Work Summary

Preliminary calculations based on second quantization of fermions in the tight-binding model.

Main Work

1. Second quantization of fermions
2. Example of 4 atom sites with 1 or 2 electrons

1 Second quantization of fermions

In order to treat the fermions properly taking into consideration the Pauli exclusion principle, second quantization is preferred. In second quantization of fermions, the creation and annihilation operators are $\hat{c}_i^\dagger$ and $\hat{c}_i$ respectively, where i denotes the label of atom/site. It is important to keep in mind the commutation relationships as Equation 1.

$$\begin{aligned} \left\{\hat{c}_i, \hat{c}_j\right\} &= 0 \\ \left\{\hat{c}_i^\dagger, \hat{c}_j^\dagger\right\} &= 0 \\ \left\{\hat{c}_i^\dagger, \hat{c}_j\right\} &= \delta_{i,j} \end{aligned} \tag{1}$$

In convention, the state should be labelled as $|\psi\rangle = \hat{c}_{i_1}^\dagger \cdots \hat{c}_{i_n}^\dagger \hat{c}_{j_1} \cdots \hat{c}_{j_n} |0\rangle$, where $i_1 > \cdots > i_n$ and $j_1 > \cdots > j_n$. The Hamiltonian for nearest neighbor and second nearest neighbor hopping are given as H_1 and H_2 in Equation 2.

$$\begin{aligned} \hat{H}_1 &= -J_1 \sum_j \left(\hat{c}_{j+1}^\dagger \hat{c}_j + h.c.\right) \\ \hat{H}_2 &= -J_2 \sum_j \left(\hat{c}_{j+2}^\dagger \hat{c}_j + h.c.\right) \end{aligned} \tag{2}$$

2 Example of 4 sites

The sites are labelled as 1, 2, 3, 4. Here, consider periodic boundary conditions, i.e. site 1 and site 4 are adjacent. Also only consider nearest neighbor hopping.

2.1 1 electron

Expressing in the basis of $\begin{pmatrix} \hat{c}_1^\dagger|0\rangle \\ \hat{c}_2^\dagger|0\rangle \\ \hat{c}_3^\dagger|0\rangle \\ \hat{c}_4^\dagger|0\rangle \end{pmatrix}$. The Hamiltonian elements are shown in Equation 3.

$$
\begin{aligned}
H_{ij} &= \langle 0|\hat{c}_i \hat{H}_1 \hat{c}_j^\dagger|0\rangle \\
&= -J_1 \langle 0|\hat{c}_i \sum_j \left(\hat{c}_{j+1}^\dagger \hat{c}_j + h.c.\right) \hat{c}_j^\dagger|0\rangle \\
&= -J_1 \langle 0|\hat{c}_i \left(\hat{c}_{j+1}^\dagger \hat{c}_j + \hat{c}_{j-1}^\dagger \hat{c}_j\right) \hat{c}_j^\dagger|0\rangle \\
&= -J_1 \left(\delta_{i,j+1} + \delta_{i,j-1}\right) \\
&= -J_1 \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}
\end{aligned}
$$

As derived before, the eigen-wavefunction is $|\psi\rangle = \hat{d}_\theta^\dagger|0\rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^N e^{in\theta} \hat{c}_n^\dagger|0\rangle$ for N atoms. Here, values of θ is restricted by the periodic boundary conditions such that $N\theta = 2p\pi$ where p is an integer. Similar to crystal momentum, in the first Brillouin zone, $\theta \in (-\pi, \pi]$. The eigen-energy is given in Equation 4.

$$
\begin{aligned}
E_\theta|\psi\rangle &= \hat{H}_1|\psi\rangle \\
&= \left(-J_1 \sum_j \left(\hat{c}_{j+1}^\dagger \hat{c}_j + h.c.\right)\right) \left(\frac{1}{\sqrt{N}} \sum_{n=1}^N e^{in\theta} \hat{c}_n^\dagger|0\rangle\right) \\
&= \frac{-J_1}{\sqrt{N}} \sum_{n=1}^N e^{in\theta} \left(\hat{c}_{n+1}^\dagger \hat{c}_n + \hat{c}_{n-1}^\dagger \hat{c}_n\right) \hat{c}_n^\dagger|0\rangle \\
&= \frac{-J_1}{\sqrt{N}} \left(\sum_{n=1}^N e^{in\theta} \hat{c}_{n+1}^\dagger + \sum_{n=1}^N e^{in\theta} \hat{c}_{n-1}^\dagger\right) |0\rangle \\
&= -J_1 \left(e^{i\theta} + e^{-i\theta}\right) |\psi\rangle \\
&= -2J_1 \cos\theta |\psi\rangle \\
\rightarrow E_\theta &= -2J_1 \cos\theta \qquad (3)
\end{aligned}
$$

A calculation of the eigenvalues of the matrix can verify this: the eigenvalues 0, $\pm 2J_1$ correspond to $\theta = -\pi/2, 0, \pi/2, \pi$.

