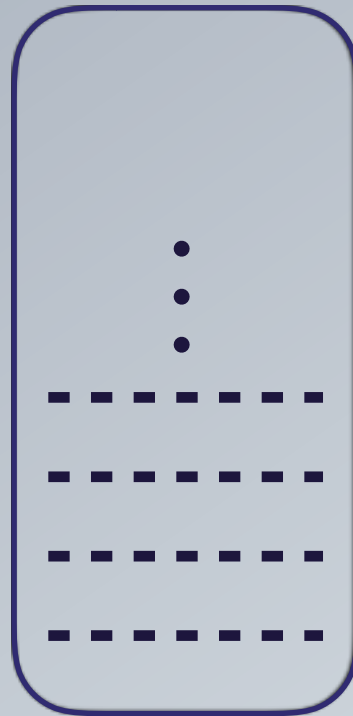


Basic idea:

Group No.5



i) basis

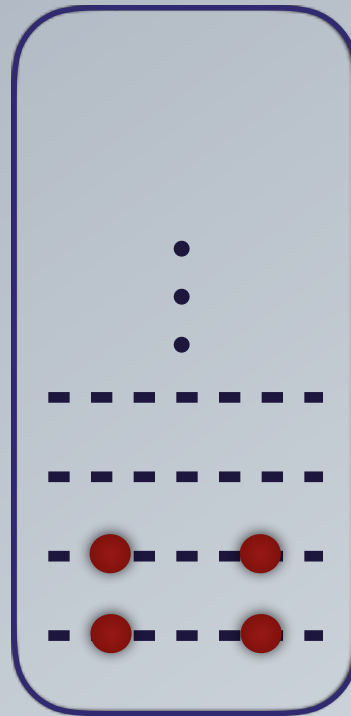


Basic idea:

Group No.5



i) basis

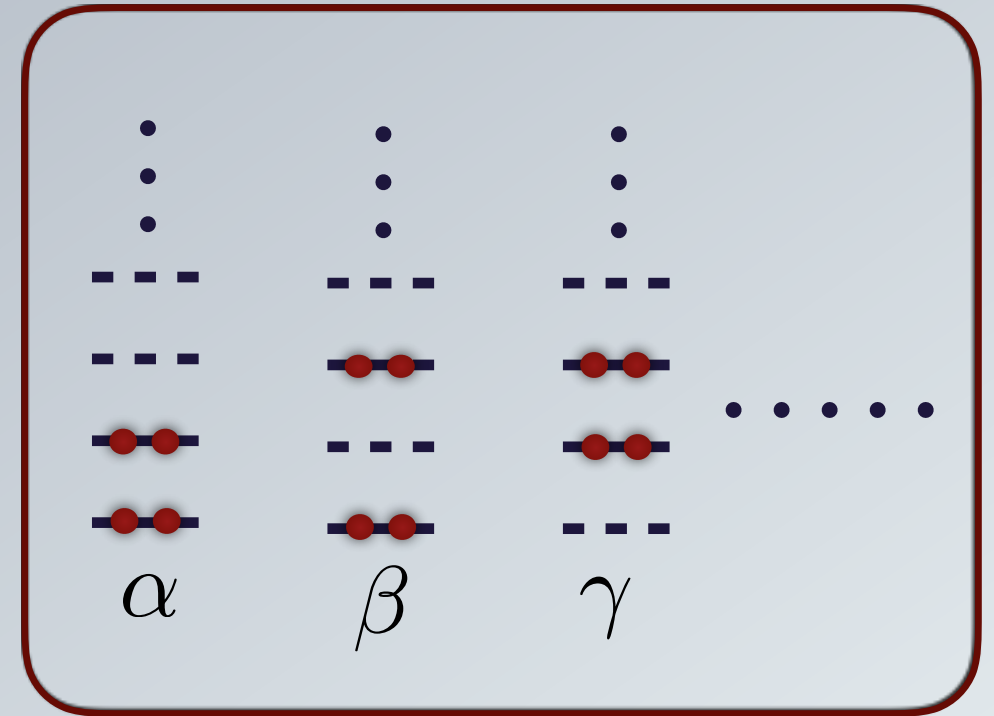
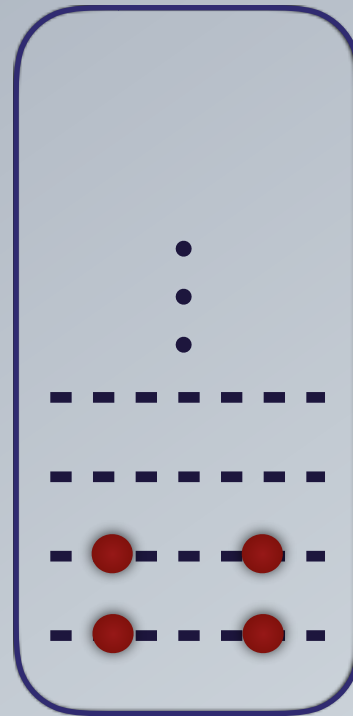


