

# Fundamentals of Nanoelectronics

**Prof. Supriyo Datta**  
ECE 453  
Purdue University

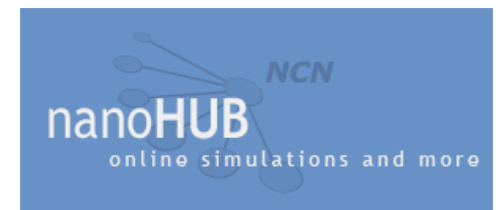
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## Lecture 22: Carbon Nanotubes

Ref. Chapter 6.1

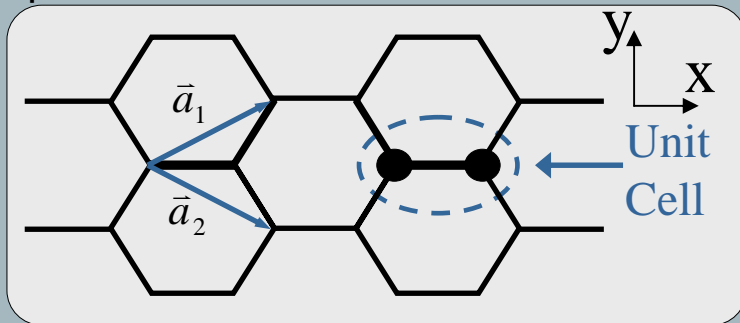


*Network for Computational Nanotechnology*



# Graphite Review

- In the last couple of sessions we've been talking about graphite. By rolling up a sheet of graphite we get a carbon nanotube which is of great interest because of its possible applications for making of transistors, electronic sensors, etc. Let's review what we've learned about graphene:



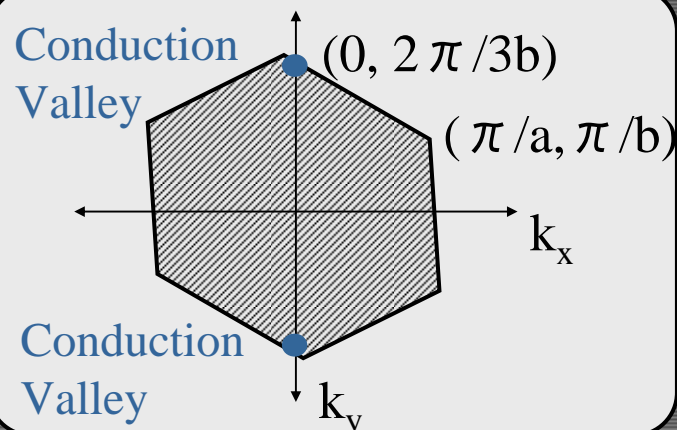
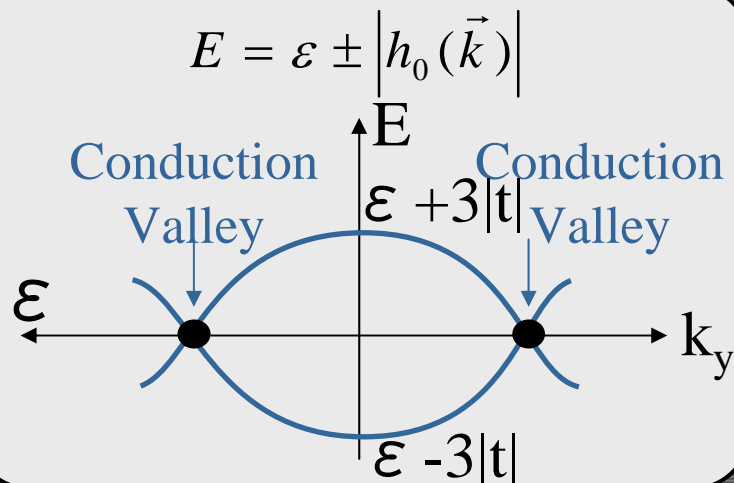
$$\vec{a}_1 = a\hat{x} + b\hat{y} = \frac{3}{2}a_0\hat{x} + \frac{\sqrt{3}}{2}a_0\hat{y}$$

