Quantum Transport:
Atom to Transistor

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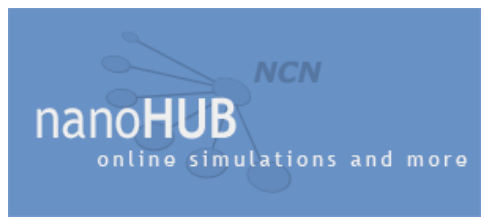
Lecture 20: Subbands: Quantum Wells, Wires, Dots and Nanotubes

Ref. Chapter 6.1

Network for Computational Nanotechnology



Introduction

00:00

- In this lecture the concept of subbands shall be introduced

- Often we are interested in low dimensional structures such as carbon nano-tubes. A low dimensional structure is that for which one or more dimension is very small.

- For the most part, if one or more dimension is on the nm scale (≈100 atoms) the conventional E-k diagram is not sufficient

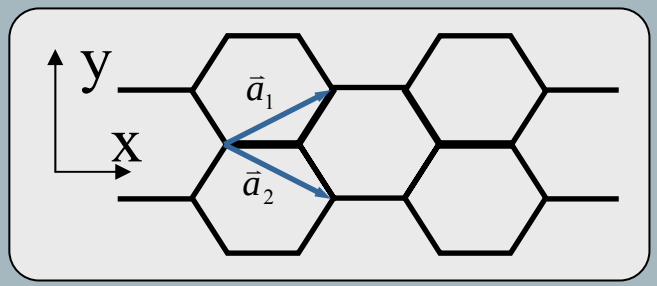
- In the succeeding lecture we will discuss how reducing a bulk solid to a low dimensional structure results in energy subbands and discrete energy levels which lead to qualitative differences and observable experimental quantities like density of states (DOS)

- The carbon nano-tube provides a particularly good illustration of the subbands because while a sheet of graphite (in x-y plane) is constraint in the z direction and has infinite wall Boundary Condition (B.C.), it can be rolled up to a nano-tube and be constraint in another dimension with 'REAL' periodic B.C.

Review of Graphite

03:00

• Remember, graphite has the structure



where, $\vec{a}_1 = a\hat{x} + b\hat{y}$ and

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

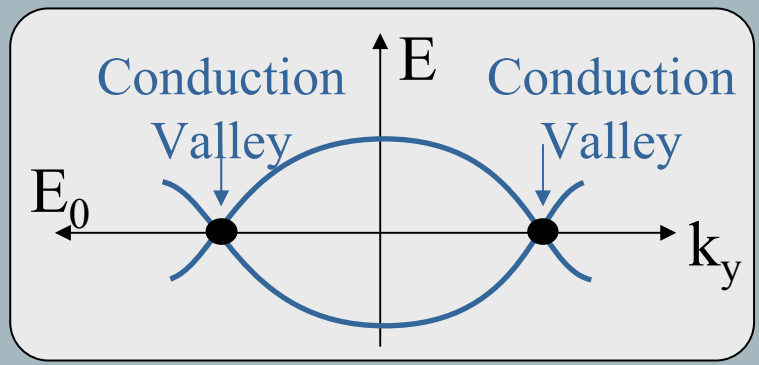
• The E-k diagram can be sound by $\left[h(\vec{k})\right] = \begin{bmatrix} E_0 & h_0 \\ h_0^* & E_0 \end{bmatrix}$

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

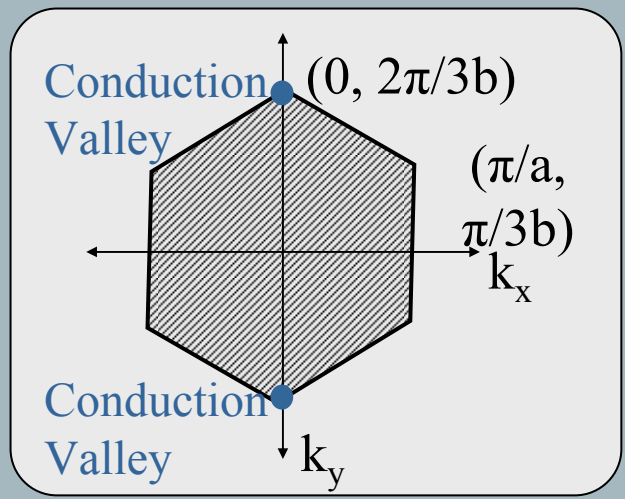
$$= -t\left(1 + 2e^{ik_x a}\cos k_y\right)$$

