Quantum Transport:
Atom to Transistor

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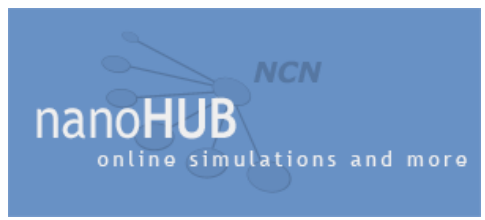
Lecture 21: Subbands: Density of States

Ref. Chapter 6.2

Network for Computational Nanotechnology



Introduction

00:00

• In this lecture we develop the concept of subbands, introducing what is known as the “Density of States” (DOS)

• We have considered how subbands are formed in low dimensional structures. It is not an abrupt process, even for bulk solids there is a quantization of the E-k space. However at this scale the granularity is extremely fine and is not experimentally perceptible.

• An excellent illustration of this process is the carbon nanotube

• The creation of subbands is not abrupt, going from nanotubes with very large diameters to those with small diameters, one would see a gradual, almost linear, process of creating experimentally discernable subbands. Remember, subbands become important experimentally only when the energy difference between them becomes greater than or comparable to the thermal energy $k_B T$

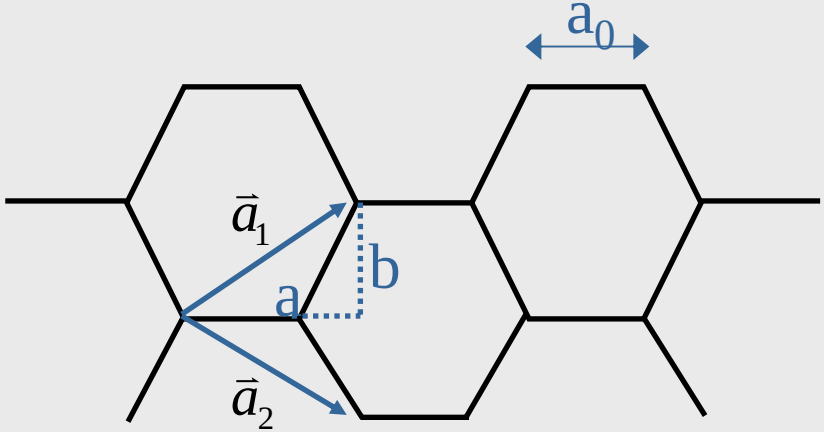
Prelude to Graphite DOS I

03:57

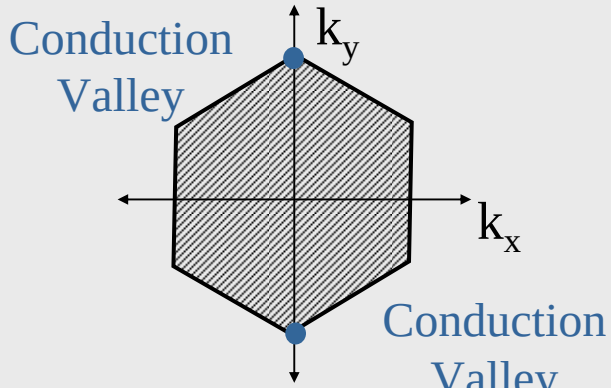
• So, how does one go from an E-k diagram to an expression for the density of states (DOS)?

• We will derive DOS for graphite but first lets review the basic properties of graphite

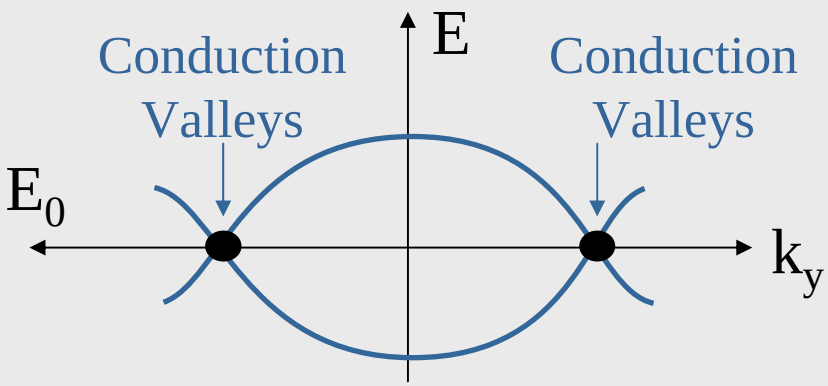
• Recall it has a structure of…



• And a Brillouin Zone of the form…



… where the above conduction points appear in the E-k diagram as…



Prelude to Graphite DOS II

07:07

• Recall, given $E = E_0 \pm h_0$ we Taylor expand h_0 about the conduction points

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

• Expanding and solving

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

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

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

• Finally we get

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

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

• The above parabolic 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.

