

Session 10

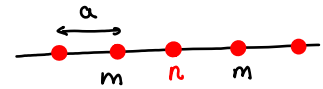
Note Title

10/15/2008

We discuss in this lecture about subbands. We learned that a periodic lattice results in a periodic Hamiltonian that greatly helps to simplify the eigenvalue matrix $h(\vec{k})$:

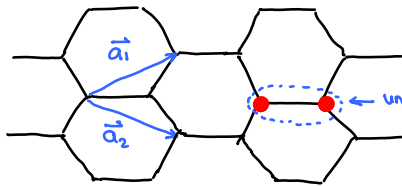
$$[h(\vec{k})] = \sum_m [H_{nm}] e^{i\vec{k} \cdot (\vec{d}_m - \vec{d}_n)}$$

\downarrow sum over neighbors, m
 \downarrow a given unit cell, n



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

For graphite, we had a 2D structure due to base coupling between the planes.



← we need a two atom unit cell to define the whole lattice in a periodic way. we use unit vectors \vec{a}_1 and \vec{a}_2 . Any site may be located by:

$$\vec{R} = m\vec{a}_1 + n\vec{a}_2 \quad m, n \text{ are integers.}$$

In general one may use 4 basis orbitals per Carbon atom: S, P_x, P_y, P_z .

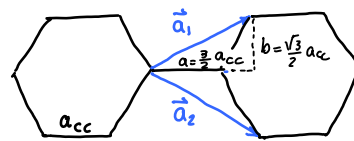
So 4 orbitals \times 2 atoms per unit cell gives an 8×8 $[h(\vec{k})]$.

If we simply only use P_z , as what we did before, we get: $[h(\vec{k})] = \begin{bmatrix} E_0 & h_0 \\ h_0 & E_0 \end{bmatrix}$ 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:

$$a_1 = a\hat{x} + b\hat{y} = \frac{3}{2} a_{cc} \hat{x} + \frac{\sqrt{3}}{2} a_{cc} \hat{y}$$

$$a_2 = a\hat{x} - b\hat{y} = \frac{3}{2} a_{cc} \hat{x} - \frac{\sqrt{3}}{2} a_{cc} \hat{y}$$



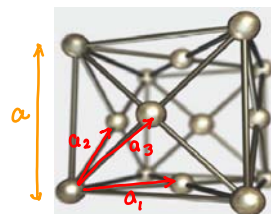
All common semiconductors have a diamond lattice structure consisting of 2 interpenetrating FCC lattices.

The basis vectors for fcc are:

$$a_1 = \frac{a}{2} (\hat{x} + \hat{y})$$

$$a_2 = \frac{a}{2} (\hat{y} + \hat{z})$$

$$a_3 = \frac{a}{2} (\hat{x} + \hat{z})$$



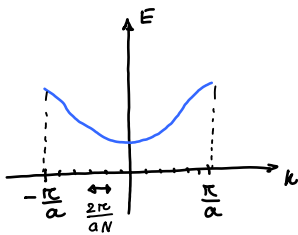
FCC lattice (face centered cubic)

In diamond (two interpenetrating FCC), the spacing between the atoms in each unit cell is $(\frac{a}{4}, \frac{a}{4}, \frac{a}{4})$.

Using 4 ($s3p$) or 5 ($s3ps^*$) basis orbitals we can describe the bandstructure of common semiconductors.

Where the Fermi energy E_f is in relation to the energy levels?

Remember for a simple 1D we had a band diagram that looked like:

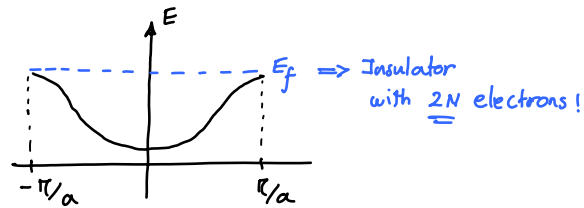
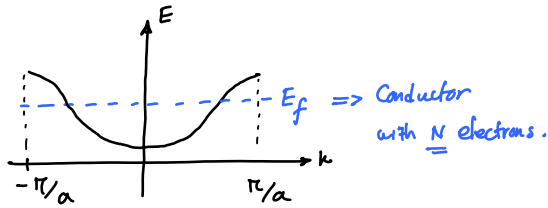


if we have N lattice points in a solid, there will be N values along the k -axis between $(-\frac{\pi}{a}, \frac{\pi}{a})$. So including spin, these levels can hold $2N$ electrons.

