

Quantum Transport:

ATOM TO TRANSISTOR

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Lecture 19: Bandstructure: Prelude to Sub-Bands

Ref. Chapter 5.2



Network for Computational Nanotechnology

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online simulations and more

- Next lecture we will move onto the topic of sub-bands, in this lecture we will continue our general discussion of bandstructure.

- To summarize

→ Whenever there exists periodicity in a solid, there will be periodicity in the Hamiltonian Matrix of that solid.

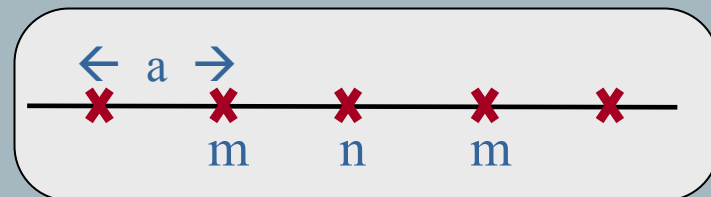
→ This fact may be used to simplify eigenvalue calculations.

- The simplified eigenvalue matrix is

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

where a given unit cell “n” is summed over all neighboring “m” unit cells

- In 1D our “n” and “m” unit cells are

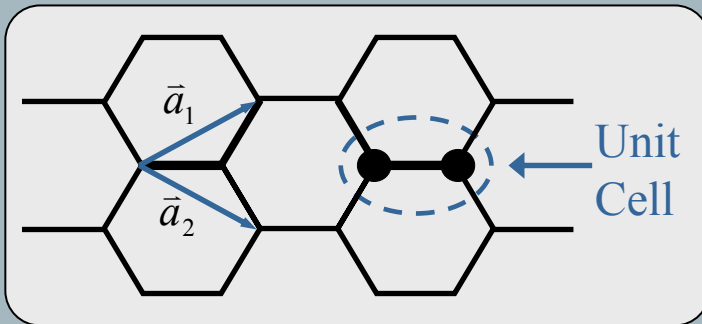


- The size of $h(\vec{k})$ depends on the number of basis functions per unit cell.
i.e. - b basis functions per unit cell gives a bxb $[h(\vec{k})]$ matrix

Graphite

03:00

- Previously, we went through the 2-D structure of graphite



- The “one” atom unit cell was not sufficient, a unit cell of two atoms had to be constructed
- We used the unit vectors \vec{a}_1 and \vec{a}_2 such that any site may be located by

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

(m and n are integers)

- In general one might use 4 basis orbitals per carbon atom (8 per unit cell). However, for graphite, as shown last time, we can get away with simply using the p_z orbital because it encompasses most of the optical and electrical properties of graphite. Nonetheless, even for graphite, to describe the full range of carbon-carbon bonding energetics one must use at least the first four basis orbitals (s, p_x , p_y , p_z).
- Note: 4 orbitals x 2 atoms per unit cell gives an 8×8 $\begin{bmatrix} h & \vec{k} \end{bmatrix}$

Graphite with just p_z

- So, using only p_z an analysis of graphite gives (see last time)...

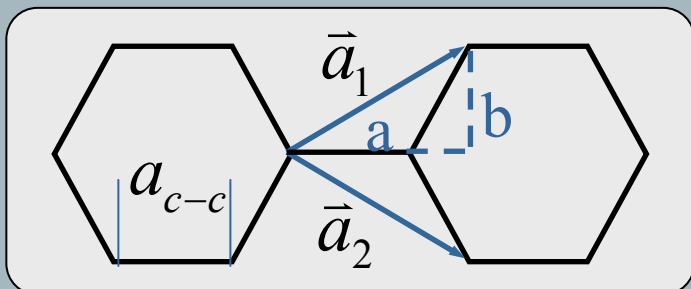
$$[h(\vec{k})] = \begin{bmatrix} E_0 & h_0^* \\ h_0 & E_0 \end{bmatrix}$$

where $h_0 = t(1 + e^{i\vec{k}\cdot\vec{a}_1} + e^{i\vec{k}\cdot\vec{a}_2})$
and $t \approx 2.5\text{eV}$ for C-C bonds

- Unit vectors are defined as:

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

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

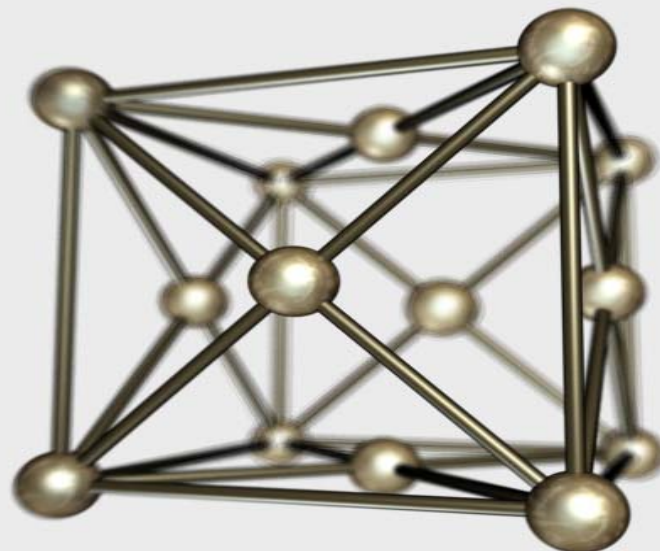


- This same methodology can be extended into 3 dimensions to describe semiconductor bandstructure.

- All common semiconductors have a diamond lattice structure consisting of 2 interpenetrating face centered cubic (fcc) atomic lattices

FCC

a



- The basis vectors are:

$$\vec{a}_1 = (\hat{x} + \hat{y})a/2$$

$$\vec{a}_2 = (\hat{y} + \hat{z})a/2$$

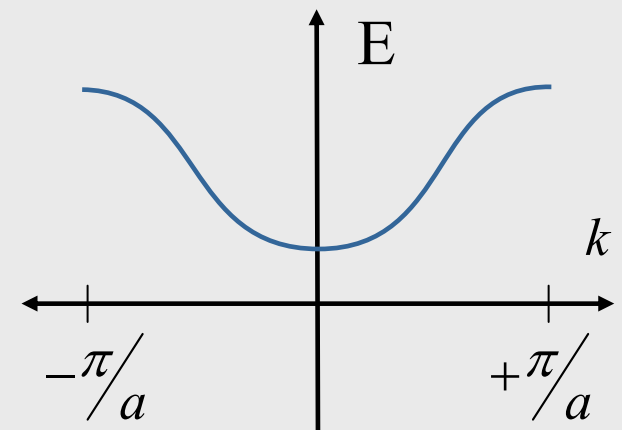
$$\vec{a}_3 = (\hat{x} + \hat{z})a/2$$

Note: with two interpenetrating FCC lattices the spacing between the atoms in each unit cell is $(a/4, a/4, a/4)$

- Using 4 (s3p) or 5 (s3ps*) basis orbitals we can describe the bandstructure of common semiconductors following the same methodology shown for graphite. Namely, looking at basis orbital overlap with nearest neighbor atoms to derive $h(\vec{k})$ and from $h(\vec{k})$ solving for the eigenvalue energies that provide the familiar bandstructure

- Next, a very important concept... consider where the Fermi energy is in relation to the energy levels

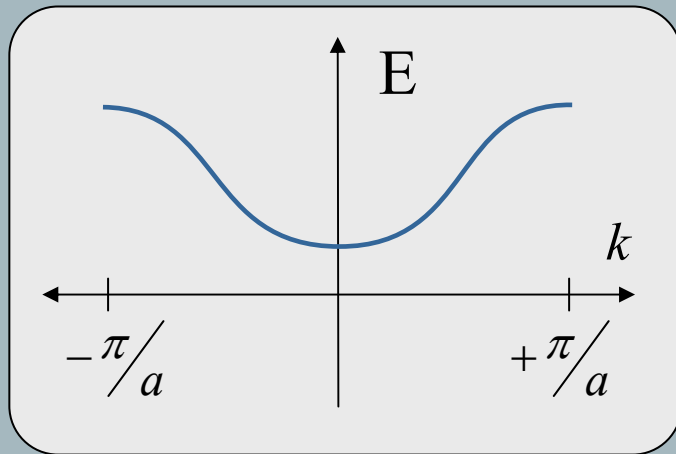
- Recall, for a simple 1D solid we get a band diagram something like:



