

# Mapping fermions to qubits

## Activity 2.1

QSciTech-QuantumBC virtual workshop  
on gate-based quantum computing

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# Disclaimer

## qiskit has already done it!

A full, optimized and robust implementation Molecule Simulation using VQE is already done in qiskit.

The method is described here :

[https://qiskit.org/documentation/tutorials/algorithms/02\\_vqe\\_advanced\\_options.html](https://qiskit.org/documentation/tutorials/algorithms/02_vqe_advanced_options.html)

and here :

[https://qiskit.org/documentation/tutorials/algorithms/03\\_vqe\\_simulation\\_with\\_noise.html](https://qiskit.org/documentation/tutorials/algorithms/03_vqe_simulation_with_noise.html)

The purpose of the present lectures is that you implement and **understand as much as possible** your own rough and un-optimized version of VQE.

# Topics

- 1. A recall of the Molecular Hamiltonian**
- 2. Fermions to qubits mapping**
- 3. Pauli Strings**
- 4. Linear Combinaison of Pauli Strings**
- 5. Complete the mapping**

# Molecular Hamiltonian Summary

The sum of the **kinetic** and **potential** from electrons/nucleus :

$$\hat{\mathcal{H}} = - \sum_i^n \frac{1}{2} \hat{\nabla}_i^2 - \sum_{i,\alpha}^{n,A} \frac{Z_\alpha}{|\hat{\mathbf{r}}_i - \mathbf{R}_\alpha|} + \sum_{i < j} \frac{1}{|\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j|} + \sum_{\alpha < \beta} \frac{Z_\alpha Z_\beta}{|\mathbf{R}_\alpha - \mathbf{R}_\beta|}$$

Transformed with **second quantization** as a weighted sums of **creation** and **annihilation** operators

$$\hat{\mathcal{H}} = \sum_{i,j} h_{ij}^{(1)} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \sum_{i,j,k,l} h_{ijkl}^{(2)} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l.$$

The weights (or integrals) are obtained from the  $n$  one-body wave functions (orbitals)

$$h_{ij}^{(1)} = \int d\mathbf{x} \phi_i^*(\mathbf{x}) \left( -\frac{1}{2} \nabla^2 - \sum_\alpha \frac{1}{|\mathbf{x} - \mathbf{R}_\alpha|} \right) \phi_j(\mathbf{x}) \quad h_{ijkl}^{(2)} = \iint d\mathbf{x} d\mathbf{x}' \frac{\phi_i^*(\mathbf{x}) \phi_j^*(\mathbf{x}') \phi_k(\mathbf{x}') \phi_l(\mathbf{x})}{|\mathbf{x} - \mathbf{x}'|}$$

$n \times n$

$n \times n \times n \times n$

# Molecular Hamiltonian

## The atomic basis

- The **atomic orbitals** (1s, 2s, 2p, ...) form a basis.

- It is **not** an **orthogonal** basis.

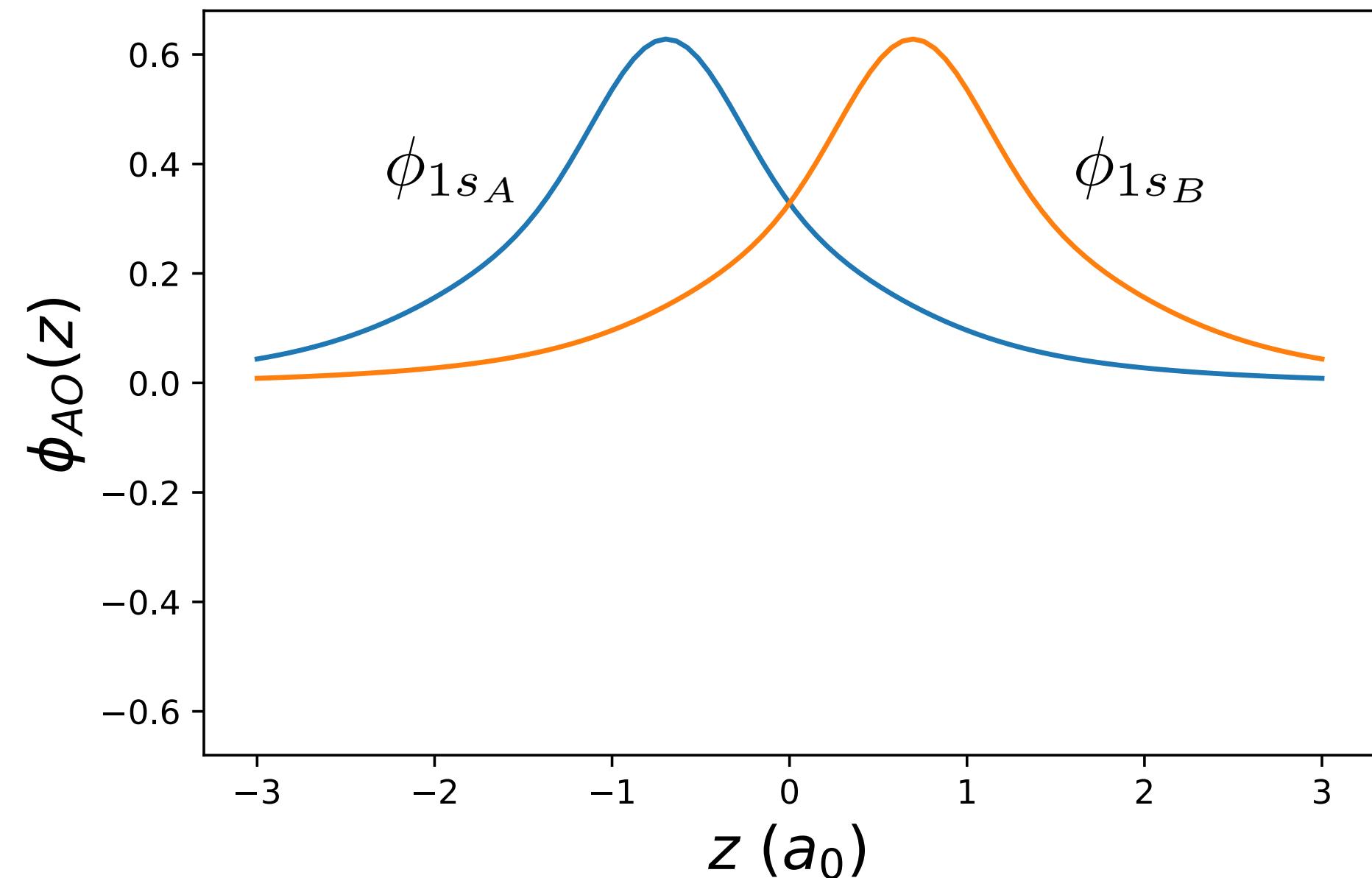
$$s_{ij} = \int d\mathbf{x} \phi_i^*(\mathbf{x}) \phi_j(\mathbf{x}) \neq \delta_{ij}$$

- **Atomic orbitals** are usually **approximated** with few **gaussians** (ex : STO-3g).