N lattice points $\Rightarrow 2N$ energy levels available for electrons.

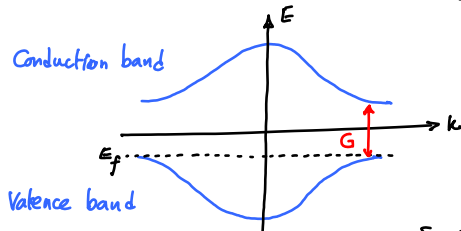
The position of E_f is determined by the number of electrons. E_f (and not the number of electrons) determines the conduction/insulation properties of a solid.

For example:



Another Example:

Take a lattice with 2 atoms per unit cell and 1 electron per atom. So given N lattice sites we have $2N$ electrons and the Fermi energy appears between the valence and conduction bands.



2 atoms per unit cell
1 basis func. per atom \rightarrow 2 basis functions \rightarrow 2 bands

N lattice points $\rightarrow 2(\text{spin}) \times N$ energy levels at each band

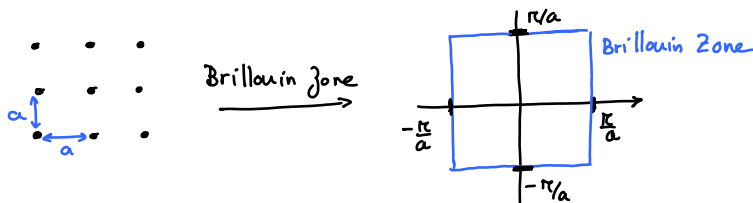
So $2N$ electrons fill only the valence band.

G is the energy gap. It determines the conduction properties of the material.

Big $G \Rightarrow$ insulator Small $G \Rightarrow$ Conductor

Where is the Brillouin Zone?

Note that $e^{i(k + \frac{2\pi}{a})na} = e^{ikna}$ for all n . Now let's consider a 2D square lattice:



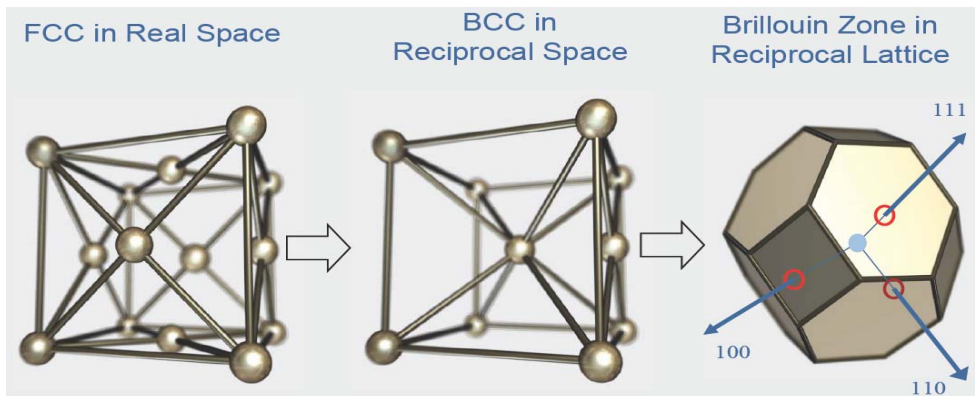
In general, given a real-space basis $R = m\vec{a}_1 + n\vec{a}_2 + p\vec{a}_3$ $m, n, p = 0, 1, 2, \dots$

the reciprocal k -space lattice is formed by: $K = M\vec{A}_1 + N\vec{A}_2 + P\vec{A}_3$ $M, N, P = 0, 1, 2, \dots$

and $\vec{A}_j \cdot \vec{a}_i = 2\pi \delta_{ij} \Rightarrow$

$$A_1 = \frac{2\pi (\vec{a}_2 \times \vec{a}_3)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \quad A_2 = \frac{2\pi (\vec{a}_3 \times \vec{a}_1)}{\vec{a}_2 \cdot (\vec{a}_3 \times \vec{a}_1)} \quad A_3 = \frac{2\pi (\vec{a}_1 \times \vec{a}_2)}{\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)}$$