with eigenvalues $E = E_0 \pm |h_0|$

• So, plotted along the k_y line we get an energy curve like



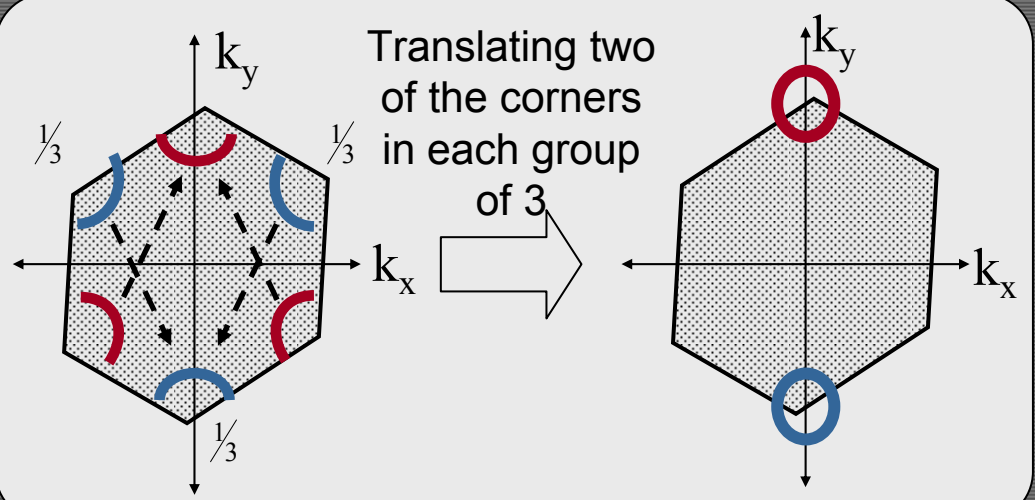
• With the conduction valleys appearing at the corners of the graphite Brillouin Zone…



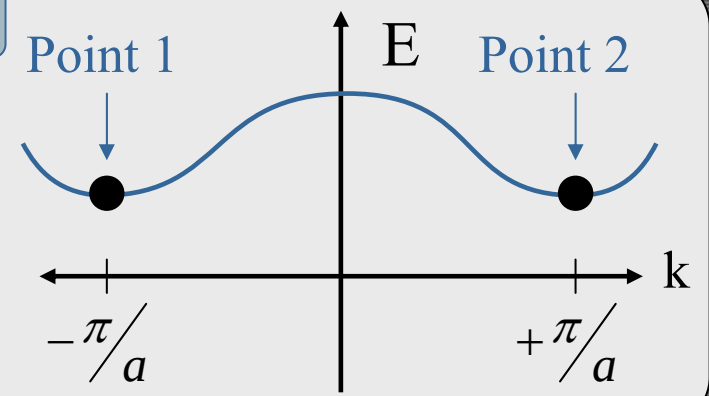
Review of Graphite

07:15

• 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 form 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 x 6 = 2(Left). Alternatively we can translate two of the corners in each group to get the full valleys on the right.



Recall 1d



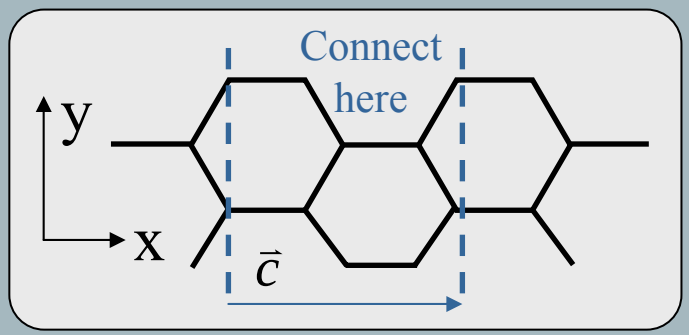
Points 1 and 2 are separated by 2π/a, so they really are one and the same point. Graphically, we visualize 1 and 2 as ½ points in k-space

Rolling up Graphite

09:00

• When we roll up graphite we get carbon nano-tube and in the process we constrain the already 1-D constraint sheet (in the z direction) yet in another dimension. Different ways of rolling will result in different E-k diagrams.

• An initial simple example is to roll in the $\hat{x}$ direction. For instance, create a tube with circumference 2a:



• We use the circumferential vector $\vec{c}$ to denote the direction and length. Here, $\vec{c} = 2a\hat{x}$ 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 $\vec{c}$ gives you the circumference of a cross section of the tube hence the name circumferential vector.)