- This basis is very useful to **compute integrals**.

$$h_{ij}^{(1)} = \int d\mathbf{x} \phi_i^*(\mathbf{x}) \left( -\frac{1}{2} \nabla^2 - \sum_{\alpha} \frac{1}{|\mathbf{x} - \mathbf{R}_{\alpha}|} \right) \phi_j(\mathbf{x})$$

$$h_{ijkl}^{(2)} = \iint d\mathbf{x} d\mathbf{x}' \frac{\phi_i^*(\mathbf{x}) \phi_j^*(\mathbf{x}') \phi_k(\mathbf{x}') \phi_l(\mathbf{x})}{|\mathbf{x} - \mathbf{x}'|}$$



# Molecular Hamiltonian

## The molecular basis

- The **molecular orbitals** are **linear combinaisons of atomic orbitals**.
- They form an **orthonormal basis**.  $s_{ij} = \int d\mathbf{x} \phi_i^*(\mathbf{x})\phi_j(\mathbf{x}) = \delta_{ij}$
- The **transformation** that goes from **atomic to molecular** can be applied on the integrals as well.

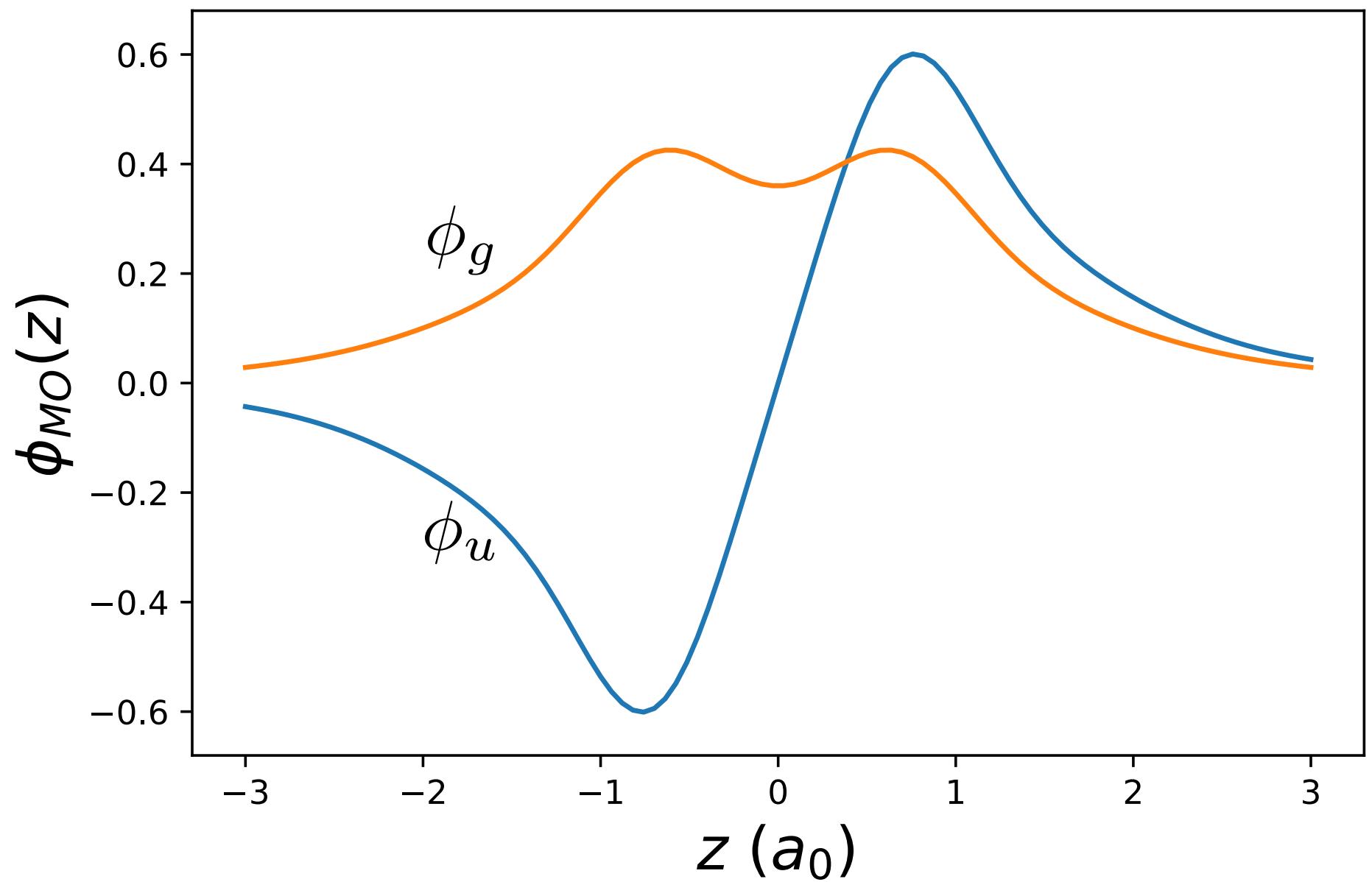
$$\phi_g \propto \phi_{1s_A} + \phi_{1s_B}$$

$$\phi_u \propto \phi_{1s_A} - \phi_{1s_B}$$

$$\phi_i^{(\text{MO})} = R_{ip}\phi_p^{(\text{AO})}$$

$$h_{ij}^{(\text{MO})} = R_{ip}R_{jq}^*h_{pq}^{(\text{AO})}$$

$$h_{ijkl}^{(\text{MO})} = R_{ip}R_{jq}R_{kr}^*R_{ls}^*h_{pqrs}^{(\text{AO})}$$



# Molecular Hamiltonian

## The transformation

We start with a **non diagonal overlap**

$$s_{ij}^{(\text{AO})} = \int d\mathbf{x} \phi_i^{(\text{AO})*}(\mathbf{x}) \phi_j^{(\text{AO})}(\mathbf{x}) \neq \delta_{ij}$$