Basic idea:

Group No.5

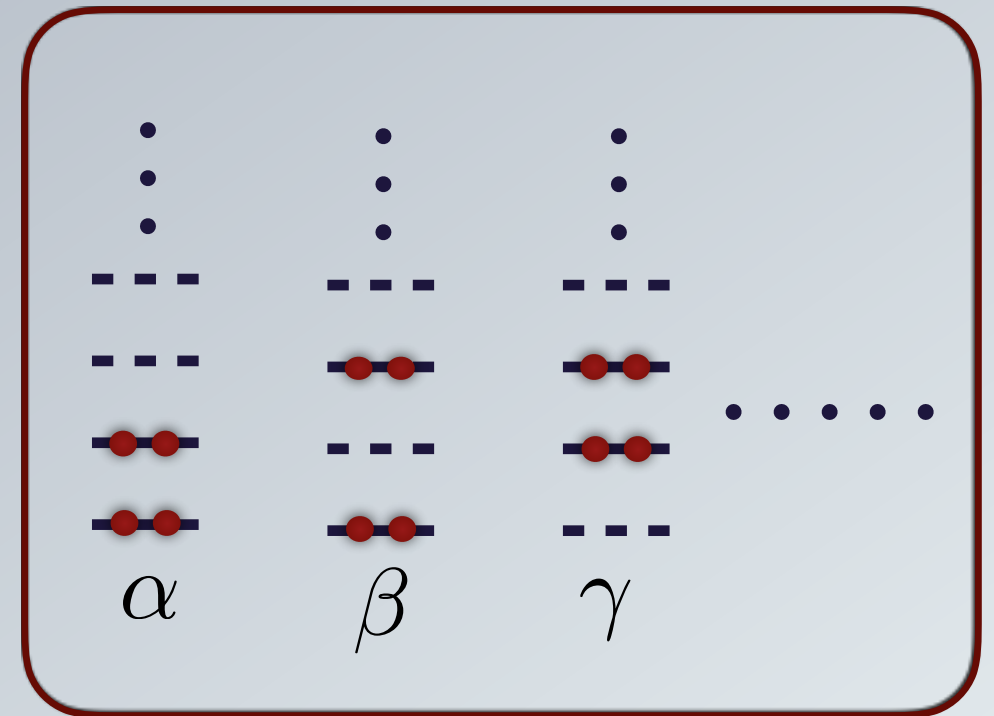
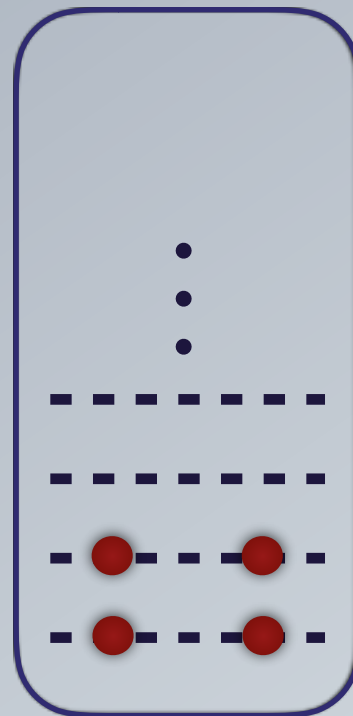