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

$$k_x \cdot 2am = 2\pi v \Rightarrow k_x = \frac{2\pi v}{2am}$$

• For the provided example, we have:

$$v = 0, \pm 1, \pm 2, \pm 3 \ldots$$

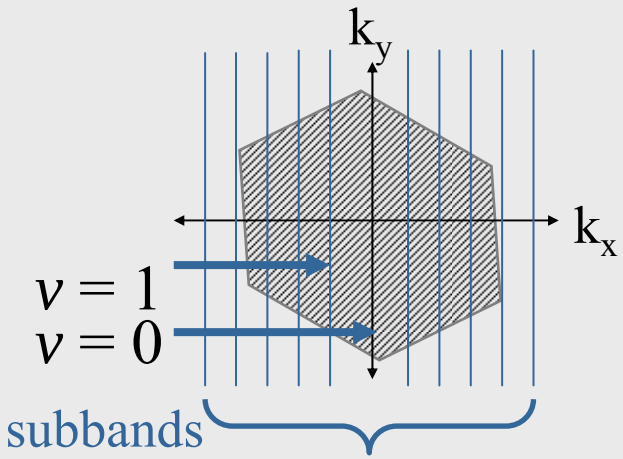
$$m = 1, 2, 3, 4 \ldots$$

• Here k_x's are series lines parallel to ky.

Carbon Nano-Tube Subbands

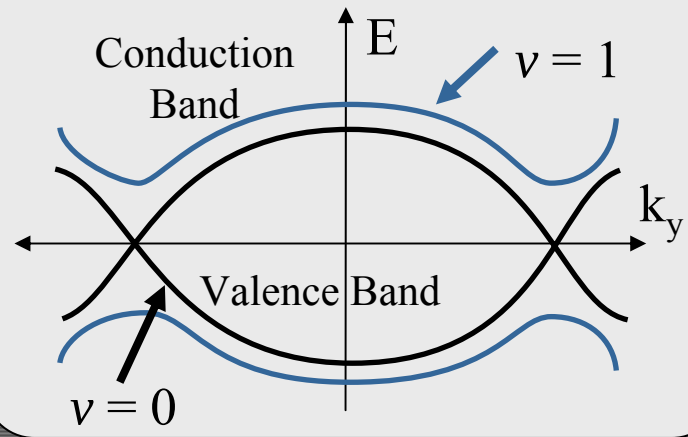
13:45

Carbon Nano-tube k_x Subbands



• This is how constraints along a given dimension result in subbands. *Note: For carbon nano-tubes with a very large circumference, the number of subbands in the Brillouin Zone can be so great that its behavior is indistinguishable from that of graphite*

• Along the k_y-axis the first two k_x subbands look like



• For ***v*** = 1 and ***v*** = 0 the Fermi energy lies above the valence band. *Note:* Only subbands passing through conduction valleys in the Brillouin Zone corners

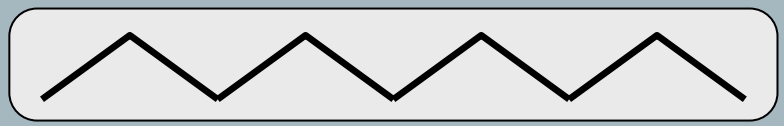
conduct, such as ***V*** = 0,the others will either semi-conduct or insulate

Nano-Tube Folding

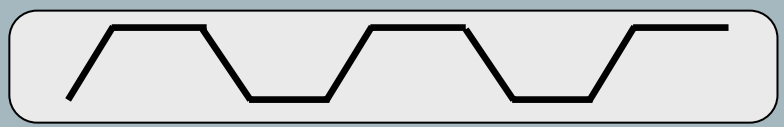
18:00

• It is possible to fold a nano-tube such that it has no subband passing thought the conduction valleys (i.e.. by folding in the $\hat{y}$ direction)

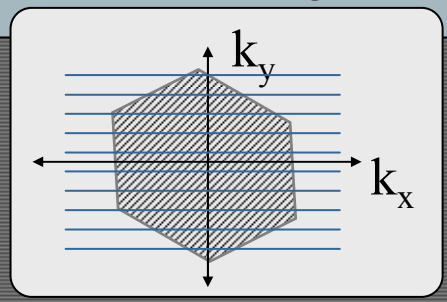
• For the most part only two types of folding are of interest. The first, a fold in the $\hat{y}$ direction resulting in the zig-zag nano-tube



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



• 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…



• A nano-tube will only conduct if one of its subbands pass through the six corners of the Brillouin Zone. So condition for conduction is

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

Therefore a zig-zag nano-tube will be like a conductor iff ***m*** is a multiple of 3!