Conductor & Insulator Band Diagrams

14:05

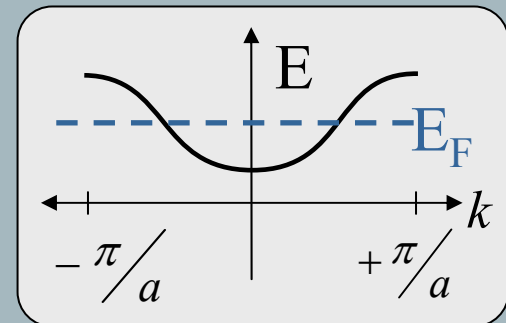
- In general, if we have N lattice points in a solid then there will be a resulting N values along the k -axis between $(-\pi/a, \pi/a)$. So a 1D diagram of the form



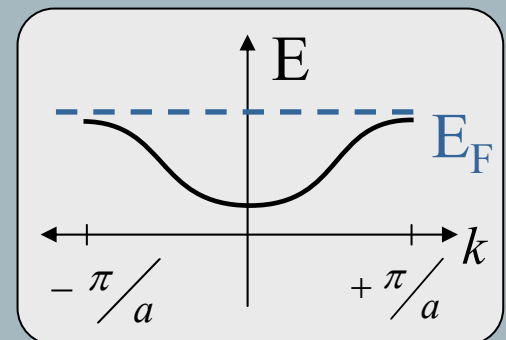
Will have $2N$ energy levels to hold electrons (spin included)

- The position of the Fermi energy is determined by the number of electrons. Likewise, the position of the Fermi energy determines the conduction/insulation properties of a solid. For example...

- Conductor, N electrons:



- Insulator, $2N$ electrons:

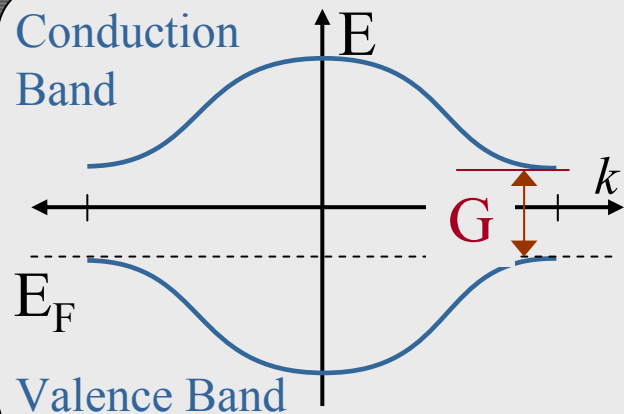


Conduction Properties and on to k-space

16:00

- Look at another example, take a lattice with 2 atoms per unit cell and 1 electron per atom. Therefore, given N lattice sites we have $2N$ electrons and the Fermi energy appears between the valence and conduction bands.

2 atoms/unit cell, 1 Basis fcn/atom



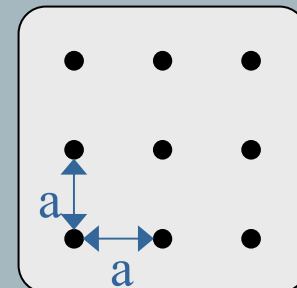
- Importantly, the energy gap between the conduction and valence bands, G , determines the conduction properties of the material. Big gap results in an insulator while a small one results in a conductor.

- Now move onto a discussion of k-space. A question often asked, *where is the Brillouin Zone?*

- Important point:

$$e^{i(k+2\pi/a)na} \text{ is equal to } e^{ikna} \text{ for all } n.$$

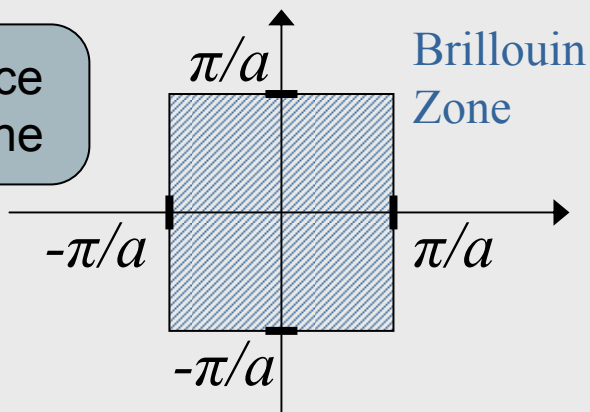
Now, let's consider the 2-D square lattice,



The k-space Brillouin zone is...