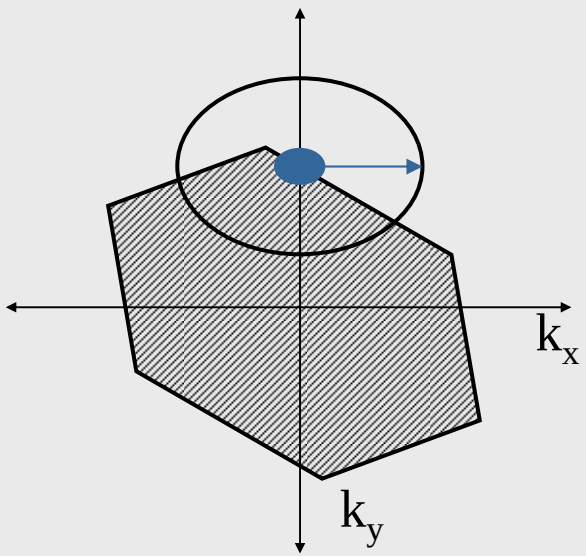
Prelude to Graphite DOS III

13:00

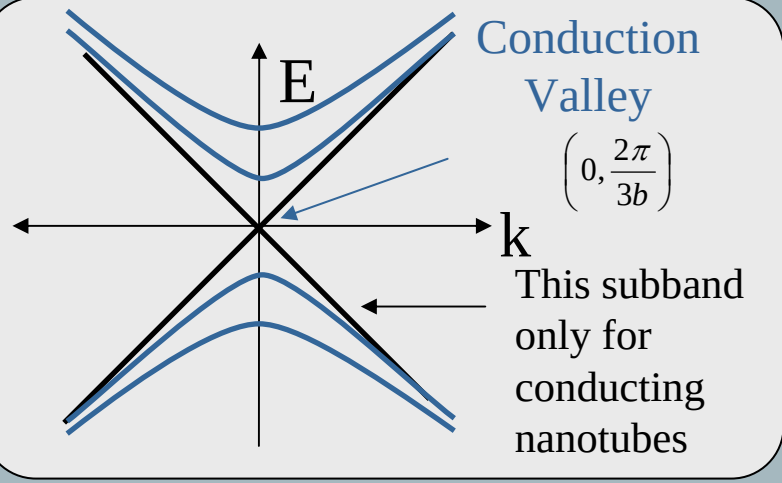
• The approximation, as shown,

$$h_0(\vec{k}) \approx at\left(ik_x + \beta_y\right)$$

is a Taylor expansion about the upper most conduction point…



• The resulting eigenvalues give rise to subband diagrams of the form (for discretized k_x or k_y in a nanotube)



• Recall, the same is done for silicon, we implement a parabolic expansion about the lowest point in the conduction band

Counting Graphite Electron States

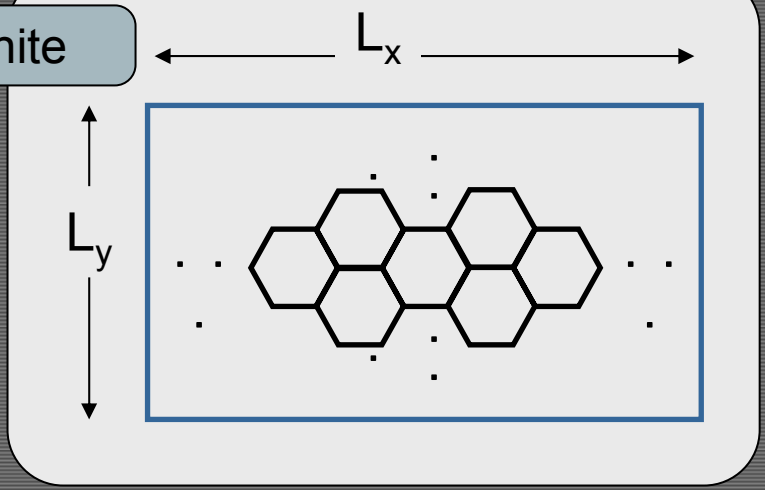
18:33

- Now, let's move onto a derivation of the density of states in graphite

- To begin, how do we count the number of states?

- First assume graphite is a large sheet of dimensions L_x by L_y. Therefore, the surface area of the solid is L_xL_y.

