Next we would like to study more general problems than spin systems.

Most often in non-relativistic quantum mechanics pb – one writes the Hami in second quantization.

Parenthesis on second quantization

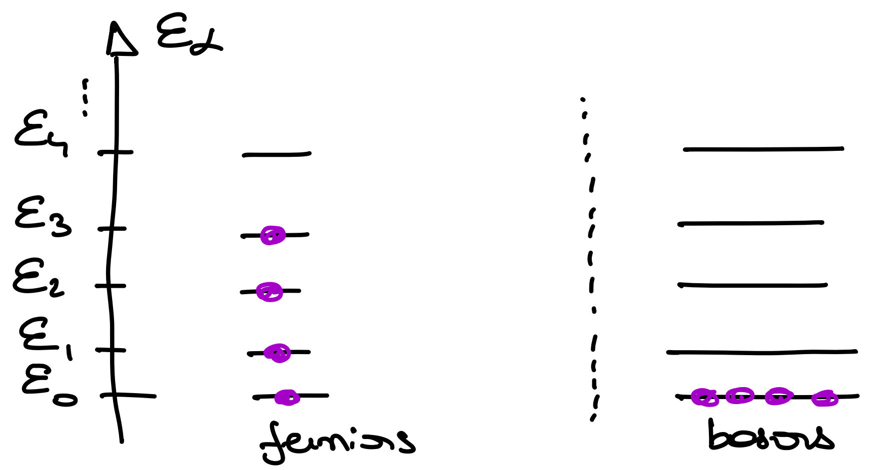
Let's consider a system of N identical particles governed by a Hamiltonian

$$\mathcal{H}_{syst} = \underbrace{H_0}_{\substack{\text{single-particle} \\ \text{Hamiltonian} \\ \text{(kinetic energy +} \\ \text{possibly single-particle} \\ \text{potential)}}} + \underbrace{V}_{\text{interaction}}$$

Let us denote $|\chi_i\rangle$ the eigenstates of H_0:

$$H_0 |\chi_i\rangle = \varepsilon\, |\chi_i\rangle$$

Without interaction V, the state of the N-particle system corresponds to a single configuration of the N particles in single-particle states $|\chi_i\rangle$. For example:



Due to undistinguishability, the state of the N-particle system is described by the symmetric (bosons) or antisymmetric (fermions) combinations of tensor products of single-particle states $|\chi_\alpha\rangle$.
In first quantization:

$$|\Phi\rangle = \frac{1}{\sqrt{N! \prod_\alpha n_i!}} \sum_P \xi^P |\chi_{i_{P_1}}\rangle \otimes \dots \otimes |\chi_{i_{P_N}}\rangle$$

where P denotes the N! permutations of all single-particle states, and

$$\begin{cases} \xi = +1 \text{ for bosons}, \ -1 \text{ for fermions} \\ n_i = \# \text{ of particles in state } \chi_i = 0,1 \text{ for fermions} \end{cases}$$

⇝ example for a 2-fermion system:

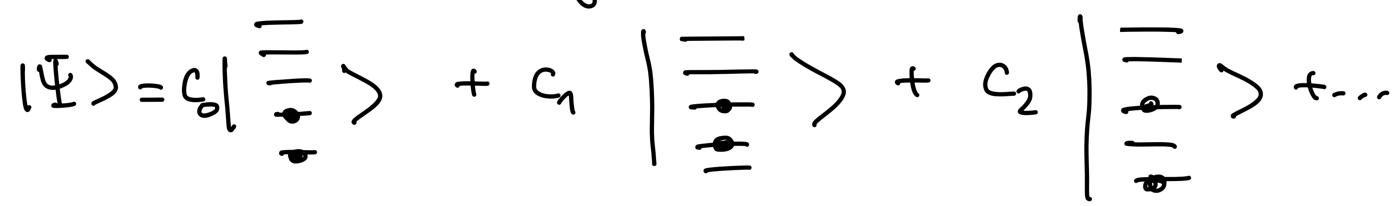
$$|\Phi\rangle = \frac{1}{\sqrt{2}} \left[|\chi_1\rangle \otimes |\chi_2\rangle - |\chi_2\rangle \otimes |\chi_1\rangle \right]$$

$|\Phi\rangle$ for a fermionic system is called a Slater determinant.

