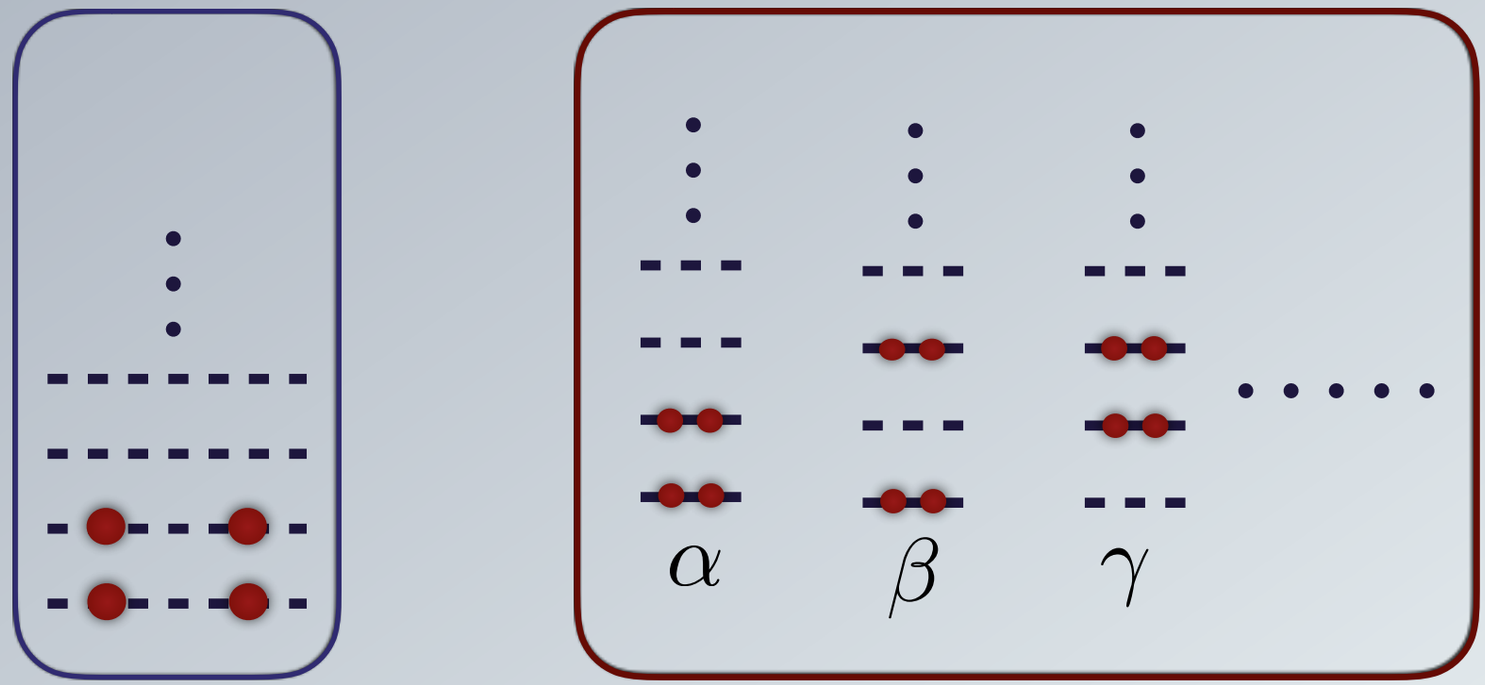
Basic idea:

Group No.5

i) basis



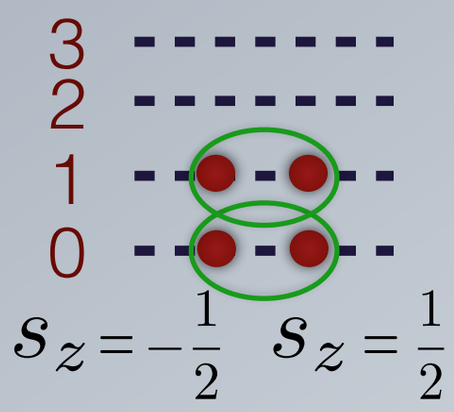
ii)Hamiltonian

$$\mathcal{H} = \begin{pmatrix} H_{\alpha\alpha} & H_{\alpha\beta} & H_{\alpha\gamma} & \cdots \\ H_{\beta\alpha} & H_{\beta\beta} & H_{\beta\gamma} & \cdots \\ H_{\gamma\alpha} & H_{\gamma\beta} & H_{\gamma\gamma} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

