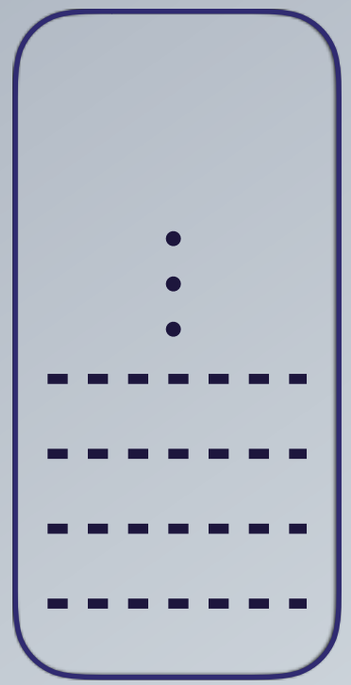
# Basic idea:

# Group No.5

## i) basis



# Basic idea:

# Group No.5

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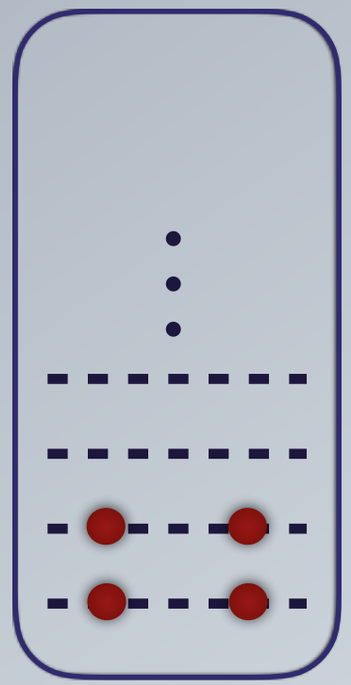
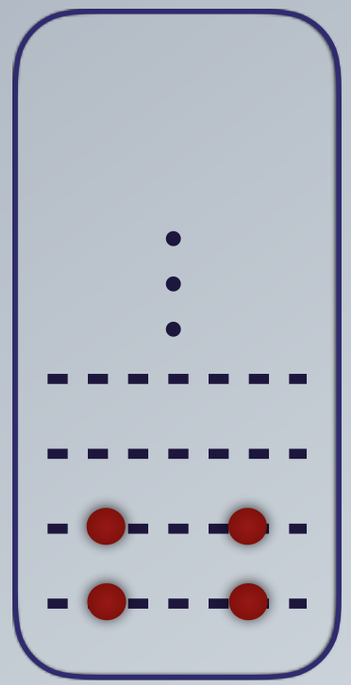
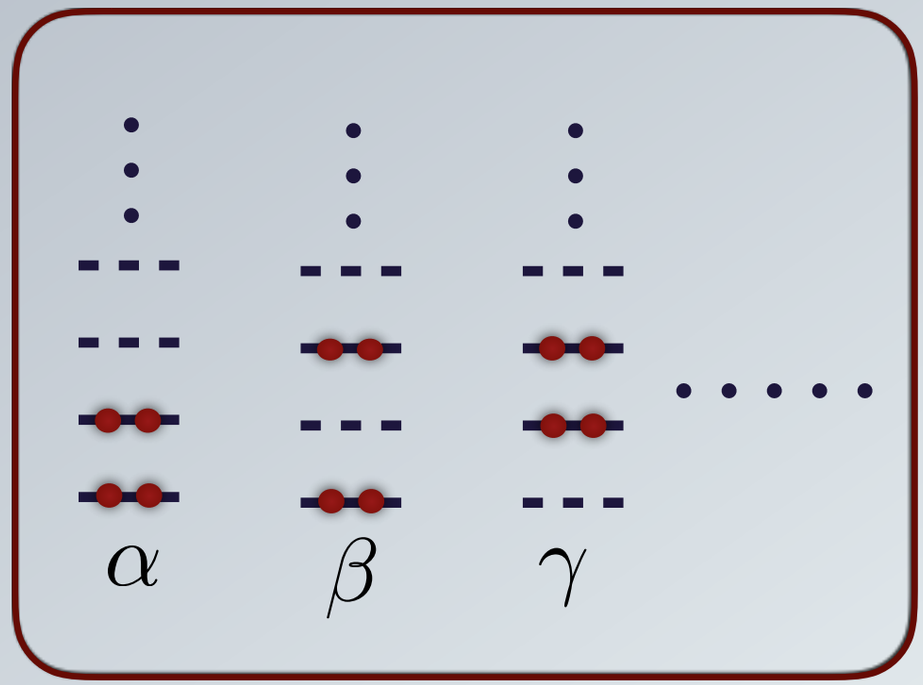