i) basis





i) basis



ii) Hamiltonian

 $\mathcal{H} =$

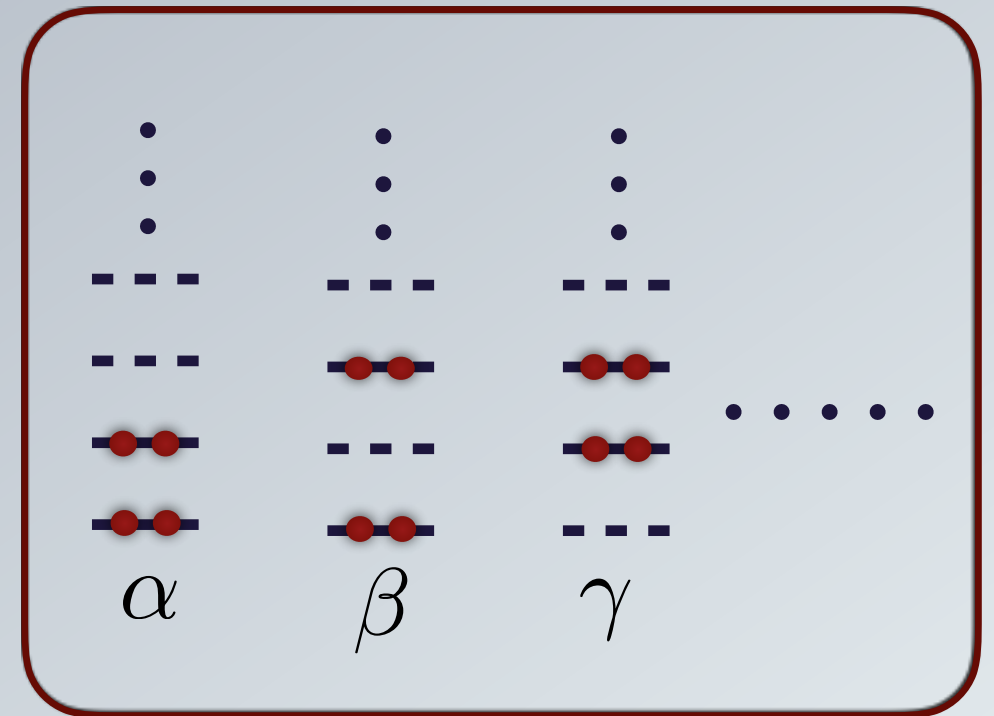
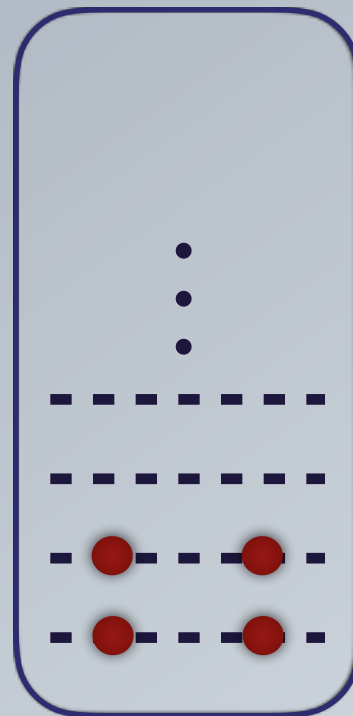
$$\begin{array}{cccc}
 H_{\alpha\alpha} & H_{\alpha\beta} & H_{\alpha\gamma} & \dots \\
 H_{\beta\alpha} & H_{\beta\beta} & H_{\beta\gamma} & \dots \\
 H_{\gamma\alpha} & H_{\gamma\beta} & H_{\gamma\gamma} & \dots \\
 \vdots & \vdots & \vdots & \ddots
 \end{array}$$

Basic idea:

Group No.5



i) basis



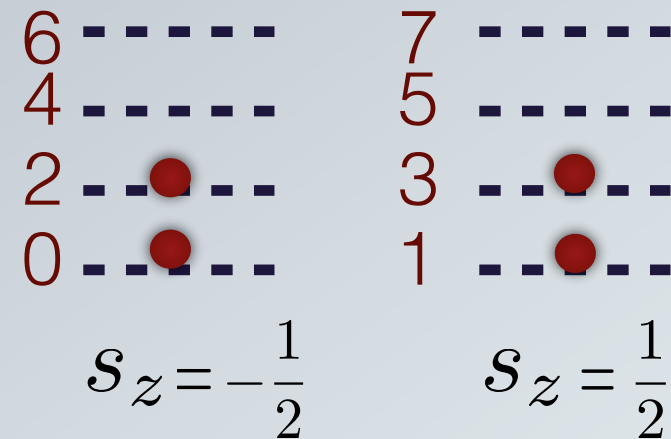
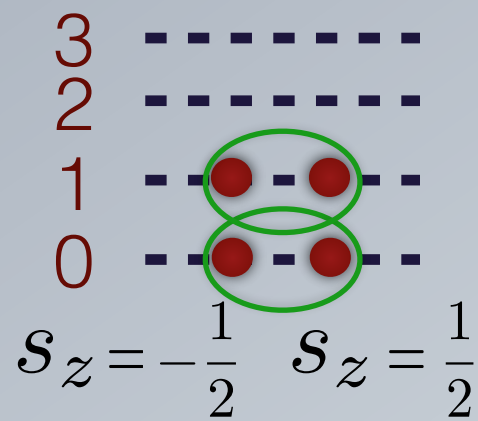
ii) Hamiltonian

