Fundamentals of Nanoelectronics

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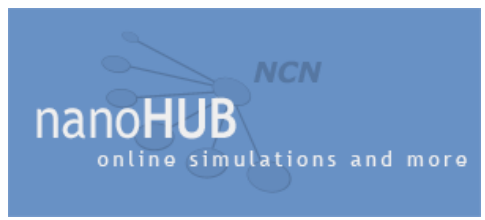
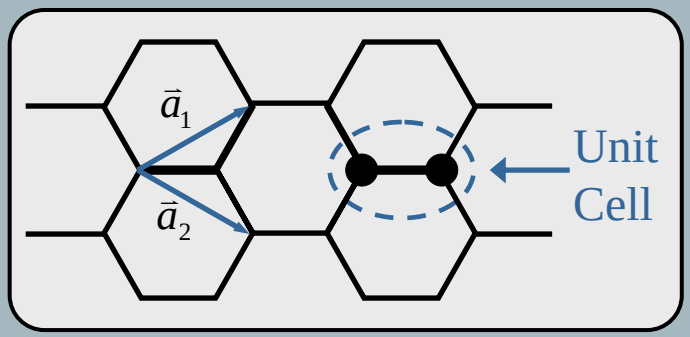
Lecture 23: Subbands

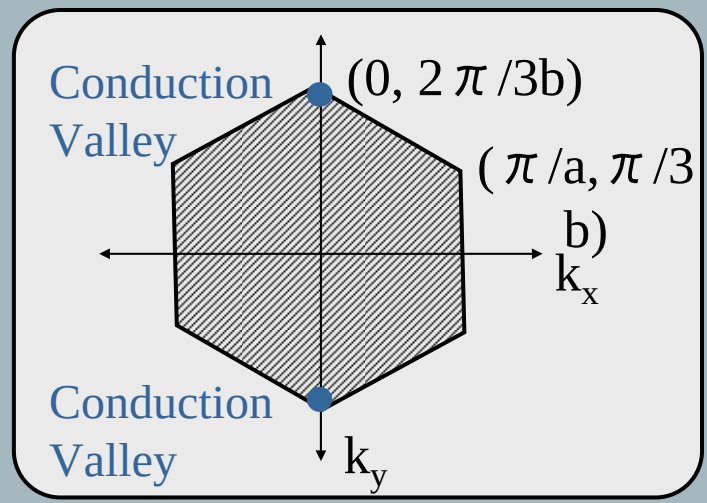
Ref. Chapter 6.1

Network for Computational Nanotechnology



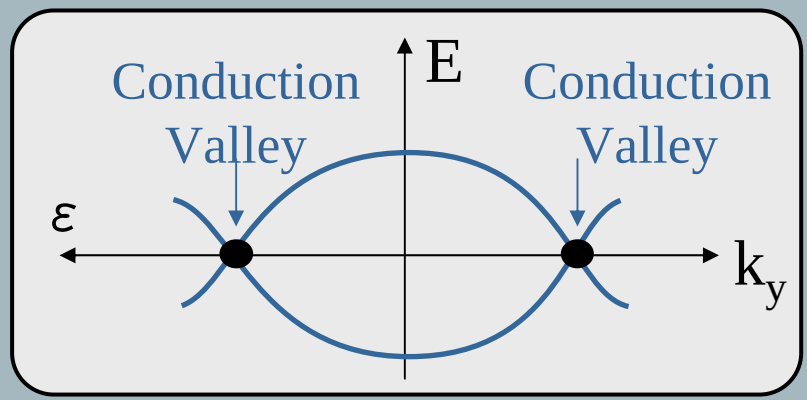


$$\vec{a}_1 = a\hat{x} + b\hat{y}$$
$$\vec{a}_2 = a\hat{x} - b\hat{y}$$



$$[h(\vec{k})] = \begin{bmatrix} E_0 & h_0 \\ h_0^* & E_0 \end{bmatrix} \Rightarrow E_{1,2} = \varepsilon \pm \left| h_0(\vec{k}) \right|$$

$$h_0(\vec{k}) = -t\left(1 + e^{i\vec{k}.\vec{a}_1} + e^{i\vec{k}.\vec{a}_2}\right) = -t\left(1 + 2e^{ik_x a}\cos k_y\right) \approx iatk_x + at\left(k_y - \frac{2\pi}{3b}\right)$$