More K-Space

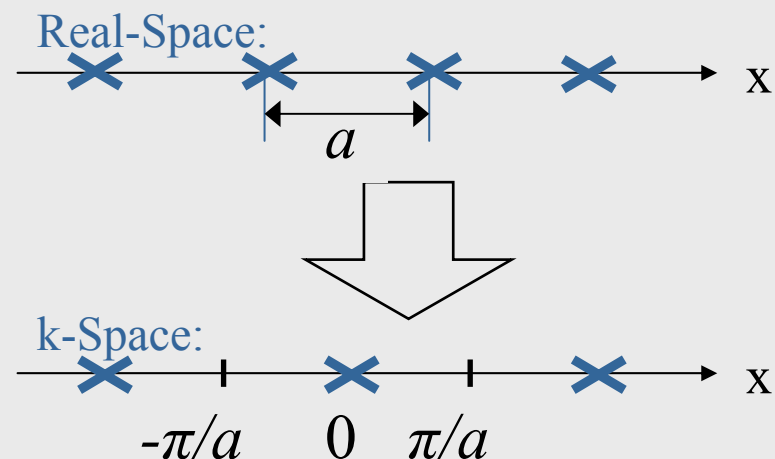
Square lattice
Brillouin Zone



- However, Brillouin Zone structure becomes more abstract for more complex 2-D and 3-D lattice structures
- In general, given a real-space basis of the form $\vec{R} = m \vec{a}_1 + n \vec{a}_2 + p \vec{a}_3$ (m, n and p are integers) we form the reciprocal k-space such that

$$\vec{K} = M\vec{A}_1 + N\vec{A}_2 + P\vec{A}_3 \text{ and } \vec{A}_j \cdot \vec{a}_i = 2\pi\delta_{ij}$$

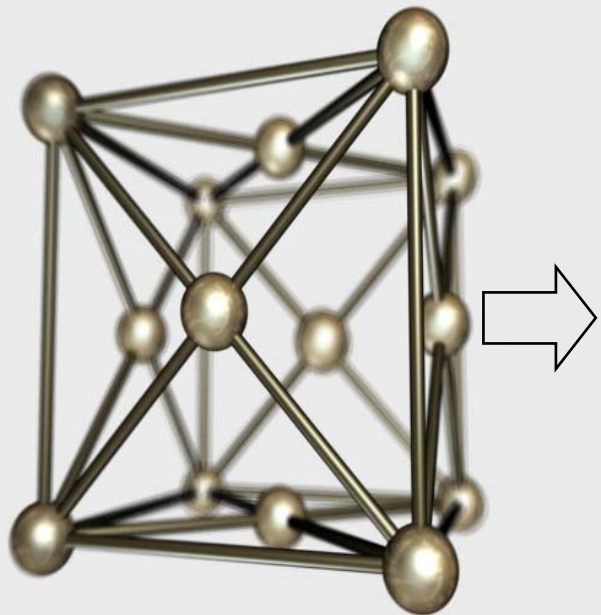
- For 1-D we have:



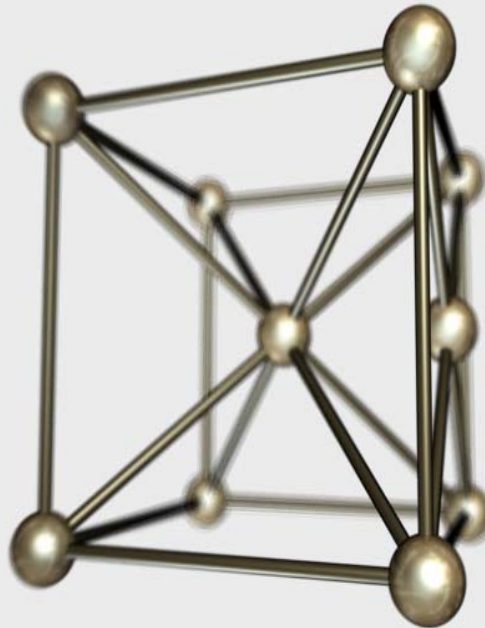
...a non-trivial example is that of semiconductors. The FCC real-space lattice of semiconductors produces a BCC (Body Centered Cubic) lattice in reciprocal space.
Diagram on next slide

