Summer Project on Condensed Matter Physics - IISc, Bangalore 2023

Lecture 3: SSH Model

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This lecture started off with a discussion about the multi-electron systems (tight-binding) and then moved on to the Su-Schrieffer-Heeger model.

1 Multi-Electron Systems

In Lecture 2, we solved the tight-binding Hamiltonian given by:

$$H = \sum_{n=1}^{\infty} E_0 c_n^\dagger c_n - \sum_{n=1}^{\infty} \gamma (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_{n+1}) \tag{1}$$

Now, using the new creation and annihilation operators we defined last lecture, the Hamiltonian becomes:

$$H = \sum_p c_p^\dagger c_p \tag{2}$$

This Hamiltonian is of the very familiar harmonic oscillator form. Actually, what we did by changing the operators by taking a Fourier transform is called diagonalization of the Hamiltonian; and this particular scheme worked because of the translational invariance of the Hamiltonian.
$\rightarrow$What is the ground state of the system? (A difficult question, for now.)

First off, let us consider a single mode defined by the operators: c_1 and $c_1^\dagger$. Then we can have two states:

$$|vac\rangle$$
$$c_1^\dagger |vac\rangle = |1\rangle$$

Also,

$$c_1^\dagger c_1 |vac\rangle = 0$$
$$c_1^\dagger c_1 |1\rangle = |1\rangle$$

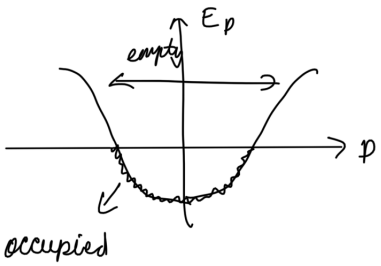
Correspondingly, for two modes given by: c_1, $c_1^\dagger$, c_2, $c_2^\dagger$, we get 4 states and it can be easily worked out.
$\therefore$ *For N fermion modes, number of states* = 2^N

Going back to the case of single mode, the Hamiltonian becomes: $H = E_1 c_1^\dagger c_1$. And its action on the two states is given below:

$$H\,|vac\rangle = 0 \tag{3}$$
$$H\,|1\rangle = E_1\,|1\rangle \tag{4}$$

$\rightarrow$What is the ground state of the system?
It depends on the sign of E_1.

In general, remembering the plot of E_p vs. p from Lecture 2, we can say that the ground state of the system is the one in which all the negative energy states are occupied and the rest are unoccupied.



$\rightarrow$How can we control the filling of states?
Experimentally: Use a battery or some voltage source!
Theoretically: Change the parameter E_0 in the Hamiltonian, which is actually the Fermi energy.

The fact that E_0 is the Fermi energy can be more clearly seen in the following way. Look at the Hamiltonian:

$$H = \sum_{n=1}^{\infty} E_0 c_n^\dagger c_n - \sum_{n=1}^{\infty} \gamma(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_{n+1}) \tag{5}$$

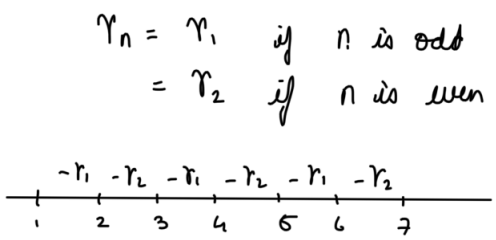
Now we know $\sum_n c_n^\dagger c_n = N$, is the number operator. So, the grnd partition function for such a system will be written as:

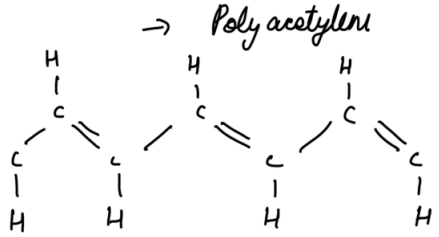
$$\mathcal{Q} = \sum e^{-\beta \mathcal{H}} = \sum_s e^{\beta(E_s - \mu N_s)} \tag{6}$$

From the above comparison, it clear that E_0 is the Fermi energy.

2 Su-Schrieffer-Heeger (SSH) Model

Till now the tight-binding Hamiltonian was being studied. Now let us think of a system which has different values of the hopping amplitude at different sites. It is important to note that such a thought is not purely theoretical and there *are* systems such as polyacetylene which has two values of the hopping amplitude which alternates between sites.





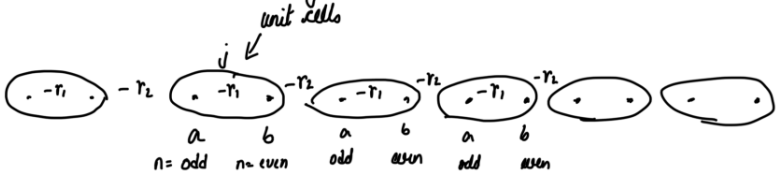
Double bonds are shorter → more overlap ⇒ hopping amplitude is larger

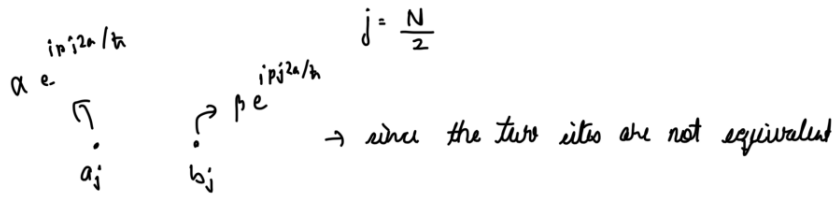
The Hamiltonian for such a system[1] will be:

$$H = -\mu \sum_{n=1}^{\infty} c_n^\dagger c_n - \sum_{n=1}^{\infty} \gamma_n (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_{n+1}) \tag{7}$$

→How to find energy levels?
It is important to understand that since we have broken translational symmetry under a translation by 1 site, we must think of a way to get it back. We will consider unit cells of two lattice points such that translational symmetry is present under translation by 2 lattice sites.

