Summer Project on Condensed Matter Physics - IISc, Bangalore 2023

Lecture 1: Introduction

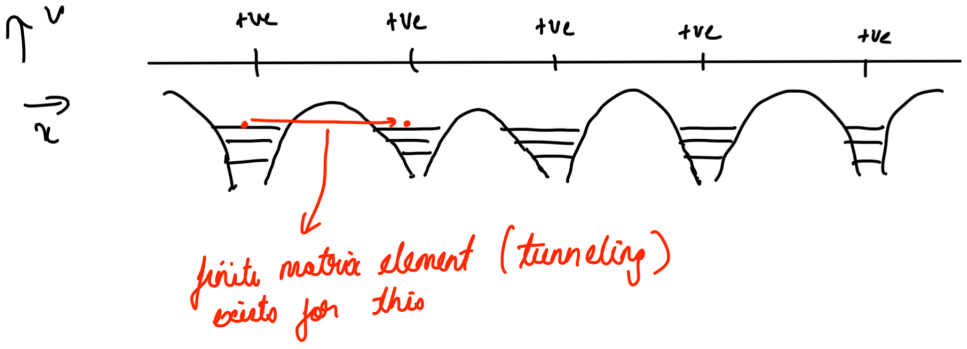
1st May, 2023

Lecturer: Prof. Diptiman Sen *Scribe: Phanindra Dewan*

This lecture gave a brief introduction to tight-binding model and the fermionic anticommutation relations

1 Tight-Binding Model

So the tight-binding model is a sort of bottom-up approach to getting the band structure of materials. Let us consider a one-dimensional lattice with lattice spacing a, such that each position is labelled by $x_n = na$. It is good to remind ourselves that in such a case, there can be two types of boundary conditions: a) Periodic and b) Open.
So in the case that there are atoms at each of these sites, we will get a situation as given below:



Due to quantum mechanical tunneling, the matrix element of a transition from one site to the next is non-zero. We will call this event "hopping", from one site to the next.
There is another way to look at it. We will consider only two sites; let's call those sites n and $n+1$. In absence of hopping, we would expect the Hamiltonian to be:

$$H = \begin{pmatrix} E_0 & 0 \\ 0 & E_0 \end{pmatrix} \tag{1}$$

And the eigenstates will be: (notice degeneracy)

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} : E_0, n \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} : E_0, n+1 \tag{2}$$

With tunneling/hopping, the effective Hamiltonian becomes ($\gamma > 0$ is the hopping amplitude for electron to jump from n $\leftrightarrow$ n+1):

$$H_{eff} = \begin{pmatrix} E_0 & -\gamma \\ -\gamma & E_0 \end{pmatrix} \tag{3}$$

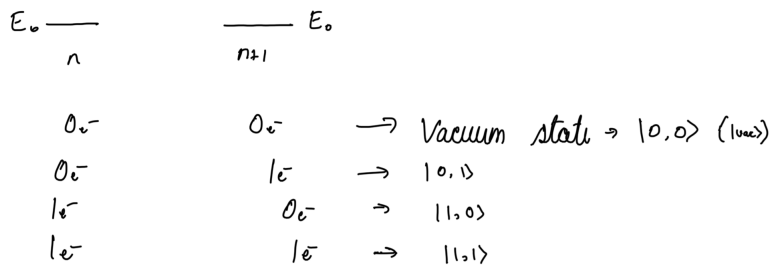
And the eigenstates will be (upto normalization factors, and notice that degeneracy is broken):

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix} : E_0 - \gamma \quad \begin{pmatrix} 1 \\ -1 \end{pmatrix} : E_0 + \gamma \tag{4}$$

These eigenstates can be considered to be a linear combination of the eigenstates localized at the n and $n+1$ sites we found before. The one with the lower energy is the $\psi_n + \psi_{n+1}$ symmetric state, and the one with the higher energy is the $\psi_n - \psi_{n+1}$ antisymmetric state.

2 Onto Second Quantization

So the possible states of the n and $n+1$ sites are:



Now seems to be a good time to introduce some operators to move between these possible states!

Creation Operator: $c_n^\dagger$, creates an electron at site n. Example:

$$\begin{aligned} c_n^\dagger |0,0\rangle &= |1,0\rangle \\ c_n^\dagger |0,1\rangle &= |1,1\rangle \\ c_n^\dagger |1,1\rangle &= 0 \\ c_{n+1}^\dagger |0,0\rangle &= |0,1\rangle \\ c_{n+1}^\dagger |1,1\rangle &= 0 \end{aligned} \tag{5}$$

Now look at this

$$c_{n+1}^\dagger |1,0\rangle = |1,1\rangle$$

Is it true?

