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
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.
• Remember, graphite has the structure

where, \( \bar{a}_1 = a\hat{x} + b\hat{y} \) and \( \bar{a}_2 = a\hat{x} - b\hat{y} \).

• The E-k diagram can be sound by

\[
\begin{bmatrix}
E_0 & h_0 \\
h_0^* & E_0
\end{bmatrix}
\]

\[
h_0 = -t \left( 1 + e^{ik_x \bar{a}_1} + e^{ik_x \bar{a}_2} \right) = -t \left( 1 + 2e^{ik_x a} \cos k_y \right)
\]

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…
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 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.

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.
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

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

- This is how constraints along a given dimension result in subbands. \textit{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.}

- For $v = 1$ and $v = 0$ the Fermi energy lies above the valence band. \textit{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.}
It is possible to fold a nano-tube such that it has no subband passing through 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!
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.

Subbands in direction \( \vec{c} = m\vec{a}_1 + n\vec{a}_2 \):

As stated earlier, subbands discretize k-space and lead to a finite number of E-k diagrams corresponding to specific values of \( \nu \). 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.

Assume an isotropic k-space near the Fermi level.
• 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 $k_z = (v 2\pi) / L_z$ 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 $k_y = (\nu' 2\pi)/L_y$ and the E-k function

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

Note: a carbon nano-tube is really, in the general sense, a form of quantum wire!
• Finally, confinement in the x-direction as well leads to a quantum dot

\[ k_x = \left( v'' \cdot 2\pi \right) / L_x \]

such that the E-k behavior is given by

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

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 \( k_B T \). Because the thermal energy tends to smooth out the difference between energy levels, the discretization corresponding to

\[ k_{x/y/z} = (q \cdot 2\pi) / L_{x/y/z} \]

must be bigger than or comparable to \( k_B T \) to experimentally show itself.

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

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

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

$$E = \frac{\hbar^2(k_x^2 + k_y^2)}{2m^*} + \frac{\hbar^2v^24\pi^2}{L_z^22m^*} \left(k_z = \frac{v2\pi}{L_z}\right)$$

• For nano-tubes we can derive a similar parabolic expression via a Taylor series expansion that approximates the subbands near the conduction valleys.
In carbon nano-tubes recall the expression for energy $E = E_0 \pm h_0$, where

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

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

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

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

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

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 discretized carbon nano-tubes (e.g. Let $k_y = \sqrt{2\pi/2mb}$)

Furthermore, this model accurately estimates conduction characteristics for folding in any direction.
Commonly, the carbon nanotube E-k diagrams, about the conduction points, given by this model look like.

Next Lecture: Density of States (DOS)