We **diagonalize** it, but it's not the identity

$$U_{mi} s_{ij}^{(\text{AO})} (U^\dagger)_{jn} = \sigma_m \delta_{mn} \neq \delta_{mn}$$

We use this trick

$$\sigma_m \delta_{mn} = \sigma_m^{1/2} \delta_{mn} \sigma_n^{1/2}$$

To write down

$$(\sigma_m^{-1/2} U_{mi}) s_{ij}^{(\text{AO})} ((U^\dagger)_{jn} \sigma_n^{-1/2}) = \delta_{mn}$$

so this transformation can produce a MO basis

$$\sigma_m^{-1/2} U_{mi}$$

But we can also do that

$$((U^\dagger)_{pm} \sigma_m^{-1/2} U_{mi}) s_{ij}^{(\text{AO})} ((U^\dagger)_{nj} \sigma_n^{-1/2} U_{nq}) = \delta_{pq}$$

to produce an other **valid transformation**

$$R_{pi} = (U^\dagger)_{pm} \sigma_m^{-1/2} U_{mi} = \sigma_m^{-1/2} U_{mp}^* U_{mi}$$

In both cases, we can use the transformation

$$R_{mi} s_{ij}^{(\text{AO})} R_{jn} = \delta_{mn} = s_{mn}^{(\text{MO})}$$

Finally, just note that

$$R_{jq} = R_{qj}^*$$

so we can apply the transformation like this

$$R_{mi} R_{nj}^* s_{ij}^{(\text{AO})} = \delta_{mn} = s_{mn}^{(\text{MO})}$$

# Molecular Hamiltonian

## The second quantization

To summarize second quantization, let's say that the **wave function** is just the **spatial description of a quantum state**.

$$\phi_g(\mathbf{r}) = \langle \mathbf{r} | g \rangle$$

$$\phi_u(\mathbf{r}) = \langle \mathbf{r} | u \rangle$$

We can now refer to these two states with their **kets**

$$|g\rangle, |u\rangle$$

Adding the **spin** degree of freedom, we make two copies of each state to form a **spin orbital basis states**.

$$|g, \uparrow\rangle, |u, \uparrow\rangle, |g, \downarrow\rangle, |u, \downarrow\rangle$$

# Molecular Hamiltonian

## Occupation basis

The spin orbitals basis states are the 4 states that can be occupied by 1 electron. The **occupation basis** identifies if one state is **occupied or not**.

$ g, \uparrow\rangle$		$ 0001\rangle$	
$ u, \uparrow\rangle$		$ 0010\rangle$	$ u_\downarrow, g_\downarrow, u_\uparrow, g_\uparrow\rangle$
$ g, \downarrow\rangle$		$ 0100\rangle$	$ f_3, f_2, f_1, f_0\rangle$
$ u, \downarrow\rangle$		$ 1000\rangle$	

This allows us to identify states with **more than one electron**.

$|0101\rangle$

The total number of states in the occupational basis of our  $H_2$  is  $2^4 = 16$ .

# Molecular Hamiltonian

## Occupational basis

The general state of the system is a **superposition** of all the **basis states**. The quantum state describe **how the electrons occupy** the different orbitals.

$$|\psi\rangle = \sum_i \alpha_i |\phi_i\rangle$$

State vector :

$$\begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \\ \alpha_5 \\ \alpha_6 \\ \alpha_7 \\ \alpha_8 \\ \alpha_9 \\ \alpha_{10} \\ \alpha_{11} \\ \alpha_{12} \\ \alpha_{13} \\ \alpha_{14} \\ \alpha_{15} \end{pmatrix} = \begin{pmatrix} \alpha_{0000} \\ \alpha_{0001} \\ \alpha_{0010} \\ \alpha_{0011} \\ \alpha_{0100} \\ \alpha_{0101} \\ \alpha_{0110} \\ \alpha_{0111} \\ \alpha_{1000} \\ \alpha_{1001} \\ \alpha_{1010} \\ \alpha_{1011} \\ \alpha_{1100} \\ \alpha_{1101} \\ \alpha_{1110} \\ \alpha_{1111} \end{pmatrix}$$

Basis :

$ 0000\rangle$	$ 0\rangle$
$ 0001\rangle$	$ 1\rangle$
$ 0010\rangle$	$ 2\rangle$
$ 0011\rangle$	$ 3\rangle$
$ 0100\rangle$	$ 4\rangle$
$ 0101\rangle$	$ 5\rangle$
$ 0110\rangle$	$ 6\rangle$
$ 0111\rangle$	$ 7\rangle$
$ 1000\rangle$	$ 8\rangle$
$ 1001\rangle$	$ 9\rangle$
$ 1010\rangle$	$ 10\rangle$
$ 1011\rangle$	$ 11\rangle$
$ 1100\rangle$	$ 12\rangle$
$ 1101\rangle$	$ 13\rangle$
$ 1110\rangle$	$ 14\rangle$
$ 1111\rangle$	$ 15\rangle$

# Our goal

## A glimpse into the future

In order to find the **ground state** we need to be able to **evaluate** the energy of a specific state.

$$E_\psi = \langle \psi | \hat{\mathcal{H}} | \psi \rangle$$

The **mapping** will be to find ways to translate a **fermionic Hamiltonian** (and quantum state) into a **qubit Hamiltonian**.

