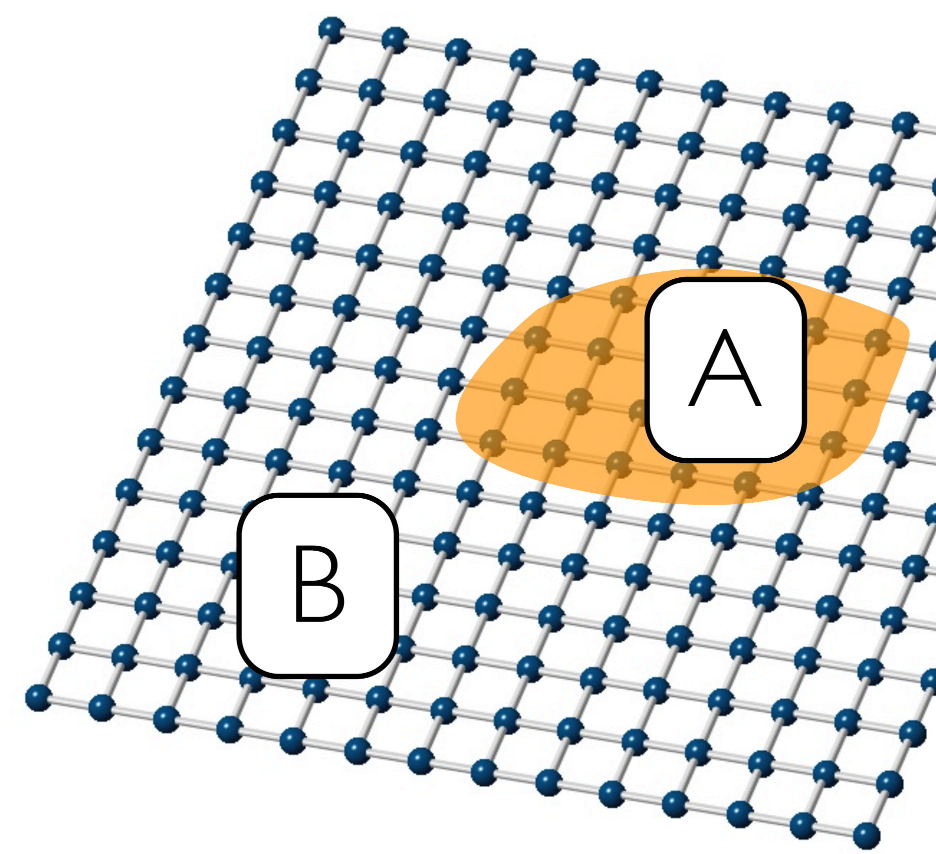
Von Neumann Entanglement Entropy

$$S(A) = -\,\mathrm{tr}\left[\rho_A \ln\left(\rho_A\right)\right] = -\sum_i p_i \ln p_i = S(B)$$

- Measures how entangled subregions A and B are.

- The number of states to keep, m, scales with S:

$$m \sim e^{S(A)}$$



Scaling of entanglement entropy

1D gapped : $S(L) \sim \ln(\xi) \Rightarrow \lim_{L\to\infty} m \sim$ **const**

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

DMRG Works

2D gapped and gapless : Area Law

$$S(L) \sim L^{d-1} \Rightarrow \lim_{L\to\infty} m \sim e^{L^{d-1}}$$

RG transformation

- Diagonalization of the reduced density matrix gives you the RG transformation.

- Truncation is done by truncating the transformation matrix.

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

$$U = \begin{array}{c} \begin{array}{cccc} |1_A\rangle & |2_A\rangle & & |N_{\lambda,A}\rangle \end{array} \\ \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1N_\lambda} \\ u_{21} & u_{22} & \cdots & u_{2N_\lambda} \\ \vdots & \vdots & \ddots & \vdots \\ u_{N_\lambda 1} & u_{N_\lambda 2} & \cdots & u_{N_\lambda N_\lambda} \end{pmatrix} \end{array}$$

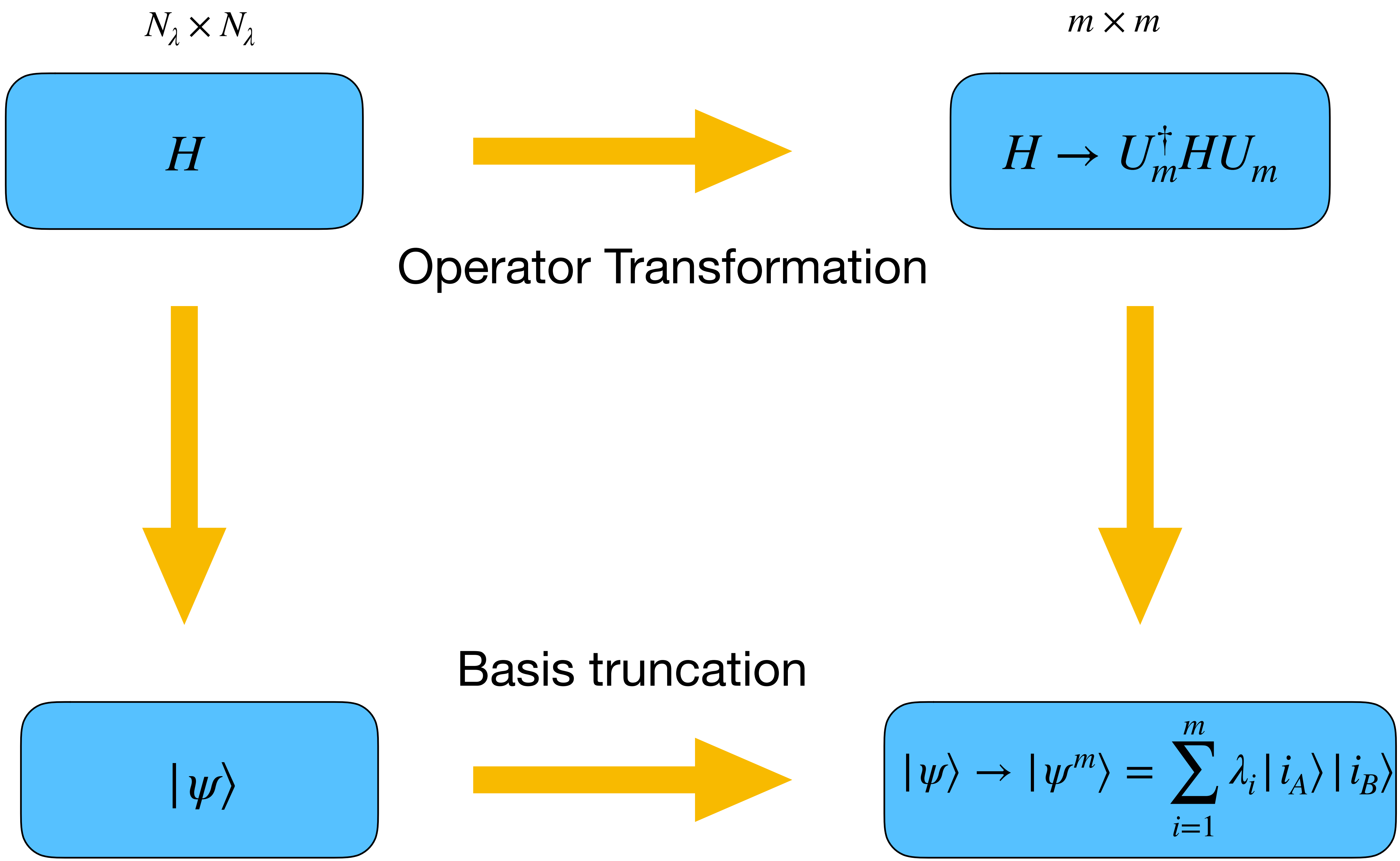
RG transformation

- Diagonalization of the reduced density matrix gives you the RG transformation.