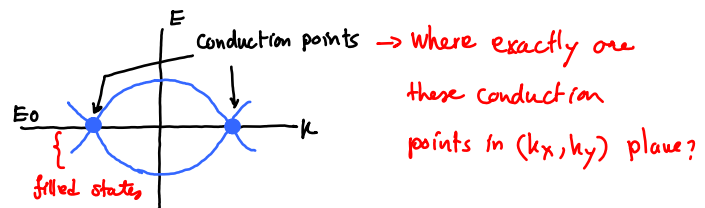
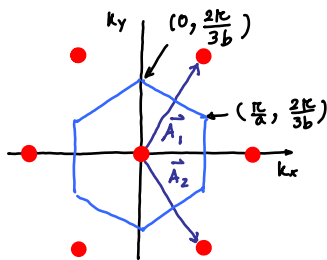
For example, FCC in real space becomes a BCC in k-space:



For example, for graphite we have:

$$\left\{ \begin{array}{l} \vec{a}_1 = \frac{3}{2} a_c \hat{x} + \frac{\sqrt{3}}{2} a_c \hat{y} \\ \vec{a}_2 = \frac{3}{2} a_c \hat{x} - \frac{\sqrt{3}}{2} a_c \hat{y} \\ \vec{a}_3 = \hat{z} \end{array} \right. \rightarrow \left\{ \begin{array}{l} \vec{A}_1 = \frac{\pi}{a} \hat{x} + \frac{\pi}{b} \hat{y} \\ \vec{A}_2 = \frac{\pi}{a} \hat{x} - \frac{\pi}{b} \hat{y} \\ \vec{A}_3 = c \hat{z} \end{array} \right.$$

So the reciprocal lattice & Brillouin zone look like:

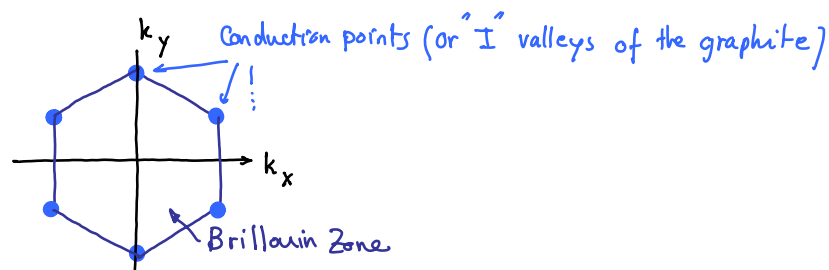


We know $E = E_0 \pm |h_0|$. Conduction happens when $E = E_0$ or $h_0 = 0$. So:

$$h_0 = t(1 + e^{ik_x a} + e^{ik_y b}) = t(1 + e^{ik_x a} (e^{iky b} + e^{-iky b})) = t(1 + 2e^{ik_x a} \cos ky b) = 0$$

$$1 + 2 \cos ky b (\cos k_x a + i \sin k_x a) = 0 \Rightarrow \underbrace{1 + 2 \cos ky b \cos k_x a}_0 + i \underbrace{\cos ky b \sin k_x a}_0 = 0 \Rightarrow$$

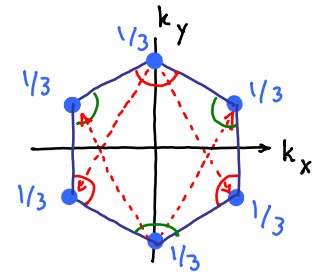
$\Rightarrow (k_x a, k_y b) = (0, \pm \frac{2\pi}{3}) (\pi, \pm \frac{\pi}{3}) (-\pi, \pm \frac{\pi}{3})$ which are the six corners of the BZ:



Notice that there are actually 2-valleys (NOT 6!).