# Our goal

**Two computers to rule them all!**

Integral terms depend only on the **nucleus configuration**. They are calculated classically.

$$h_{ij}^{(1)} = h_{ij}^{(1)}(\{\mathbf{R}_\alpha\}) \quad \propto n^2$$

$$h_{ijkl}^{(2)} = h_{ijkl}^{(2)}(\{\mathbf{R}_\alpha\}) \quad \propto n^4$$

The quantum computer will be used to evaluate the **expected values** of the operator parts.

$$\langle \psi | \hat{\mathcal{H}} | \psi \rangle = \sum_{i,j} h_{ij}^{(1)} \langle \psi | \hat{a}_i^\dagger \hat{a}_j | \psi \rangle + \frac{1}{2} \sum_{i,j,k,l} h_{ijkl}^{(2)} \langle \psi | \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l | \psi \rangle \quad \propto 2^n$$

# Mapping Fermions to Qubits

a link between two spaces

# Jordan-Wigner Mapping States

Map the **fermionic states** into **qubit states**.

$$|f_3 f_2 f_1 f_0\rangle \xrightarrow{\hspace{1cm}} |q_3 q_2 q_1 q_0\rangle$$

The **Jordan-Wigner** mapping is a direct mapping. The state of each **qubit** represents an **orbital** occupation.

$$f_i = q_i$$

For example, the one electron states map like this:

$$\begin{array}{ccc} |0001\rangle & \xrightarrow{\hspace{1cm}} & |0001\rangle \\ |0010\rangle & & |0010\rangle \\ |0100\rangle & & |0100\rangle \\ |1000\rangle & & |1000\rangle \end{array}$$

# Jordan-Wigner mapping

## Operators

**Fermionic states** are modified by the **creation** and **annihilation** operators

$$\hat{a}^\dagger \quad \hat{a}$$

**Qubit states** are modified by **Pauli** operators

$$\hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = |0\rangle\langle 0| + |1\rangle\langle 1| \quad \hat{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = |0\rangle\langle 1| + |1\rangle\langle 0|$$

$$\hat{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = |0\rangle\langle 0| - |1\rangle\langle 1| \quad \hat{Y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = -i |0\rangle\langle 1| + i |1\rangle\langle 0|$$

We need to make the **translation** between these two worlds.

# Jordan-Wigner mapping

## Operators

Let's start with the **annihilation** for the  $f_0$  ( $q_0$ ) state.

$ f_3 f_2 f_1 f_0\rangle$ $\hat{a}_0  0001\rangle =  0000\rangle$ $\hat{a}_0  0000\rangle = 0$	$ q_3 q_2 q_1 q_0\rangle$ $\hat{X}_0  0001\rangle =  0000\rangle$ $\hat{X}_0  0000\rangle =  0001\rangle$ <b>? No !</b>
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$$\hat{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = |0\rangle\langle 1| + |1\rangle\langle 0|$$

$$i\hat{Y} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = |0\rangle\langle 1| - |1\rangle\langle 0|$$

$$\frac{X + i\hat{Y}}{2} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = |0\rangle\langle 1|$$

# Jordan-Wigner mapping

## Operators

$$\frac{X + i\hat{Y}}{2} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = |0\rangle\langle 1|$$

Let's start with the **annihilation** for the  $f_0$  ( $q_0$ ) state.

$ f_3 f_2 f_1 f_0\rangle$	$ q_3 q_2 q_1 q_0\rangle$
$\hat{a}_0  0001\rangle =  0000\rangle$	$ 0\rangle\langle 1 _0  0001\rangle =  0000\rangle$
$\hat{a}_0  0000\rangle = 0$	$ 0\rangle\langle 1 _0  0000\rangle = 0$

We mapped our first **fermionic operator** to a **qubit operator**!

$$\hat{a}_0 = \frac{1}{2} (\hat{X}_0 + i\hat{Y}_0)$$

# Jordan-Wigner mapping

## Operators

$$\frac{X + i\hat{Y}}{2} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = |0\rangle\langle 1|$$

Now the **annihilation** for the  $f_1$  ( $q_1$ ) state. These operators anti-commute.

$ f_3 f_2 f_1 f_0\rangle$ $\hat{a}_1  0010\rangle =  0000\rangle$ $\hat{a}_1  0000\rangle = 0$ $\hat{a}_0 \hat{a}_1 = -\hat{a}_1 \hat{a}_0$	$ q_3 q_2 q_1 q_0\rangle$ $\hat{a}_1 = \frac{1}{2} (\hat{X}_1 + i\hat{Y}_1)$ ? No ! $(\hat{X}_0 + i\hat{Y}_0)(\hat{X}_1 + i\hat{Y}_1) = (\hat{X}_1 + i\hat{Y}_1)(\hat{X}_0 + i\hat{Y}_0)$
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There is **anti-commutation** in the Pauli group.

$$\hat{X}\hat{Z} = -\hat{Z}\hat{X} \quad \hat{Y}\hat{Z} = -\hat{Z}\hat{Y}$$

# Jordan-Wigner mapping

## Operators

Now the **annihilation** for the  $f_1$  ( $q_1$ ) state. These operators anti-commute.

$ f_3 f_2 f_1 f_0\rangle$ $\hat{a}_1  0010\rangle =  0000\rangle$ $\hat{a}_1  0000\rangle = 0$ $\hat{a}_0 \hat{a}_1 = -\hat{a}_1 \hat{a}_0$	$ q_3 q_2 q_1 q_0\rangle$ $\hat{a}_1 = \frac{1}{2} (\hat{X}_1 + i\hat{Y}_1) \hat{Z}_0$
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These operators do anti-commute.

$$\begin{aligned}
 (\hat{X}_0 + i\hat{Y}_0)(\hat{X}_1 + i\hat{Y}_1)\hat{Z}_0 &= (\hat{X}_1 + i\hat{Y}_1)(\hat{X}_0 + i\hat{Y}_0)\hat{Z}_0 \\
 &= -(\hat{X}_1 + i\hat{Y}_1)\hat{Z}_0(\hat{X}_0 + i\hat{Y}_0)
 \end{aligned}$$

$$\begin{aligned}
 \hat{X}\hat{Z} &= -\hat{Z}\hat{X} \\
 \hat{Y}\hat{Z} &= -\hat{Z}\hat{Y}
 \end{aligned}$$

# Jordan-Wigner mapping

## Operators

For a 4 states system we generalize the **annihilation operators** so that they **anti-commute** with each other.