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

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

- Dispersion relation:  

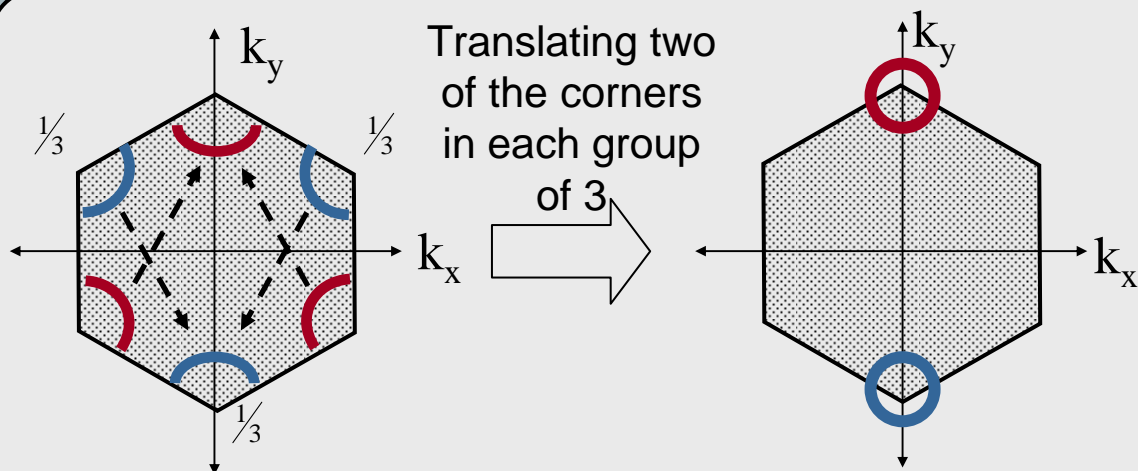
$$h_0 = t(1 + 2 \cos k_y b) \text{ for } k_x = 0$$



# Graphite Review

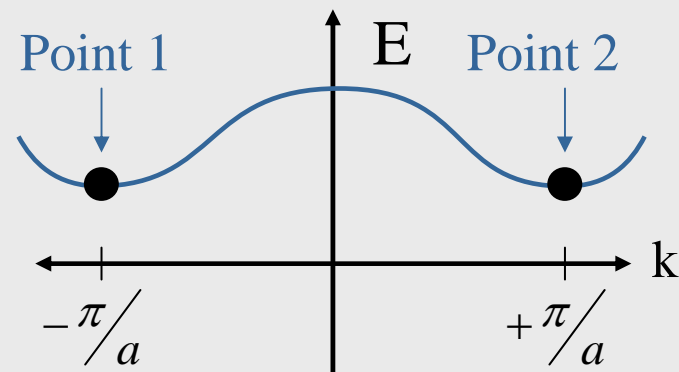
- Recall, the six Brillouin valleys really only give 2 independent valleys, e.g. in each group of 3 that are in the picture two of the valleys are away from the other by a reciprocal lattice unit vector; hence represent the same state. One can think that each corner in the 1<sup>st</sup> Brillouin zone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

$$h_0(\vec{k}) = -t(1 + 2e^{ik_x a} \cos k_y b)$$



RECALL: 1 D

Points 1 and 2 are separated by  $2\pi/a$ , so they really are one and the same point. Graphically, we visualize 1 and 2 as  $\frac{1}{2}$  points in  $k$ -space



# Carbon Nanotube Boundary Conditions

11:02

- For a sheet of material or a 2D surface, the correct boundary conditions are the infinite potentials at the edges but for mathematical convenience people usually use periodic boundary conditions. What saves us is that if one is interested in the bulk properties at the center of the sheet will not depend what's happening at the edges. But for nanostructures this cannot be done because what's happening at the edges can effect the middle of the solid so Periodic Boundary Conditions (PBC) cannot be used.
- Carbon nanotubes are a case where PBC is real because we roll up Graphene and in doing so boundary points at one edge overlap with the boundary points at the other edge; hence the periodicity.