**Basic idea:** **Group No.5**

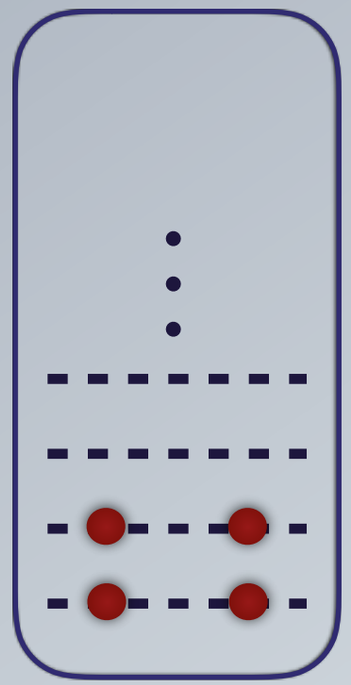
## i) basis

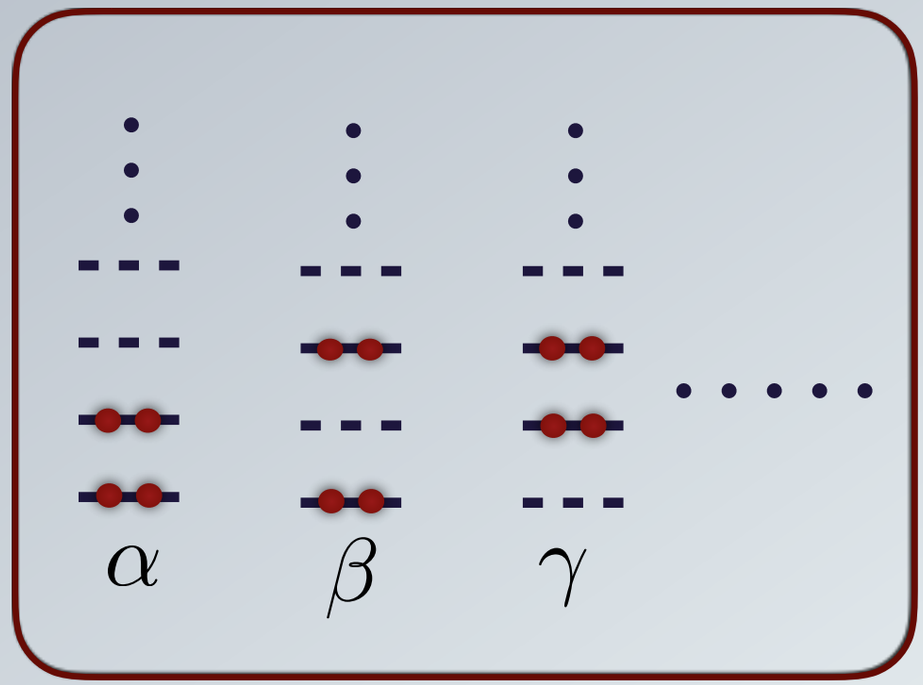




**Basic idea:** **Group No.5**

## i) basis





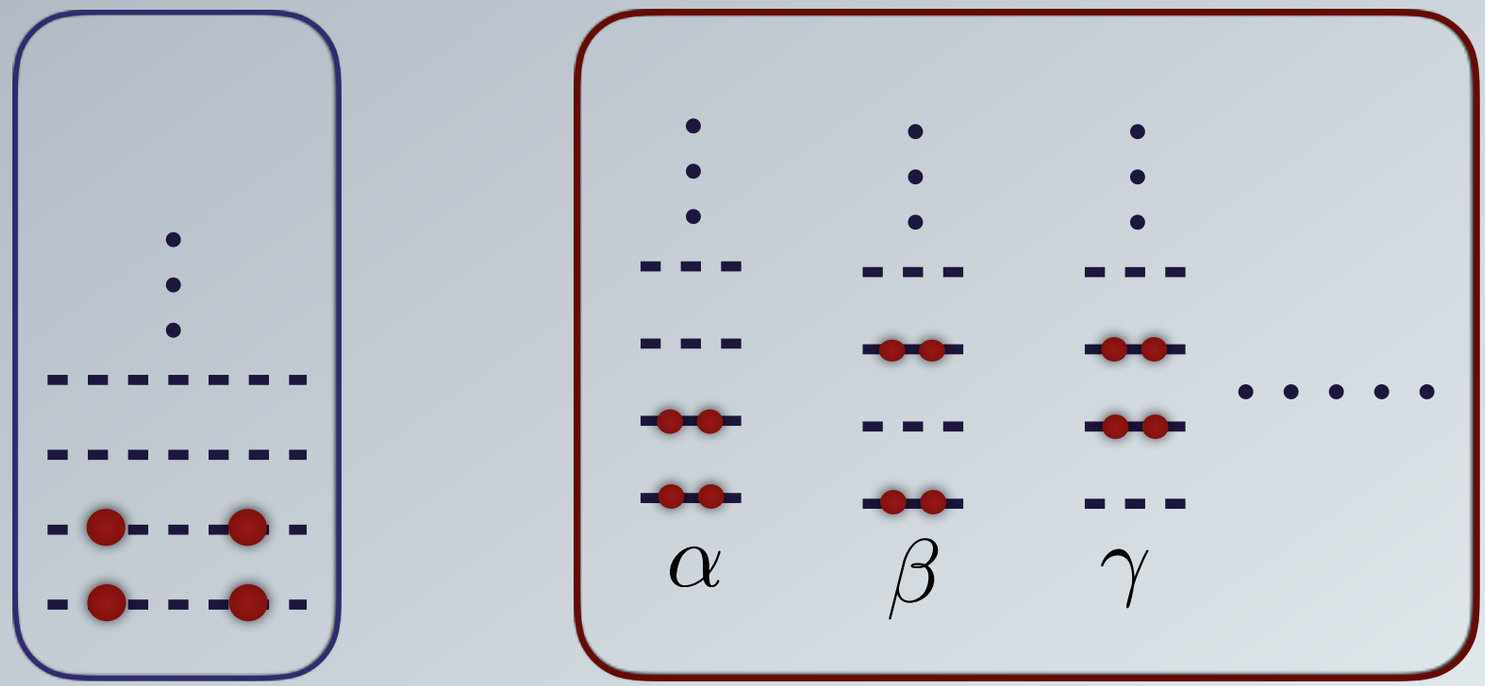