When the interaction $\hat{V}$ turns on, the particles interact and can be scattered between single-particle states, so that the state $|\Psi\rangle$ of the interacting N-particle system can be written as a superposition of N-particle configurations $|\Phi\rangle$.

$$|\Psi\rangle = \sum_{\alpha} c_{\alpha} |\Phi_{\alpha}\rangle$$

example for a 2-fermion system:



It is clear that the expression for the $|\Phi\rangle$'s above is impractical for large N. It is also not usable when one wants to describe processes with varying number of particles.

What we understand is that for system of identical particles, it only matters how many particles occupy a certain single-particle state $|x_i\rangle$ -

Thus each configuration $|\Phi\rangle$ can be written in much simpler way, in terms of occupation numbers.

If we have M single-particle states:

$$|\Phi\rangle \equiv |n_{M-1}\, n_{M-2} \,\dots\, n_1\, n_0\rangle$$

where n_α = # of particles in state $|\chi_\alpha\rangle$

and $\sum_{i=0}^{M-1} n_i = N$

For fermionic systems $n_i = 0$ or 1 due to the Pauli exclusion principle.
Thus fermionic systems can be easily mapped to qubits, since the configurations $|\Phi\rangle = |0\,1\,0 \dots 1\,1\rangle$ can be identified with computational-basis states.

In what follows we will focus on fermionic systems.

The configurations $|\Phi\rangle$ can be obtained from the vacuum state $|\emptyset\rangle = |000\ldots0\rangle$ by applying successively creation operators $a_i^\dagger$:

$$|\Phi\rangle = \left(a_{M-1}^\dagger\right)^{n_{M-1}} \left(a_{M-2}^\dagger\right)^{n_{M-2}} \cdots \left(a_1^\dagger\right)^{n_1} \left(a_0^\dagger\right)^{n_0} |\emptyset\rangle \quad (*)$$

$a_\alpha^\dagger$ creates a fermion in state $|\chi_\alpha\rangle$
the associated destruction operator a_α destroys a fermion in state $|\chi_\alpha\rangle$.

Thus $\quad a_i |\emptyset\rangle = 0 \quad \forall i$

These operators satisfy anti-commutation relations specific to fermionic op:

$$\begin{cases} \{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0 \\ \{a_i^\dagger, a_j\} = \delta_{ij} \end{cases}$$

$$\{A, B\} = AB + BA \quad \text{(anticommutator)}$$

$\Rightarrow$ writing the state as in $(*)$ automatically takes care of the antisymm.

The action of these operators on N-particle configurations are:

$$\boxed{a_i |n_{M-1} \dots n_i \dots n_0\rangle = \underbrace{\varphi_i}_{\text{phase}} \underline{\underline{n_i}} \, |n_{M-1} \dots n_i - 1 \dots n_0\rangle}$$

$|\chi_i\rangle$ must be occupied, otherwise $a_i |n_{M-1} \dots n_0\rangle = 0$

$$\varphi_i = (-1)^{\sum_{j=M-1}^{i+1} n_j}$$

due to anti-commutation rule of fermionic ops.

(ex $a_2 |1101\rangle$ with n_3, n_2, n_1, n_0

$$= a_2 \, a_3^\dagger a_2^\dagger a_0^\dagger \overbrace{|0000\rangle}^{|\phi\rangle}$$

$$= - a_3^\dagger a_2 a_2^\dagger a_0^\dagger |\phi\rangle$$

$$= - a_3^\dagger (1 - a_2^\dagger a_2) a_0^\dagger |\phi\rangle$$

$$= - a_3^\dagger a_0^\dagger |\phi\rangle + \underbrace{a_3^\dagger a_2^\dagger a_2 a_0^\dagger |\phi\rangle}_{-a_3^\dagger a_2^\dagger a_0^\dagger \underbrace{a_2 |\phi\rangle}_{0}}$$

where we used:

$\{a_i, a_j^\dagger\} = \delta_{ij}$

$\Rightarrow$
- $a_i a_j^\dagger = - a_j^\dagger a_i$ if $i \neq j$.
- $a_i a_i^\dagger = \{a_i, a_i^\dagger\} - a_i^\dagger a_i$
  $= 1 - a_i^\dagger a_i$.)