Taylor Expansion

$$h_0(\vec{k}) = -t\left(1 + 2e^{ik_x a}\cos k_y\right) \approx iatk_x + at\left(k_y - \frac{2\pi}{3b}\right)$$

- Recall, given $E = \varepsilon_0 \pm h_0$ we Taylor expand h_0 about the conduction points

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

- Expanding and solving

$$\frac{\partial h_0}{\partial k_x} = -2t(ia)e^{+ik_x a}\cos k_y b, \quad \frac{\partial h_0}{\partial k_y} = 2tbe^{+ik_x a}\sin k_y b$$

$$\therefore \left[\frac{\partial h_0}{\partial k_x}\right]_{(0,2\pi/3b)} = -i2t\left(\frac{3a_0}{2}\right)\left(-\frac{1}{2}\right) = ita$$

$$\left[\frac{\partial h_0}{\partial k_y}\right]_{(0,2\pi/3b)} = 2tb\left(\frac{\sqrt{3}}{2}\right) = tb\sqrt{3} = t\left(\frac{\sqrt{3}a_0}{2}\right)\sqrt{3} = ta$$

- Finally we get

$$h_0(\vec{k}) = ta(ik_x + \beta_y)$$

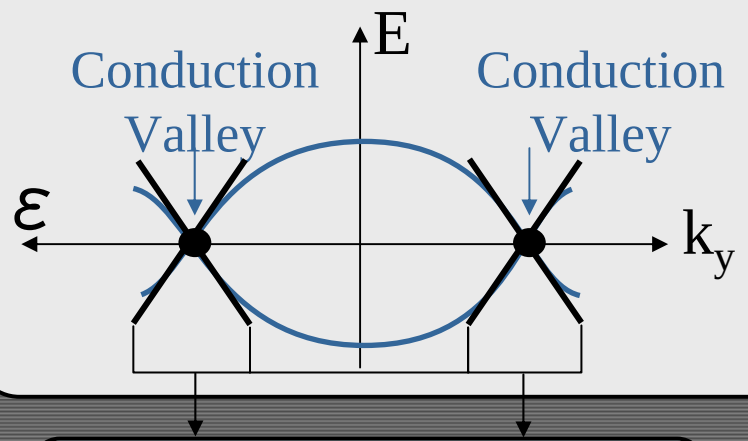
$$\text{where } \beta_y = k_y - \frac{2\pi}{3b}$$

- The above approximation describes quite well the behavior of semiconducting and conducting nanotubes. This, of course, is true because all the “action” (electrical and optical effects) tend to occur at or close to the conduction point.

Taylor Approximation

09:02

$$h_0(\vec{k}) = -t\left(1 + 2e^{ik_x a}\cos k_y\right) \approx iatk_x + at\left(k_y - \frac{2\pi}{3b}\right)$$



$$E = \varepsilon \pm \frac{3ta_0}{2}\sqrt{k_x^2 + \left(k_y - \frac{2\pi}{3b}\right)^2}$$

This approximation works quit well and will result in these tangent lines close to the conduction valleys. This, of course, is true because all the "action" (electrical and optical effects) tend to occur at or close to the conduction point.

Folding Graphene / Zigzag Nanotube

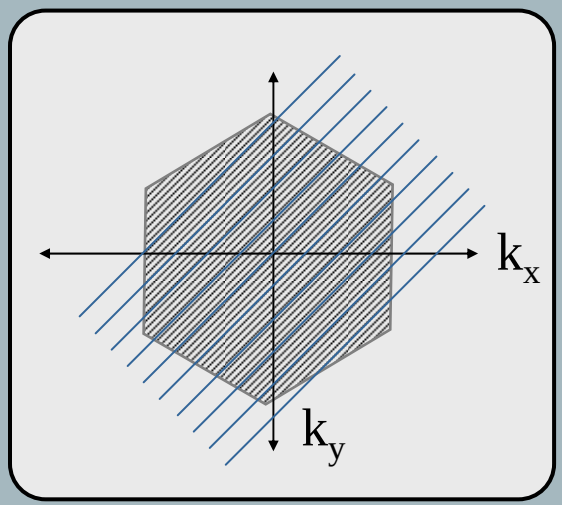
12:30

• The periodic boundary conditions along the circumference requires that $\vec{k} \cdot \vec{c} = 2\pi\nu$ where ν is an integer.