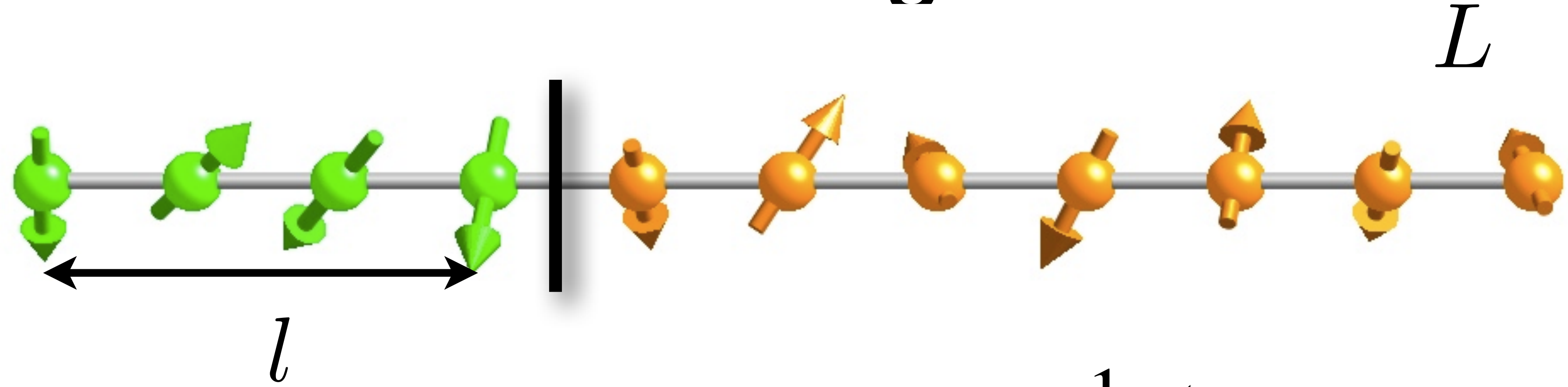
- Truncation is done by truncating the transformation matrix.

$$U \to U_m = \begin{array}{c} \begin{array}{cccc} |1_A\rangle & |2_A\rangle & & |m_A\rangle \end{array} \\ \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1m} \\ u_{21} & u_{22} & \cdots & u_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ u_{N_\lambda 1} & u_{N_\lambda 2} & \cdots & u_{N_\lambda m} \end{pmatrix}_{m \times N_\lambda} \end{array} \qquad |\psi\rangle \to |\psi_m\rangle$$

RG transformation



Heisenberg model



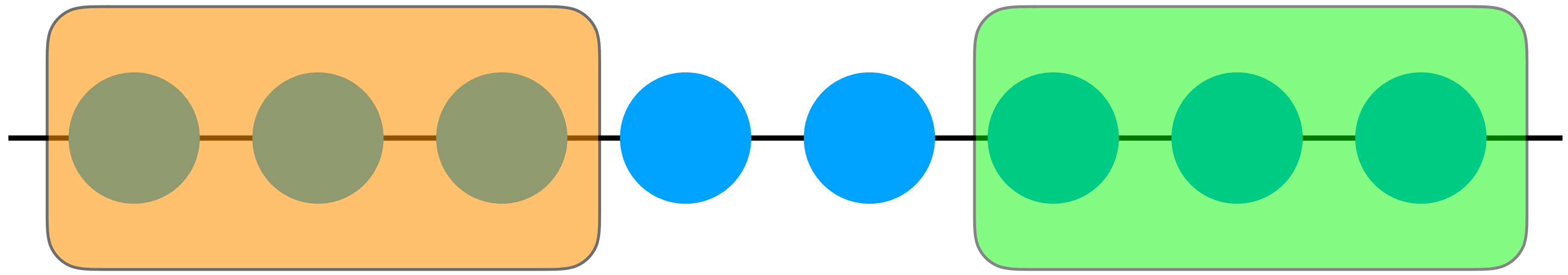
$$H = \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} = \sum_i S_i^z S_{i+1}^z + \frac{1}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right)$$

$$S^z = \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix} \quad S^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad S^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

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

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

Split chain into blocks



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

Block Hamiltonian

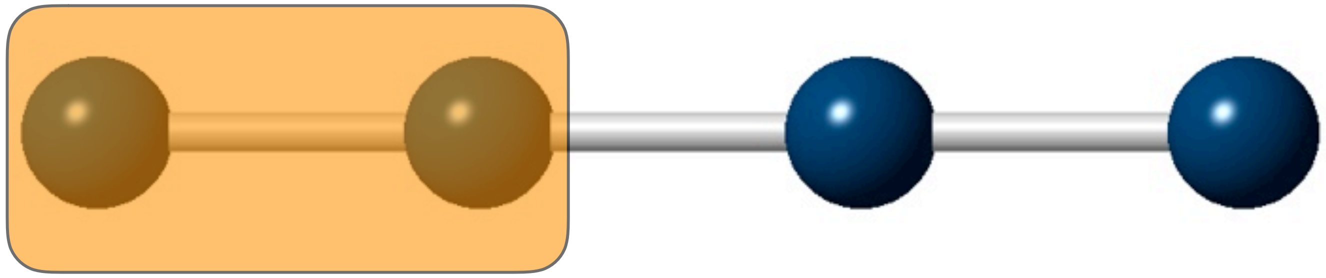
Block Hamiltonian

system

environment

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

Building the Hamiltonian

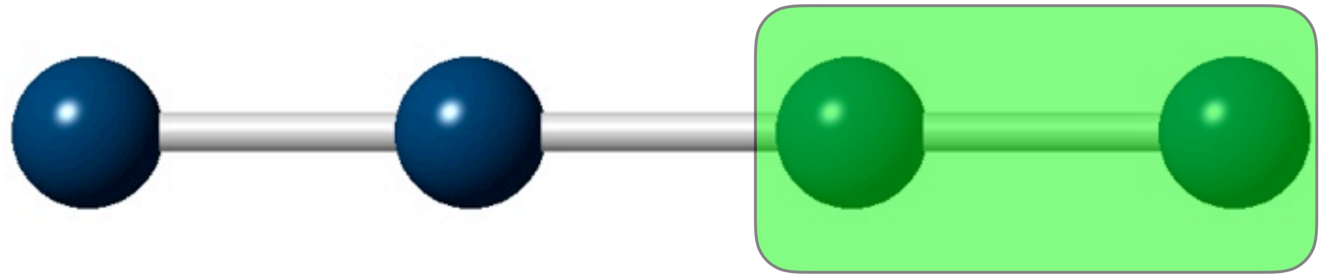


$$H_b^{(s)} = \frac{1}{2}\left(S_{s,1}^{+} \otimes S_{s,2}^{-} + S_{s,1}^{-} \otimes S_{s,2}^{+}\right) + S_{s,1}^{z} \otimes S_{s,2}^{z}$$