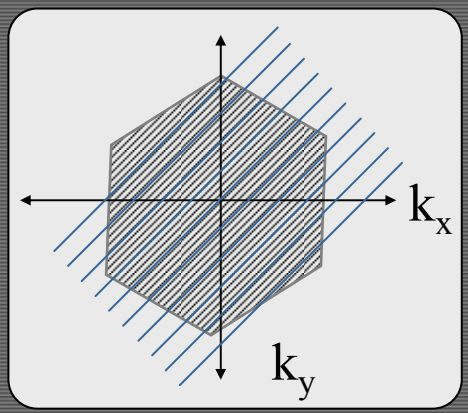
General Folding

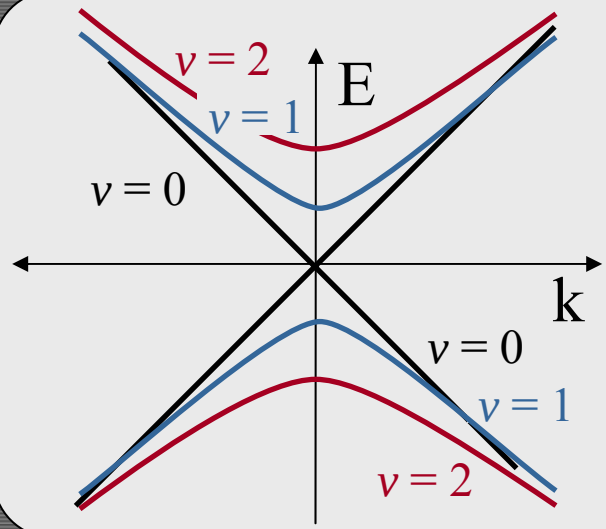
• In general, it is possible to fold a carbon nano-tube along any circumferential vector of the form $\vec{c} = m\vec{a}_1 + n\vec{a}_2$

•where ***m*** and ***n*** are integers, and (***m*** – ***n***) must be a multiple of three in order for metallic properties to exist

• As stated earlier, subbands discretize k-space and lead to a finite number of E-k diagrams corresponding to specific values of ***v***. In general we are most concerned with the behavior of a material near the Fermi level, so we consider the dispersion relations along each subband close to this level.

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





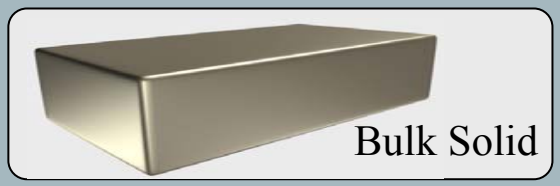
Assume an isotropic k-space near the Fermi level.

Return to Dimensional Confinement

30:40

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

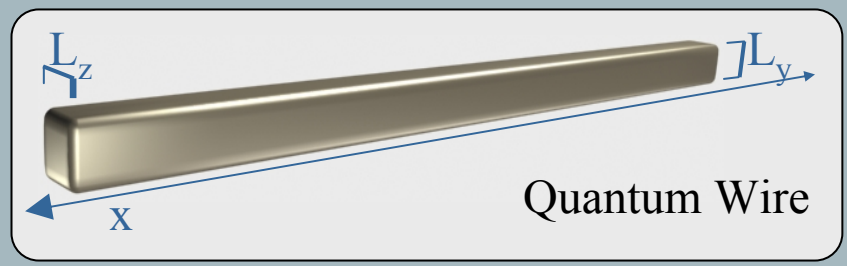
Consider the well known bulk solid



without any constraints, very long, wide and deep. It has a general E-k behavior expressed by the function $E(k_x, k_y, k_z)$ but 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 and k_z will **be forced to have discrete values.**

• 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

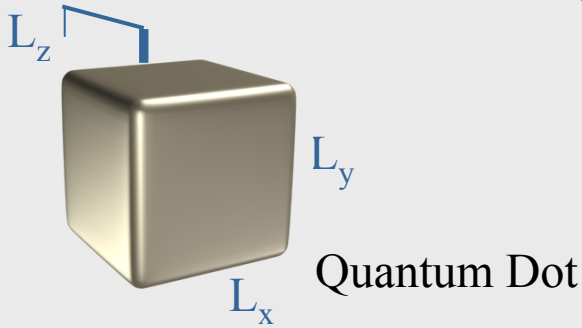
$$E_{v,v'}(k_x) = E\left(k_x, k_y = \frac{v'2\pi}{L_y}, k_z = \frac{v2\pi}{L_z}\right)$$

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

More on Dimensional Confinement

35:00

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



• The quantum dot has $k_x = (v''2\pi)/L_x$ 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 lead to experimental observables?* Essentially, quantization must be compared to 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 bigger than or comparable to k_BT to experimentally show itself.