## ii)Hamiltonian

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

# Basic idea:

# Group No.5

## i) basis

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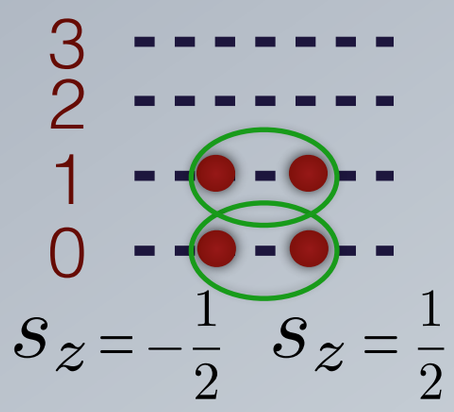
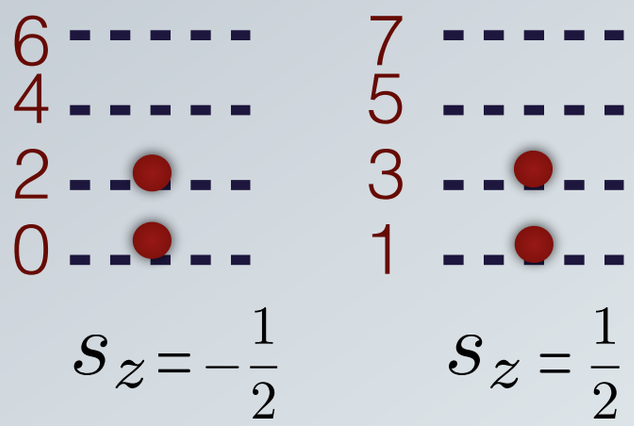
## iii)Diagonalization