To understand this question, let us remind ourselves of the action of creation operators in the case of photons, when quantization of EM field is done.

$$\begin{aligned} a^\dagger_{\vec{k_1}} \left|vac\right\rangle &= \left|\vec{k_1}\right\rangle \\ a^\dagger_{\vec{k_2}} \left|\vec{k_1}\right\rangle &= \left|\vec{k_1}, \vec{k_2}\right\rangle, (k_1 \neq k_2) \end{aligned} \tag{6}$$

The curious thing about the above equations is that we could've done it in any other way i.e., we could've created a photon with k_2 before k_1, and it wouldn't have changed the final state. Now the question is whether this is true for electrons as well. The short answer to that question is that it is not so. For electrons the ordering of the creation and annihilation operators does matter. And the answer to why it must be so is that electrons are fermions and photons are bosons. The standard way of ordering the creation and annihilation operators is to create from left to right. So in that ordering, we get:

$$c^\dagger_n c^\dagger_{n+1} \left|0,0\right\rangle = \left|1,1\right\rangle \implies c^\dagger_{n+1} c^\dagger_n \left|0,0\right\rangle = -c^\dagger_n c^\dagger_{n+1} \left|0,0\right\rangle = -\left|1,1\right\rangle$$

But wait! How did we get to the last step? We have implicitly invoked the anticommutation relations satisfied by the creation operators of electrons. Quite generally, the fermionic creation operators satisfy the following anticommutation relation:

$$\{c^\dagger_n, c^\dagger_{n+1}\} = c^\dagger_n c^\dagger_{n+1} + c^\dagger_{n+1} c^\dagger_n = 0$$

For two different sites n and m,

$$\begin{aligned} c^\dagger_m c^\dagger_n &= -c^\dagger_n c^\dagger_m \\ \{c^\dagger_m, c^\dagger_n\} &= 0 \end{aligned} \tag{7}$$

Annhilation Operator: c_n, annihilates an electron at site n. Example:

$$\begin{aligned} c_n \left|0,0\right\rangle &= 0 \\ c_n \left|1,0\right\rangle &= \left|0,0\right\rangle \end{aligned} \tag{8}$$

What sort of relations do these two operators satisfy?
For a single site n,

$$\begin{aligned} c_n c^\dagger_n + c^\dagger_n c_n &= ? \\ (c_n c^\dagger_n + c^\dagger_n c_n) \left|0,0\right\rangle &= \left|0,0\right\rangle \\ (c_n c^\dagger_n + c^\dagger_n c_n) \left|1,0\right\rangle &= \left|1,0\right\rangle \\ \implies \{c_n, c^\dagger_n\} &= 1 \end{aligned} \tag{9}$$

What about at different sites? ($n < m$) Consider these states:

$$\begin{aligned} \left|0,0\right\rangle &= \left|vac\right\rangle \\ \left|0,1\right\rangle &= c^\dagger_m \left|vac\right\rangle \\ \left|1,0\right\rangle &= c^\dagger_n \left|vac\right\rangle \\ \left|1,1\right\rangle &= c^\dagger_n c^\dagger_m \left|vac\right\rangle \end{aligned} \tag{10}$$

Then we get:

$$\begin{aligned}
(c_n c_m^\dagger + c_m^\dagger c_n)\,|vac\rangle &= 0 \\
(c_n c_m^\dagger + c_m^\dagger c_n)\,|1,0\rangle &= c_n c_m^\dagger\,|1,0\rangle + c_m^\dagger c_n\,|1,0\rangle \\
&= c_n c_m^\dagger c_n^\dagger\,|vac\rangle + c_m^\dagger c_n c_n^\dagger\,|vac\rangle \\
&= -c_n c_n^\dagger\,|0,1\rangle + |0,1\rangle \\
&= -\,|0,1\rangle + |0,1\rangle \\
&= 0
\end{aligned}$$

Thus, working the same for other states,

$$\{c_n, c_m^\dagger\} = \delta_{nm} \tag{11}$$

3 Back to Tight-Binding

We will claim that the tight-binding hamiltonian introduced in section 1 can be written as:

$$H_{eff} = \begin{pmatrix} E_0 & -\gamma \\ -\gamma & E_0 \end{pmatrix} = E_0(c_n^\dagger c_n + c_{n+1}^\dagger c_{n+1}) - \gamma(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_{n+1}) \tag{12}$$

Now let us act this Hamiltonian on the known states:

$$\begin{aligned}
H\,|0,0\rangle &= 0 \\
H\,|1,0\rangle &= E_0(|1,0\rangle + 0) - \gamma(0 + |0,1\rangle) \\
&= E_0\,|1,0\rangle - \gamma\,|0,1\rangle \\
H\,|0,1\rangle &= E_0\,|0,1\rangle - \gamma\,|1,0\rangle \\
H\,|1,1\rangle &= E_0(|1,1\rangle + |1,1\rangle) - \gamma(0+0) \\
&= 2E_0\,|1,1\rangle
\end{aligned}$$

So, we know,

$$\begin{aligned}
H(|1,0\rangle + |0,1\rangle) &= (E_0 - \gamma)(|1,0\rangle + |0,1\rangle) \\
H(|1,0\rangle - |0,1\rangle) &= (E_0 + \gamma)(|1,0\rangle - |0,1\rangle)
\end{aligned} \tag{13}$$