FCC in Direct Lattice to BCC in reciprocal Lattice

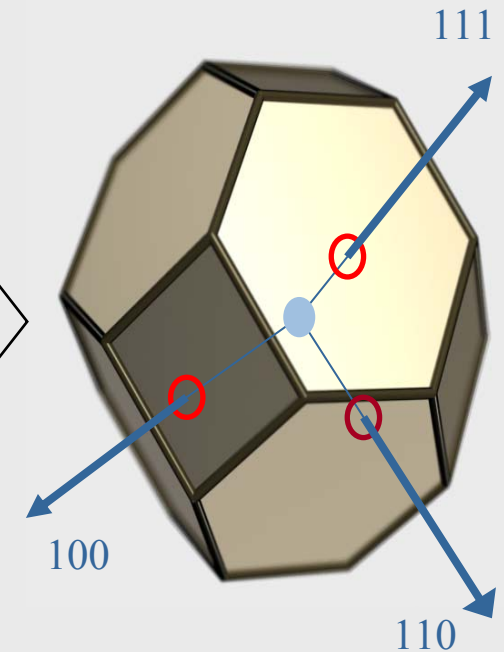
FCC in Real Space



BCC in
Reciprocal Space



Brillouin Zone in
Reciprocal Lattice

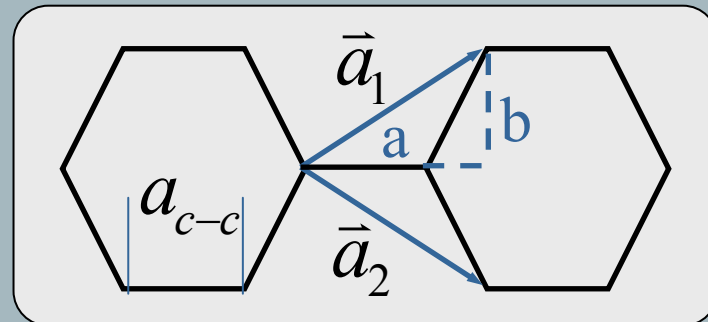


Recall basis vectors in Direct lattice of graphite:

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

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

$$\vec{a}_3 = \hat{z} \text{ Perpendicular to the plane of paper}$$



• To get the basis vectors in the reciprocal space we use: $\vec{A}_j \cdot \vec{a}_i = 2\pi\delta_{ij}$ (1)

• Using 1,
we have:

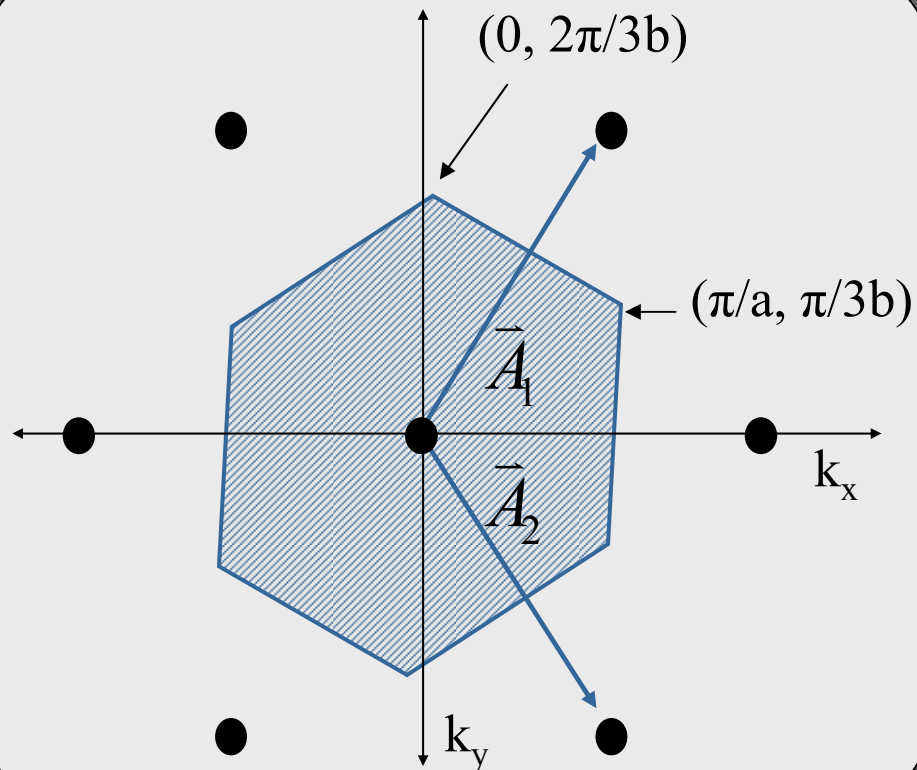
$$\vec{A}_1 = \frac{2\pi(\vec{a}_2 \times \vec{a}_3)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{\pi}{a}\hat{x} + \frac{\pi}{b}\hat{y}$$

