

Fundamentals of Nanoelectronics

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Lecture 21 : Graphene Bandstructure

Ref. Chapter 6.1



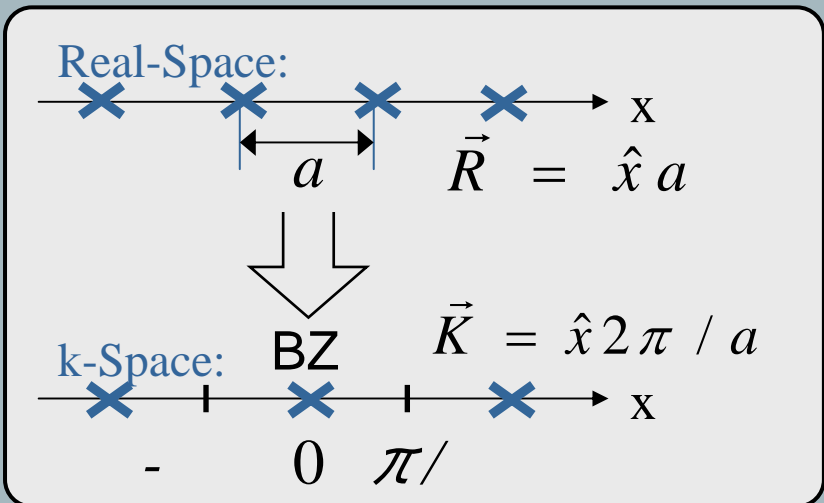
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Review of Reciprocal Lattice

00:05

- In the last class we learned how to construct the reciprocal lattice.
- For 1D we have:



- In general for periodic structures we can write 3 basis vectors such that any point in the lattice can be written as a linear combination of them with the condition that the coefficients must be integers.

$$\vec{R} = m \vec{a}_1 + n \vec{a}_2 + p \vec{a}_3$$

- Similarly any point in the reciprocal lattice can be written as:

$$\vec{K} = M \vec{A}_1 + N \vec{A}_2 + P \vec{A}_3$$

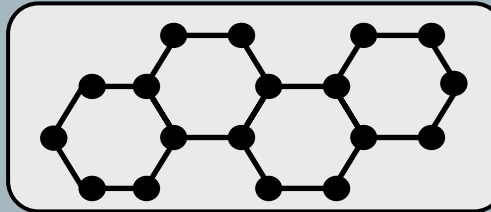
- How are the vectors “A” related to vectors “a”? The defining condition is:

$$\vec{A}_j \cdot \vec{a}_i = 2\pi \delta_{ij} \begin{cases} \delta_{ij} = 0 \text{ for } i \neq j \\ \delta_{ij} = 1 \text{ for } i = j \end{cases}$$

- The significance of reciprocal lattice vectors “A” is that points in k space which are apart from each other by an integer multiple of “Ai’s”, give is the same wavefunction solution.

Graphene

06:50



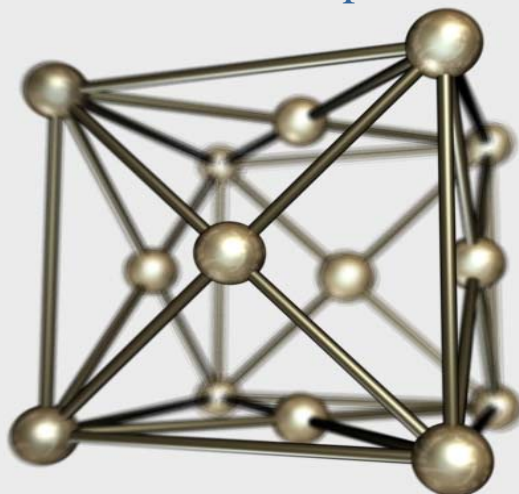
Graphene is made up of carbon atoms bonded in a hexagonal 2D plane.

Graphite is 3D structure that is made up of weakly coupled Graphene sheets.