Similarly for creation operators:

$$\boxed{a_i^\dagger \, |n_{M-1} \dots n_i \dots n_0\rangle = \varphi_i \underbrace{(1-n_i)}_{} |n_{M-1} \dots n_i + 1 \dots n_0\rangle}$$

$|x_i\rangle$ must be empty to create a fermion in it.

Note: The op. $n_i = a_i^\dagger a_i$ counts the number of particles in state $|x_i\rangle$.

The Hamiltonians can also be written in terms of these creation / annihilation operators.

One-particle operators such as H_0 take the form:

$$\boxed{\hat{H}_0 = \sum_{ij} \langle x_i | \hat{H}_0 | x_j\rangle \, a_i^\dagger a_j}$$

Two-particle operators take the form:

$$\boxed{\hat{V} = \frac{1}{4} \sum_{ijkl} \langle x_i x_j | \hat{V} | \overline{x_k x_l}\rangle \, a_i^\dagger a_j^\dagger a_l a_k}$$

where $\langle \chi_i \chi_j | \hat{V} | \overline{\chi_k \chi_\ell} \rangle = \langle \chi_i \chi_j | \hat{V} | \chi_k \chi_\ell \rangle - \langle \chi_i \chi_j | \hat{V} | \chi_\ell \chi_k \rangle$

(antisymmetrized interaction matrix element).

(Note: we will consider in this course only 2-particle interaction $\hat{V}$ as above - This can be generalized to 3-particle interactions with $a^\dagger a^\dagger a^\dagger a a a$ etc...)

The formalism of second quantization is detailed in many books dealing with many-body physics.

In system relevant to quantum chemistry, condensed matter, (low-energy) nuclear physics the Hamiltonians are usually written in the generic second-quantized form as above.

We will encounter a few examples in this course.

$\rightsquigarrow$ How can we simulate such systems on quantum computers?

There are different ways to do that. One of the most popular mapping is the Jordan-Wigner mapping.

* Jordan-Wigner mapping :

(Jordan, Wigner, Z. Phys, 47 631 (1928))

As mentionned above, N-fermion system in the occupation-number representation can be intuitively mapped to qubits since

$$|\Psi\rangle_{syst} = \sum_{\alpha} c_{\alpha} |\Phi_{\alpha}\rangle$$

$$= \sum_{\substack{n_0=0,1 \\ \vdots \\ n_{M-1}=0,1 \\ \text{with} \\ \sum_i n_i = N}} c_{n_{M-1} \cdots n_0} |n_{M-1} n_{M-2} \ldots n_1 n_0\rangle$$

This can be identified with a state of a n-qubit system where the single-particle occupations are mapped to the qubits :

single-partic state $\qquad\qquad$ qubit

$$|n_i = 0\rangle \leftrightarrow |0 \equiv \uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix}$$

$$|n_i = 1\rangle \leftrightarrow |1 \equiv \downarrow\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

many-body states $|n_{M-1} \dots n_0\rangle \leftrightarrow |x_{M-1} \dots x_0\rangle$.

(⚠ sometimes the other convention (less intuitive)

$$|n_i - 1\rangle \leftrightarrow |0 \equiv \uparrow\rangle$$
$$|n_i = 0\rangle \leftrightarrow |1 \equiv \downarrow\rangle$$

is used).

The number of qubits needed to describe the system is equal to the number of single-particle states.

The number of config contributing to $|\Psi\rangle$ is is the # of ways of distributing the N fermions among M single-partic. states

ie $\binom{N}{M}$.

Now the next step is to map the Hamiltonian in second quantization to Pauli operators.

we want qubit operators acting like $a^\dagger$ and a .

we know that the "ladder operator"

$$\sigma^+ = \frac{X+iY}{2} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

acts on one-qubit states as:

$$\begin{cases} \sigma^+ |0\rangle = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0 \\ \sigma^+ |1\rangle = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle \end{cases}$$

Similarly $\sigma^- = \frac{X-iY}{2} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$

acts as

$$\begin{cases} \sigma^- |0\rangle = |1\rangle \\ \sigma^- |1\rangle = |0\rangle \end{cases}$$

Thus σ^+ and σ^- act on one-qubit states in the same way as a and a^+ act on one-particle states.