Single spin operator in the block

$$I \otimes \mathbf{S}$$

Building the Hamiltonian

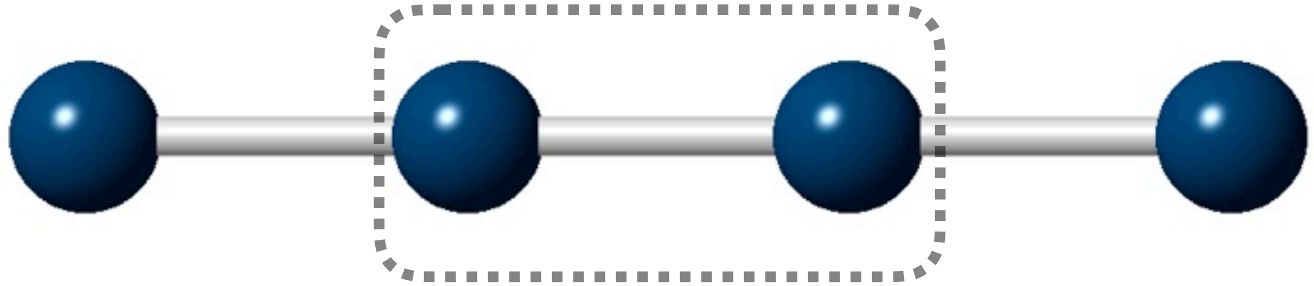


$$H_b^{(e)} = \frac{1}{2}\left(S_{s,3}^{+} \otimes S_{s,4}^{-} + S_{s,3}^{-} \otimes S_{s,4}^{+}\right) + S_{s,3}^{z} \otimes S_{s,4}^{z}$$

Single spin operator in the block

$$\mathbf{S} \otimes I$$

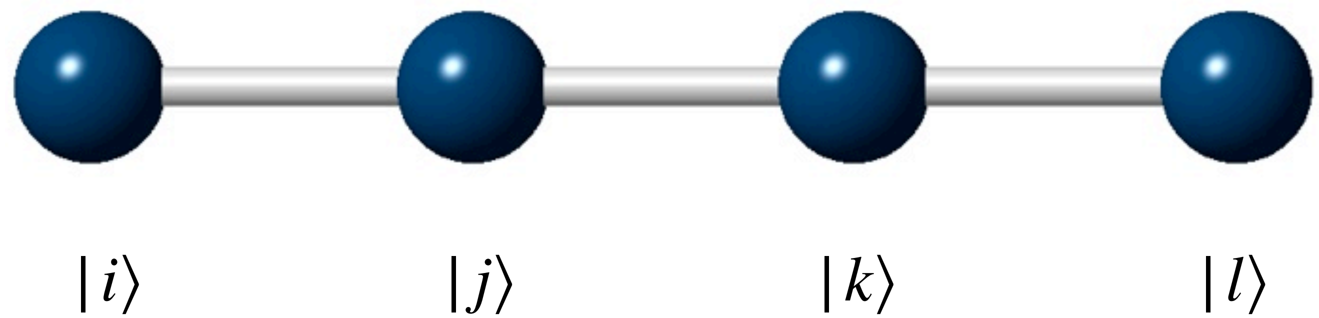
Building the Hamiltonian



$$H_{se} = \frac{1}{2}\left(S^{+}_{s,2} \otimes S^{-}_{s,3} + S^{-}_{s,2} \otimes S^{+}_{s,3}\right) + S^{z}_{s,2} \otimes S^{z}_{s,3}$$

$$S^{z} = \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix} \quad S^{+} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad S^{-} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Building the Hamiltonian



$$H = H_b^{(s)} \otimes I + I \otimes H_b^{(e)} +$$
$$(S_x \otimes S_x + S_y \otimes S_y + S_z \otimes S_z)$$

Find the ground state

$|i\rangle$ $|j\rangle$ $|k\rangle$ $|l\rangle$

$$H = H_b^{(s)} \otimes I + I \otimes H_b^{(e)} + H_{se}$$

- Find the ground state $|\psi_0\rangle$ of H
- Construct the density matrix $\rho = |\psi_0\rangle\langle\psi_0|$
- Construct the reduced density matrix

$$\rho_s = \sum_{kl} \langle k|\langle l|\psi_0\rangle\langle\psi_0|k\rangle|l\rangle$$

- Keeping m eigenstates $\{|\phi_i\rangle\}$ with largest eigenvalues $\{\Lambda_i\}$ of ρ_s

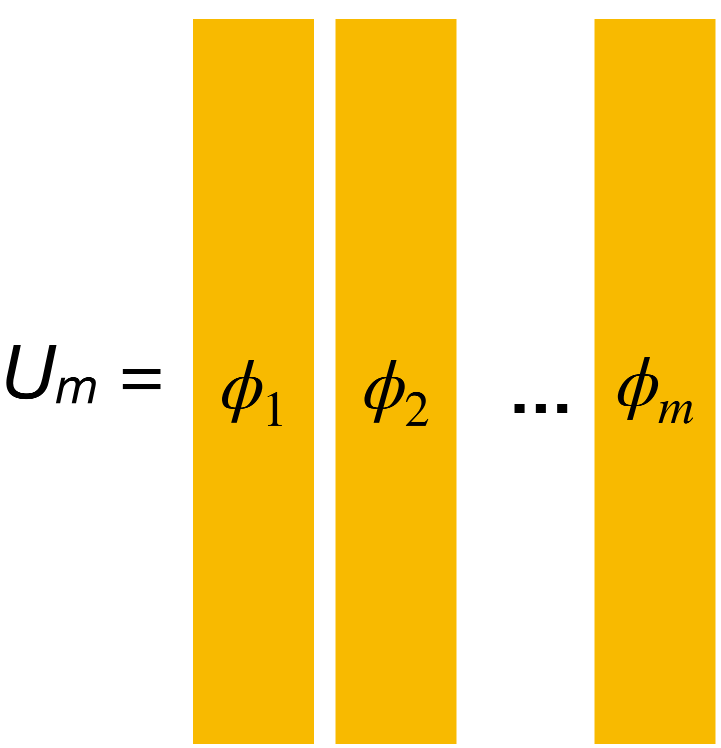
RG transformation

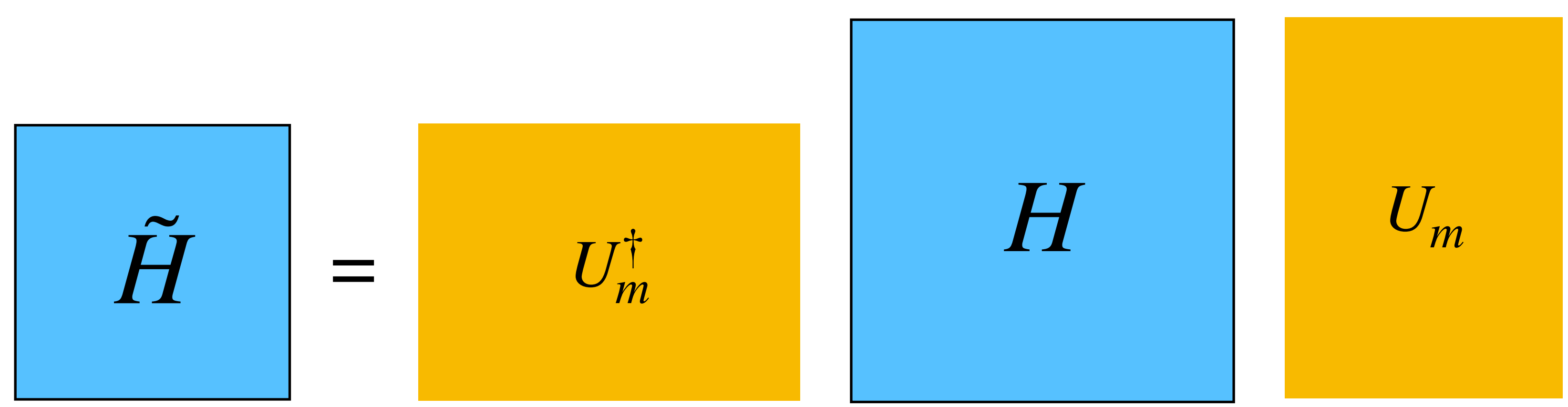
- Construct transformation matrix

$$U_m = \left(|\phi_1\rangle \quad |\phi_2\rangle \quad \dots \quad |\phi_m\rangle \right)$$