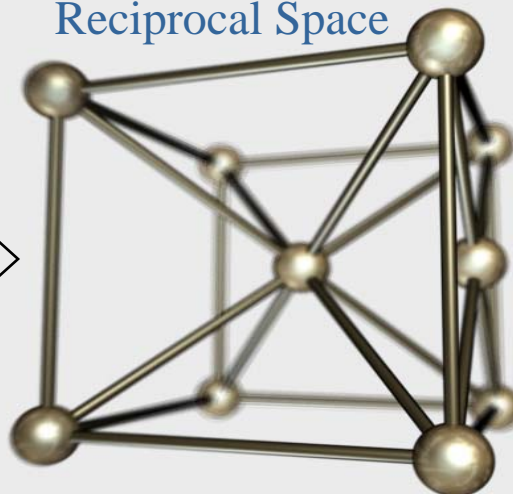
This is of particular importance because carbon nanotubes are made up of a Graphene sheet that is rolled up like cylinder. Carbon nanotubes themselves are of interest because people believe they can make all kinds of Nano devices with them.

- Semiconductors of interest to us have what is called a diamond structure. The diamond structure is composed of two interpenetrating FCC lattices the following way: Imagine two FCC lattices such that each atom of each lattice is on top of the corresponding atom of the other lattice. You should only be seeing 1 FCC lattice as of now. Then fix one lattice and move the other one in the direction of the body diagonal of the fixed one by $\frac{1}{4}$ of the body diagonal. Now you've yourself a diamond lattice. If the two FCC lattices are made up of two different types of atoms, the structure is then called a Zincblend lattice.
- To visualize the reciprocal lattice **focus only on one FCC lattice** in the diamond structure.