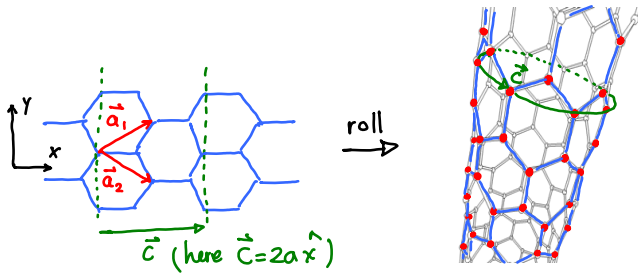
This is because for 4 of the valleys can be formed by reciprocal lattice vector from the other two. \rightarrow

So each corner contributes $1/3$ of the conduction.



Subbands in nanostructures

Consider rolling up graphite and making a nanotube.



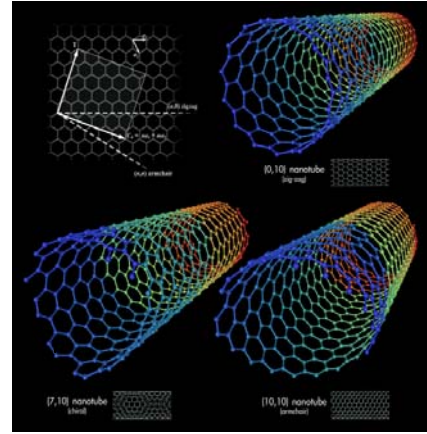
\vec{C} : Circumferential vector denote the direction and length.

In general $\vec{C} = 2am\hat{x}$ $m=1, 2, 3, \dots$

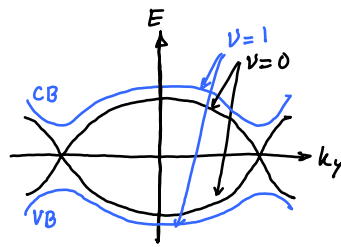
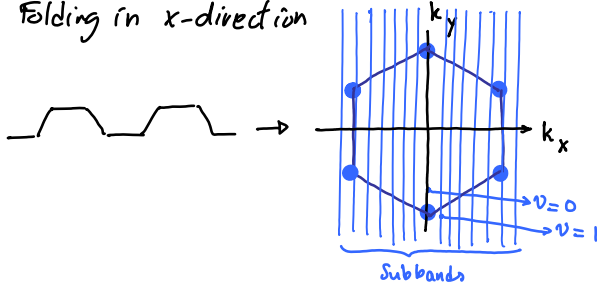
This results in real periodic BCs (perhaps the only real periodic BC!).

So we have: $\vec{k} \cdot \vec{C} = 2\pi v$ $v=0, \pm 1, \pm 2, \dots$

$k_x \cdot 2am = 2\pi v \rightarrow k_x = \frac{2\pi v}{2am}$ these are parallel lines to k_y :



Folding in x-direction



E_f lies above the VB.

So for $v=0$, CNT

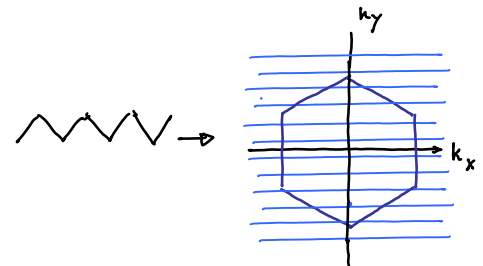
is conductor and for $v=1$

it is either semiconductor or insulator.

It is also possible to fold a nano-tube such that no subband passes through the conduction valleys, like by folding in \hat{y} direction:

A CNT will only conduct if one of the subbands passes through one of the six corners of the BZ.

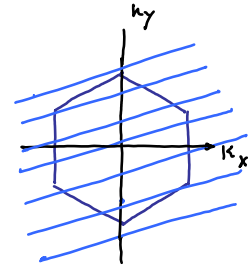
So condition for conduction is:



$$\frac{2\pi v}{2mb} = \frac{2\pi}{3b} \text{ or } \frac{v}{2m} = \frac{1}{3} \rightarrow \text{a Zig-Zag CNT will be conductor iff } m \text{ is a multiple of } 3!$$

In general we can fold CNT in any direction:

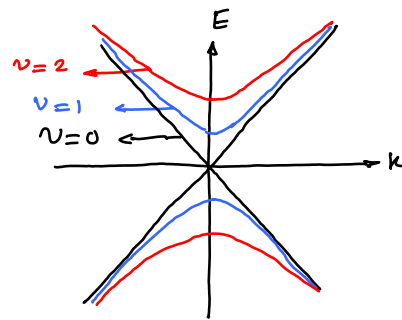
$$\vec{C} = m\vec{a}_1 + n\vec{a}_2 \quad m, n = 0, \pm 1, \pm 2, \dots$$



and $(m-n)$ must be a multiple of three for metallic properties to happen.