For the action on n-qubit states we also need the phase due to anticommutation of fermionic operators.

$$a_i^+ |n_{N-1} \dots n_0\rangle = (-)^{n_{N-1}+\dots+n_{i+1}} (1-n_i) |n_{N-1} \dots 1+n_i \dots n_0\rangle$$

$$a_i |n_{N-1} \dots n_0\rangle = (-)^{n_{N-1}+\dots+n_{i+1}} n_i |n_{N-1} \dots 1-n_i \dots n_0\rangle$$

This phase can be obtained with Z operators since

$$\begin{cases} Z|0\rangle = |0\rangle \\ Z|1\rangle = -|1\rangle . \end{cases}$$

$\Rightarrow$ the operator $\prod_{j=M-1}^{i+1} Z_j$ will pick up a (-1) for each occupied state between n_{M-1} & n_{i+1} and thus provides the desired phase.

Thus we have

$$\boxed{\begin{aligned} a_i^{\dagger} &\equiv \left(\prod_{j=M-1}^{i+1} Z_j \right) \sigma_i^{-} \\ a_i &\equiv \left(\prod_{j=M-1}^{i+1} Z_j \right) \sigma_i^{+} \end{aligned}}$$

With this we write the second-quantized Hamiltonian in terms of Pauli operators σ^+, σ^- and Z.

JW mapping is intuitive but requires many Z gates if the interaction acts btw "distant" qubits (in terms of ordering in the basis).

If have M sp states $\rightarrow$ $a_i^{(+)}$ requires $O(M)$ gates

- **Parity mapping**

Instead of storing the occupation numbers of each orbital into the qubits, one can store the "parity" p_i of the single-particle states above (or below):

$$p_i = \left(\sum_{j=n-1}^{i} n_j \right) \bmod 2$$

Example : consider the fermionic state :

$$|n_4=1, n_3=1, n_2=1, n_1=0, n_0=1\rangle \equiv |11101\rangle_{\text{fermionic}}$$

- In the JW mapping this is encoded into

$$|x_4=1, x_3=1, x_2=1, x_1=0, x_0=1\rangle \equiv |11101\rangle_{JW}$$

- In the parity mapping the fermionic state is encoded into :

$$|p_4=1, p_3=0, p_2=1, p_1=1, p_0=0\rangle \equiv |\,1 \quad 0 \quad 1 \quad 1 \quad 0\,\rangle_{\text{parity}}$$

$n_4 = 1$

$n_4 \oplus n_3 = 0$

$n_4 \oplus n_3 \oplus n_2 = 1$

$n_4 \oplus n_3 \oplus n_2 \oplus n_1 = 1$

$n_4 \oplus \dots \oplus n_0 = 0.$

The action of an annihilation operator a_i is:

$$a_i\, |n_{M-1} \dots n_i \dots n_0\rangle = (-1)^{\sum_{j>i} n_j}\, n_i\, |n_{M-1} \dots \underbrace{n_i - 1}_{0} \dots n_0\rangle$$

- In JW: the phase $(-1)^{\sum_{j>i} n_j}$ requires $\prod_{j>i} Z_j$
- In the parity mapping, $\sum_{j>i} n_j \pmod 2$ is simply the value of qubit $i+1$

$$p_{i+1} = \sum_{j>i} n_j \pmod 2$$

$\Rightarrow$ can obtain the phase by acting locally on qubit $i+1$.

However the action of annihilating a fermion has now become more complicated
↳ in state i

because

1) the way we act on qubit i depends on p_{i+1}

if $p_{i+1} = 0$ $(p_i = 1)$ $\overset{a_i}{\Rightarrow}$ p_i must decrease by 1 $\Rightarrow \sigma_i^+$

if $p_{i+1} = 1$ $(p_i = 0)$ $\overset{a_i}{\Rightarrow}$ p_i must increase by 1 $\Rightarrow \sigma_i^-$

2) the parity p_j of all states $j<i$ is also affected by the annihilation:
need to flip all the p_j $(j<i)$ with X.