$$\vec{A}_2 = \frac{2\pi(\vec{a}_3 \times \vec{a}_1)}{\vec{a}_2 \cdot (\vec{a}_3 \times \vec{a}_1)} = \frac{\pi}{a}\hat{x} - \frac{\pi}{b}\hat{y}$$

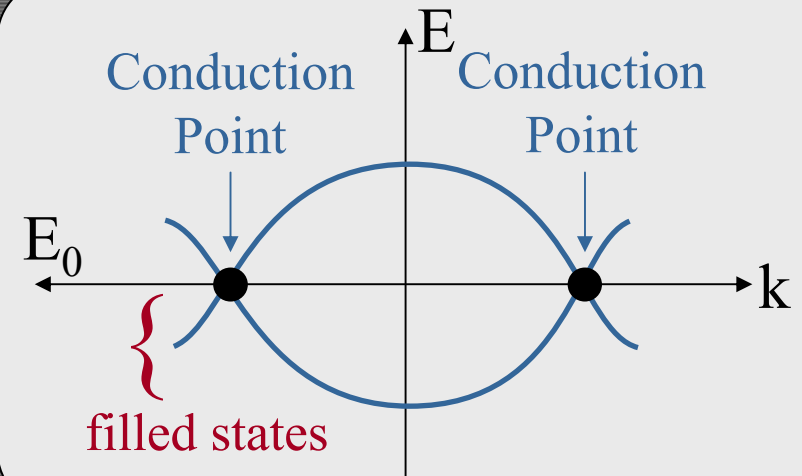
$$\vec{A}_3 = c\hat{z}$$

Reciprocal Graphite Lattice

- Thus, the reciprocal lattice and Brillouin zone of graphite look like:



- Now, we know from previous lectures that if we plot in a particular k -direction we get a diagram something like:



- So: "Where exactly are these conduction points in the (k_x, k_y) plane?"

Conduction Points

- We know that $E = E_0 \pm |h_0|$, therefore our conduction points occur at $|h_0| = 0$, or simply $h_0 = 0$. So,

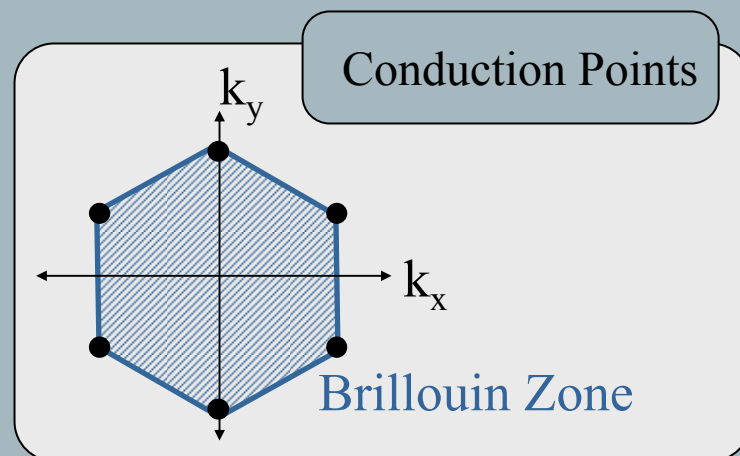
$$\begin{aligned} h_0 &= t \left(1 + e^{i\bar{k} \cdot \bar{a}_1} + e^{i\bar{k} \cdot \bar{a}_2} \right) \\ &= t \left[1 + e^{ik_x a} \left(e^{+ik_y b} + e^{-ik_y b} \right) \right] \\ &= 0 \end{aligned}$$