So subbands discretize k -space and lead to finite number of E - k diagrams corresponding to each value of v .

We are often 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.



Consider now a nanowire in the x direction:

periodic BC for L_z and L_y results in:

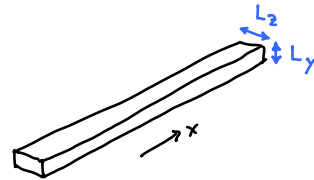
$$k_z = \frac{2\pi}{L_z} v \quad k_y = \frac{2\pi}{L_y} v'$$

So the energy is: $E_{v,v'}(k_x) = E(k_x, k_y = \frac{2\pi}{L_y} v', k_z = \frac{2\pi}{L_z} v)$

For a quantum dot we also have discretization in k_x :

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

quantum dots are often referred as **artificial atoms**.



Question: When do constraints lead to experimental observables?

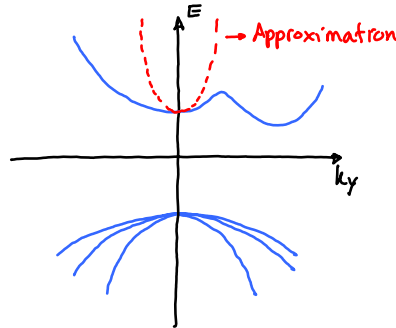
Answer: Quantization must be compared to thermal energy, $k_B T$. because the thermal energy tends to smooth out the difference between energy levels, quantization

of $k_{x,y,z} = \frac{2\pi v}{L_{x,y,z}}$ must be larger or comparable to $k_B T$ to experimentally show itself.

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

For example, for Silicon using parabolic approximation:

$$E(k_x, k_y, k_z) = \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2}{2m^*} (k_x^2 + k_y^2 + k_z^2) \quad \text{where } m^* \text{ is the effective mass.}$$



With z confinement we get a Quantum well and have:

$$E = \frac{\hbar^2}{2m^*} (k_x^2 + k_y^2) + \frac{\hbar^2}{2m^*} \left(\frac{2\pi v}{L_z} \right)^2$$

With z and y confinement we have a Quantum wire:

$$E = \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2 4\pi^2}{2m^*} \left(\frac{v^2}{L_z^2} + \frac{v'^2}{L_y^2} \right)$$

and for $x, y,$ and z confinement we have a Quantum dot:

$$E = \frac{\hbar^2 4\pi^2}{2m^*} \left(\frac{v^2}{L_z^2} + \frac{v''^2}{L_y^2} + \frac{v'''^2}{L_x^2} \right)$$

For example for CNT, we can derive a parabolic expression via Taylor expansion.

$$E = E_0 \pm \hbar \omega$$

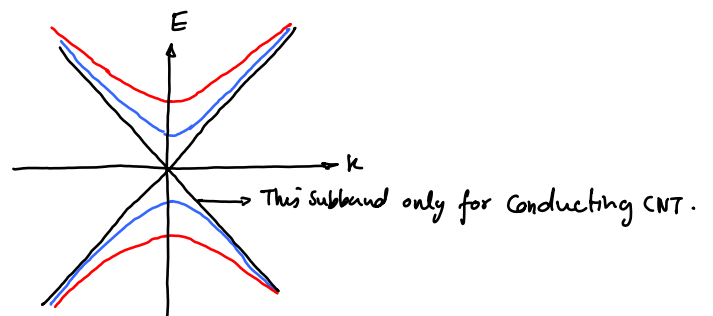
$$\hbar \omega = -t \left(1 + 2e^{ik_x a} \cos k_y b \right) \quad \text{expand } \hbar \omega \text{ around } (k_x, k_y) = \left(0, \pm \frac{2\pi}{3b} \right)$$