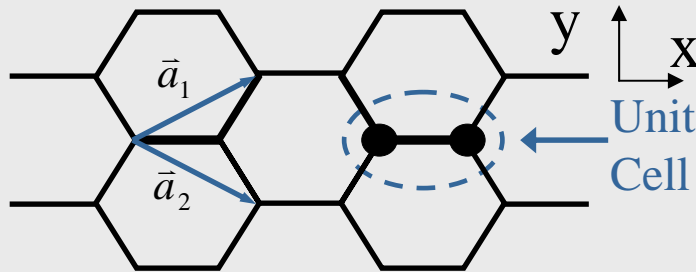
$$\text{PBC} : kL = 2\pi\nu$$



- The question is how to impose PBC in a two dimensional case.



# Rolling Up Graphite



$$\vec{a}_1 = a\hat{x} + b\hat{y} \quad \text{and} \quad \vec{a}_2 = a\hat{x} - b\hat{y}$$

- It is clear that Graphene can be rolled up into a nanotube in various ways depending on how one rolls it up. So how can we classify or define the nanotubes? The idea is that in the process of rolling up Graphene, a unit cell gets superimposed on another. One uses the vector that connects the two unit cells in Graphene to describe the corresponding nanotube. This vector is called the circumferential vector and can be written as a combination of vectors  $\vec{a}_1$  and  $\vec{a}_2$  with integer factors:  $\vec{c} = m\vec{a}_1 + n\vec{a}_2$

- Type of nanotube is described by : (m, n)

- An initial simple example is to roll in the x direction. For instance, create a tube described as: (10,10)
- We use the circumferential vector  $\vec{c}$  to denote the direction and length. Here,  $\vec{c} = 20a\hat{x}$  but in general  $\vec{c} = 2am\hat{x}$  where  $m$  is an integer. This will result in 'REAL' periodic B.Cs because each point on graphite will coincide with a similar one after being rolled up. (Notice that the magnitude of gives you the circumference of a cross section of the tube hence the name circumferential vector.)

- For the most part only two types of folding are of interest. The first, a fold in the  $\hat{y}$  direction resulting in the zig-zag nano-tube

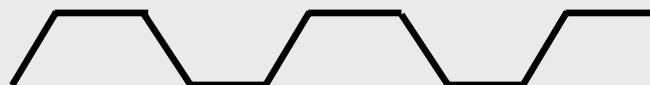
Zigzag



$(m, 0)$

since the circumferential edge looks like a zig-zag. The second, a fold in the  $\hat{x}$  direction resulting in the arm-chair nano-tube

Armchair



$(m, m)$

# PBC $\rightarrow$ Subbands $\rightarrow$ Discrete Energy Levels

22:52

- The periodic B.C along the circumference requires that  $\vec{k} \cdot \vec{c} = 2\pi\nu$  ( $\nu$  is an integer)

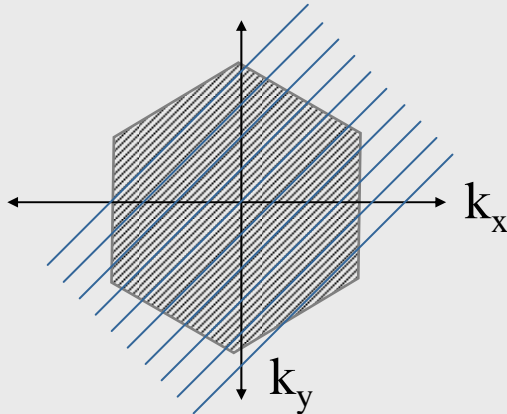
$$\vec{c} = m\vec{a}_1 + n\vec{a}_2 = \hat{x}a(m+n) + \hat{y}b(m-n)$$