$\Rightarrow$ the action of a_i is mapped into

$$Q_i = (-1)^{p_{i+1}} \Big\{ |1\rangle\langle 1|_{i+1} \otimes \sigma_i^- \otimes \Big(\prod_{j<i} X_j\Big)$$

$$+ |0\rangle\langle 0|_{i+1} \otimes \sigma_i^+ \otimes \Big(\prod_{j<i} X_j\Big) \Big\}$$

$$= \Big\{ - |1\rangle\langle 1|_{i+1} \otimes \sigma_i^- \otimes \Big(\prod_{j<i} X_j\Big)$$

$$+ |0\rangle\langle 0|_{i+1} \otimes \sigma_i^+ \otimes \prod_{j<i} X_j \Big\}.$$

Similarly the action of a_i^+ is mapped into

$$a_i^+ = \Big\{ -|1\rangle\langle 1|_{i+1} \otimes \sigma_i^+ \otimes \prod_{j<i} X_j$$

$$+ |0\rangle\langle 0|_{i+1} \otimes \sigma_i^- \otimes \prod_{j<i} X_j \Big\}$$

⇒ Now the annihilation / creation of fermions require acting on all qubits.

We have traded the non-locality of computing the parity for non-locality of annihilating / creating.

⇒ $a_i^{(+)}$ still requires $O(M)$ gates

Since the parity encoding is less intuitive than the JW mapping, and offers no gain in terms of gate counts, it is typically not used.

There is another mapping, however, which is in between JW and parity, which requires only $O(\log M)$ gates.

Bravyi- Kitaev (BK) mapping

(Annals of Phys. 298 210 (2002))

Here the fermionic state $|n_{M-1} \dots n_0\rangle$ is encoded into $|b_{M-1} \dots b_0\rangle$ where (for ex)

$$b_i = \begin{cases} n_i & \text{if } i \text{ is odd} \\ \tilde{p}_i = \left(\sum_j n_j \right) \bmod 2 & \text{, if } i \text{ even} \end{cases}$$

$j \in$ set of orbitals adjacent to i (& $j \geq i$)

more precisely the transfo btw $|n_{M-1} \dots n_0\rangle$ & $|b_{M-1} \dots b_0\rangle$ is given by

$$\beta_{2^x} = \left(\begin{array}{c|c} \beta_{2^{x-1}} & 0 \\ \hline \underset{\leftarrow 1 \rightarrow}{0} & \beta_{2^{x-1}} \end{array} \right)$$

where $\beta_1 = (1)$ and "$\leftarrow 1 \rightarrow$" = row of 1's.

example : $|n\rangle \equiv |n_7 \dots n_0\rangle$

$$x = 0 \longrightarrow \beta_1 = 1$$

$$x = 1 \longrightarrow \beta_2 = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$$

$$x = 2 \longrightarrow \beta_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{pmatrix}$$

$$x = 3 \longrightarrow \beta_8 = \begin{pmatrix} \begin{matrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{matrix} & 0 \\ \begin{matrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \end{matrix} & \begin{matrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{matrix} \end{pmatrix}$$

$$\beta_8 \, |n\rangle = |b\rangle$$

$$\Leftrightarrow \begin{pmatrix} & & \\ & \beta_8 & \\ & & \end{pmatrix} \begin{pmatrix} n_7 \\ n_6 \\ \vdots \\ n_0 \end{pmatrix} = \begin{pmatrix} b_7 \\ b_6 \\ \vdots \\ b_0 \end{pmatrix}$$

$$\Rightarrow \begin{cases} b_7 = n_7 \\ b_6 = n_7 + n_6 \\ b_5 = n_5 \\ b_4 = n_7 + n_6 + n_5 + n_4 \\ b_3 = n_3 \\ b_2 = n_3 + n_2 \\ b_1 = n_1 \\ b_0 = n_7 + n_6 + \dots + n_1 + n_0 . \end{cases}$$

Now: the parity $(-)^{\sum_{j>i} n_j} \equiv p_i$ is contained in a few partial sums (ex: for $i = \cancel{5}4$: $n_7 + n_6 + n_5 = b_6 + b_5$) ...

Similarly we don't need to update all the qubits when annihilating / creating $a_{(i)}^{+}$ but only those which contain n_i.

It can be shown that the overall cost for $a_i^{(+)}$ is now $O(\log M)$.

Due to the complicated nature of the BK encoding, this mapping is in fact rarely used, and we will not go into more details of it in this course.

It is important to emphasize, that optimal mappings can often be tailored to the system of interest.
In particular, using symmetries (e.g particle-number conservation etc...) often allow for more efficient mappings.