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

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

$$\vec{k} \cdot \vec{c} = 2\pi\nu$$

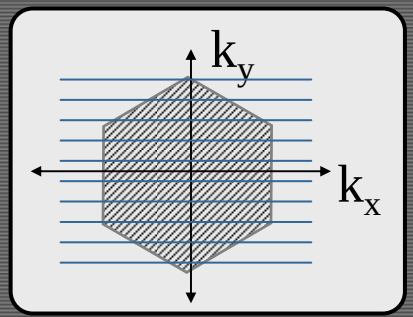


Zigzag nanotube

• A fold in the $\hat{y}$ direction has the circumferential vector $\vec{c} = 2mb\,\hat{y}$, where ***m*** is an integer, and the resulting subbands look something like…

$$k_y \cdot (2bm) = 2\pi\upsilon$$

$$k_y = \frac{2\pi\upsilon}{2bm}$$



Zigzag Nanotube: E-k Plot

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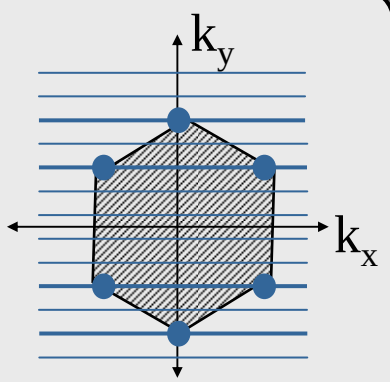


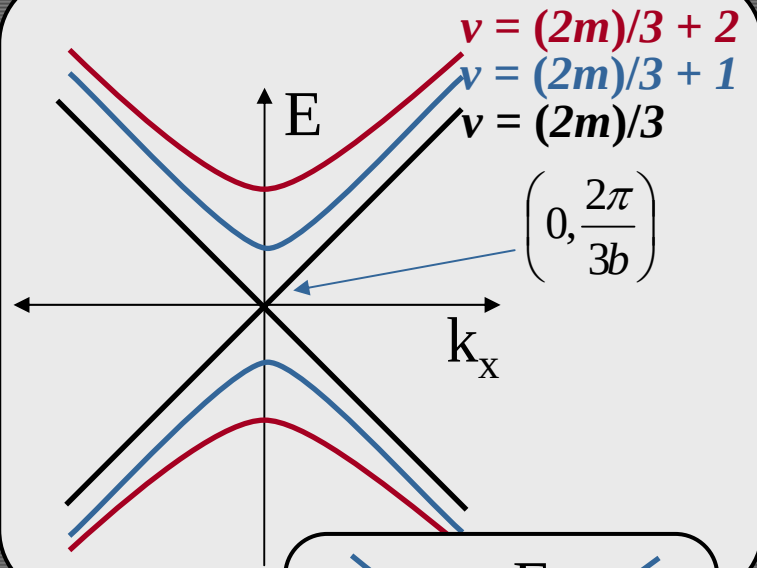
• A general energy expression for a $\hat{y}$ fold, zigzag, nanotube is:

$$E_v(k_x) = \varepsilon \pm at\sqrt{k_x^{\,2} + k_v^{\,2}}$$

$$\text{where } k_v = \frac{2\pi}{3b}\left(\frac{3v}{2m} - 1\right)$$

Conducting Nanotube

$$m = 3\upsilon$$

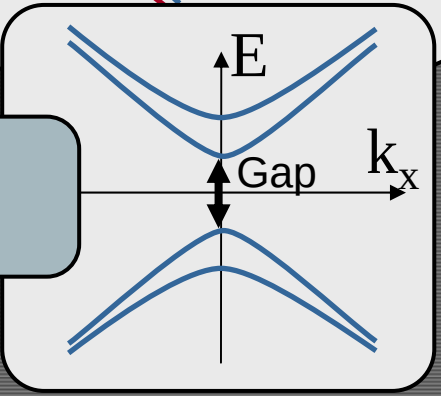


• A nanotube will only conduct if one of its subbands pass through the six corners of the Brillouin Zone. The condition for conduction is

$$\frac{2\pi v}{2mb} = \frac{2\pi}{3b} \text{ or } \frac{v}{2m} = \frac{1}{3}$$

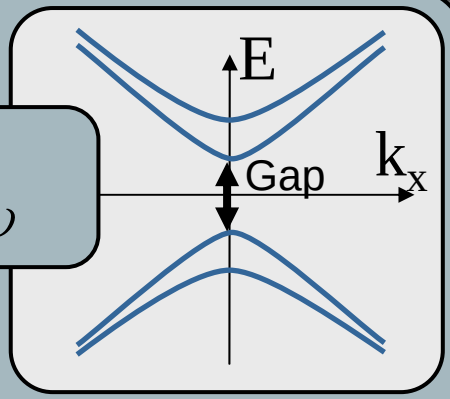
Therefore only if ***m*** is a multiple of 3 then conduction will in a zigzag nanotube.