2.2 2 electrons

When there are 2 electrons, the Pauli exclusion principle come into play. Therefore, it is restricted that there should not be two electrons resting on the same atom. The basis should be $|i,j\rangle = \hat{c}_i^\dagger \hat{c}_j^\dagger|0\rangle$, where i > j as convention.

$$
\begin{aligned}
\hat{H}_1|i,j\rangle &= \left(-J_1\sum_j\left(\hat{c}^\dagger_{j+1}\hat{c}_j+h.c.\right)\right)\hat{c}^\dagger_i\hat{c}^\dagger_j|0\rangle \\
&= -J_1\left(\hat{c}^\dagger_{i+1}\hat{c}_i+\hat{c}^\dagger_{i-1}\hat{c}_i+\hat{c}^\dagger_{j+1}\hat{c}_j+\hat{c}^\dagger_{j-1}\hat{c}_j\right)\hat{c}^\dagger_i\hat{c}^\dagger_j|0\rangle \\
&= -J_1\left(\Delta_{i+1,j}\hat{c}^\dagger_{i+1}\hat{c}^\dagger_j+\Delta_{i-1,j}\hat{c}^\dagger_{i-1}\hat{c}^\dagger_j+(-1)^2\,\Delta_{i,j+1}\hat{c}^\dagger_i\hat{c}^\dagger_{j+1}+(-1)^2\,\Delta_{i,j-1}\hat{c}^\dagger_i\hat{c}^\dagger_{j-1}\right)|0\rangle \quad (4)\\
&\text{here define } \Delta_{i,j}=1-\delta_{i,j},\ \text{where } \delta \text{ is the kronecker delta}
\end{aligned}
$$

As examples, see Equation 5.

$$
\begin{aligned}
\hat{H}_1|21\rangle &= -J_1\left(\hat{c}^\dagger_3\hat{c}^\dagger_1+\hat{c}^\dagger_2\hat{c}^\dagger_4\right)|0\rangle \\
&= -J_1\left(\hat{c}^\dagger_3\hat{c}^\dagger_1-\hat{c}^\dagger_4\hat{c}^\dagger_2\right)|0\rangle \\
&= -J_1\left(|31\rangle-|42\rangle\right) \\
\hat{H}_1|31\rangle &= -J_1\left(\hat{c}^\dagger_4\hat{c}^\dagger_1+\hat{c}^\dagger_2\hat{c}^\dagger_1+\hat{c}^\dagger_3\hat{c}^\dagger_2+\hat{c}^\dagger_3\hat{c}^\dagger_4\right)|0\rangle \\
&= -J_1\left(\hat{c}^\dagger_4\hat{c}^\dagger_1+\hat{c}^\dagger_2\hat{c}^\dagger_1+\hat{c}^\dagger_3\hat{c}^\dagger_2-\hat{c}^\dagger_4\hat{c}^\dagger_3\right)|0\rangle \\
&= -J_1\left(|41\rangle+|21\rangle+|32\rangle-|43\rangle\right) \quad (5)
\end{aligned}
$$

With the basis $\begin{pmatrix}|21\rangle\\|41\rangle\\|31\rangle\\|42\rangle\\|32\rangle\\|43\rangle\end{pmatrix}$, the Hamiltonian can be written as Equation 6.

$$
\hat{H}_{hop} = -J_1\begin{pmatrix}0&0&1&-1&0&0\\0&0&1&1&0&0\\1&1&0&0&1&-1\\-1&1&0&0&1&1\\0&0&1&1&0&0\\0&0&-1&1&0&0\end{pmatrix} \quad (6)
$$

The eigen-energy can be calculated as given in Equation 7.

$$
\begin{aligned}
E_\theta \left(\hat{d}^\dagger_{\theta_2} \hat{d}^\dagger_{\theta_1} |0\rangle \right) &= \hat{H}_1 \left(\hat{d}^\dagger_{\theta_2} \hat{d}^\dagger_{\theta_1} |0\rangle \right) \\
&= \left(-J_1 \sum_j \left(\hat{c}^\dagger_{j+1} \hat{c}_j + h.c. \right) \right) \left(\frac{1}{N} \sum_{n,m=1}^{N} e^{i(n\theta_1 + m\theta_2)} \hat{c}^\dagger_m \hat{c}^\dagger_n |0\rangle \right) \\
&= \frac{-J_1}{N} \sum_{n,m=1}^{N} e^{i(n\theta_1 + m\theta_2)} \left(\hat{c}^\dagger_{n+1} \hat{c}_n + \hat{c}^\dagger_{n-1} \hat{c}_n + \hat{c}^\dagger_{m+1} \hat{c}_m + \hat{c}^\dagger_{m-1} \hat{c}_m \right) \hat{c}^\dagger_m \hat{c}^\dagger_n |0\rangle \\
&= \frac{-J_1}{N} \sum_{n,m=1}^{N} e^{i(n\theta_1 + m\theta_2)} \left(\hat{c}^\dagger_m \hat{c}_{n+1} + \hat{c}^\dagger_m \hat{c}_{n-1} + \hat{c}^\dagger_{m+1} \hat{c}_n + \hat{c}^\dagger_{m-1} \hat{c}_n \right) |0\rangle \\
&= -J_1 \left(e^{i\theta_1} + e^{-i\theta_1} + e^{i\theta_2} + e^{-i\theta_2} \right) \left(\hat{d}^\dagger_{\theta_2} \hat{d}^\dagger_{\theta_1} |0\rangle \right) \\
&= -2J_1 \left(\cos\theta_1 + \cos\theta_2 \right) \left(\hat{d}^\dagger_{\theta_2} \hat{d}^\dagger_{\theta_1} |0\rangle \right) \\
\rightarrow E_\theta &= -2J_1 \left(\cos\theta_1 + \cos\theta_2 \right)
\end{aligned}
\tag{7}
$$

To verify, calculate the eigenvalues of the matrix form, which gives 0 and ± 2. This is valid because the two fermions can't occupy the same momentum state in the phase space, i.e. $\theta_1 \neq \theta_2$.