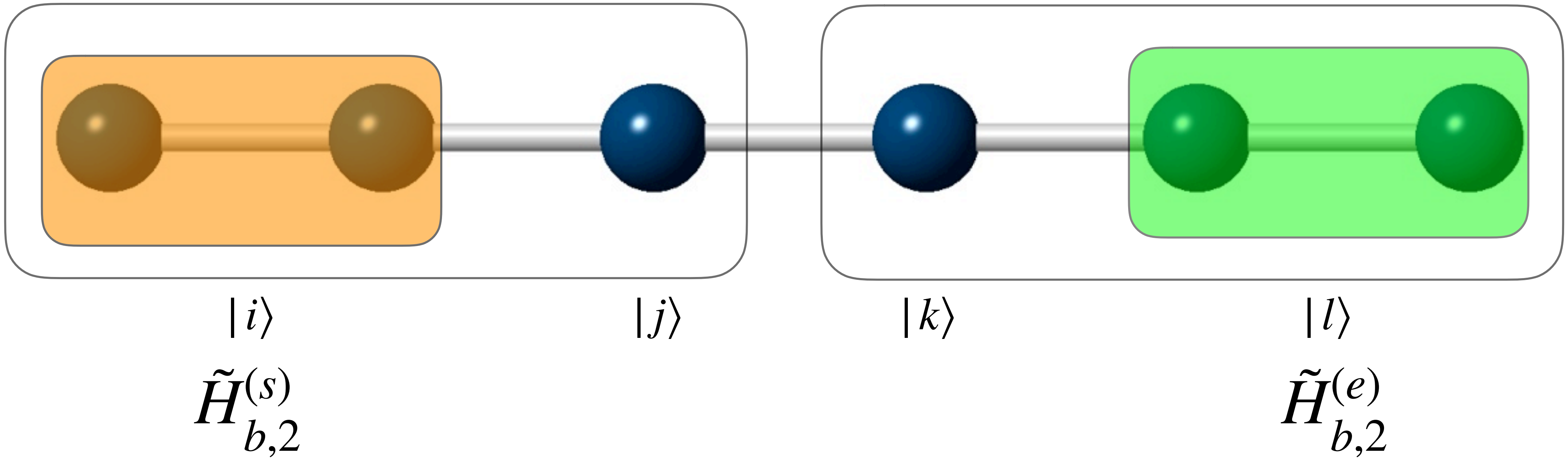
- Transform the block Hamiltonian and operators

$$\tilde{H}_b^{(s)} = U_m^\dagger H_b^{(s)} U_m \,, \tilde{\mathbf{S}} = U_m^\dagger (I \otimes \mathbf{S}) U_m$$





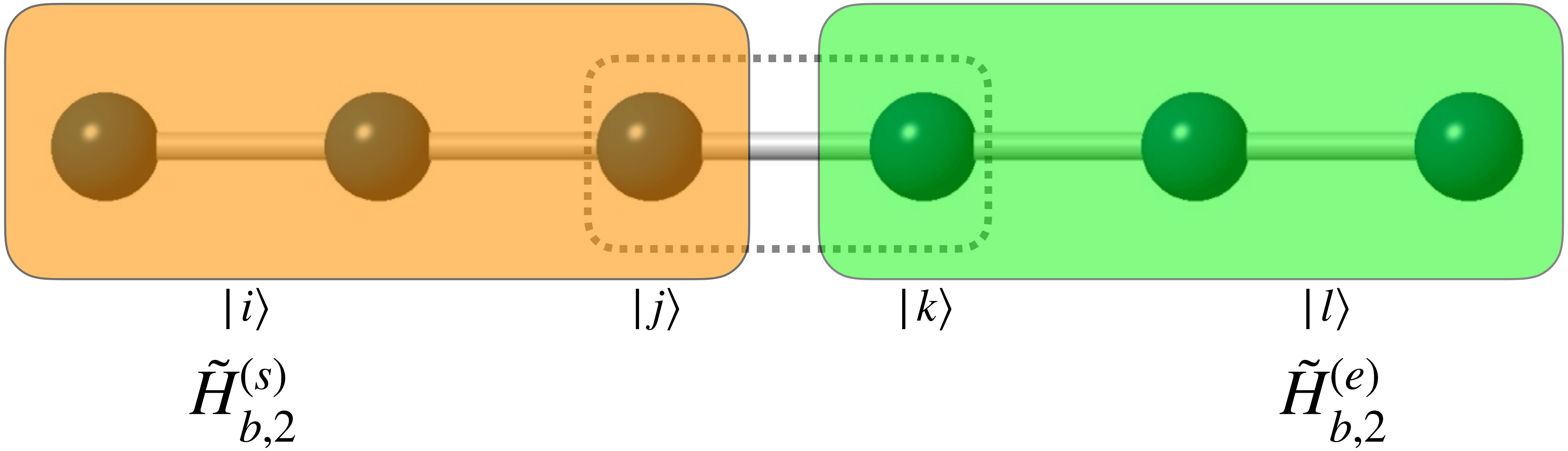
Building the Hamiltonian



$$H^{(s)}_{b,3} = \tilde{H}^{(s)}_{b,2} + (\tilde{\mathbf{S}} \otimes I) \cdot (I \otimes \mathbf{S})$$

$$H^{(e)}_{b,3} = \tilde{H}^{(e)}_{b,2} + (I \otimes \mathbf{S}) \cdot (\tilde{\mathbf{S}} \otimes I)$$

Building the Hamiltonian

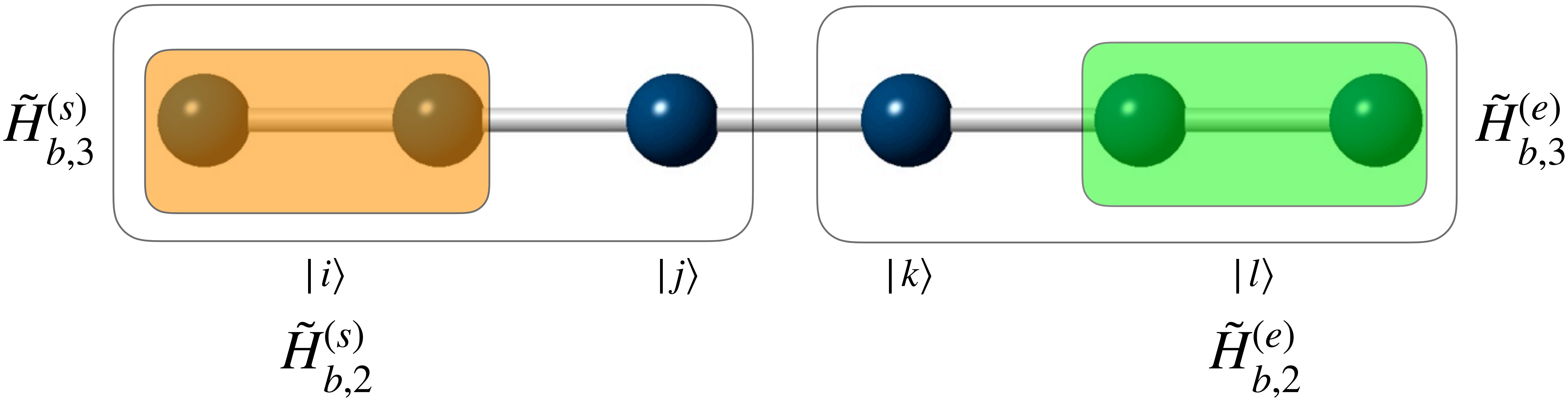


$$H^{(s)}_{b,3} = \tilde{H}^{(s)}_{b,2} + (\tilde{\mathbf{S}} \otimes I) \cdot (I \otimes \mathbf{S})$$