$$\hbar \omega \approx k_x \left. \frac{\partial \hbar \omega}{\partial k_x} \right|_{\left(0, \pm \frac{2\pi}{3b} \right)} + \left(k_y \pm \frac{2\pi}{3b} \right) \left. \frac{\partial \hbar \omega}{\partial k_y} \right|_{\left(0, \pm \frac{2\pi}{3b} \right)} = \frac{i3a_0 t}{2} k_x \pm \frac{3a_0 t}{2} \left(k_y \pm \frac{2\pi}{3b} \right) = \frac{i3a_0 t}{2} (k_x \pm i\beta_y) \quad \text{where } \beta_y = k_y \pm \frac{2\pi}{3b}$$

Thus:

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

$$\left(a = \frac{3}{2} a_0 \right)$$



Density of states

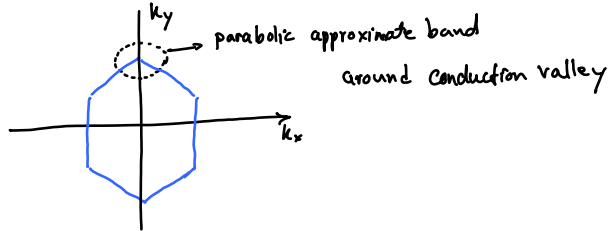
We learned how subbands are formed in nanostructures. In fact, subband formation is not sudden. Even in bulk material we have subbands. But as we make the material smaller, the subbands' separation increases. But the question now is how do we find DOS from E-k diagram?

Let's again consider graphite. We derived an approximate parabolic band with:

$$h_0(\vec{k}) \cong t a (i k_x + \beta_y)$$

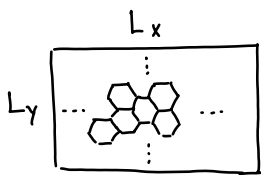
$$\text{where } \beta_y = k_y - \frac{2\pi}{3b}$$

$$E(k) = E_0 \pm |h_0|$$



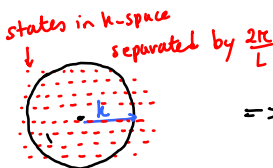
We want to know how many states are available per unit energy:

$$\text{DOS} = \# \text{ of state / unit energy}$$



$$\begin{aligned} \text{k-space} \rightarrow \frac{2\pi}{L_x} \times \frac{2\pi}{L_y} \Rightarrow \# \text{ state in region } d k_x d k_y &= \frac{d k_x d k_y}{\frac{2\pi}{L_x} \frac{2\pi}{L_y}} \times 2 = \frac{S}{2\pi^2} d k_x d k_y \\ & \text{spin} \quad \text{2D area in real space} \end{aligned}$$

usually we like to know how many states are in a region of radius k:



$$\Rightarrow N(k) = \frac{\pi k^2}{\frac{2\pi}{L_x} \frac{2\pi}{L_y}} \times 2 = 2\pi k^2 \frac{S}{4\pi^2}$$

we wish to express $N(k)$ in terms of energy:

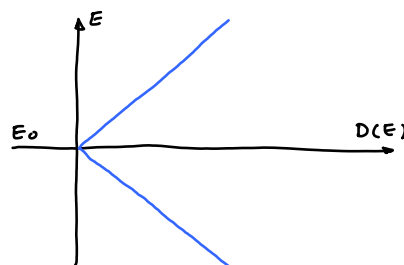
$$E = E_0 \pm a t \sqrt{k_x^2 + \beta_y^2}$$

$$k \cong \sqrt{k_x^2 + \beta_y^2} \rightarrow N(E) = \frac{S}{2\pi} (k_x^2 + \beta_y^2) = \frac{S}{2\pi} \left(\frac{E - E_0}{a t} \right)^2$$

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

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

This is exactly what people measure experimentally using a scanning tunneling microscope!



So what happens to the graphite DOS when we roll a graphite sheet into a CNT?