$\mathcal{H} =$

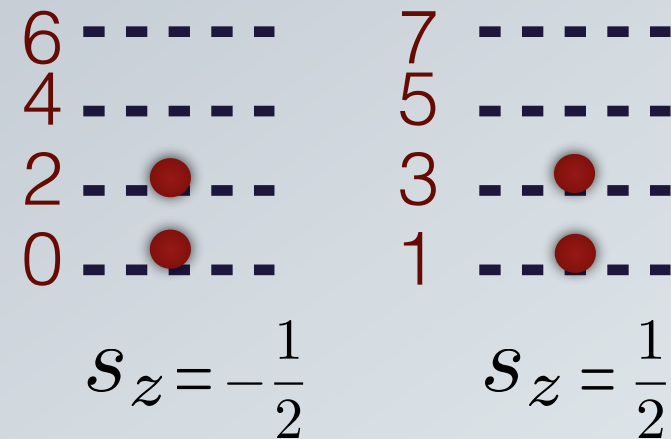
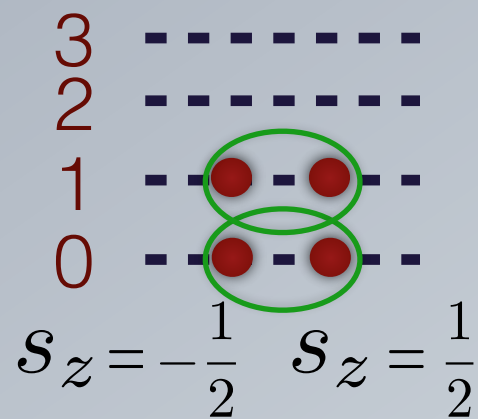
$$\begin{array}{cccc} H_{\alpha\alpha} & H_{\alpha\beta} & H_{\alpha\gamma} & \dots \\ H_{\beta\alpha} & H_{\beta\beta} & H_{\beta\gamma} & \dots \\ H_{\gamma\alpha} & H_{\gamma\beta} & H_{\gamma\gamma} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{array}$$

iii) Diagonalization

Different strategy:

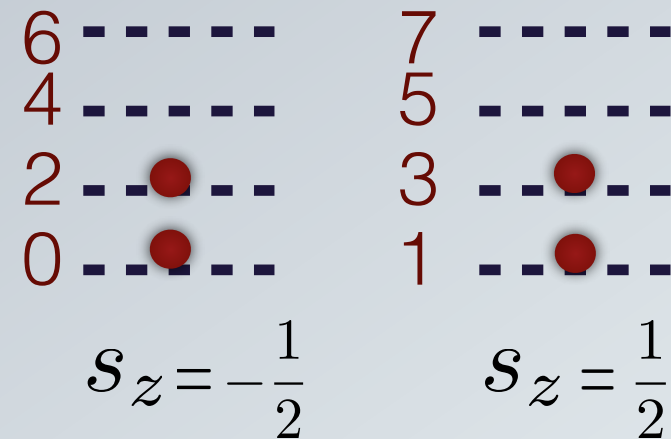
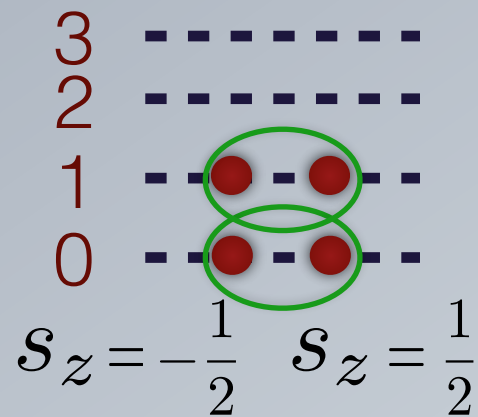


Different strategy:



C++ vs Python

Different strategy:



C++ vs Python

Windows vs Linux vs MacOs

Configuration & Hamiltonian:



step 1:

2p2h

0 h : (0, 1) p : (4, 5)