$$H_{se} = (\mathbf{S} \otimes I) \cdot (I \otimes \mathbf{S})$$

$$H = H^{(s)}_{b,3} \otimes I + I \otimes H^{(e)}_{b,3} + H_{se}$$

RG transformation

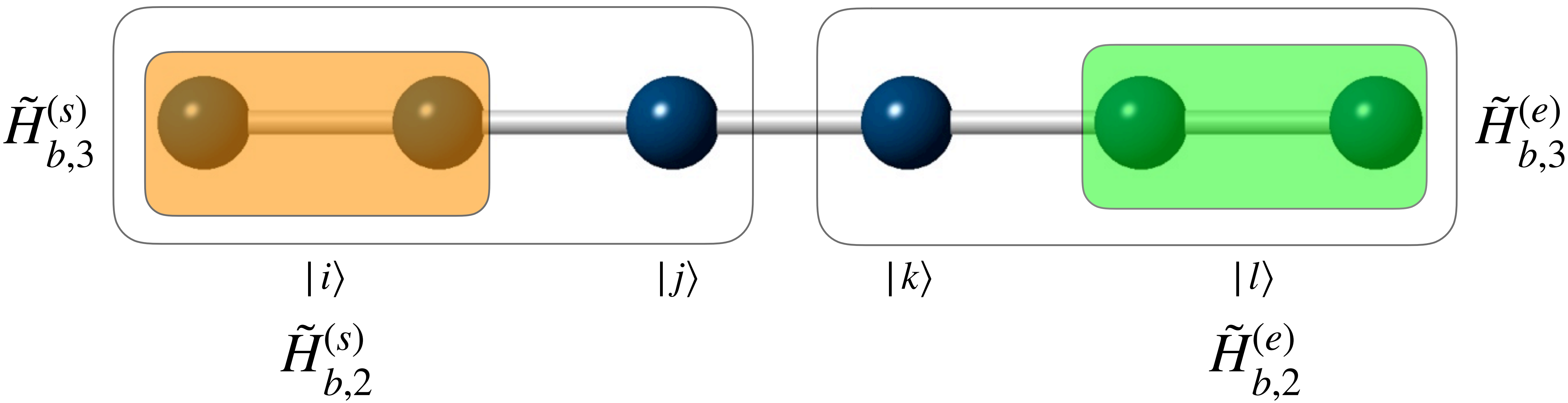


- Find the ground state $|\psi_0\rangle$ of H
- Construct the density matrix $\rho = |\psi_0\rangle\langle\psi_0|$
- Construct the reduced density matrix

$$\rho_s = \sum_{kl} \langle k|\langle l|\psi_0\rangle\langle\psi_0|k\rangle|l\rangle$$

- Keeping m eigenstates $\{|\phi_i\rangle\}$ with largest eigenvalues $\{\Lambda_i\}$ of ρ_s

RG transformation



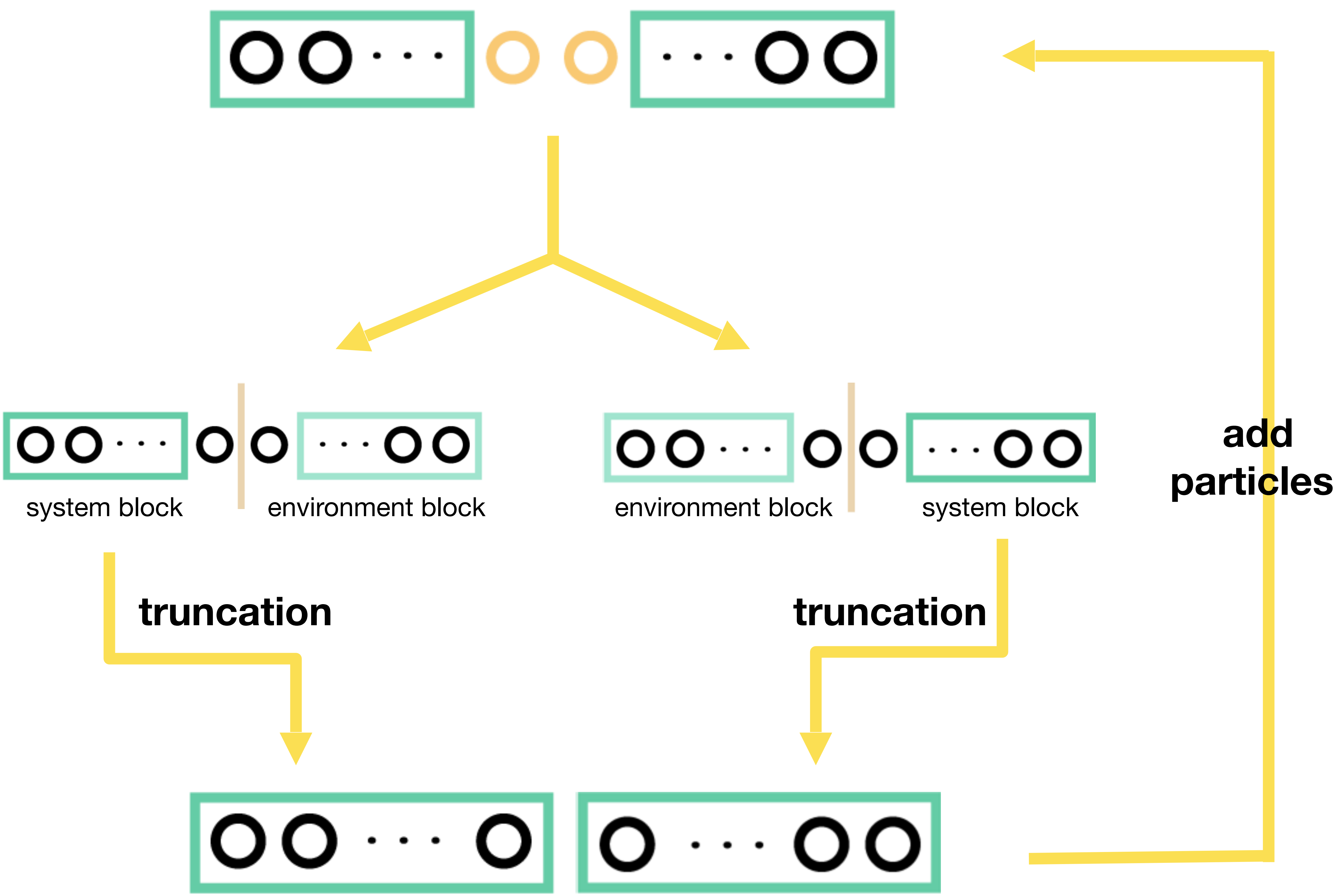
- Construct transformation matrix

$$U_m = \begin{pmatrix} |\phi_1\rangle & |\phi_2\rangle & \dots & |\phi_m\rangle \end{pmatrix}$$