# Different strategies:

## Y

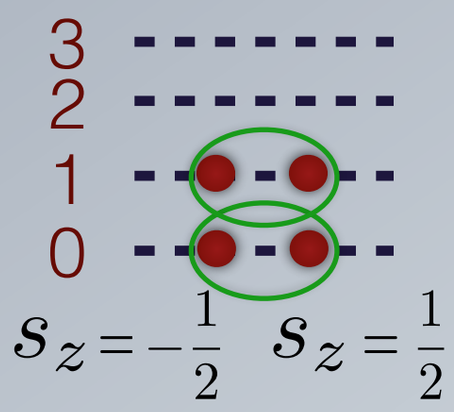



## AY

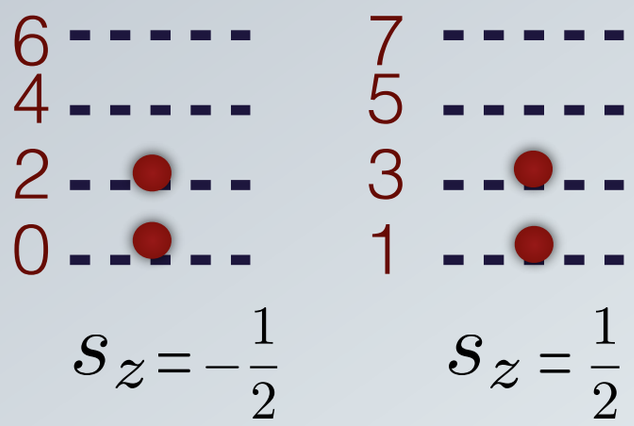


# Different strategies:

## Y



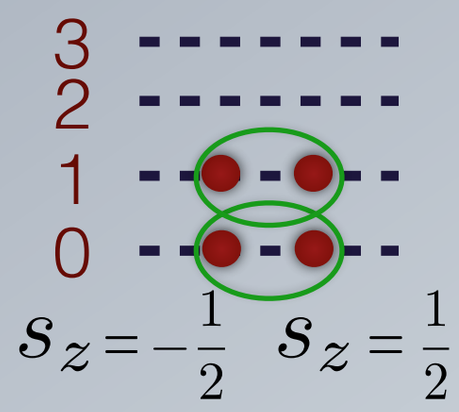

## AY



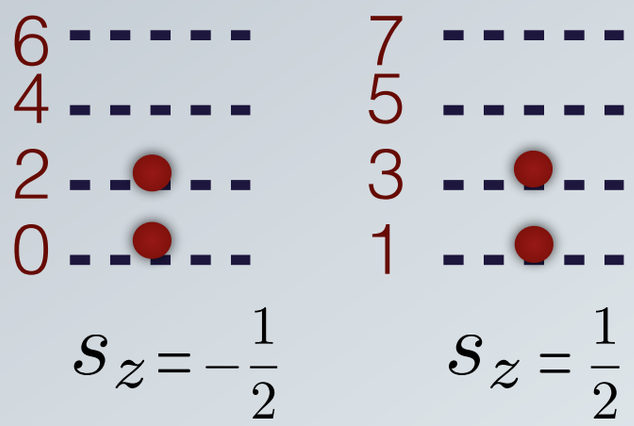

**C++ vs Python**

# Different strategies:

## Y




## AY




**C++ vs Python**

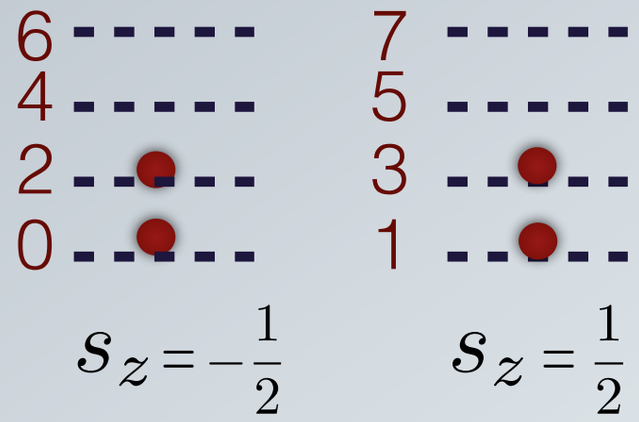
**Windows vs Linux vs MacOs**

# 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) |