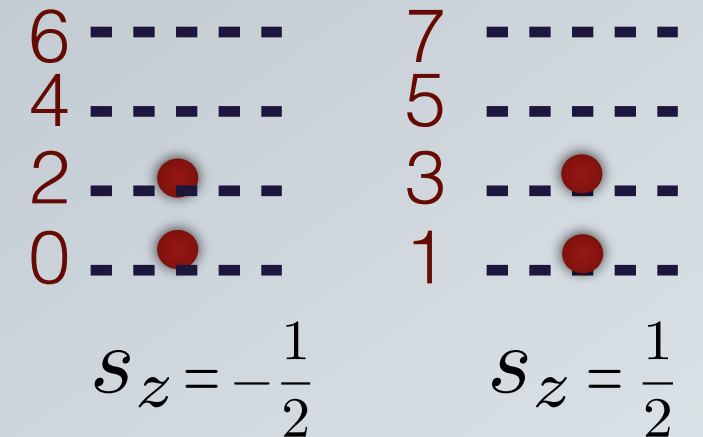
1 h : (0, 1) p : (6, 7)

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)



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

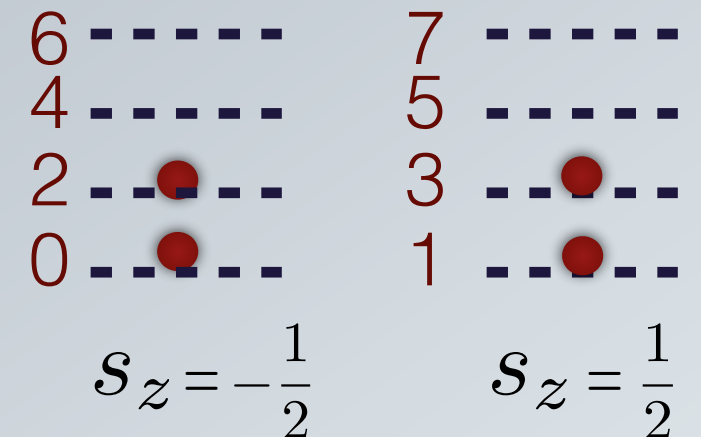
0 h : (0, 1, 2, 3) p : (4, 5, 6, 7)

step 2:

0p0h: 11110000

2p2h: 00111100, 00110011...

4p4h: 00001111



Configuration & Hamiltonian:



step 1:

2p2h

0 h : (0, 1) p : (4, 5)

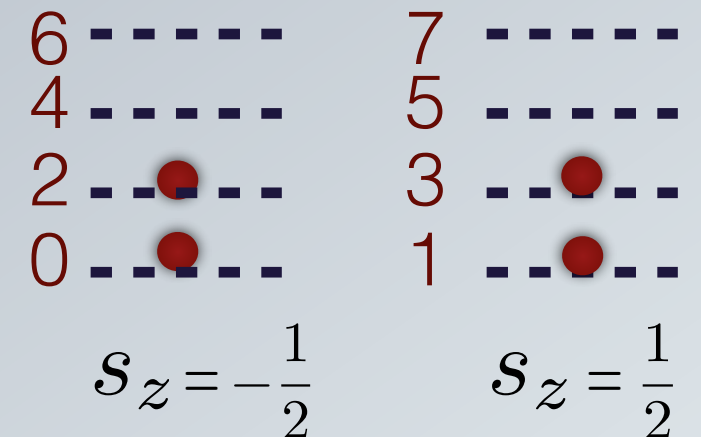
1 h : (0, 1) p : (6, 7)

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:

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

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



Configuration & Hamiltonian:

step 1:

2p2h

0 h : (0, 1) p : (4, 5)

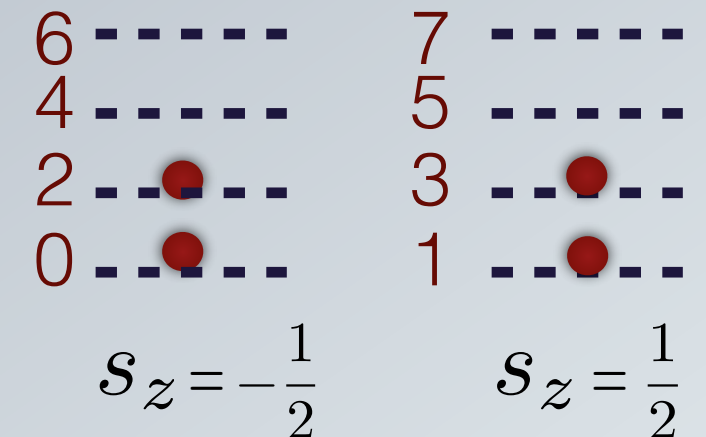
1 h : (0, 1) p : (6, 7)