$$\left. \begin{aligned} \hat{a}_0 &= \frac{1}{2} (\hat{X}_0 + i\hat{Y}_0) \\ \hat{a}_1 &= \frac{1}{2} (\hat{X}_1 + i\hat{Y}_1) \hat{Z}_0 \\ \hat{a}_2 &= \frac{1}{2} (\hat{X}_2 + i\hat{Y}_2) \hat{Z}_1 \hat{Z}_0 \\ \hat{a}_3 &= \frac{1}{2} (\hat{X}_3 + i\hat{Y}_3) \hat{Z}_2 \hat{Z}_1 \hat{Z}_0 \end{aligned} \right\} \quad \hat{a}_i = \frac{1}{2} (\hat{X}_i + i\hat{Y}_i) \bigotimes_{j < i} \hat{Z}_j$$

# Jordan-Wigner mapping

## Operators

What about **creation operators**?

$$|f_3 f_2 f_1 f_0\rangle$$

$$\hat{a}_0^\dagger |0000\rangle = |0001\rangle$$

$$\hat{a}_0^\dagger |0001\rangle = 0$$

$$\{a_0, a_0^\dagger\} = \hat{I}_0$$

$$|q_3 q_2 q_1 q_0\rangle$$

$$|1\rangle\langle 0|_0 |0000\rangle = |0001\rangle$$

$$|1\rangle\langle 0|_0 |0001\rangle = 0$$

$$|0\rangle\langle 1|1\rangle\langle 0| + |1\rangle\langle 0|0\rangle\langle 1| = |0\rangle\langle 0| + |1\rangle\langle 1| = \hat{I}$$

$$\hat{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = |0\rangle\langle 1| + |1\rangle\langle 0|$$

$$i\hat{Y} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = |0\rangle\langle 1| - |1\rangle\langle 0|$$

$$\frac{X - i\hat{Y}}{2} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = |1\rangle\langle 0|$$

# Jordan-Wigner mapping

## Operators

We get a general expression to translate any **Fermionic operator** to a **qubit operator** using the **Jordan-Wigner** mapping.

$$\left. \begin{array}{l} \hat{a}_0 = \frac{1}{2}(\hat{X}_0 + i\hat{Y}_0) \\ \hat{a}_1 = \frac{1}{2}(\hat{X}_1 + i\hat{Y}_1)\hat{Z}_0 \\ \hat{a}_2 = \frac{1}{2}(\hat{X}_2 + i\hat{Y}_2)\hat{Z}_1\hat{Z}_0 \\ \hat{a}_3 = \frac{1}{2}(\hat{X}_3 + i\hat{Y}_3)\hat{Z}_2\hat{Z}_1\hat{Z}_0 \end{array} \right\} \quad \left. \begin{array}{l} \hat{a}_i = \frac{1}{2}(\hat{X}_i + i\hat{Y}_i) \bigotimes_{j < i} \hat{Z}_j \\ \hat{a}_i^\dagger = \frac{1}{2}(\hat{X}_i - i\hat{Y}_i) \bigotimes_{j < i} \hat{Z}_j \\ \hat{a}_i^\dagger = \frac{1}{2}(\hat{X}_i - i\hat{Y}_i) \bigotimes_{j < i} \hat{Z}_j \end{array} \right\}$$

$$\left. \begin{array}{l} \hat{a}_0^\dagger = \frac{1}{2}(\hat{X}_0 - i\hat{Y}_0) \\ \hat{a}_1^\dagger = \frac{1}{2}(\hat{X}_1 - i\hat{Y}_1)\hat{Z}_0 \\ \hat{a}_2^\dagger = \frac{1}{2}(\hat{X}_2 - i\hat{Y}_2)\hat{Z}_1\hat{Z}_0 \\ \hat{a}_3^\dagger = \frac{1}{2}(\hat{X}_3 - i\hat{Y}_3)\hat{Z}_2\hat{Z}_1\hat{Z}_0 \end{array} \right\}$$

$$\left. \begin{array}{l} \{\hat{a}_i, \hat{a}_j\} = 0 \\ \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0 \\ \{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{ij} \end{array} \right.$$

$$\hat{a}_i^\mp = \frac{1}{2}(\hat{X}_i \pm i\hat{Y}_i) \bigotimes_{j < i} \hat{Z}_j$$

# Jordan-Wigner mapping Hamiltonian

We have mapped the **fermionic operators**. Now we need to map the whole **Hamiltonian**.

$$\hat{\mathcal{H}} = \sum_{i,j} h_{ij}^{(1)} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \sum_{i,j,k,l} h_{ijkl}^{(2)} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l.$$

Example : term  $i=0, j=1$  of the one body leads to 4 terms.

$$h_{01} \hat{a}_0^\dagger \hat{a}_1 = h_{01} \frac{1}{2} \left( \hat{X}_0 - i \hat{Y}_0 \right) \times \frac{1}{2} \left( \hat{X}_1 + i \hat{Y}_1 \right) \hat{Z}_0$$

There will be  $64 + 4096$  terms in total. We need good tools to carry this out.  
Let's introduce **Pauli Strings** and **Linear Combinations of Pauli Strings**.

# **Pauli Strings and Operators (Linear Combinaison of Pauli Strings)**

# Pauli Strings

## Definition

A Pauli String of length  $n$  is an operator acting on  $n$  qubits with either a **Pauli Operator** or the **Identity** on each qubit.

$$\hat{\mathcal{P}} \equiv \bigotimes_{i=0}^n \hat{\sigma}_i \quad \hat{\sigma}_i \in \left\{ \hat{I}_i, \hat{X}_i, \hat{Y}_i, \hat{Z}_i \right\}$$

Example :

$$\hat{a}_2 = \frac{1}{2} (\hat{X}_2 + i\hat{Y}_2) \hat{Z}_1 \hat{Z}_0$$

$$\hat{a}_2 = \frac{1}{2} \hat{I}_3 \hat{X}_2 \hat{Z}_1 \hat{Z}_0 + \frac{i}{2} \hat{I}_3 \hat{Y}_2 \hat{Z}_1 \hat{Z}_0$$

$$\hat{a}_2 = \frac{1}{2} \hat{I} \hat{X} \hat{Z} \hat{Z} + \frac{i}{2} \hat{I} \hat{Y} \hat{Z} \hat{Z}$$

Confusing notation if taken out of context

# Pauli Strings

## Product

A **product** of 2 Pauli Strings is a Pauli String (and a **phase**). Pauli operators acting on different qubits always commute.