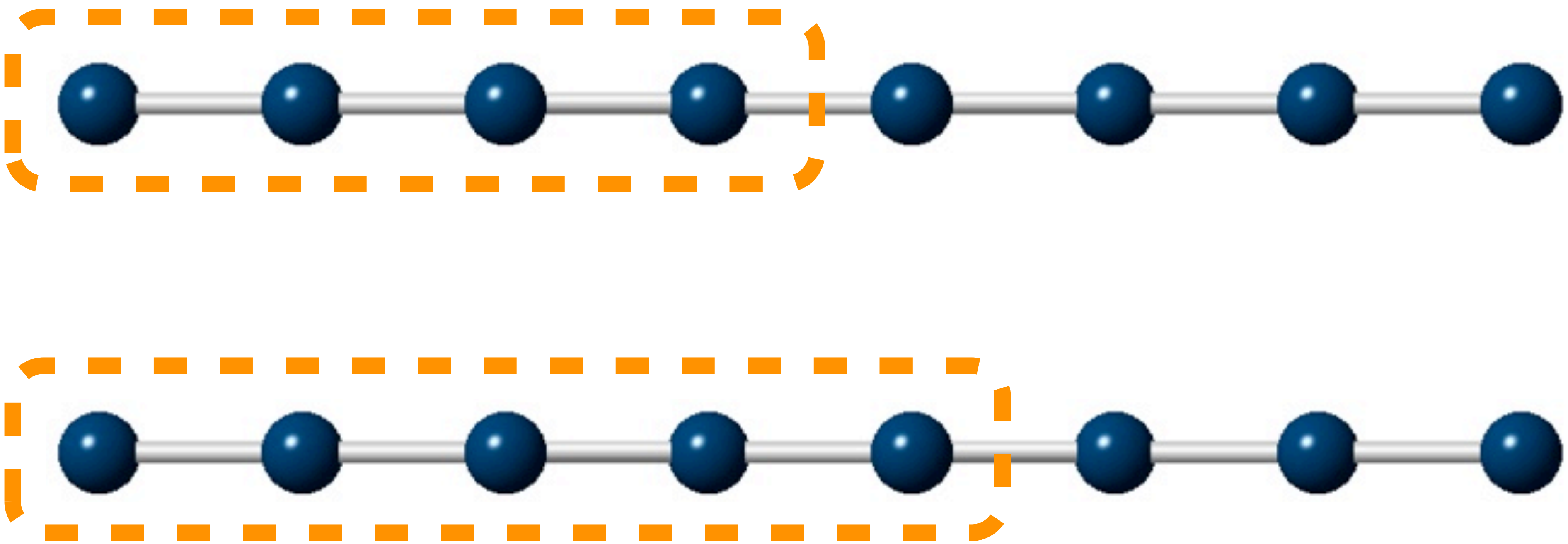
- Transform the block Hamiltonian and operators

$$\tilde{H}^{(s)}_{b,3} = U_m^\dagger H^{(s)}_{b,3} U_m \, , \tilde{\mathbf{S}} = U_m^\dagger (I \otimes \mathbf{S}) U_m$$