When rolling in \hat{y} direction, k_y becomes discrete:

$\vec{C} = 2mb\hat{y} \rightarrow$ Zig Zag CNT \rightarrow conducting only if m is a multiple of 3, since:

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

A general energy expression for a \hat{y} -fold, zig-zag CNT is:

$$E_v(k_x) = E_0 \pm \sqrt{k_x^2 + k_v^2} \quad \text{where } k_v = \frac{2\pi}{3b} \left(\frac{3v}{2m} - 1 \right)$$

Since CNT is a 1D structure, or a nanowire, we look at the number states that lie in a distance k from the origin. For zig-zag CNT:

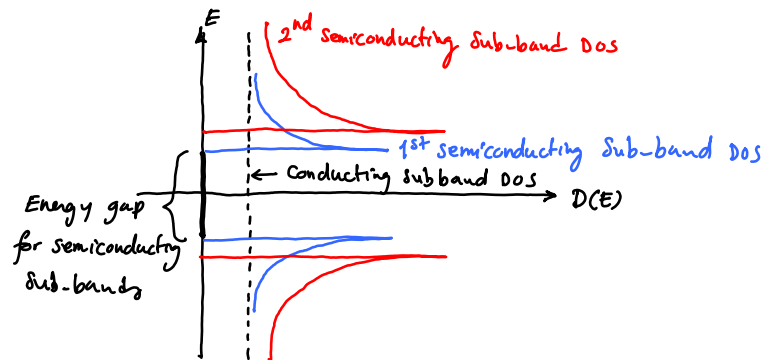
$$N(k_x) = 2 \frac{k_x}{\frac{2\pi}{L}} = \frac{L}{\pi} k_x$$

And in terms of energy assume E_0 , such that

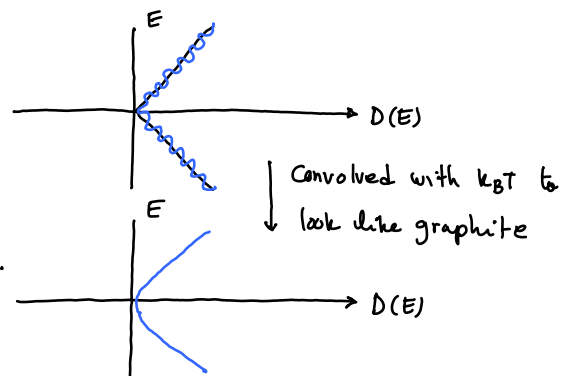
$$N_v(E) = \frac{L}{\pi} k_x = \frac{L}{\pi} \sqrt{\frac{E^2}{a^2 t^2} - k_v^2} = \frac{L}{\pi a t} \sqrt{E - a^2 t^2 k_v^2}$$

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

To get the total DOS, we must sum over all sub-bands: $D(E) = \sum_v D_v(E)$




The semiconducting DOS gap depends on the size of the CNT. For small diameter CNTs, the gap is large and for large CNTs, it is small. CNT with large diameter start to look like graphite! This is specially true at high Temperature. The jagged DOS is made smooth via convolution with $k_B T$.



Subbands and Conductance

Recall we discussed the minimum resistance in the FET channel. The minimum resistance comes from the contact resistance. For smaller devices this resistance becomes more important.

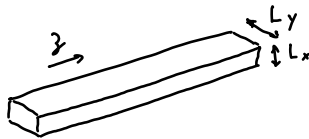
$$R_{min} = \frac{h}{2e^2} \approx 12.9 \text{ k}\Omega$$


Note that this resistance can not be reduced by improving the contact. *There is a minimum contact resistance.*

But shouldn't the resistance decrease as the cross section area increases? Yes, as we increase the channel cross section, the number of modes increases, so the resistance decreases:

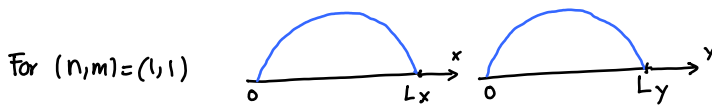
$$R_{min} = \frac{h}{2e^2} \frac{1}{M} \quad \text{M is the number modes available at given Fermi energy, i.e. } M(E_f)$$

Example: What does the density of states and modes distribution look like for a quantum wire?