$$\therefore 1 + 2e^{ik_x a} \cos k_y b = 0$$

This occurs for the following coordinates:

$$(k_x a, k_y b) = \left\{ \begin{array}{l} \left(0, 2\pi/3 \right), \left(0, -2\pi/3 \right), \left(+\pi, \pi/3 \right), \\ \left(+\pi, -\pi/3 \right), \left(-\pi, \pi/3 \right), \left(-\pi, -\pi/3 \right) \end{array} \right\}$$

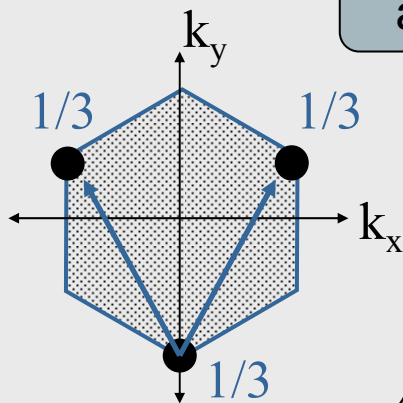
- On the (k_x, k_y) plane these points appear at the six corners of the Brillouin zone.



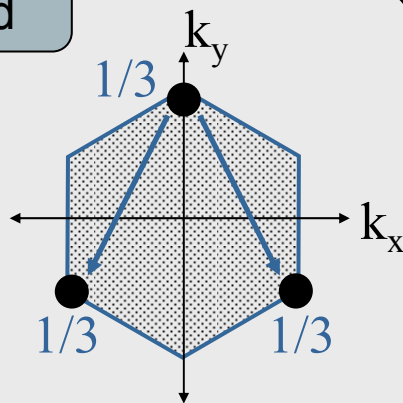
- Often we refer to these conduction points as “ Γ ” valleys which control the conduction properties.

How Many Conduction Points

- Does this mean that there are 6 valleys? **NO!** In reality, each corner of the Brillouin Zone only contributes $1/3^{\text{rd}}$ of a conduction point. Each $1/3^{\text{rd}}$ is associated to its other $2/3^{\text{rds}}$ by 2 lattice unit vectors. For example:

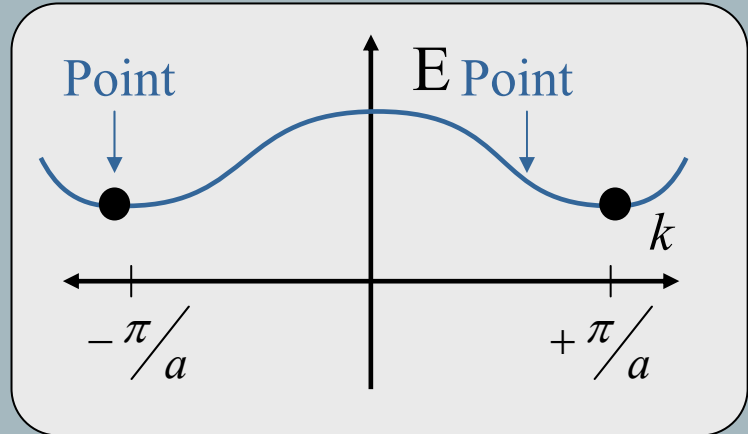


and



Two Full Valleys

- Perhaps a simpler way to think about it is to consider a point at the boundary of a 1-D Brillouin Zone...



- Is this 1 or 2 valleys? Clearly, it is one and the same point, since they are separated by a distance of $2\pi/a$. So we can think of the points on the graph as two $1/2$ points ($1/2 + 1/2 = 1$)!

Next Lecture: Start Sub-Bands