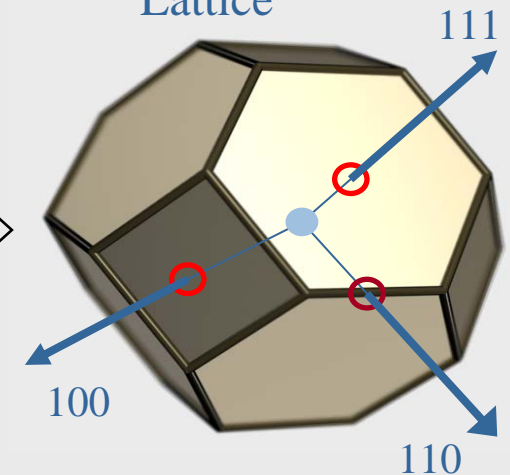
FCC in Real Space



BCC in Reciprocal Space



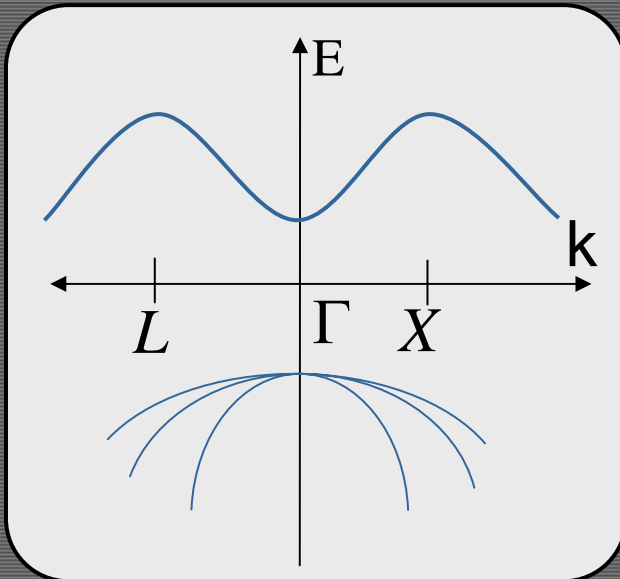
Brillouin Zone in Reciprocal Lattice



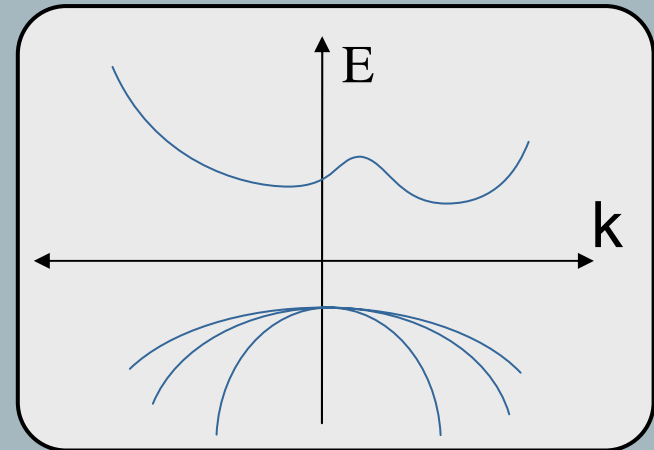
E-k Diagrams for 3D Reciprocal Lattices

11:16

- Since the reciprocal space is now 3 dimensional, to draw the E-k diagram we have choose particular directions and draw E-k diagram along those directions:



- Some useful information:
- The top of the valence band usually occurs at the Gamma point ($k=0$). The bottom of conduction band however does not always lie at $k=0$. For example consider Silicon:



- If both conduction band minimum and the valence band maximum lie at the same value of k , the material is called a direction bandgap semiconductor. Other wise the material is indirect like Si.

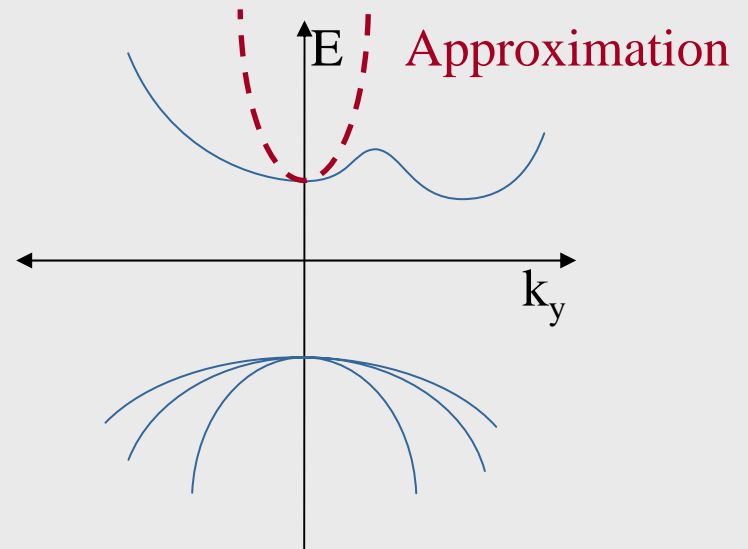
- Usually, it is necessary to derive an expression for $E(k_x, k_y, k_z)$ about the conduction points of a bulk solid
- For silicon, use the parabolic approximation

$$E = E_c + \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2 (k_x^2 + k_y^2 + k_z^2)}{2m^*}$$

where m^* is the effective mass.

