Fermion to qubit mappings:

In these notes, we will try to understand some of the mappings that exist between fermionic bases & qubit basis. These are very useful in variety of problems:

1. Solve some interacting spin systems exactly by mapping them to non-interacting fermionic systems.
2. Solve a quantum Chemistry Hamiltonian on a quantum Computer.

Before diving into these mappings let's look at fermionic orbital basis (Fock basis)

- Fock basis and fermionic creation / anhilation operators

Suppose, we have some finite single particle fermionic modes, say 'n'. Then the system of M fermions ($M \leq n$) can be described by the subspace spanned by the vectors of the form:

$$|\alpha\rangle = |f_0 f_1 \dots f_{n-2} f_{n-1}\rangle \quad \text{where} \quad f_i = \{0, 1\} \qquad - (1)$$

Clearly, the dimension of this subspace $= 2^n$.

What does a particular $|\alpha\rangle$ mean physically? Let us take an example:

Suppose, $n = 4$ and we have $M - 3$. One of the allowed state $|\alpha\rangle$ is given by

$$|\alpha\rangle = |\underbrace{1110}_{\text{4 digits indicate 4 single particle modes}}\rangle$$

the first mode has one fermion

the last mode has no fermion

The $\{f_i\}$ are termed as occupations and the basis describing the subspace is termed as occupation basis.

Clearly, the values of $\{f_i\}$ are limited to $\{0, 1\}$. The underlying reason for this is the Pauli's exclusion principle.

Creation / anhilation operators:

Let $a_1, a_2, \dots a_n$ denote the set of operators acting on the Hilbert space of M particles ($M \leq n$). The set $a_1^+, a_2^+, \dots, a_n^+$ denote the adjoint operators. Due to the Pauli's exclusion principle, these operators satisfy certain algebra given as follows:

$$\{a_j, a_k^+\} = \delta_{jk} \quad ; \quad \{a_j, a_k\} = 0 \qquad - (2)$$

where $\{A, B\} = AB + BA$ (Anti commutator)

Using the CACs (canonical anti-commutation relations), we can derive the following action on the basis described in 1.

Creation operator: $a_j^{+}|\alpha\rangle = (-1)^{S_j}(1-f_j)|\alpha'\rangle$

where $|\alpha\rangle = |f_0 f_1 \ldots f_j \ldots f_{n-1}\rangle$ & $|\alpha'\rangle = |f_0 f_1 \ldots f_j{+}1 \ldots f_{n-1}\rangle$ — (3)

Anhilation operator: $a_j|\alpha\rangle = (-1)^{S_j} f_j |\alpha'\rangle$

where $|\alpha\rangle = |f_0 f_1 \ldots f_j \ldots f_{n-1}\rangle$ & $|\alpha'\rangle = |f_0 f_1 \ldots f_j{-}1 \ldots f_{n-1}\rangle$ — (4)

and $S_j = \sum_{i<j} f_i$

- The operators in (3) & (4) are called creation & anhilation operators because they either create or destroy a fermion in the 'j'th mode respectively!
- The reason for the prefactor $(-1)^{S_j}$ is the antisymmetric nature of the wavefunction induced by the algebra of these operators. (Parity)

An important statement regarding these operators is that they can be used to represent many-body operators!

Fermion → qubit mapping!

There are 3 widely used mapping between fermionic occupation number basis to qubit basis. The key requirement of such maps: Bijection!

Any such map need to preserve the following information:
1. Occupation numbers
2. Parity

With the above information, we also need to work out the equivalent operators of $\{a_j\}$ and $\{a_j^{+}\}$ in the qubit basis. Let us carry out this task with 3 different mappings:

1. Jordan-Wigner transformation 2. Parity transformation 3. Bravyi-Kitaev transformation

However, before going into the details of the transformation, it is convenient define certain sets of qubit! Namely,

1. **Update set, $U(i)$:** The set of qubit indices that needs to be updated when the occupation of i^{th} qubit changes excluding the qubit 'i' itself.

2. **Parity set, $P(i)$:** The set of qubits indices that store the same parity of fermions upto i^{th} orbital (excluding i^{th} orbital).

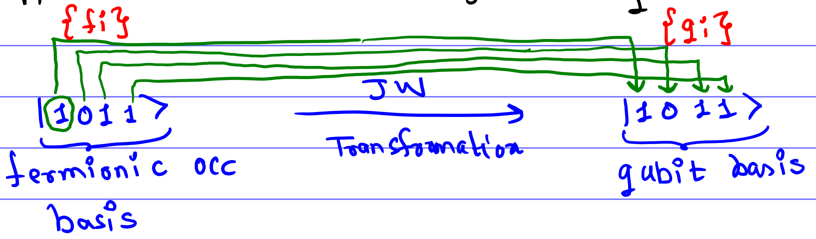
3. Flip set, $F(i)$: The qubit indices which tells us whether the qubit 'i' is same as f_i or $\bar{f_i}$.