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

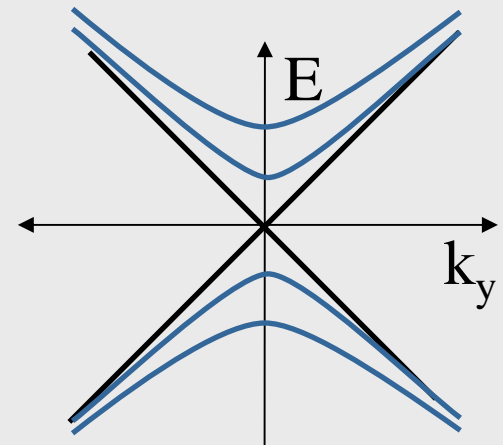
$$\vec{k} \cdot \vec{c} = k_x a(m+n) + k_y b(m-n) = 2\pi\nu$$

Subbands in Direction

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



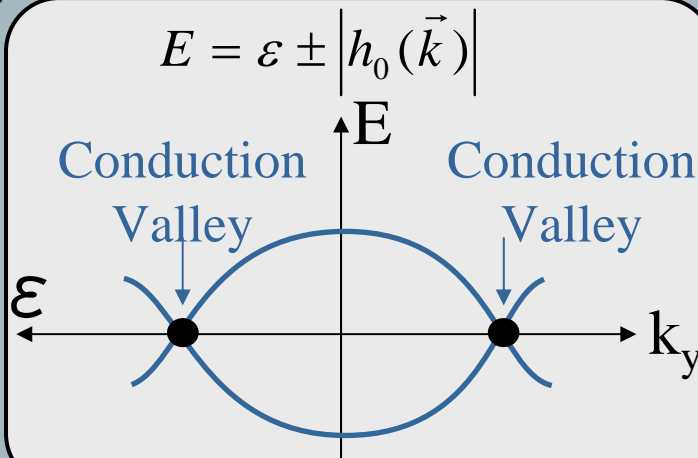
- Commonly, the carbon nano-tube E-k diagrams, about the conduction points, given by this model look like:



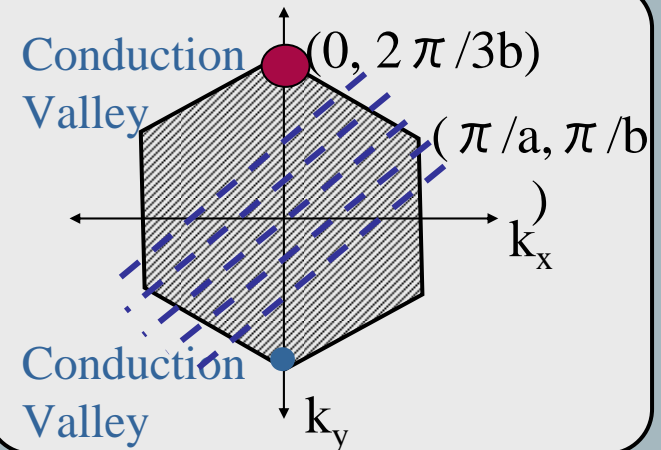
# Carbon Nanotube: Electrical Conduction

28:10

- A nano-tube will only conduct if one of its subbands passes through the six corners of the Brillouin Zone. In particular consider the corner marked by the red dot:



A nanotube is described by the pair of integers  $(m, n)$



$$\left. \begin{aligned} h_0(\vec{k}) &= -t(1 + 2e^{ik_x a} \cos k_y b) = 0 \\ k_x &= 0 \end{aligned} \right\} \Rightarrow (0, 2\pi/3b): \text{coordinate of the corner}$$

• Equation of the line:  $\vec{k} \cdot \vec{c} = k_x a(m+n) + k_y b(m-n) = 2\pi v$

$$\frac{2\pi}{3b} b(m-n) = 2\pi v \Rightarrow \frac{m-n}{3} = v : \text{integer}$$