$$\hat{\mathcal{P}}^{(1)} = \bigotimes_{i=0}^n \hat{\sigma}_i^{(1)} \quad \hat{\mathcal{P}}^{(2)} = \bigotimes_{i=0}^n \hat{\sigma}_i^{(2)} \quad \hat{\sigma}_i \in \left\{ \hat{I}_i, \hat{X}_i, \hat{Y}_i, \hat{Z}_i \right\}$$

$$\hat{\mathcal{P}}^{(2)} \hat{\mathcal{P}}^{(1)} = \bigotimes_{i=0}^n \hat{\sigma}_i^{(2)} \hat{\sigma}_i^{(1)}$$

We use the Pauli Operator relations to get the result of the product

$$\hat{X}\hat{Y} = i\hat{Z}$$

$$\hat{Y}\hat{Z} = i\hat{X}$$

$$\hat{Z}\hat{X} = i\hat{Y}$$

# Pauli Strings

## Product

Examples :

$$(\hat{I}_3 \hat{I}_2 \hat{I}_1 \hat{X}_0) (\hat{I}_3 \hat{I}_2 \hat{X}_1 \hat{Z}_0) = -i (\hat{I}_3 \hat{I}_2 \hat{X}_1 \hat{Y}_0)$$

$$(\hat{I}_3 \hat{I}_2 \hat{Z}_1 \hat{Z}_0) (\hat{I}_3 \hat{I}_2 \hat{Y}_1 \hat{Y}_0) = (-i)^2 (\hat{I}_3 \hat{I}_2 \hat{X}_1 \hat{X}_0) = - (\hat{I}_3 \hat{I}_2 \hat{X}_1 \hat{X}_0)$$

$$\begin{aligned}\hat{X} \hat{Y} &= i \hat{Z} \\ \hat{Y} \hat{Z} &= i \hat{X} \\ \hat{Z} \hat{X} &= i \hat{Y}\end{aligned}$$

# Pauli Strings in the computer ZX representation

Any **Pauli string** can be written as

$$\hat{\mathcal{P}} = (-i)^{\mathbf{z} \cdot \mathbf{x}} \hat{Z}^{\mathbf{z}} \hat{X}^{\mathbf{x}}$$

With **z** and **x** arrays of **(mod 2) integers**. Why is there a **phase** in front?

$$\begin{aligned} \hat{Z}^{(1,1,1,0)} \hat{X}^{(0,1,1,1)} &= (\hat{Z}_0 \hat{Z}_1 \hat{Z}_2 \hat{I}_3) (\hat{I}_0 \hat{X}_1 \hat{X}_2 \hat{X}_3) \\ &= (\hat{I}_3 \hat{Z}_2 \hat{Z}_1 \hat{Z}_0) (\hat{X}_3 \hat{X}_2 \hat{X}_1 \hat{I}_0) \\ &= i^2 \hat{X}_3 \hat{Y}_2 \hat{Y}_1 \hat{Z}_0 \end{aligned} \quad \hat{Z}\hat{X} = i\hat{Y}$$

Including the phase, we always end up with a **pure Pauli string**.

$$(-i)^{(1,1,1,0) \cdot (0,1,1,1)} \hat{Z}^{(1,1,1,0)} \hat{X}^{(0,1,1,1)} = (-i)^2 i^2 \hat{X}_3 \hat{Y}_2 \hat{Y}_1 \hat{Z}_0 = \hat{X}_3 \hat{Y}_2 \hat{Y}_1 \hat{Z}_0$$

# Pauli Strings in the computer ZX representation

Beware of your implementation!

$$\hat{\mathcal{P}} = (-i)^{\mathbf{z} \cdot \mathbf{x}} \hat{Z}^{\mathbf{z}} \hat{X}^{\mathbf{x}}$$

Pauli matrices are their own inverse. Therefore, the components of  $\mathbf{z}$  and  $\mathbf{x}$  should be considered as **(mod 2) integers**, not **booleans**; the boolean addition correspond to "OR", whereas the **(mod 2)** addition correspond to "XOR".

The imaginary number has a 4-fold symmetry. Therefore, the result of  $\mathbf{z} \cdot \mathbf{x}$  should be considered as a **(mod 4) integer**.

# Pauli Strings in the computer ZX product

We can **multiply** 2 Pauli strings using the ZX representation. The result needs to follow the **ZX representation**.

$$\begin{aligned} \hat{\mathcal{P}}_1 &= (-i)^{\mathbf{z}_1 \cdot \mathbf{x}_1} \hat{Z}^{\mathbf{z}_1} \hat{X}^{\mathbf{x}_1} & \longrightarrow & \hat{\mathcal{P}}_3 = (-i)^{\mathbf{z}_3 \cdot \mathbf{x}_3} \hat{Z}^{\mathbf{z}_3} \hat{X}^{\mathbf{x}_3} \\ \hat{\mathcal{P}}_2 &= (-i)^{\mathbf{z}_2 \cdot \mathbf{x}_2} \hat{Z}^{\mathbf{z}_2} \hat{X}^{\mathbf{x}_2} \end{aligned}$$

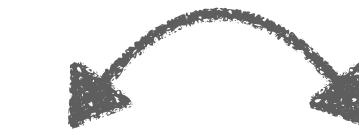
$$\hat{\mathcal{P}}_1 \hat{\mathcal{P}}_2 = (-i)^w \hat{\mathcal{P}}_3 = (-i)^{w + \mathbf{z}_3 \cdot \mathbf{x}_3} \hat{Z}^{\mathbf{z}_3} \hat{X}^{\mathbf{x}_3}$$

# Pauli Strings in the computer

## ZX product

At first the ZX order is not respected.

$$\hat{\mathcal{P}}_1 \hat{\mathcal{P}}_2 = (-i)^{\mathbf{z}_1 \cdot \mathbf{x}_1 + \mathbf{z}_2 \cdot \mathbf{x}_2} \hat{Z}^{\mathbf{z}_1} \hat{X}^{\mathbf{x}_1} \hat{Z}^{\mathbf{z}_2} \hat{X}^{\mathbf{x}_2}$$



Reordering introduces an **extra phase (-1)** **every time** there is both **Z** and **X** acting on the **same qubit**.