Sheet of Graphite



- All states in this structure will be separated by the unit distances $2\pi/L_x$ and $2\pi/L_y$ (k-space)
- How many states will lie in a given k-space area "A_k"?

let $A_k = dk_x dk_y$, $\therefore$ # of states $= N(k) = \dfrac{dk_x dk_y}{2\pi/L_x \cdot 2\pi/L_y}$

Note: Multiply by 2 to include spin degeneracy

Graphite Density of States

22:44

• Usually, we are interested in how many states lie within a region of radius k, such that

$$N(k) = \pi k^2 \, S/4\pi^2$$

where s is the surface area of a 2-D material such as graphite

• By nature, of course, we wish to express N in terms of energy. For graphite we use

$$k \approx \sqrt{k_x^2 + \beta_y^2} \text{ and}$$

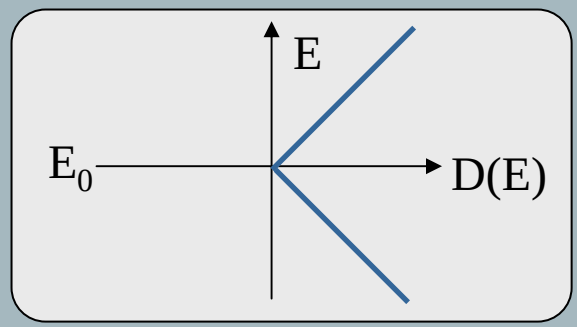
$$E = E_0 \pm at\sqrt{k_x^2 + \beta_y^2}$$

$$\therefore N(E) = \frac{S}{4\pi}\left(\frac{E - E_0}{at}\right)^2$$

• To get the density of states simply take the derivative of N(E) with respect to E

$$D(E) = \frac{\partial N(E)}{\partial E} = \frac{S}{2\pi a^2 t^2}(E - E_0)$$

• Thus, for graphite D(E) is linear with respect to energy

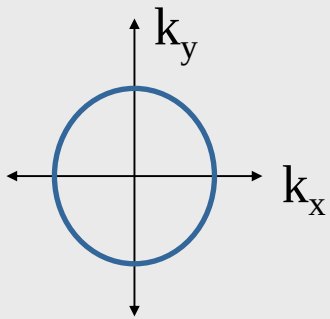


… this is exactly what people measure experimentally using a scanning tunneling microscope.

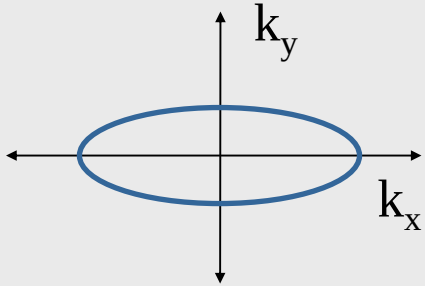
Carbon Nanotube DOS I

27:00

• *Note: In the case of graphite an isotropic constant energy contour was assumed (circle)*



• This need not necessarily be the case, for Silicon the energy contour is an ellipse



and with some complication, D(E) may be solved in much the same manner.

• So, what happens to the graphite DOS when we roll a graphite sheet into a carbon nanotube?

• Recall, when rolling in the $\hat{y}$ direction k_y becomes discrete. Such that for the circumferential vector it is required that $\vec{C} = 2mb\hat{y}$

$$\vec{k} \cdot \vec{C} = k_y 2mb = 2\pi v$$

And the resulting 'zig-zag' nanotube is only conducting if m is a multiple of 3, since