Infinite-size DMRG

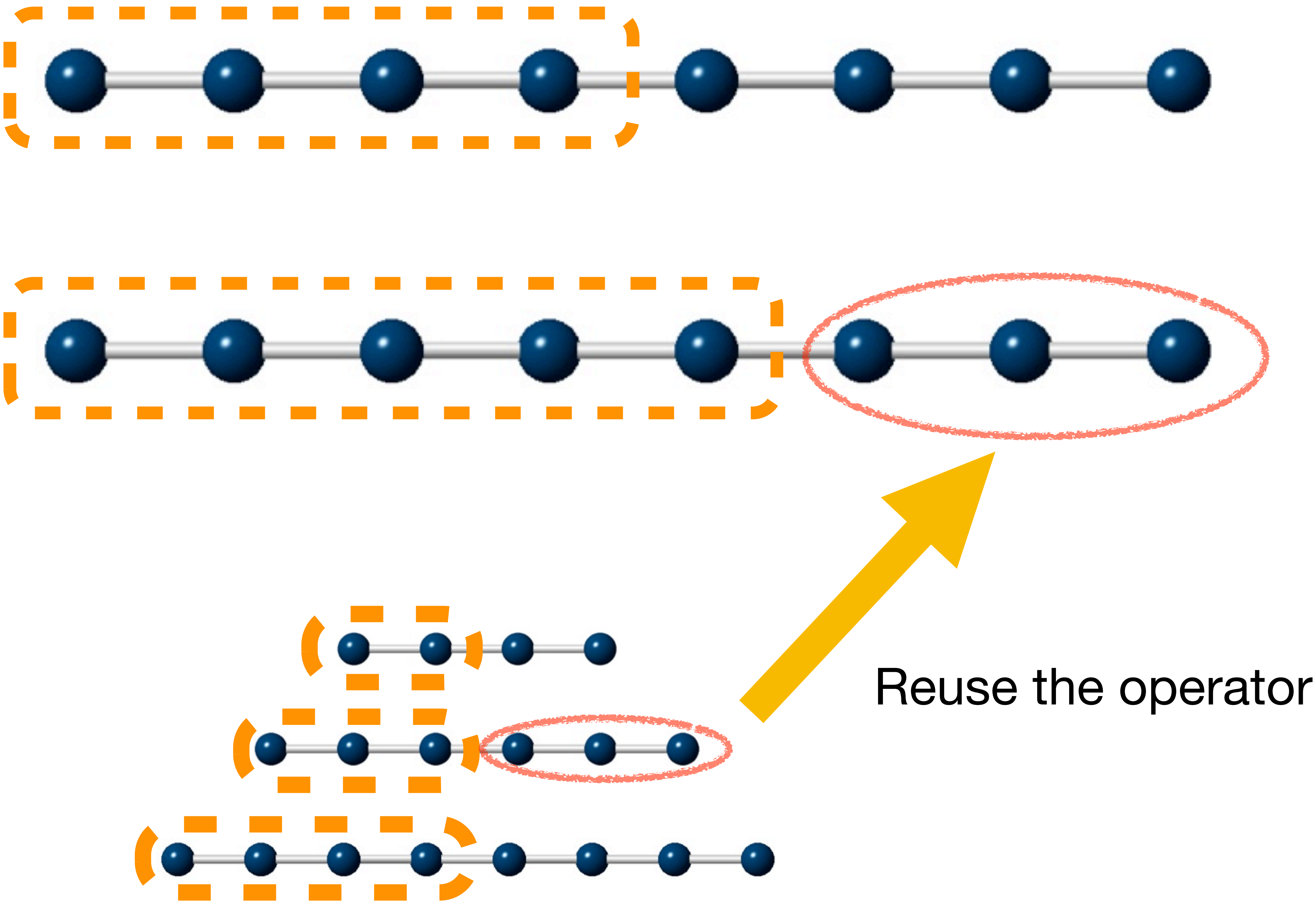


Finite-size DMRG

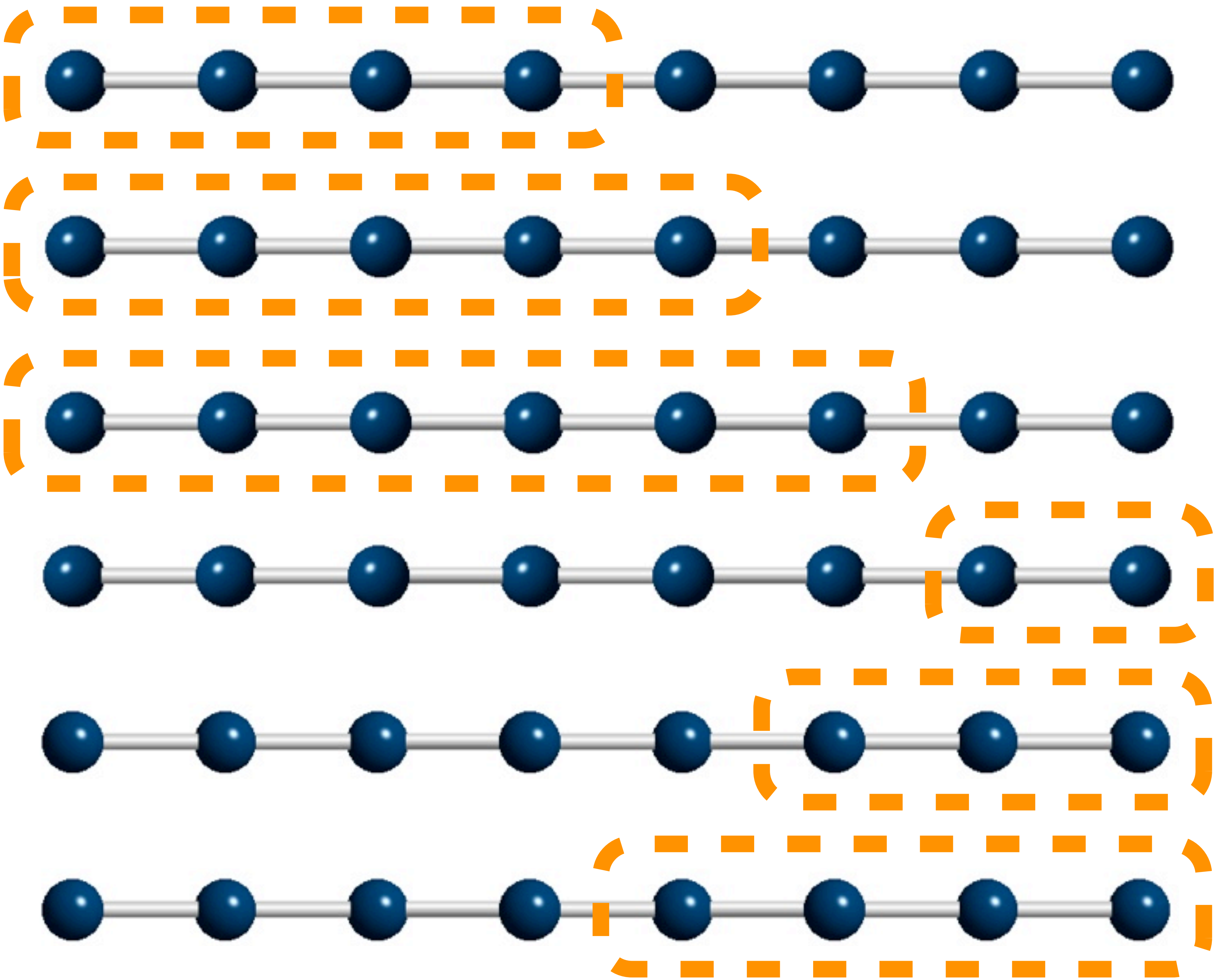


- Grow the chain to the desired size
- Improve ground state (energy) by sweeping

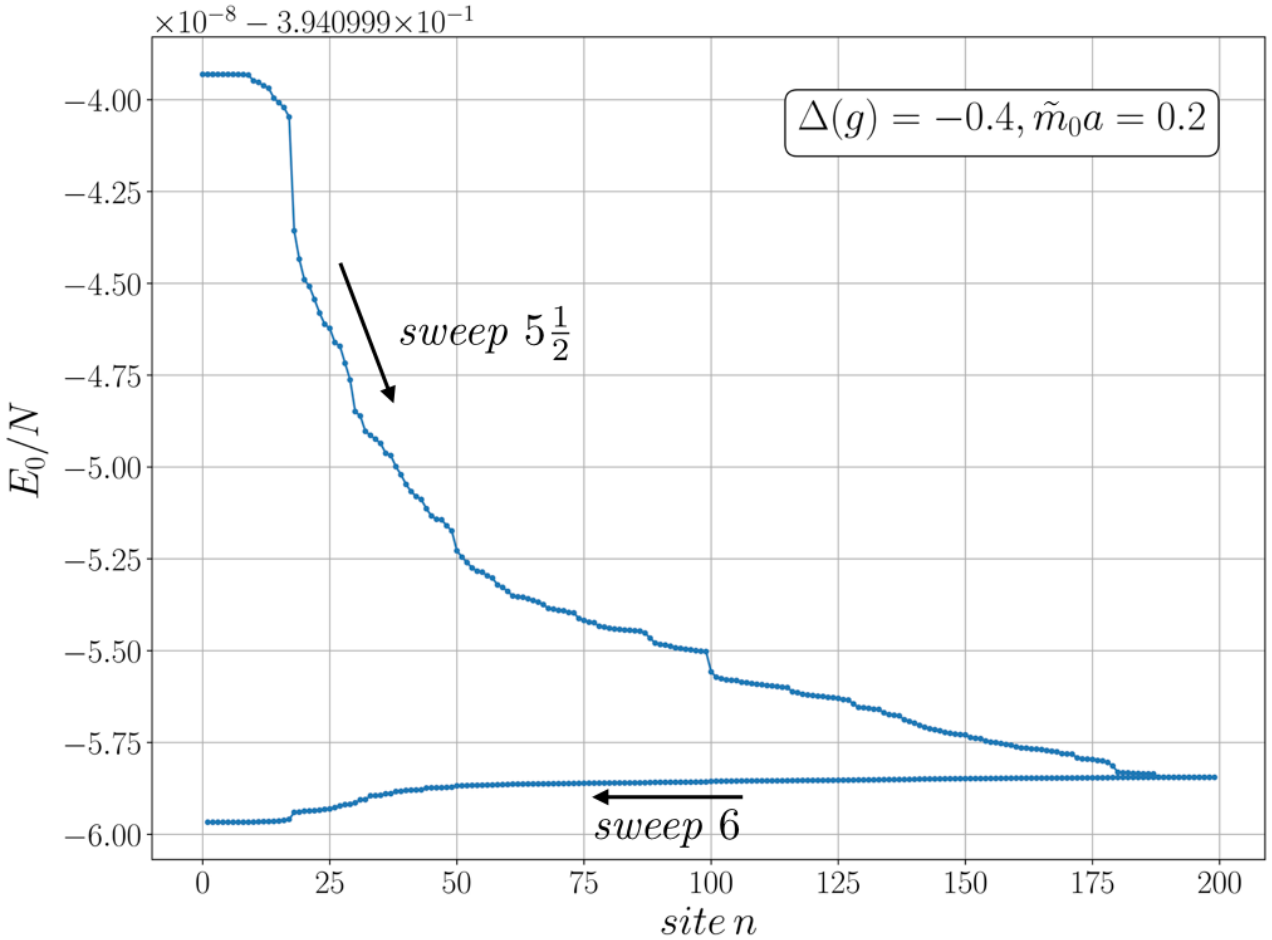
Sweeping



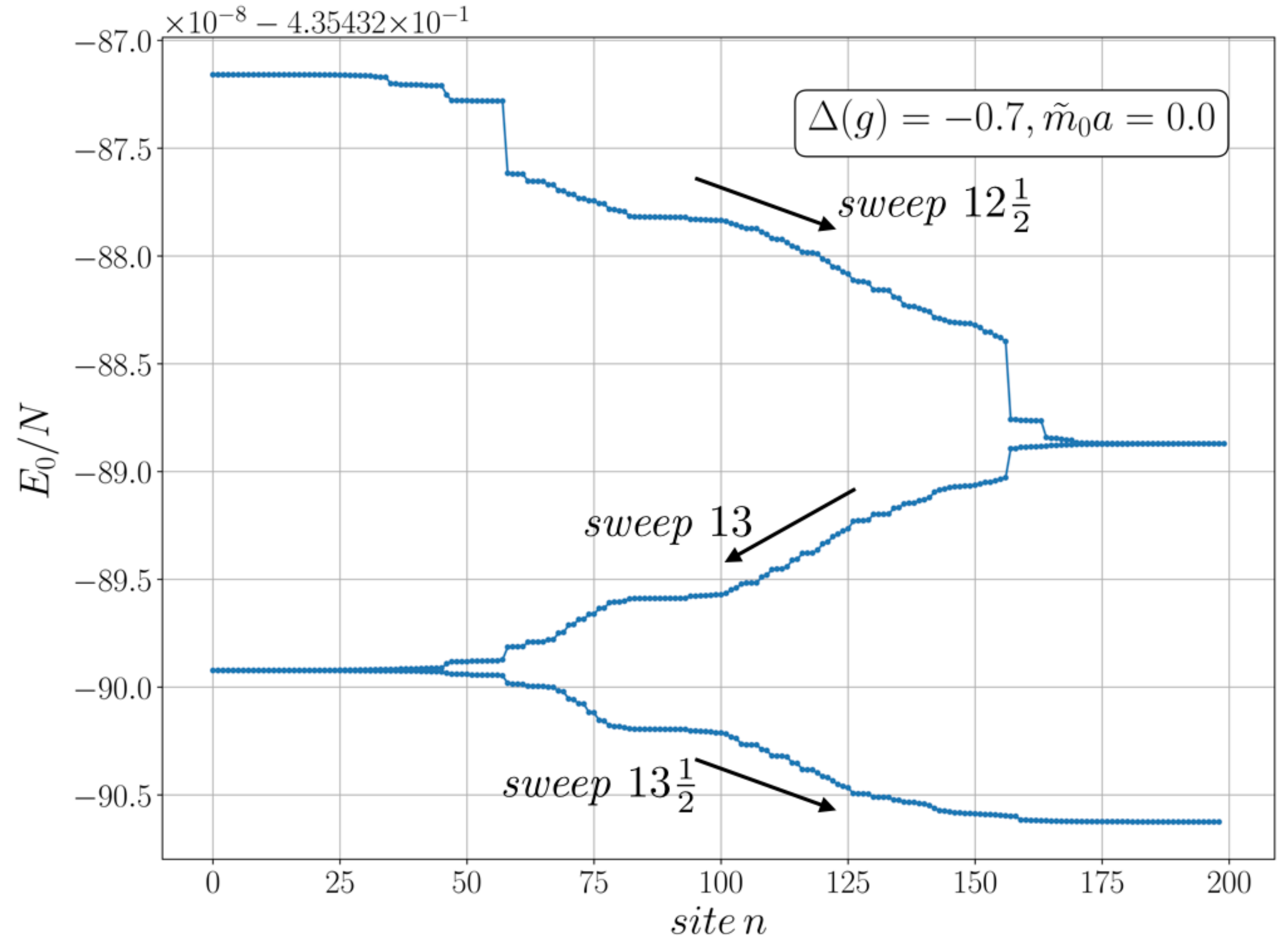
Finite-size DMRG



Sweeping

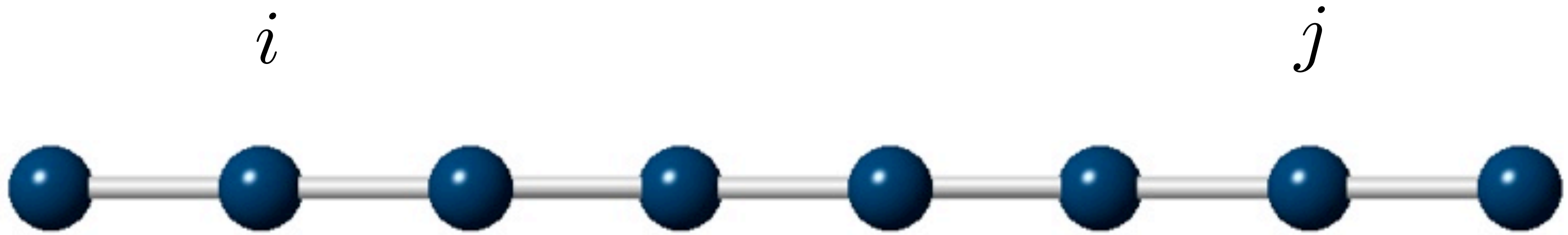


$\times 10^{-8} - 3.940999 \times 10^{-1}$
$\Delta(g) = -0.4, \tilde{m}_0 a = 0.2$
$sweep\ 5\frac{1}{2}$
$sweep\ 6$
E_0/N
$site\ n$
−4.00
−4.25
−4.50
−4.75
−5.00
−5.25
−5.50
−5.75
−6.00
0
25
50
75
100
125
150
175
200



$\times 10^{-8} - 4.35432 \times 10^{-1}$
$\Delta(g) = -0.7, \tilde{m}_0 a = 0.0$
$sweep\ 12\frac{1}{2}$
$sweep\ 13$
$sweep\ 13\frac{1}{2}$
E_0/N
$site\ n$
−87.0
−87.5
−88.0