Semi-Conducting Nanotube $m \neq 3\upsilon$



Semi-Conducting Gap

Semi-Conducting Nanotube $m \neq 3\upsilon$



$$E_v(k_x) = \varepsilon \pm at\sqrt{k_x^{\,2} + \left(\frac{2\pi}{3b}\left(\frac{3v}{2m} - 1\right)\right)^2}$$

- How can we estimate the semi-conducting band gap?
- This can be done by finding the smallest value of the second term in the equation above:

$$at\sqrt{k_x^{\,2} + \left(\frac{2\pi}{3b}\left(\frac{3v - 2m}{2m}\right)\right)^2}$$

is minimized if: $3v - 2m = 1$

- The minimum is then:

$$at\sqrt{k_x^{\,2} + \left(\frac{2\pi}{3b \cdot 2m}\right)^2} \quad \text{where} \quad a = \frac{3a_0}{2}$$

- The quantity above represents half of the band gap shown in the figure given that kx=0.

$$E_g = \frac{3a_0 t}{2} \times \frac{4}{3d}$$ d: diameter of nanotube

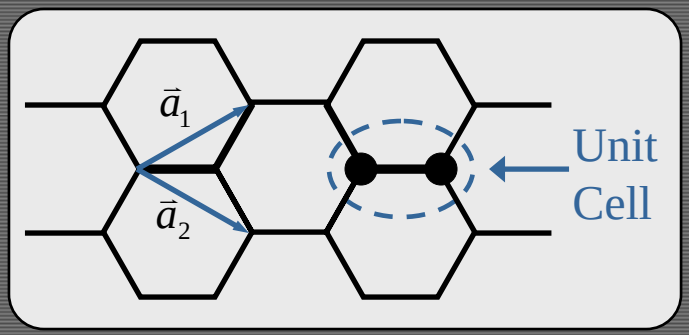
$$\boxed{E_g = \frac{2a_0 t}{d}}$$

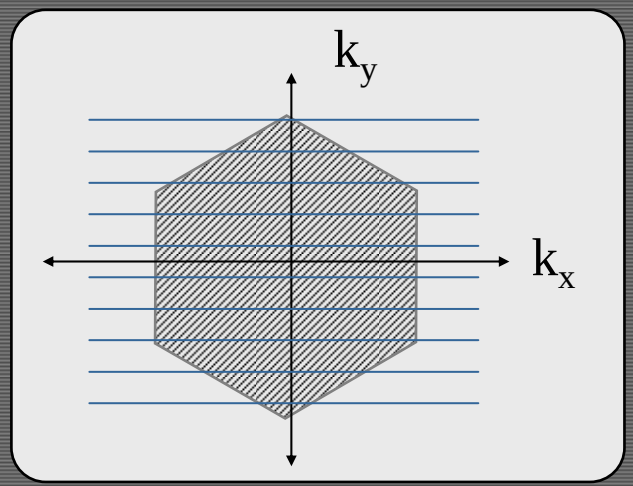
- Let's put some numbers in to find Eg for a carbon nanotube with diameter: d=28 Å.

$$E_g = \frac{2\left(1.4\times10^{-10}\,m\right)\left(2.5eV\right)}{\left(28\times10^{-10}\,m\right)} = 0.25eV$$

Confinement → Subbands

33:53





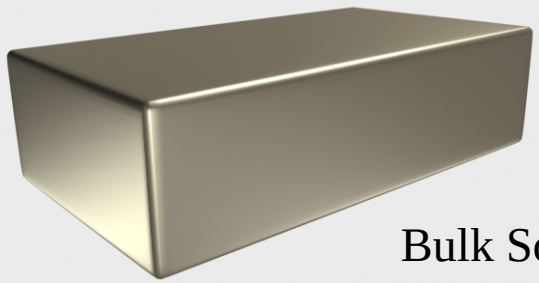
$$k_y = \frac{2\pi\upsilon}{2bm}$$

- As long as we have a sheet of a material, the confinement is only in 1 dimension. Then all k values on the kx, ky plane are allowed. The E-k plot will then be 3 dimensional because at each point in the k plane, there is a corresponding energy value.
- The imposition of periodic boundary conditions by folding a sheet of graphite to a carbon nanotube -for example a zigzag nanotube- makes only certain values of “ky” acceptable. These are the horizontal lines shown in the figure.
- Increasing the diameter of nanotube will make the lines closer to each other and decreasing the diameter will make the lines further apart. In the limit of very big diameters, we get the same thing as a sheet of graphite: the acceptable lines get really close to each other and it starts to look like a bulk piece of graphite sheet namely: Graphene.