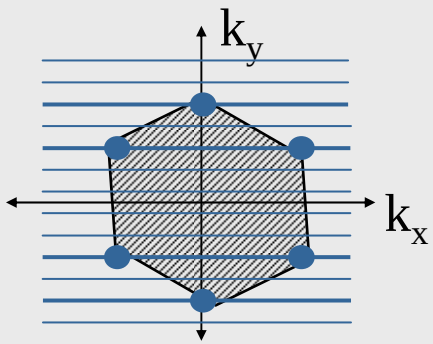
$$k_y = \frac{2\pi}{3b}\frac{3v}{2m}$$

Carbon Nanotube DOS II

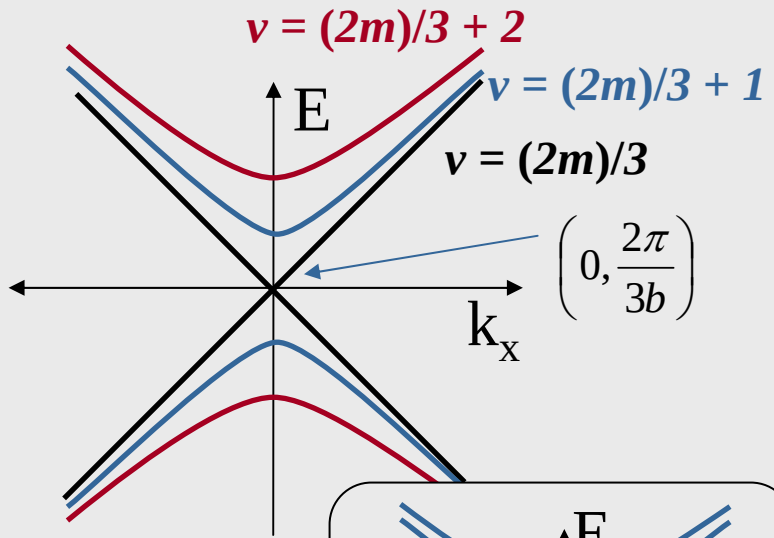
32:15

Zig-Zag Conducting Carbon Nanotube k-Space

• As shown in previous lectures, we can draw the subbands for various values of *v*…



Conducting Nanotube (m=3n)
n: integer

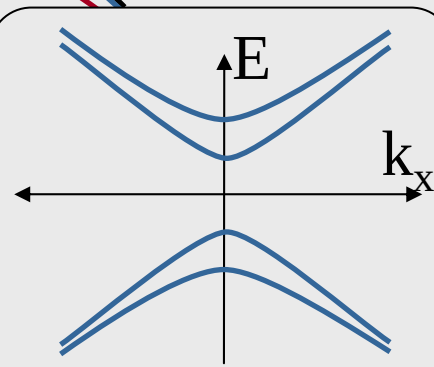


• A general energy expression for a $\hat{y}$ fold, zig-zag, nanotube is

$$E_v(k_x) = E_0 \pm \sqrt{k_x^{\,2} + k_v^{\,2}}$$

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

Semi-Conducting Nanotube (m≠3n)



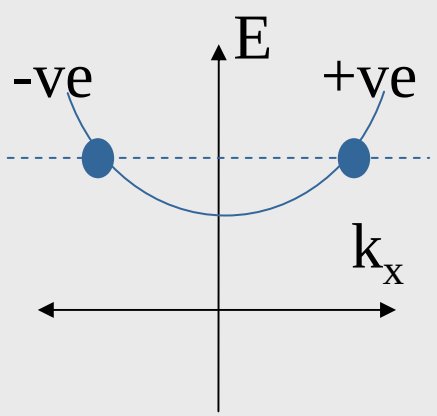
Counting Nanotube States

39:00

• Because the nanotube is a 1-D structure, or quantum wire, to count the number of states we look at how many states lie in a distance k from the origin. Formally, for the zig-zag nanotube, this is

$$N(k_x) = 2\left(L/2\pi\right)k_x$$

Note: The extra factor of 2 is added to count the +ve and –ve k states



• To express the number of states as a function of energy assume $E_0 = 0$, such that

$$N(E) = \frac{L}{\pi}\sqrt{\frac{E^2}{a^2t^2} - k_v} = \frac{L}{\pi at}\sqrt{E - a^2t^2k_v^{\,2}}$$

• Finally the density of states for a particular sub-band is

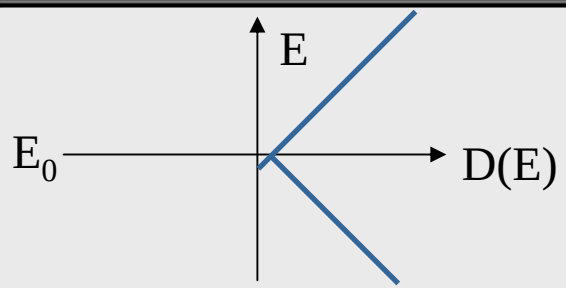
$$D_v(E) = \frac{\partial N_v(E)}{\partial E} = \frac{L}{\pi at}\frac{E}{\sqrt{E^2 - a^2t^2k_v^2}}$$