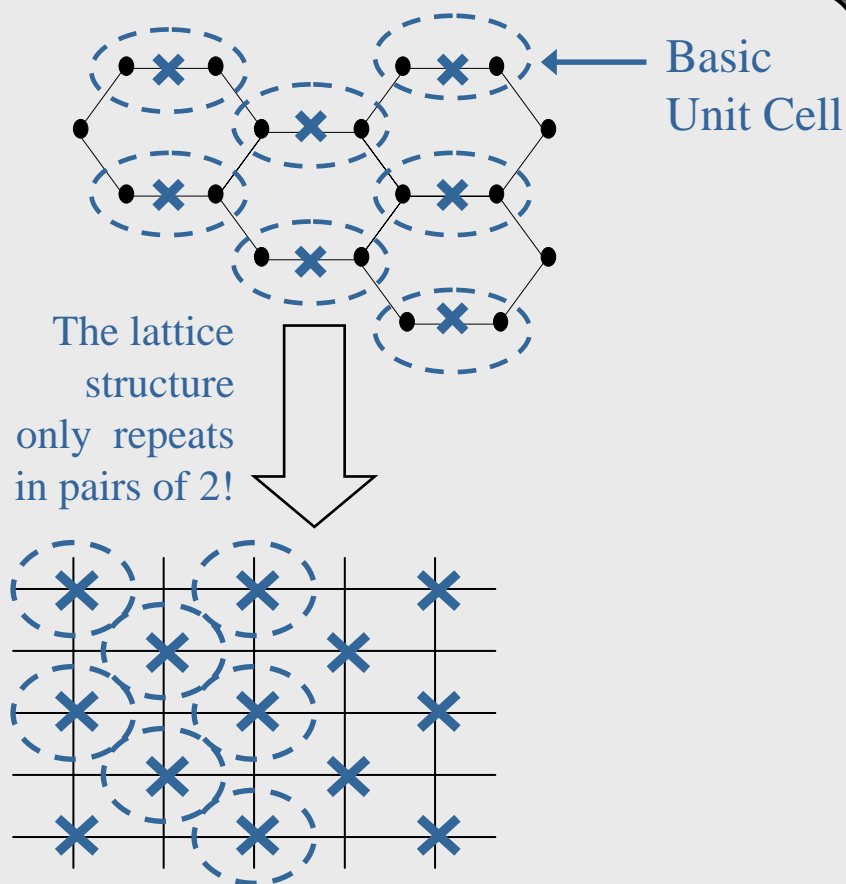
- For nanotubes we can derive a similar parabolic expression via a Taylor series expansion that approximates the subbands near the conduction valleys

Silicon Parabolic Conduction Band Approximation



E-k Relation for Graphene

- Let's get back to Graphene. First identify the basic unit cell

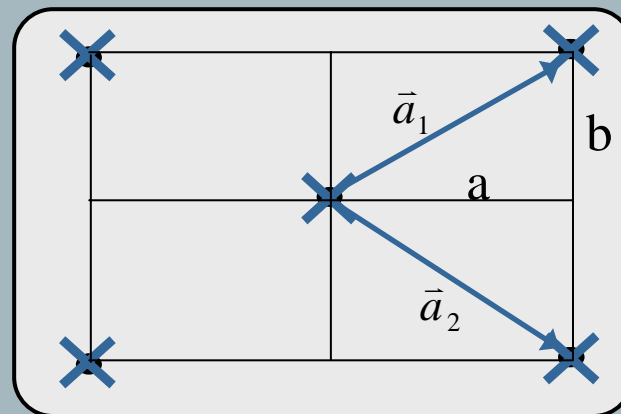


- Remember the general result of principle of bandstructure:

$$E\{\phi_0\} = [h(\vec{k})]\{\phi_0\}$$

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

- To write $h(k)$ consider one unit cell and its nearest neighbors. Figure shows that there will be 5 terms in the summation for $h(k)$.



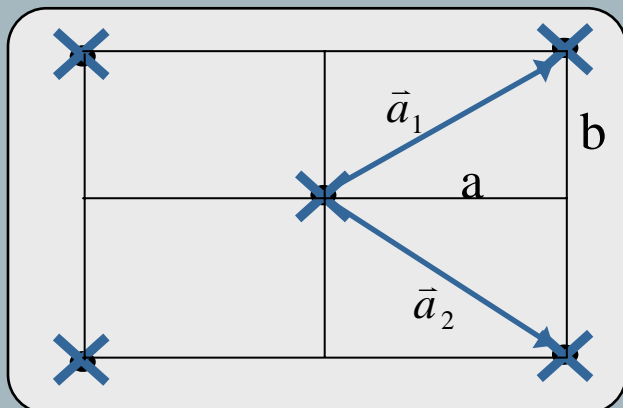
Graphene E-k Diagram

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- Writing the summation terms and adding them up we get:

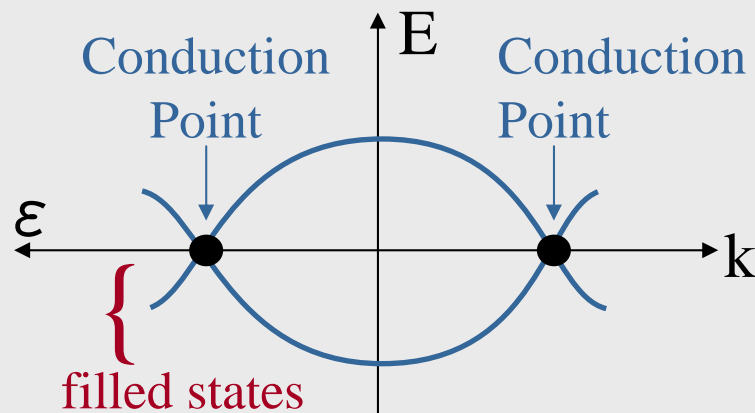
$$h(\vec{k}) = \begin{bmatrix} \varepsilon & h_0^* \\ h_0 & \varepsilon \end{bmatrix}$$

- Where

$$h_0 = t \left(1 + e^{i\vec{k}\cdot\vec{a}_1} + e^{i\vec{k}\cdot\vec{a}_2} \right)$$

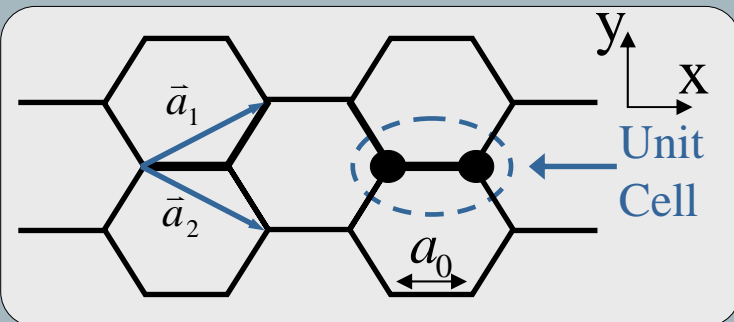
- The eigenvalues of this matrix are given by:

$$E(\vec{k}) = \varepsilon \pm |h_0(\vec{k})|$$



Magnitude of $h(\mathbf{k})$

- Next we like to locate the conduction points in the 2 dimensional \mathbf{k} space:



$$\vec{a}_1 = a\hat{x} + b\hat{y} = \frac{3}{2}a_0\hat{x} + \frac{\sqrt{3}}{2}a_0\hat{y}$$

$$\vec{a}_2 = a\hat{x} - b\hat{y} = \frac{3}{2}a_0\hat{x} - \frac{\sqrt{3}}{2}a_0\hat{y}$$

$$\vec{k} = k_x\hat{x} + k_y\hat{y}$$

$$h_0 = t\left(1 + e^{i\vec{k}\cdot\vec{a}_1} + e^{i\vec{k}\cdot\vec{a}_2}\right) = t\left(1 + e^{i(k_x a + k_y b)} + e^{i(k_x a - k_y b)}\right) = t\left(1 + 2e^{ik_x a} \cos k_y b\right)$$

- To find the conduction points we need to set $|h(\mathbf{k})|=0$. So we need to find $|h(\mathbf{k})|$:

$$\therefore |h_0|^2 = h_0 h_0^* = t^2 \left(1 + 4 \cos k_x a \cos k_y b + 4 \cos^2 k_y b\right)$$