$$\hat{X}^{\mathbf{x}_1} \hat{Z}^{\mathbf{z}_2} = (-1)^{\mathbf{z}_2 \cdot \mathbf{x}_1} \hat{Z}^{\mathbf{z}_2} \hat{X}^{\mathbf{x}_1} = (-i)^{2\mathbf{z}_2 \cdot \mathbf{x}_1} \hat{Z}^{\mathbf{z}_2} \hat{X}^{\mathbf{x}_1}$$

$$\hat{X} \hat{Z} = -\hat{Z} \hat{X}$$

$$(-i)^2 = -1$$

At this point we have :

$$\hat{\mathcal{P}}_1 \hat{\mathcal{P}}_2 = (-i)^{2\mathbf{z}_2 \cdot \mathbf{x}_1 + \mathbf{z}_1 \cdot \mathbf{x}_1 + \mathbf{z}_2 \cdot \mathbf{x}_2} \hat{Z}^{\mathbf{z}_1} \hat{Z}^{\mathbf{z}_2} \hat{X}^{\mathbf{x}_1} \hat{X}^{\mathbf{x}_2}$$

# Pauli Strings in the computer ZX product

We are not very far from a proper ZX representation

$$\hat{\mathcal{P}}_1 \hat{\mathcal{P}}_2 = (-i)^{2\mathbf{z}_2 \cdot \mathbf{x}_1 + \mathbf{z}_1 \cdot \mathbf{x}_1 + \mathbf{z}_2 \cdot \mathbf{x}_2} \hat{Z}^{\mathbf{z}_1} \hat{X}^{\mathbf{x}_1 + \mathbf{x}_2}$$

$$\hat{\mathcal{P}}_1 \hat{\mathcal{P}}_2 = (-i)^w \hat{\mathcal{P}}_3 = (-i)^{w + \mathbf{z}_3 \cdot \mathbf{x}_3} \hat{Z}^{\mathbf{z}_3} \hat{X}^{\mathbf{x}_3}$$

Let's identify  $\mathbf{z}_3$  and  $\mathbf{x}_3$  remembering the components are **(mod 2) integers**.

$$\mathbf{z}_3 = \mathbf{z}_1 + \mathbf{z}_2 \pmod{2} \quad \mathbf{x}_3 = \mathbf{x}_1 + \mathbf{x}_2 \pmod{2}$$

We can now express the product phase remembering it is a **(mod 4) integer**.

$$w = 2\mathbf{z}_2 \cdot \mathbf{x}_1 + \mathbf{z}_1 \cdot \mathbf{x}_1 + \mathbf{z}_2 \cdot \mathbf{x}_2 - \mathbf{z}_3 \cdot \mathbf{x}_3 \pmod{4}$$

# Operators (Linear combinaison of Pauli Strings)

## Definition

We already encountered **linear combinaisons of Pauli strings** (LCPS).

$$\hat{\mathcal{H}} = \sum_i h_i \hat{\mathcal{P}}_i$$

$$\hat{a}_2 = \frac{1}{2} \hat{I}_3 \hat{X}_2 \hat{Z}_1 \hat{Z}_0 + \frac{i}{2} \hat{I}_3 \hat{Y}_2 \hat{Z}_1 \hat{Z}_0$$

We can define any operator as a LCPS

$$\hat{A} = \sum_i c_i \hat{\mathcal{P}}_i$$

# Operators (Linear combinaison of Pauli Strings)

## Addition

Consider 2 LCPS with different numbers of Pauli Strings.

$$\hat{A}_1 = \sum_i^{n_1} c_i^{(1)} \hat{\mathcal{P}}_i^{(1)}$$

$$\hat{A}_2 = \sum_i^{n_2} c_i^{(2)} \hat{\mathcal{P}}_i^{(2)}$$

The **sum** of two LCPS is simply the union of the two LCPS.

$$\hat{A}_1 + \hat{A}_2 = \hat{A}_3$$

$$\hat{A}_3 = \sum_i^{n_3} c_i^{(3)} \hat{\mathcal{P}}_i^{(3)}$$

$$n_3 = n_1 + n_2$$

# Operators (Linear combinaison of Pauli Strings)

## Product

Consider 2 LCPS with different numbers of Pauli Strings.

$$\hat{A}_1 = \sum_i^{n_1} c_i^{(1)} \hat{\mathcal{P}}_i^{(1)}$$

$$\hat{A}_2 = \sum_i^{n_2} c_i^{(2)} \hat{\mathcal{P}}_i^{(2)}$$

The **product** of two LCPS is also a LCPS. The **phase** from the product of Pauli strings can be absorbed in the **coefficients**.

$$\hat{A}_1 \hat{A}_2 = \sum_{i,j}^{n_1, n_2} c_i^{(1)} c_j^{(2)} \hat{\mathcal{P}}_i^{(1)} \hat{\mathcal{P}}_j^{(2)}$$

$$\hat{A}_3 = \sum_k^{n_3} c_k^{(3)} \hat{\mathcal{P}}_k^{(3)}$$

$$n_3 = n_1 \times n_2$$

$$k = j + i n_2$$

$$\hat{\mathcal{P}}_i^{(1)} \hat{\mathcal{P}}_j^{(2)} = (-i)^{w_k} \hat{\mathcal{P}}_k^{(3)}$$

$$c_i^{(1)} c_j^{(2)} (-i)^{w_k} = c_k^{(3)}$$

# Operators (Linear combinaison of Pauli Strings)

## Combinaison

The **product** of LCPS can produce **duplicates** of the same Pauli string. When this happens we can **combine** these terms by **summing** their respective **coefficients**. For example,

$$\hat{A}_1 = a\hat{I}\hat{I}\hat{I}\hat{Z} - b\hat{I}\hat{I}\hat{Z}\hat{Z} \quad \hat{A}_2 = a\hat{Z}\hat{Z}\hat{Z}\hat{I} + b\hat{Z}\hat{Z}\hat{I}\hat{I}$$

The product gives 4 terms, but can be combined into only 2, of which one cancels out!

$$\begin{aligned}\hat{A}_1\hat{A}_2 &= a^2\hat{Z}\hat{Z}\hat{Z}\hat{Z} + ab\hat{Z}\hat{Z}\hat{I}\hat{Z} - ba\hat{Z}\hat{Z}\hat{I}\hat{Z} - b^2\hat{Z}\hat{Z}\hat{Z}\hat{Z} \\ &= (a^2 - b^2)\hat{Z}\hat{Z}\hat{Z}\hat{Z} + (ab - ba)\hat{Z}\hat{Z}\hat{I}\hat{Z} \\ &= (a^2 - b^2)\hat{Z}\hat{Z}\hat{Z}\hat{Z}\end{aligned}$$

In practice, we will **remove** any Pauli strings with a **coefficient smaller than a given threshold**.