# Configuration & Hamiltonian:

**step 1:**

2p2h

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|---|---|---|
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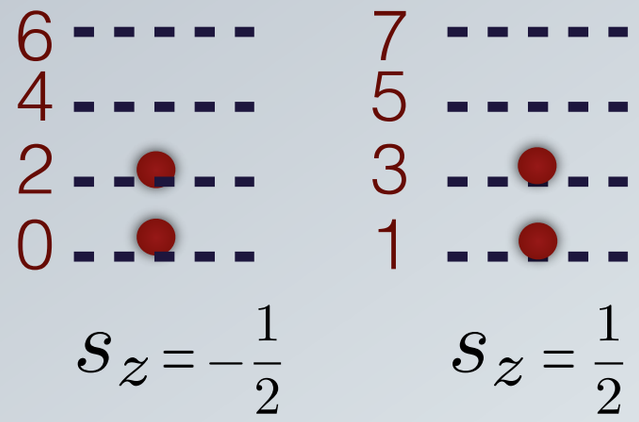


4p4h

| | | |
|---|---|---|
| 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

| | | |
|---|---|---|
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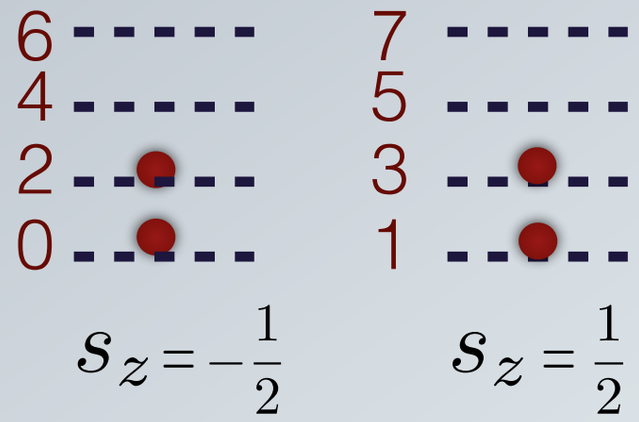