so,

$$|h_0(\vec{k})| = t \sqrt{1 + 4 \cos k_x a \cos k_y b + 4 \cos^2 k_y b}$$

Conduction Valleys

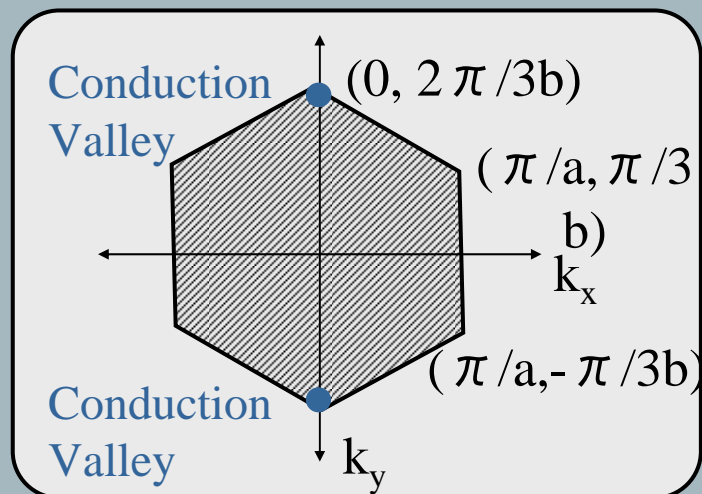
- Now let $|h_0(\vec{k})| = t\sqrt{1 + 4\cos k_x a \cos k_y b + 4\cos^2 k_y b} = 0$

- Let $k_x a = 0$ and investigate $h(k)$ as a function of k_y .

$$h_0 = t(1 + 2\cos k_y b) \text{ for } k_x = 0 \Rightarrow k_y b = \frac{2\pi}{3} \text{ to get } h_0(k) = 0$$

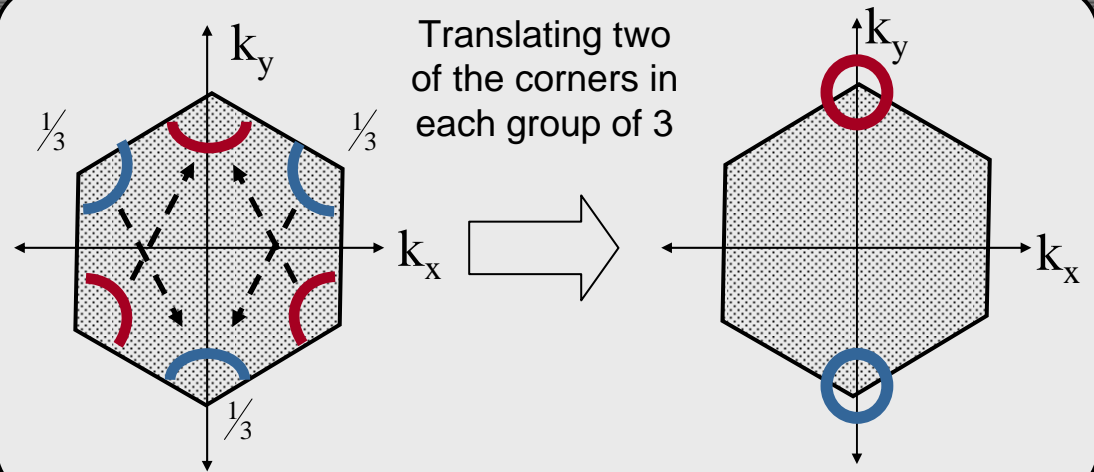
- Let $k_x a = \pi$ and investigate $h(k)$ as a function of k_y .

$$h_0 = t(1 - 2\cos k_y b) \text{ for } k_x = \pi \Rightarrow k_y b = \frac{\pi}{3} \text{ to get } h_0(k) = 0$$



Two Full Valleys

- The six Brillouin valleys really only give 2 independent valleys, e.g. in each group of 3 that are in the picture two of the valleys are away from the other by a reciprocal lattice unit vector; hence represent the same state. One can think that each corner in the 1st Brillouin zone contributes 1/3rd. $1/3 \times 6 = 2$ (left figure). Alternatively we can translate two of the corners in each group to get the full valleys on the right.



- Dispersion relation along k_y .

$$h_0 = t(1 + 2 \cos k_y b) \text{ for } k_x = 0$$