# Back to the Mapping

# Back to the Mapping

## The general idea

A **molecular Hamiltonian** can therefore be represented as a **linear combinaison of Pauli strings**.

$$\hat{\mathcal{H}} = \sum_{i,j} h_{ij}^{(1)} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \sum_{i,j,k,l} h_{ijkl}^{(2)} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l \quad \hat{\mathcal{H}} = \sum_i h_i \hat{\mathcal{P}}_i$$

The **expected value** of the Hamiltonian (aka energy) is a **weighted sum** of the expected values of the Pauli strings.

$$\langle \psi | \hat{\mathcal{H}} | \psi \rangle = \sum_i h_i \langle \psi | \hat{\mathcal{P}}_i | \psi \rangle$$

# Back to the Mapping

## ZX representation of Jordan-Wigner (4 qubits)

Fermionic operators are Linear Combinations of 2 Pauli Strings.

$$\hat{a}_i^{\mp} = \frac{1}{2} (\hat{\mathcal{P}}_i^R \pm i\hat{\mathcal{P}}_i^I)$$

In the **Jordan-Wigner** mapping with 4 qubits the ZX representations are :

$$\hat{\mathcal{P}}_i^R = \hat{X}_i \bigotimes_{j < i} \hat{Z}_j$$

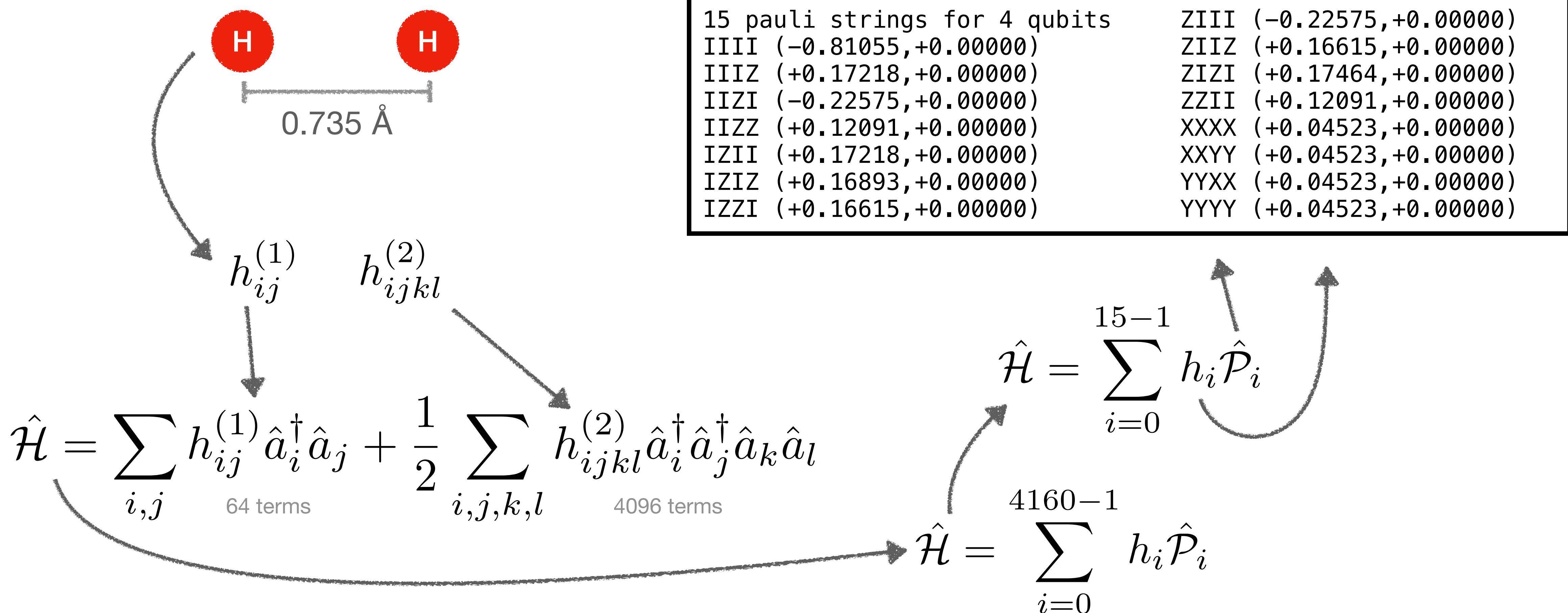
$\hat{\mathcal{P}}_i^R$	z_bits				x_bits			
	0	1	2	3	0	1	2	3
0	0.5	0	0	0	0	1	0	0
1	0.5	1	0	0	0	0	1	0
2	0.5	1	1	0	0	0	0	1
3	0.5	1	1	1	0	0	0	1

$$\hat{\mathcal{P}}_i^I = \hat{Y}_i \bigotimes_{j < i} \hat{Z}_j$$

$\hat{\mathcal{P}}_i^I$	z_bits				x_bits			
	0	1	2	3	0	1	2	3
0	0.5	1	0	0	0	0	1	0
1	0.5	1	1	0	0	0	1	0
2	0.5	1	1	1	0	0	0	1
3	0.5	1	1	1	1	0	0	1

# The Mapping of H<sub>2</sub> with Jordan-Wigner

## A summary



**Just code it!**

**Questions?**

# Some ressources

**Just 2, so you are not overwhelmed with information**

## Review

McArdle, S., Endo, S., Aspuru-Guzik, A., Benjamin, S. C., & Yuan, X. (2020). Quantum computational chemistry. *Reviews of Modern Physics*, 92(1), 15003. <https://doi.org/10.1103/RevModPhys.92.015003>, arXiv : [1808.10402](https://arxiv.org/abs/1808.10402)

## Mapping

Seeley, J. T., Richard, M. J., & Love, P. J. (2012). The Bravyi-Kitaev transformation for quantum computation of electronic structure. *Journal of Chemical Physics*, 137(22). <https://doi.org/10.1063/1.4768229>, arXiv : [1208.5986](https://arxiv.org/abs/1208.5986)