We are all set now to begin our journey of studying various maps

1. Jordan - Wigner Transformation

Recall that the number of basis elements of ferm occ basis is 2^n, where 'n' is the number of single particle modes. Also, the Hilbert space of 'n' qubits is also 2^n. The JW mapping is very simple in the sense that each fermionic basis is mapped to the exact analogue in qubit basis. For example:

$n=4$

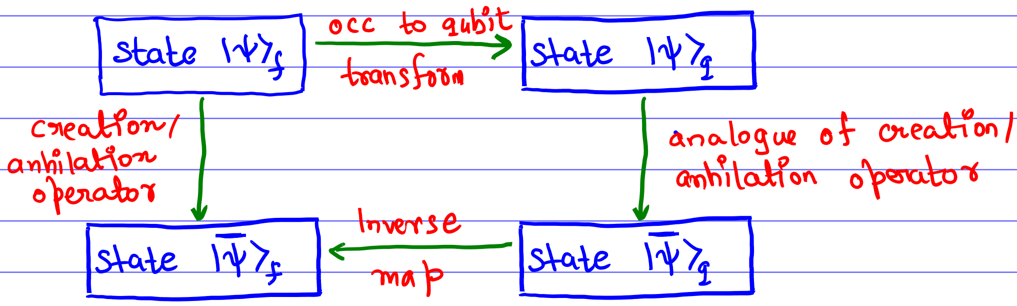


The qubit in the j^{th} position stores the occupation of the j^{th} orbital. However, the parity is still obtained by $(-1)^{S_j}$; $S_j = \sum_{i<j} q_i$. Thus, we say that in the JW transformation:

1. Occupation number information is stored locally.
2. Parity information is stored non-locally.

Creation/anhilation operators in qubit basis

Next we set out to find the analogue of C/A operators in qubit bases. In other words, what operators would act it in a same way as C/A operators for qubit basis? To understand this, let us look at the below diagram:



Thus, the analogue operators must satisfy the same algebra (CACs)! We can arrive at the results by requiring the same action in ③ & ④, which is

$$a_j^\dagger|\alpha\rangle_f = (-1)^{S_j}(1-f_j)|\alpha'\rangle_f \Rightarrow a_j^\dagger \rightarrow Q_j^\dagger \equiv \prod_{i<j}\sigma_i^z \otimes \sigma_j^+ \quad — \quad (5)$$

$$a_j|\alpha\rangle_f = (-1)^{S_j} f_j |\alpha'\rangle_f \Rightarrow a_j \rightarrow Q_j^- \equiv \prod_{i<j}\sigma_i^z \otimes \sigma_j^- \quad — \quad (6)$$

We can also check that they satisfy CACs! To understand ⑤ & ⑥, let us disect each term in $Q_j^\pm$.

$$Q_j^\pm = \underbrace{\prod_{i<j} \sigma_i^z}_{\text{Phase } (-1)^{s_j}} \otimes\, \sigma_j^\pm$$

captures the increase or decrease in occ basis.

$$\sigma_j^\pm = \frac{1}{2}(\sigma_x \mp i\sigma_y)$$

$$\sigma_j^+|0\rangle = |1\rangle \qquad \sigma_j^-|1\rangle = |0\rangle$$

$$|\alpha'\rangle_f = |f_0 f_1 \dots \boxed{f_j \pm 1} \dots f_{n-1}\rangle$$

Let us look at an example to make things clear: Suppose $|\alpha\rangle_f = |10110\rangle$

$$\rightarrow \quad a_4^+|\alpha\rangle_f = a_5^+ |\overset{0}{1}\overset{1}{0}\overset{2}{1}\overset{3}{1}\overset{4}{0}\rangle = \overset{1+0+1+1}{(-1)}\ |10111\rangle$$
$$= -1|10111\rangle_f$$

Note

Our convention: $|f_0 f_1 \dots f_{n-1}\rangle$ for occ basis

$$\rightarrow \quad Q_4^+|\alpha\rangle_b = Q_4^+ |\overset{0}{1}\overset{1}{0}\overset{2}{1}\overset{3}{1}\overset{4}{0}\rangle = \prod_{i=0}^{3} \sigma_i^z \otimes \sigma_4^+ |10110\rangle$$

$$= \sigma_0^z \sigma_1^z \sigma_2^z \sigma_3^z \sigma_4^+ |10110\rangle$$

$$= (-1)(+1)(-1)(-1)|10111\rangle = -1|10111\rangle_b$$

In JW transformation:

1. The update set, $U(i) = \phi \quad \forall i$
2. The parity set, $P(i) = \{j \mid j < i\}$
3. The flip set, $F(i) = \phi \quad \forall i$

Using these, we can rewrite the JW transformation as follows:

$$a_j^\pm \rightarrow Q_j^\pm = Z_{P(j)} \otimes \sigma_j^\pm \qquad — \quad ⑦$$

The parity set scales as $O(n)$ for JW.