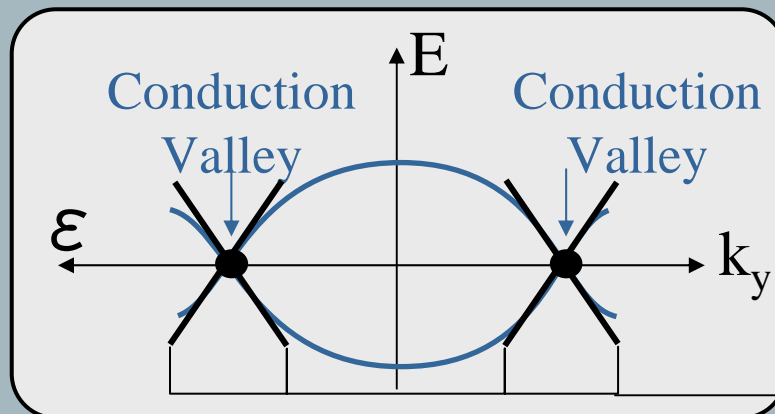
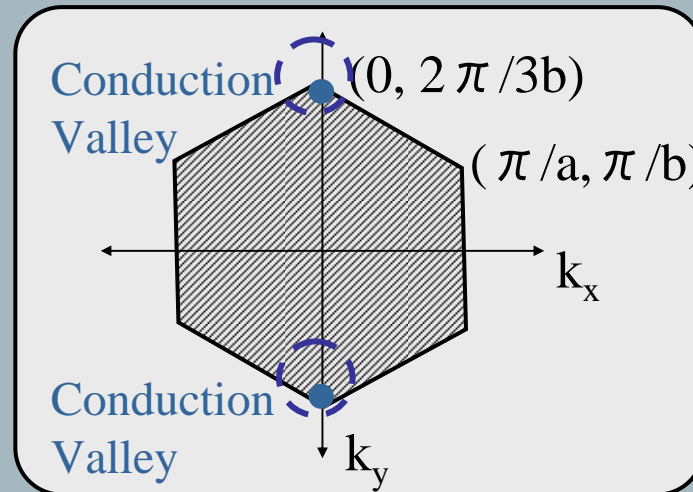
**Condition for  
Conduction**



# Taylor Approximation Overview

39:30

- Next let's try to simplify the expression for  $h(k)$ . The following simplification is based on Taylor series expansion and it is only valid close to the conduction valleys.



The approximation will result in these tangent lines close to the conduction valleys

# Taylor Approximation

40:40

- To do the approximation consider the E-k relation:

$E = \varepsilon \pm \left| h_0(\vec{k}) \right| = \varepsilon \pm t \sqrt{1 + 4 \cos k_x a \cos k_y b + 4 \cos^2 k_y b}$  which after simplification can be written as

$$E = \varepsilon \pm ta \sqrt{k_x^2 + \beta_y^2} \quad \text{where } \beta_y = k_y \pm \left(2\pi/3b\right), \quad a \equiv \frac{3a_0}{2}$$

- So, to approximate the energy expression we Taylor expand  $h_0$  about the conduction valleys

$$(k_x, k_y) = (0, \pm(2\pi)/3b)$$

$$h_0 \approx k_x \left[ \frac{\partial h_0}{\partial k_x} \right]_{(0, \pm 2\pi/3b)} + \left( k_y \pm 2\pi/3b \right) \left[ \frac{\partial h_0}{\partial k_y} \right]_{(0, \pm 2\pi/3b)}$$

$$= \frac{i3at}{2} k_x \pm \frac{3a_0 t}{2} \left( k_y \pm 2\pi/3b \right) = \frac{i3a_0 t}{2} (k_x \pm i\beta_y),$$

$$\text{where } \beta_y = k_y \pm \left(2\pi/3b\right)$$