−88.5
−89.0
−89.5
−90.0
−90.5
0
25
50
75
100
125
150
175
200

Measurements

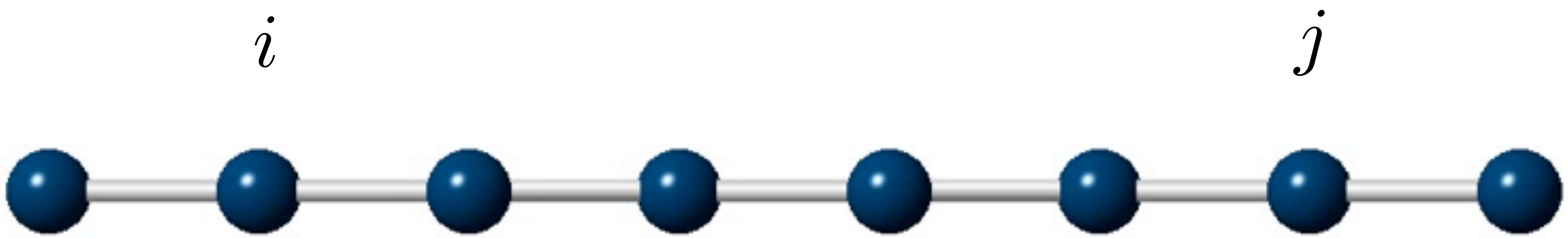


$$\Big\langle \psi \Big| S_i^z S_j^z \Big| \psi \Big\rangle \approx \Big\langle \psi_{L/2}^m \Big| \tilde{S}_i^z \tilde{S}_j^z \Big| \psi_{L/2}^m \Big\rangle$$

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

$$O(i, L/2) = U_m(i) U_m(i+1) \cdots U_m(L/2)$$

Fermionic sign



$$S_j^z = c_j^\dagger c_j - \frac{1}{2}$$

$$S_j^+ = c_j^\dagger e^{i\pi \sum_{l<j} n_l}$$

$$S_j^- = c_j e^{-i\pi \sum_{l<j} n_l}$$

$$c_i^\dagger c_j = S_i^+ e^{-i\pi \sum_{l=i+1}^{j-1} n_l} S_j$$

Jordan-Wigner transformation

Optimization

- Use symmetries
- Guess for Lanczos (wave function transformation)
- Everything under m^3
- DGEMM should be your best friend