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

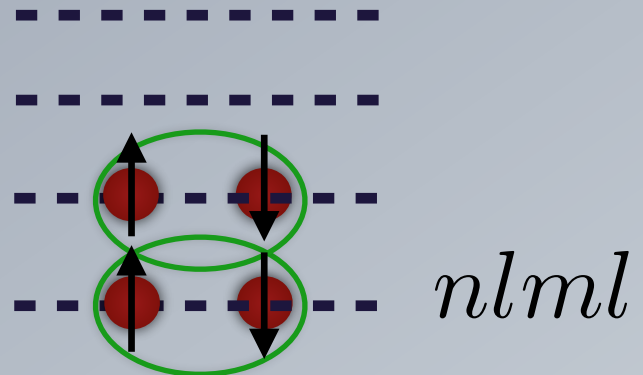
step 3:

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

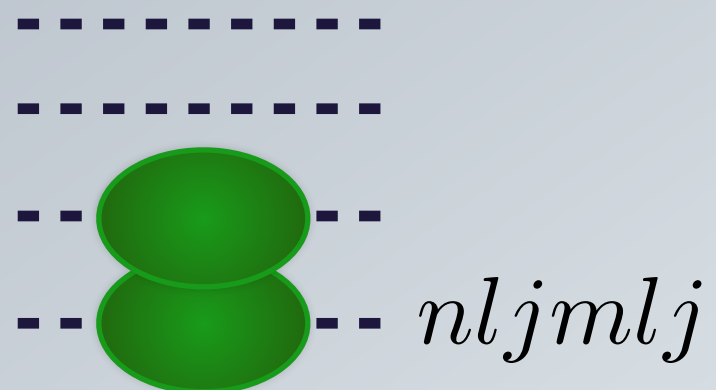
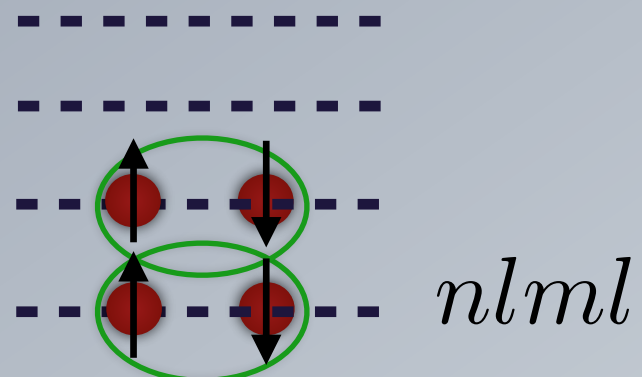
$$\langle SD | \mathcal{H} | SD_{jl}^{ik} \rangle = -G$$

$$\begin{array}{cccc} H_{\alpha\alpha} & H_{\alpha\beta} & H_{\alpha\gamma} & \dots \\ H_{\beta\alpha} & H_{\beta\beta} & H_{\beta\gamma} & \dots \\ H_{\gamma\alpha} & H_{\gamma\beta} & H_{\gamma\gamma} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{array}$$

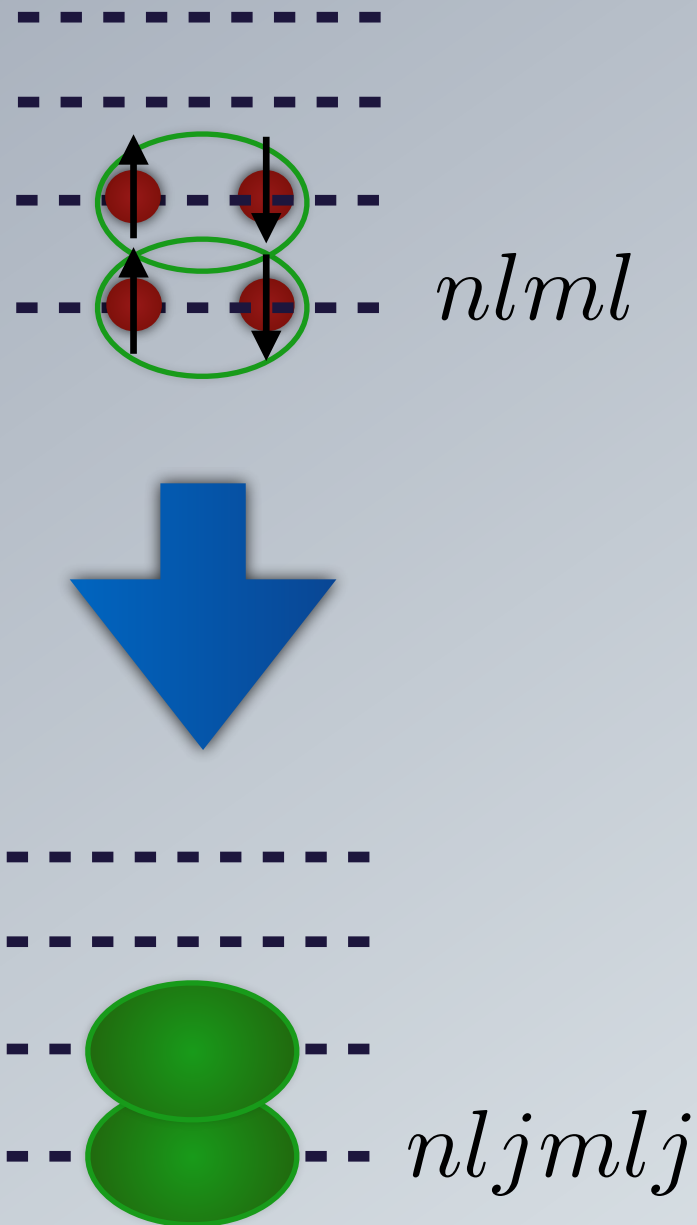
Configuration & Hamiltonian:



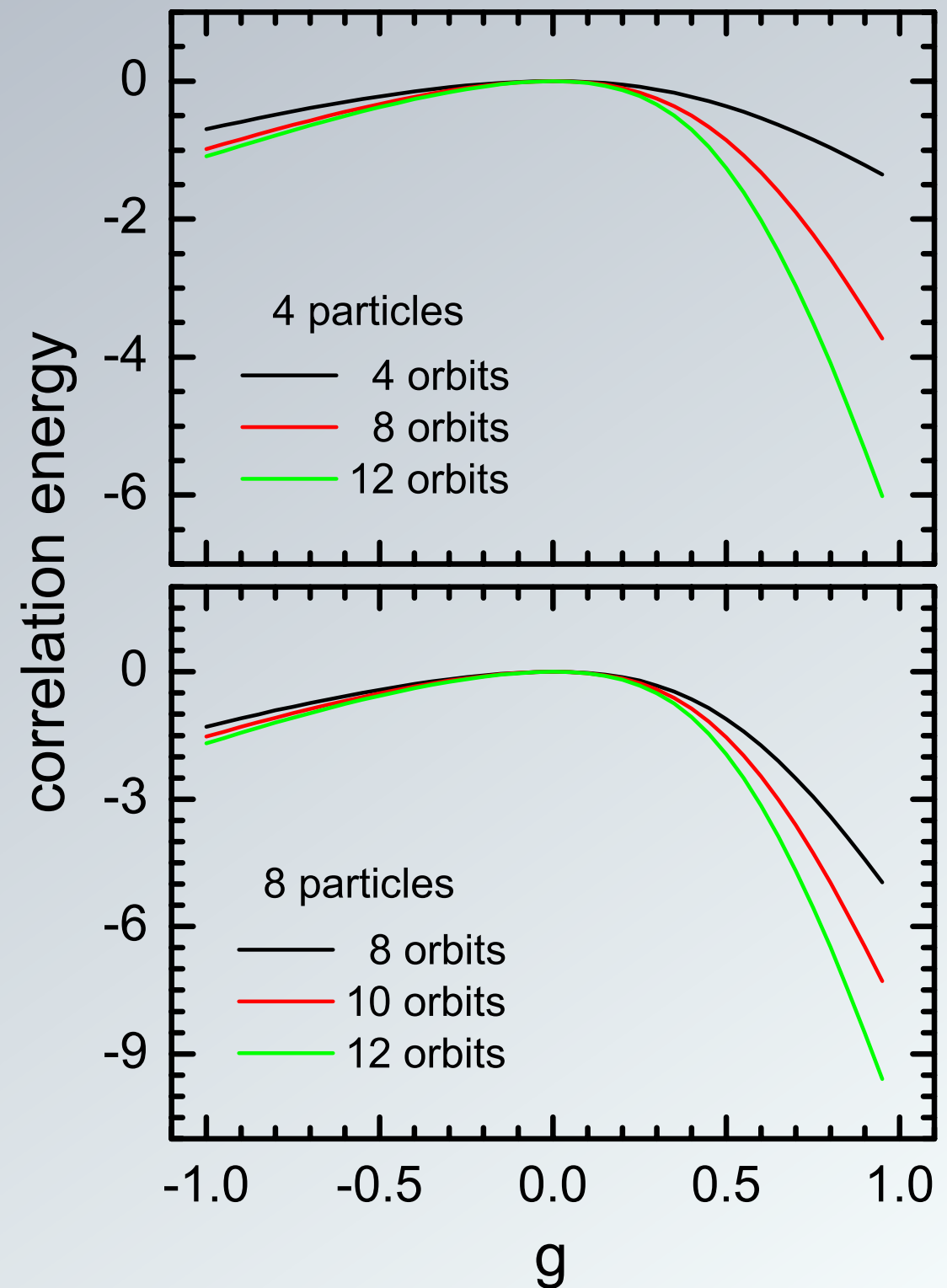
Configuration & Hamiltonian:



Configuration & Hamiltonian:



NO truncation in pair ex. number



Thank you!

Group No.5

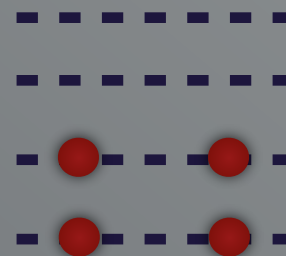
YIYUAN CHEN

ADAM VERNON

YUANZHUO MA



Group No.5



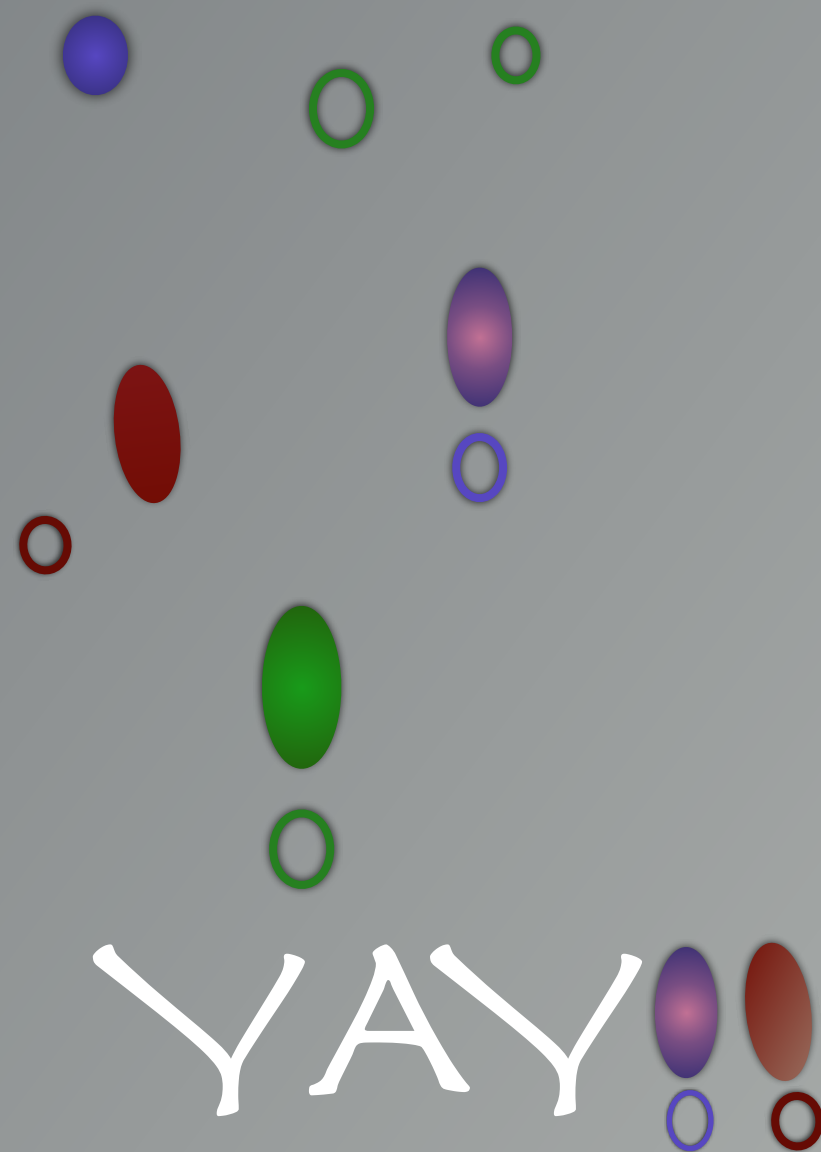
YAY

YAY

YAY

YAY

YAY



YAY YAY

YAY