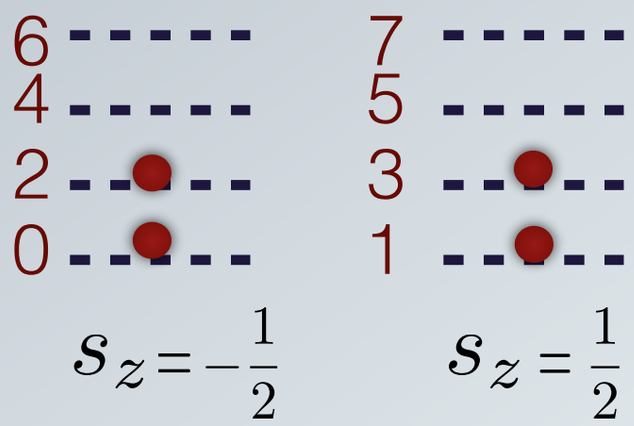
iii)Diagonalization

Different strategies:

Y



AY



C++ vs Python

Windows vs Linux vs MacOs

Configuration & Hamiltonian:

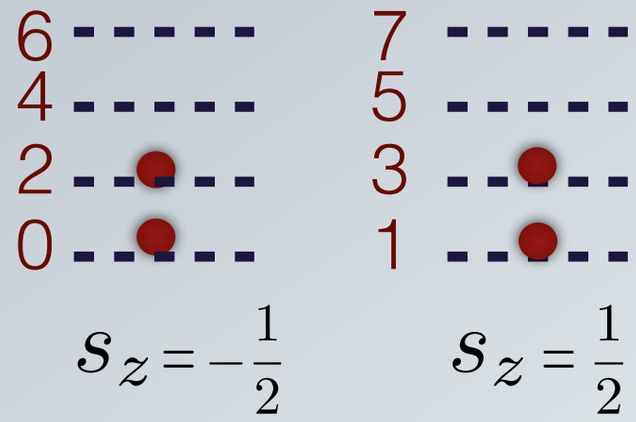
step 1:

2p2h

0	h : (0, 1)	p : (4, 5)
1	h : (0, 1)	p : (6, 7)
2	h : (2, 3)	p : (4, 5)
3	h : (2, 3)	p : (6, 7)

4p4h

0	h : (0, 1, 2, 3)	p : (4, 5, 6, 7)



step 2:

0p0h:11110000

2p2h: 00111100, 00110011…

4p4h: 00001111

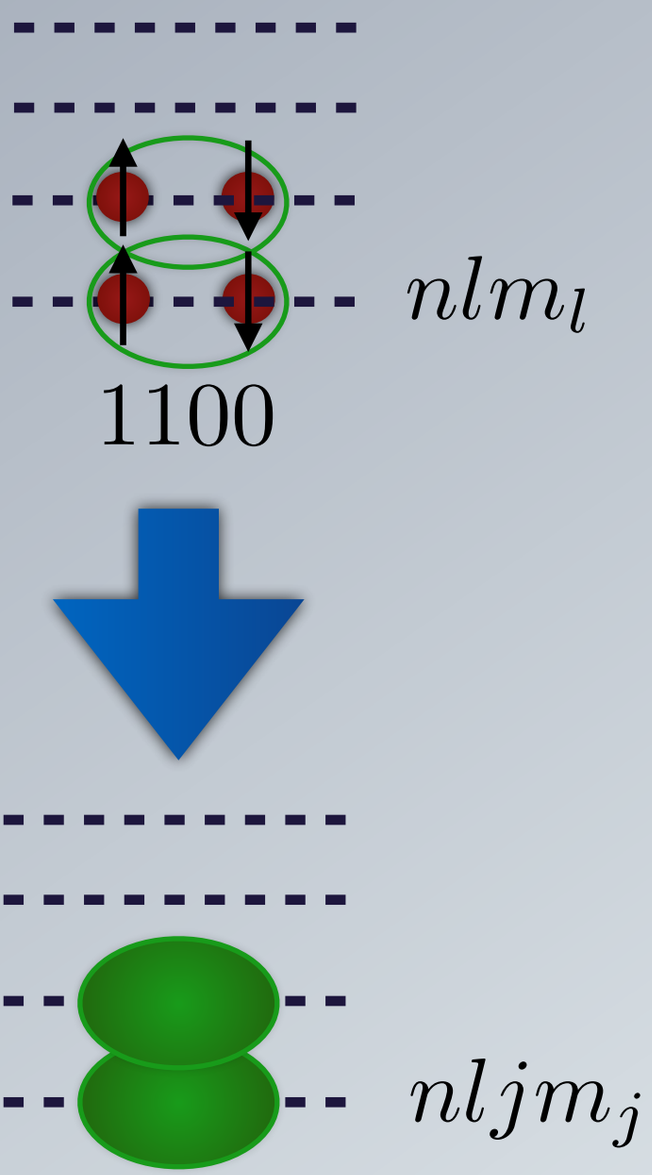
step 3:

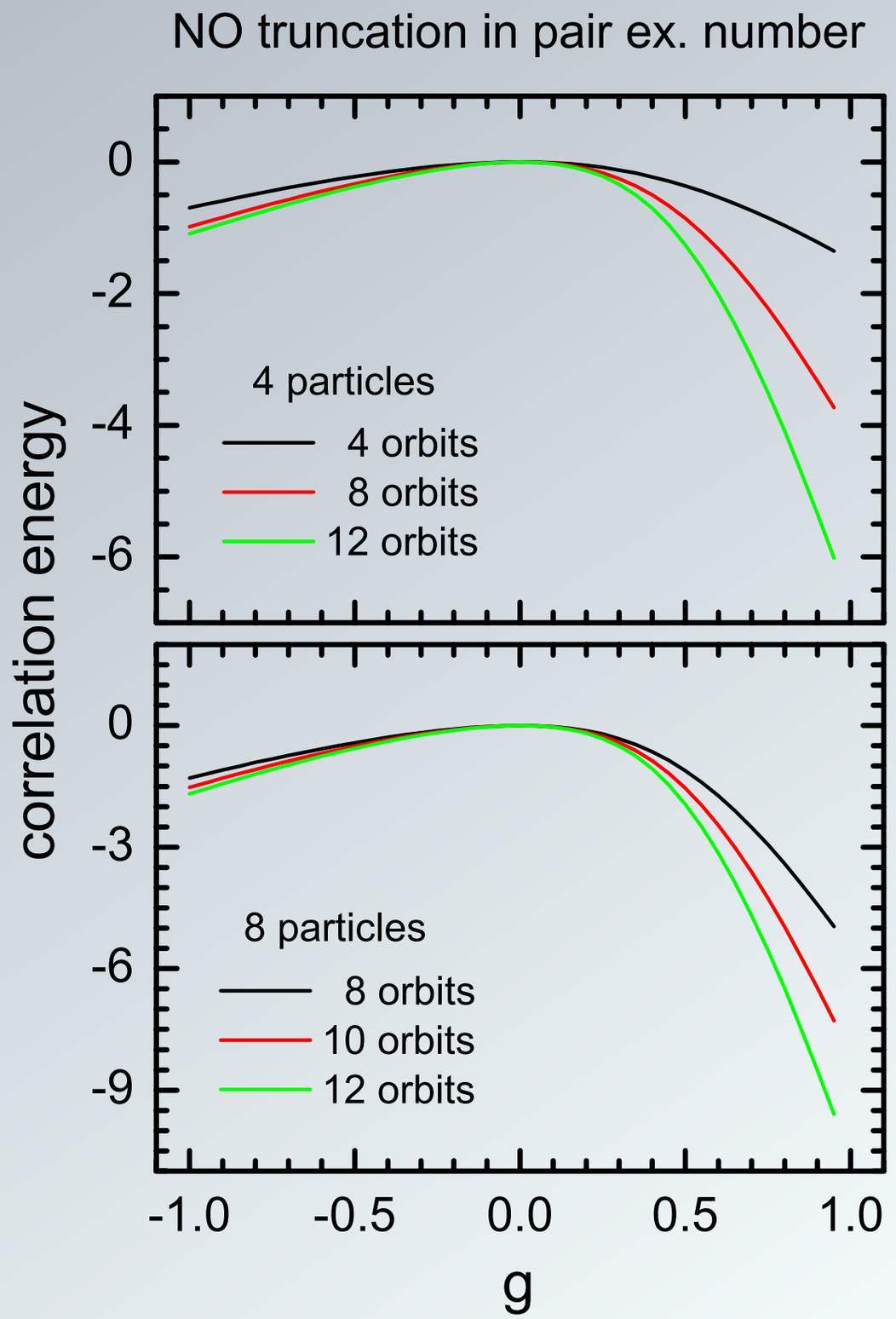
$$\langle SD|\mathcal{H}|SD\rangle = \sum_{i\in SD} \epsilon_i - n_{pair} \times G$$

$$\langle SD|\mathcal{H}|SD^{ik}_{jl}\rangle = -G$$

$$\begin{matrix} H_{\alpha\alpha} & H_{\alpha\beta} & H_{\alpha\gamma} & \cdots \\ H_{\beta\alpha} & H_{\beta\beta} & H_{\beta\gamma} & \cdots \\ H_{\gamma\alpha} & H_{\gamma\beta} & H_{\gamma\gamma} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{matrix}$$

Configuration & Hamiltonian:





Thank you!

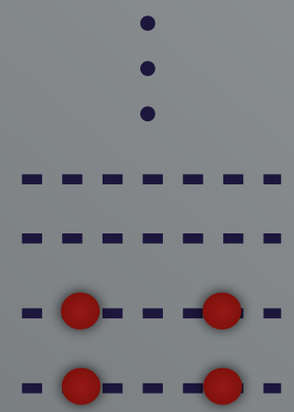
Group No.5

Yiyuan Cheng Adam Vernon Yuanzhuo Ma

Group No.5

YA

Y



YAY

YAY

YAY

YAY

YAY

YAY!!

YAY YAY YAY!