Not invariant under translation by 1 site. But is possible with translation by 2 sites.





Previously, we solved: $H|n\rangle = -\gamma(|n+1\rangle + |n-1\rangle) - \mu|n\rangle$

Next, we define states:
$|a_j\rangle \rightarrow$ 1 electron state with electron at site a of jth unit cell
$|b_j\rangle \rightarrow$ 1 electron state with electron at site b of jth unit cell
Acting with H,

$$H|a_j\rangle = -\mu|a_j\rangle - \gamma_1|b_j\rangle - \gamma_2|b_{j-1}\rangle$$

[1]Any such 1-D system will dimerise due to Peierls instability. Dimerisation means the shortening of one bond and lengthening of another due to unequal hopping amplitude (strength of bond). Check 'Surprises in Theoretical Physics'.

$$H|b_j\rangle = -\mu|b_j\rangle - \gamma_1|a_j\rangle - \gamma_2|a_{j+1}\rangle$$

Note that we have 2 equations as we have two states in the unit cell.

Next, just like in tight-binding, we can try the eigenstate given below:

$$|p\rangle = \sum_{j=1}^{N/2}\left[e^{\frac{ipj2a}{\hbar}}\alpha|a_j\rangle + e^{\frac{ipj2a}{\hbar}}\beta|b_j\rangle\right]$$

Here, $e^{\frac{ip2aN}{2\hbar}} = 1 \implies \frac{paN}{\hbar} = 2\pi \implies p = \frac{2\pi\hbar}{Na}$ times an integer
The range of p: $\frac{-\pi\hbar}{2a}$ to $\frac{\pi\hbar}{2a}$ (no. of p values = N/2)

So,

$$\begin{aligned}
H|p\rangle &= -\mu|p\rangle + \sum_{j=1}^{N/2} e^{\frac{ipj2a}{\hbar}}\left[-\gamma_1|b_j\rangle - \gamma_2|b_{j-1}\rangle - \gamma_1|a_j\rangle - \gamma_2|a_{j+1}\rangle\right] \\
&= -\mu|p\rangle + \sum_{j=1}^{N/2} e^{\frac{ipj2a}{\hbar}}\left[-\gamma_1|b_j\rangle - \gamma_2 e^{\frac{ip2a}{\hbar}}|b_j\rangle - \gamma_1|a_j\rangle - \gamma_2 e^{\frac{-ip2a}{\hbar}}|a_j\rangle\right] \\
&= -\mu|p\rangle + \sum_{j=1}^{N/2} e^{\frac{ipj2a}{\hbar}}\left[-\gamma_1|a_j\rangle - \gamma_1|b_j\rangle - \gamma_2 e^{\frac{-ip2a}{\hbar}}|a_j\rangle - \gamma_2 e^{\frac{ip2a}{\hbar}}|b_j\rangle\right]
\end{aligned}$$

Also,

$$H|p\rangle = E_p|p\rangle = E_p\sum_j\left[e^{\frac{ipj2a}{\hbar}}\alpha|a_j\rangle + e^{\frac{ipj2a}{\hbar}}\beta|b_j\rangle\right]$$

Comparing, we get:

$$E_p\alpha e^{\frac{ipj2a}{\hbar}} = -\mu e^{\frac{ipj2a}{\hbar}} - \gamma_1\beta e^{\frac{ipj2a}{\hbar}} - \gamma_2\beta e^{\frac{ip(j-1)2a}{\hbar}} \tag{8}$$

$$E_p\beta e^{\frac{ipj2a}{\hbar}} = -\mu e^{\frac{ipj2a}{\hbar}} - \gamma_1\alpha e^{\frac{ipj2a}{\hbar}} - \gamma_2\alpha e^{\frac{ip(j+1)2a}{\hbar}} \tag{9}$$

$$\begin{aligned}
\implies -\mu\alpha - \gamma_1\beta - \gamma_2\beta e^{\frac{-ip2a}{\hbar}} &= E_p\alpha \\
\mu\beta - \gamma_1\alpha - \gamma_2\alpha e^{\frac{ip2a}{\hbar}} &= E_p\beta
\end{aligned}$$

$$\implies \begin{pmatrix} -\mu & -\gamma_1 - \gamma_2 e^{\frac{-ip2a}{\hbar}} \\ -\gamma_1 - \gamma_2 e^{\frac{ip2a}{\hbar}} & -\mu \end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = E_p\begin{pmatrix}\alpha\\ \beta\end{pmatrix} \tag{10}$$

Solving this eigenvalue equation will give us the energy, $E_p(p)$[2]

[2]However, it is important to note that these are energies of "bulk states". This particular system also allows "edge" or "end" states. These will come later.