2. Parity transformation

An alternate approach exists to reduce the scaling of parity set! Instead of storing occupation f_j in qubit q_j, we can store parity of orbitals upto j (including j) in qubit q_j, i.e.,

$$q_j \equiv \underbrace{p_j}_{\text{parity basis}} = \left[\sum_{i=0}^{j} f_j\right] \bmod 2 \qquad — \quad ⑧$$

Note

The sum is followed up with a mod 2.

Further, we can also look at the matrix $[\pi_n]$ which connects 'occ basis' to 'parity' basis.

Matrix transformation: $$p_j = \sum_i [\Pi_n]_{ji} f_i \qquad - \quad (9)$$

where Π_n is given by $(n=8)$

$$\Pi_8 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

Let us work out one example:

$$\underbrace{|10101110\rangle}_{\text{fermionic basis}} \xrightarrow{\text{Parity}} |\underline{1}\ \ \underline{1+0}\ \ \underline{1+0+1}\ \ \underline{1+0+1+0}\ \ \underline{1+0+1+0+1}\ \ \underline{1+0+1+0+1+1}\ \ \underline{1+0+1+0+1+1+1}\ \ \underline{1+0+1+0+1+1+1+0}\rangle$$

$$\rightarrow \underbrace{|11001011\rangle}_{\text{parity basis}}$$

We can also look the same from the matrix Π_8 by encoding $|10101110\rangle \longrightarrow (1,0,1,0,1,1,1,0)^T$

$$\begin{array}{ccccc} \Pi_8 & & \vec{f} & & \vec{b} \\ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} & & \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ 1 \\ 1 \\ 0 \end{bmatrix} & = & \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \\ 1 \end{bmatrix} \end{array}$$

Contrast to JW transformation:

1. The parity is now stored locally.
2. However, the occupation number is stored non-locally.

We further look at how the operators are given in parity basis. Since the occupation information is non local, we cannot directly use '$\sigma_j^{\pm}$' to reflect the actual change in occupation number.

We want to figure out $a_j^{\pm}$ in parity basis. Suppose, $p_{j-1} = |0\rangle$. This tells us that the parity of orbitals upto $j-1$ is 0. This implies that p_j exactly stores the corresponding ferm occ no f_j because $p_j = p_{j-1} \oplus f_j$. However, if $p_{j-1} = |1\rangle$, then $b_j = \bar{f}_j$, i.e, it stores the flipped occ number.

Note
$\oplus$ = addition mod 2

Thus we have, $$P_j^{\pm} \equiv |0\rangle\langle 0|_{j-1}\, \sigma_j^{\pm} - |1\rangle\langle 1|_{j-1}\, \sigma_j^{\mp} \quad -(10)$$

The reason for this negative sign is that parity of orbitals till $j-1$ is 1.

Unfortunately, the story isn't complete! Since we changed the qubit j, the qubits $i>j$ must also be changed as p_j appears in the parity sum.

$$p_i = (p_0 + \dots \underline{p_j} + \dots p_i) \bmod 2 \qquad (i>j)$$

Thus the chain of σ_i^x are required to update the qubits $i>j$. Hence, the operator $a_j^{\pm}$ is given by:

$$a_j^{\pm} \equiv P_j^{\pm} \otimes \prod_{i>j} \sigma_i^x \quad -(11)$$

For the Parity transformation, we have:

1. The parity set, $P(i) = \{i-1\}$ (local)
2. The update set, $U(i) = \{j \mid j>i\}$ (non-local)
3. The Flip set, $F(i) = \{i-1\}$

In this case, the update set scales as $O(n)$! Using these sets, we can write $a_j^{\pm}$ in Parity transformation as follows:

$$a_j^{\pm} \equiv \left(|0\rangle\langle 0|_{j-1}\, \sigma_j^{\pm} - |1\rangle\langle 1|_{j-1}\, \sigma_j^{\mp}\right) \otimes \prod_{i>j} \sigma_i^x$$

$$= \left(\Pi^0_{F(j)}\, \sigma_j^{\pm} + \Pi^1_{F(j)}\, \sigma_j^{\mp}\right) \otimes Z_{P(j)} \otimes X_{U(j)}$$

where $\Pi^k = |k\rangle\langle k|$, $Z_{P(j)} = \sigma_{j-1}^z$, $X_{U(j)} = \prod_{i>j} \sigma_i^x$

As we saw, in both approaches, one of the sets grows as $O(n)$: we require $O(n)$ Pauli matrices for a single application of $a_j^{\pm}$. Is there a way to do it more efficiently? The answer is yes!! – Bravyi Kitaev mapping!