Lecture 18: Bandstructure 3
Ref. Chapter 5.1 & 5.2
• Last time we talked about the principle of bandstructure which allows one to calculate the energy levels of a periodic structure. In particular we talked about a dimerized solid which has two atoms per unit cell.

\[ \{\varphi_n\} = \{\varphi_0\} e^{i k n a} \Rightarrow E\{\varphi_0\} = [h(k)]\{\varphi_0\} \]

\[
\begin{bmatrix}
\phi_1 \\
\phi_2 \\
\vdots \\
\phi_N \\
\end{bmatrix}
= 
\begin{bmatrix}
E \\
\vdots \\
E \\
\end{bmatrix}
\]

Every row looks the same

• Today we want to expand this idea to a higher dimension: 2D.
• In particular we’ll use the principle of bandstructure to describe the energy levels of graphene…

• The dispersion relation looks like:
• The importance of this material comes in play when they roll this up to become a carbon nanotube which is of great interest nowadays. Today we’ll talk about the energy levels of a Graphene sheet.

• Remember that the starting point is the Schrödinger equation which can be turned into a matrix equation once a proper set of basis functions are has been chosen.

• How many basis functions do we need per atom? The basis functions are the atomic orbitals. There are 4 orbitals for the valence electrons of a carbon atom.

\[
\begin{array}{c}
\text{C6:} \\
2s \\
2p \\
1s
\end{array}
\]

As it turns out we can talk only one of these four orbitals for our basis set. This makes the problem easier and tractable analytically.

• The reason that we can ignore the other 3 is that the “Pz” orbital does not mix with the other ones (the structure is planar). So the problem can be separated into two parts: the one for Pz orbital; and the one for S, Px, Py. At the end of the day it turns out that only the Pz orbitals play a major role in determining the electronic and optical properties.
To construct a basis set, the next question is: how many atoms are there per unit cell? In other words, what is the minimal number of atoms that can be put together to construct a cell from which, the whole lattice can be constructed?

The answer is: we need two atoms
Schrödinger equation reads:

$$E\{\phi_n\} = \sum_m [H_{nm}]\{\phi_m\} \quad (1)$$

Equation 1 can be solved by:

$$\{\phi_n\} = \{\phi_0\} e^{i\vec{k} \cdot \vec{d}_n} \quad (2)$$

Where vector $d_n$ is:

- Putting (2) in (1):

$$E\{\phi_0\} e^{i\vec{k} \cdot \vec{d}_n} = \sum_m [H_{nm}]\{\phi_0\} e^{i\vec{k} \cdot \vec{d}_m} \Rightarrow$$

$$E\{\phi_0\} = \sum_m [H_{nm}] e^{i\vec{k} \cdot (\vec{d}_m - \vec{d}_n)} \{\phi_0\}$$
Graphene: \( h(k) \)

- Let’s rewrite \( h(k) \):

\[
[h(\vec{k})] = \sum_m \left[H_{nm}\right] e^{i\vec{k} \cdot (\vec{a}_m - \vec{a}_n)} \tag{1}
\]

- To evaluate \( h(k) \), we choose any unit cell \( n \) and then perform the summation over its nearest neighbors including \( n \) itself:

\[
m=1 & m,1 & m,2 \\
n,1 & 0 & 0 \\
n,2 & t & 0 \\
\]

- To write the phase factor notice that \( d_m-d_n \) for \( m=2 \) is Actually \( a_1 \).

Continuing like this, we can write all of the 4 terms that run through neighbors 1 to 4:

\[
\begin{bmatrix}
0 & 0 \\
t & 0 \\
0 & t \\
0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
e^{i\vec{k} \cdot \vec{a}_1} \\
e^{i\vec{k} \cdot (-\vec{a}_2)} \\
e^{i\vec{k} \cdot (-\vec{a}_1)} \\
e^{i\vec{k} \cdot \vec{a}_2} \\
\end{bmatrix}
\]

Phase factor is 1
• All together we have the following 2by2 matrix for Graphene:

\[
\begin{bmatrix}
\varepsilon & \Delta \\
\Delta^* & \varepsilon
\end{bmatrix}
\]

\[\Delta \equiv t \left(e^{-i\vec{k} \cdot \vec{a}_1} + e^{-i\vec{k} \cdot \vec{a}_2} + 1\right)\]

eigenvalues : \[E = \varepsilon \pm \Delta\]