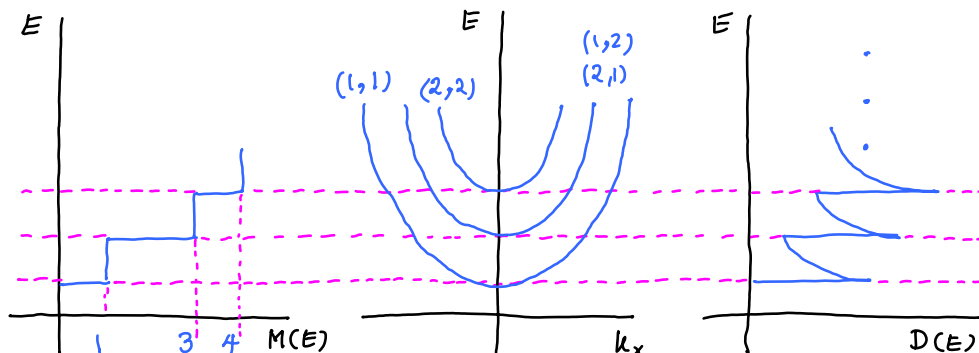


$$E = \frac{\hbar^2 k_z^2}{2m} + \frac{\hbar^2}{2m} \left(\frac{n\pi}{L_x}\right)^2 + \frac{\hbar^2}{2m} \left(\frac{m\pi}{L_y}\right)^2 \quad n, m = 1, 2, 3, \dots$$

The quantized wavefunctions in the x and y directions look like:



The DOS peaks where each subband is crossed versus energy. The mode distribution has a staircase distribution increasing by integer amounts of 1 or more depending on the degeneracy of the subband:



Example Calculate the current in a QW of length L .

First the number of electrons available for

conduction is given by:

$$n = \sum_{k_x \text{ in current}} |\phi|^2 = \sum_{k_x} \frac{1}{L}$$

$$I = env = \sum_{k_x} e \frac{1}{L} v_x = \frac{e}{L} \sum_{k_x} v_x(k_x)$$

For a long wire, this sum can be written in integral form:

$$I = \frac{e}{L} \int \frac{dk_x}{2\pi/L} v(k_x)$$

↳ Recall the spacing between two points in k -space is $\frac{2\pi}{L}$

$$\text{Velocity is also: } v_x(k_x) = \frac{\hbar k_x}{m}$$

$$\rightarrow I = \frac{e\hbar}{2\pi m} \int k_x dk_x \quad \text{to make the integral over energy, we use the } E(k):$$

$$E(k_x) = \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2}{2m} \left(\frac{n\pi}{L_y}\right)^2 + \frac{\hbar^2}{2m} \left(\frac{m\pi}{L_z}\right)^2 \quad n, m = 0, 1, 2, \dots \Rightarrow dE = \frac{\hbar^2}{m} k_x dk_x$$

$$\rightarrow I = e \int \frac{dE}{2\pi\hbar} = \frac{e}{h} \int_{\epsilon_2}^{\epsilon_1} dE = \frac{e}{h} (\epsilon_1 - \epsilon_2) = \frac{e^2}{h} v \quad \text{where } v \text{ is the bias voltage.}$$

So the current carried by electrons in a certain energy range is $\frac{e}{h}$ multiplied by that energy range.

For this example $\int dE = \epsilon_1 - \epsilon_2 = eV$. Since only positive velocity states are occupied between ϵ_1 and ϵ_2 , this represents the excess positive going electrons. Below ϵ_2 both the positive and negative velocity states are equally occupied, hence, their contributions cancel.

We also notice that the current carried by a subband is independent of the subband shape, it need not be parabolic, the relation $I = \frac{e}{h} \int dE$ holds for all cases! This is because the correct velocity is the group velocity:

$$v_x(k_x) = \frac{1}{\hbar} \frac{\partial E}{\partial k_x} \rightarrow I = e \int \frac{dk_x}{2\pi} v_x = e \int \frac{dk_x}{2\pi\hbar} \frac{\partial E}{\partial k_x} = \frac{e}{h} \int dE$$

The total current is the sum of contributions from all the modes:

$$I = \frac{e}{h} (\epsilon_1 - \epsilon_2) M(E_f)$$