• To get the total density of states we must sum over all sub-bands

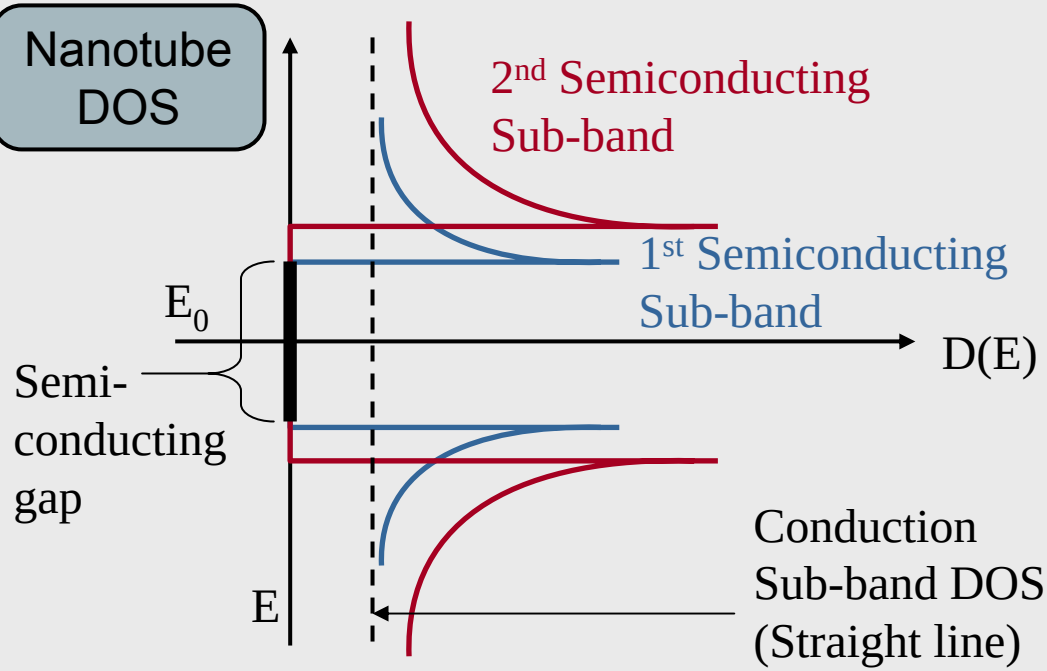
$$D(E) = \sum_v D_v(E)$$

Carbon Nanotube DOS Appearance

• Now, what does the density of states for a carbon nanotube look like?
• Recall, the linear DOS for graphite…



Nanotube DOS



• For the nanotube something similar occurs, with the exception of spikes that appear at every subband

• Note: for semiconducting nanotubes there is no subband around Fermi level and so the density of states is zero for a region about E_0 (this is marked as the “semiconducting gap” on the above diagram)

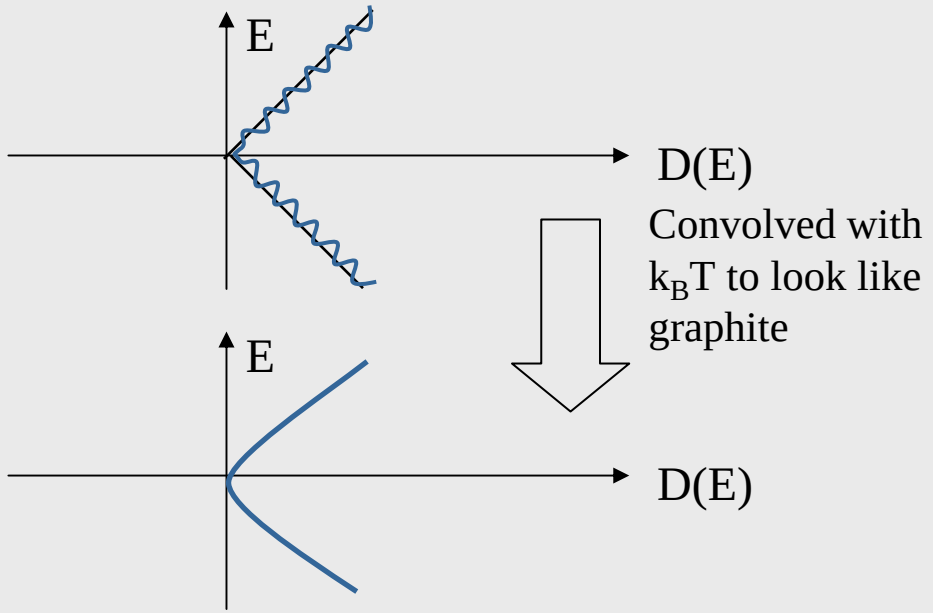
Big Nanotubes

48:30

- The semiconducting DOS gap depends on the size of a nanotube. Those with small diameters have a large gap and those with large diameters have a small gap

- Hence, nanotubes with a large diameter begin to look like graphite! This is especially true at high temperatures, the jagged appearance of D(E) is made smooth via convolution with $k_B T$

Big Nanotube DOS



Next Lecture: Minimum resistance of a wire