Dimensional Confinement

• How do we look at this process of dimensional confinement in a general manner? Where does the carbon nano-tube fit in?

• Consider the well known bulk solid



without any constraints, very long, wide and deep. It has a general E-k behavior expressed by the function $E(k_x, k_y, k_z)$

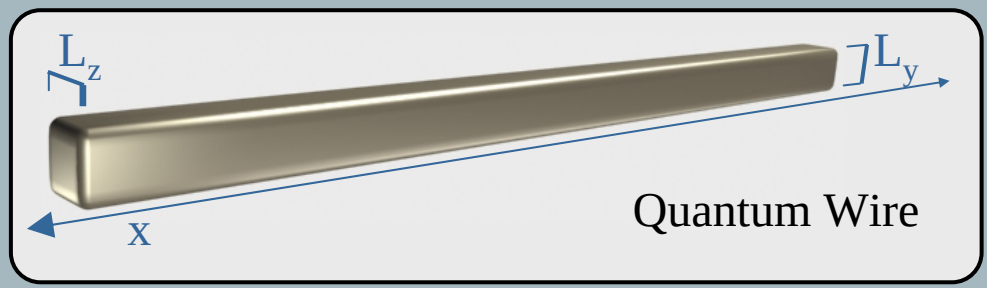
• If we constrain the bulk solid in one direction, say k_z, to a comparably short length, L_z, we get what is known as a **quantum well ...**

• **...**Assuming periodic boundary conditions for L_z, we get $k_z = (v2\pi) / L_z$ and our E-k function is

$$E_v(k_x, k_y) = E(k_x, k_y, k_{z=(2\pi v)/L_z})$$

(where v is an integer)

• Similarly, constraining along the k_y direction results in a **quantum wire**



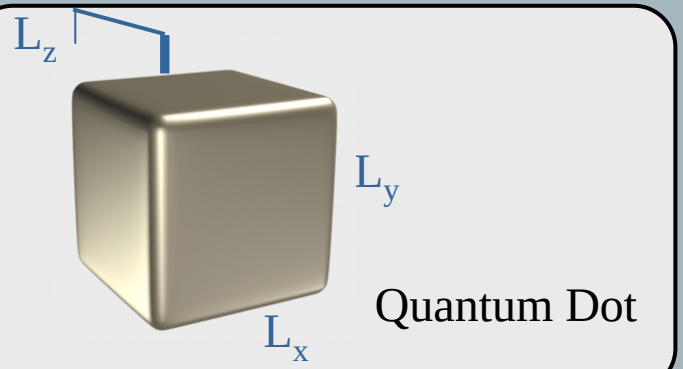
• For the quantum wire we have $k_y = (v'2\pi)/L_y$ and the E-k function

$$E_{v,v'}(k_x) = E\left(k_x, k_y = \frac{v'2\pi}{L_y}, k_z = \frac{v2\pi}{L_z}\right)$$

Note: a carbon nanotube is really, in the general sense, a form of quantum wire!

More Dimensional Confinement

• Finally, confinement in the x-direction as well leads to a quantum dot



•The quantum dot includes $k_x = (v'' 2\pi)/L_x$ such that the E-k behavior is given by

$$E_{v,v',v''} = E\left(k_x = \frac{v''2\pi}{L_x}, k_y = \frac{v'2\pi}{L_y}, k_z = \frac{v2\pi}{L_z}\right)$$

The quantum energy levels are discretized in the same way as those of an atom and so quantum dots are often referred to as artificial atoms

• One important question, *when do constraints begin to lead to quantization of the bandstructure?* Essentially, quantization depends on the thermal energy k_BT. Because the thermal energy tends to smooth out the difference between energy levels, the discretization corresponding to $k_{x/y/z} = (q2\pi)/L_{x/y/z}$ must be less than or comparable to k_BT to experimentally (and hence physically) matter.

Note: this is often the motivation for conducting experiments at very low temperatures