4p4h

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

**step 2:**

0p0h:11110000

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**step 3:**

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

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

# Configuration & Hamiltonian:

**step 1:**

2p2h

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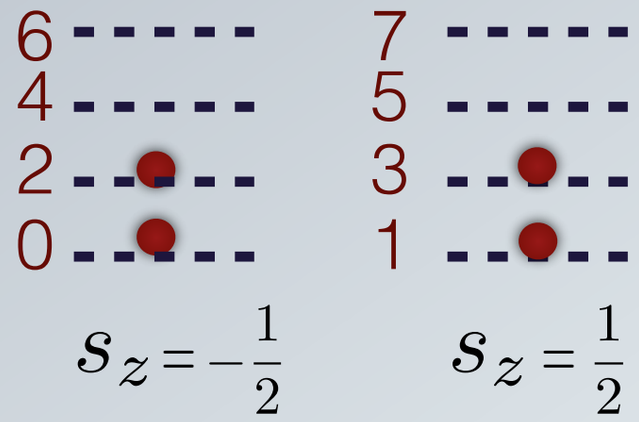


4p4h

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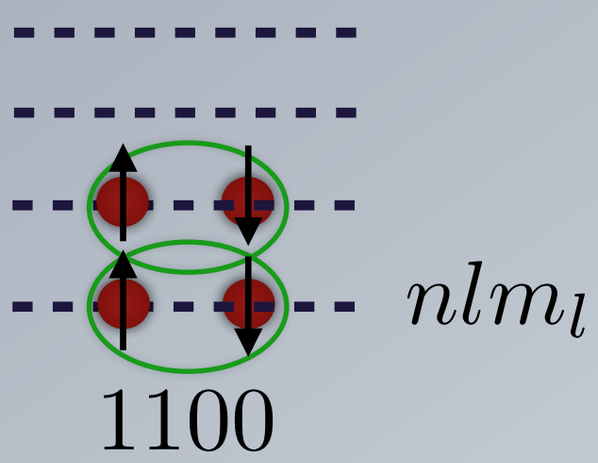
$$\begin{matrix} H_{\alpha\alpha} & H_{\alpha\beta} & H_{\alpha\gamma} & \cdots \\ H_{\beta\alpha} & H_{\beta\beta} & H_{\beta\gamma} & \cdots \\ H_{\gamma\alpha} & H_{\gamma\beta} & H_{\gamma\gamma} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{matrix}$$

# Configuration & Hamiltonian:



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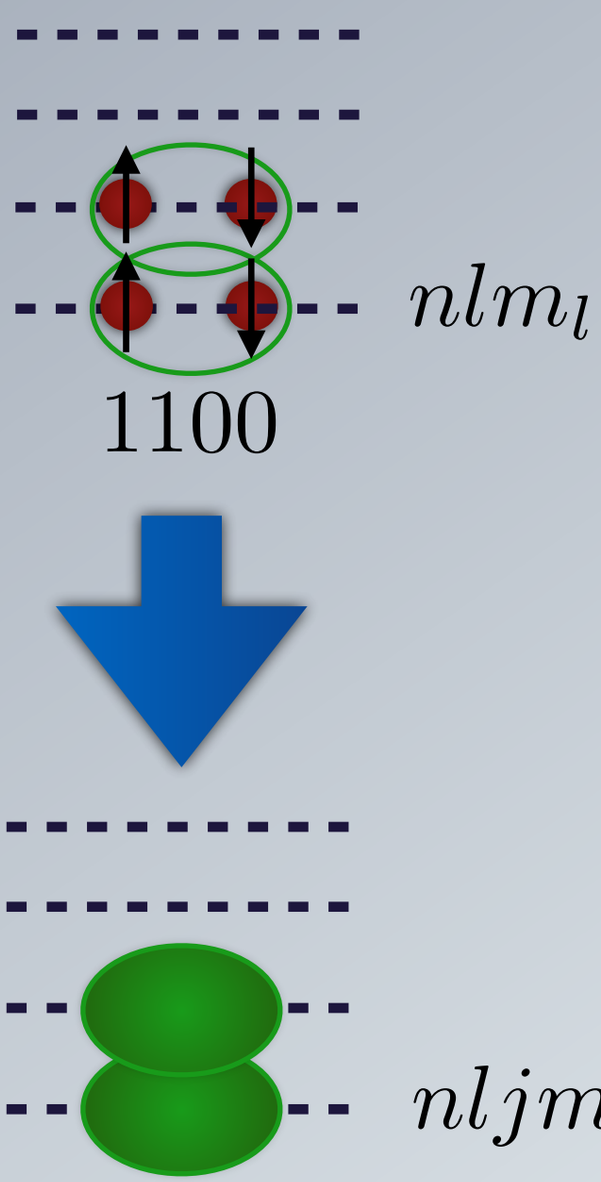