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

An Approximate Expression for $E(k_x, k_y, k_z)$

42:00

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

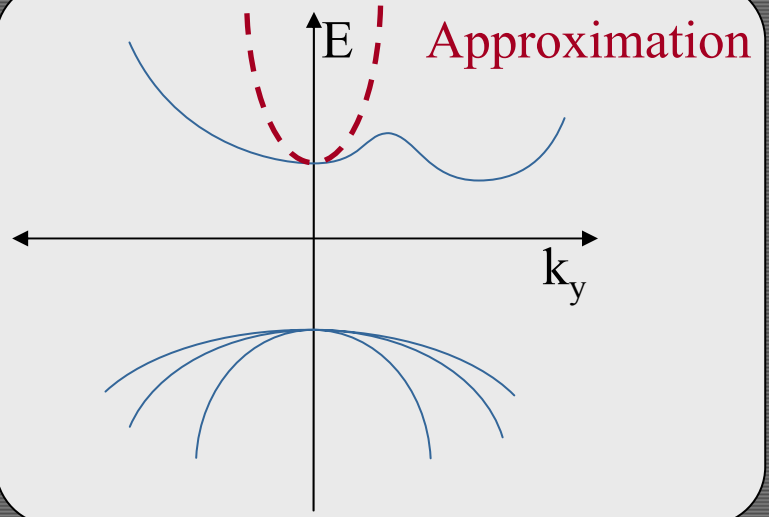
- For silicon, use the parabolic approximation

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

where m* is the effective mass. And with z confinement, we get an expression for the quantum well with the dispersion relation:

$$E=\frac{\hbar^2\left(k_x^{\,2}+k_y^{\,2}\right)}{2m^*}+\frac{\hbar^2v^2 4\pi^2}{L_z^2 2m^*}\quad\left(k_z=\frac{v2\pi}{L_Z}\right)$$

Silicon Parabolic Conduction Band Approximation



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

Taylor Approximation for Nano-Tubes

45:25

• In carbon nano-tubes recall the expression for energy $E = E_0 \pm h_0$, where

$$h_0 = -t\left(1 + 2e^{ikx^a}\cos k_y b\right)$$

• So, to approximate the energy expression we Taylor expand h_0 about the conduction valleys
$(k_x, k_y) = (0, \pm(2\pi)/3b)$

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

$$= \frac{i3a_0t}{2}k_x \pm \frac{3a_0t}{2}\left(k_y \pm 2\pi/3b\right) = \frac{i3a_0t}{2}\left(k_x \pm i\beta_y\right),$$

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

• Thus,

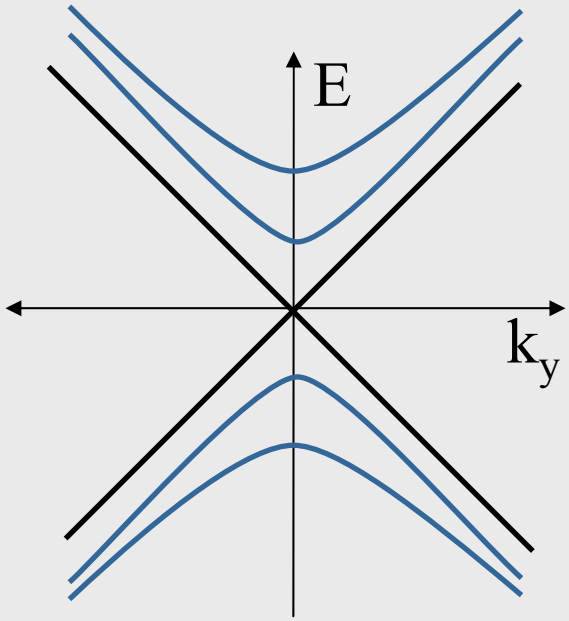
$$E = E_0 \pm \frac{3ta_0}{2}\sqrt{k_x^2 + \beta_y^2}$$

• This parabolic expression, just as with silicon, provides a good model of the conduction properties of graphite and the descretized carbon nano-tubes (e.g. Let $k_y = v2\pi/2mb$)

• Furthermore, this model accurately estimates conduction characteristics for folding in any direction.

Closing Comments

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



Next Lecture: Density of States (DOS)