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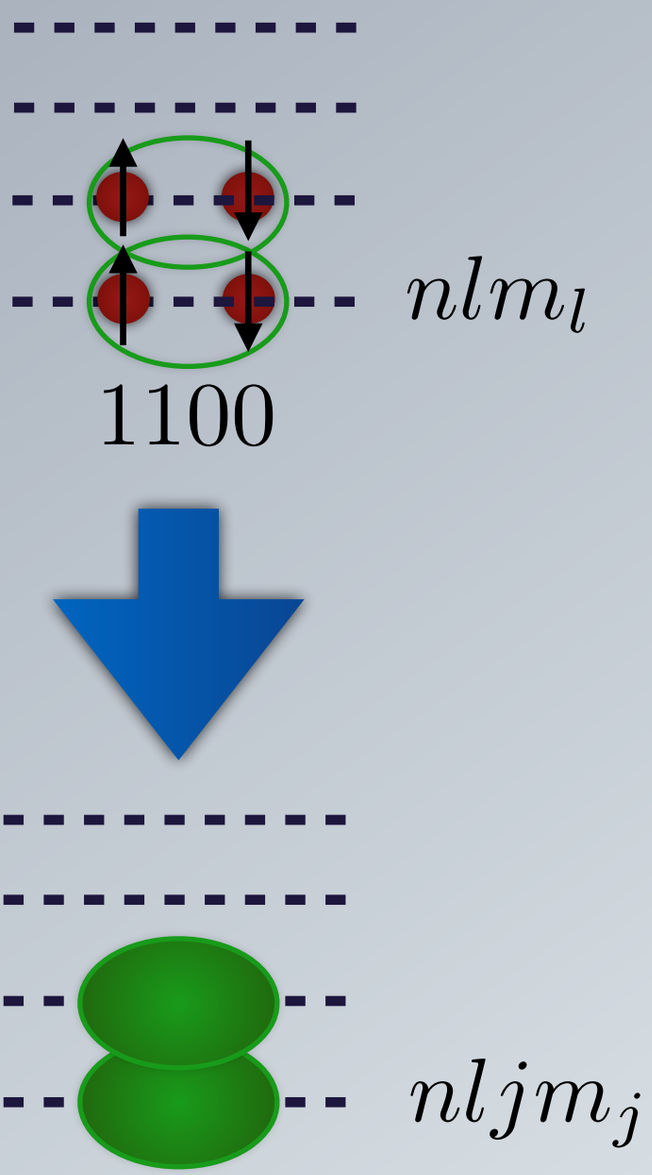
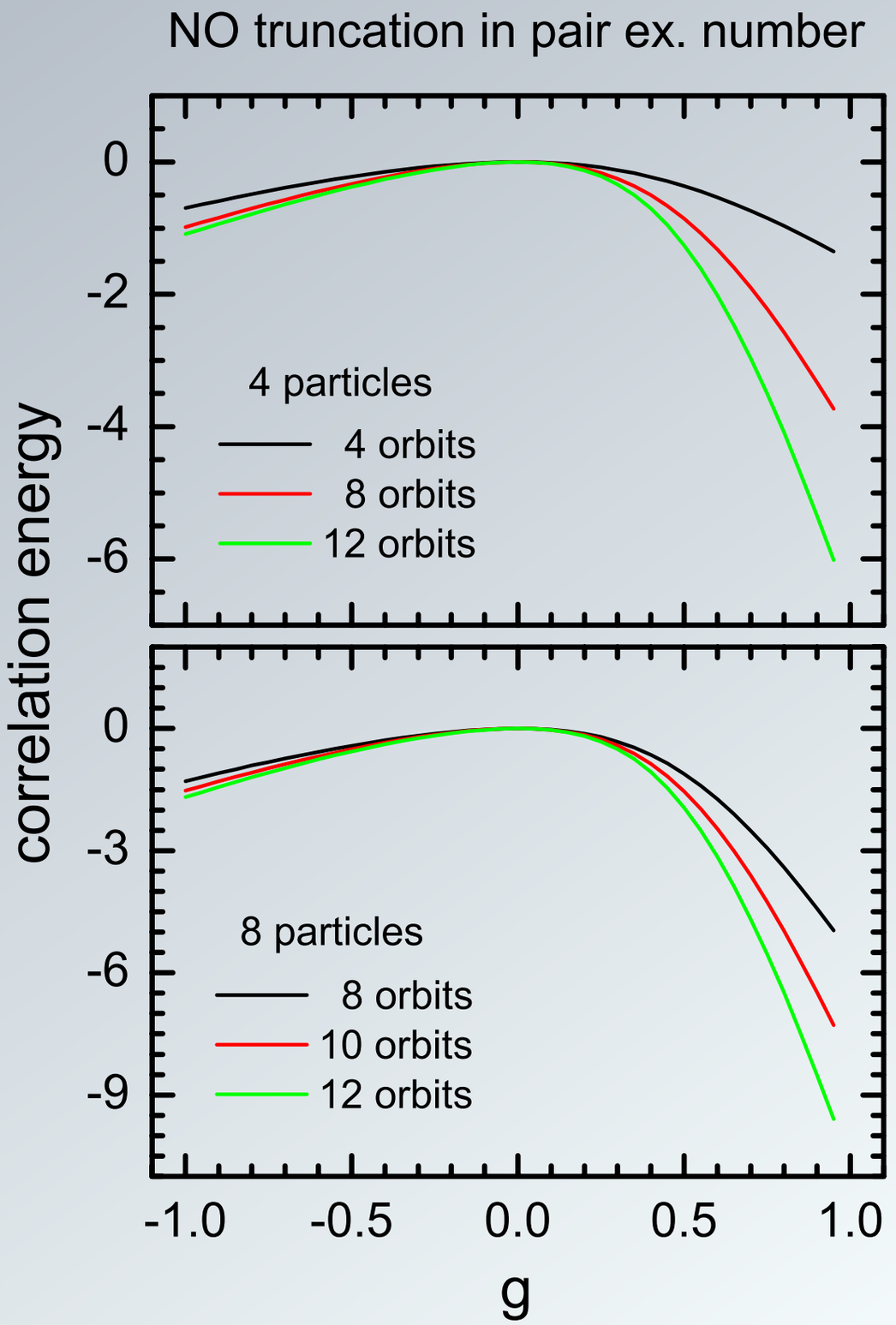


# Thank you!

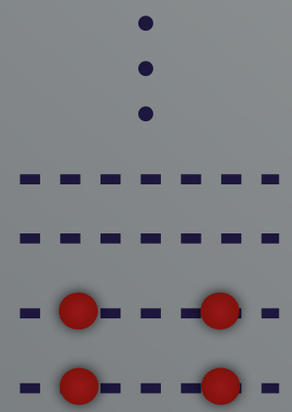
## Group No.5

Yiyuan Cheng  Adam Vernon  Yuanzhuo Ma

# Group No.5

YA

Y



YAY

YAY

YAY

YAY

YAY

YAY!!

YAY
YAY
YAY