Nanotube Calculations

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1 Density of states

The 1D dispersion relation of a nanotube is obtained by simply slicing the 2D graphene cone with a line in k space offset by some vector k_0:

$$E = \pm\hbar v_F \sqrt{k_x^2 + k_0^2}$$

where the Fermi velocity v_F is given by:

$$v_F = \frac{3\gamma_0 a_0}{2\hbar}$$

a_0 is the C-C bond length and γ_0 is the tight binding nearest neighbour energy overlap integral. (Note: similar formulas appear with a $\sqrt{3}$ when a_0 is defined as lattice constant instead of the bond length.) The relation between the offset k_0 and the bandgap E_g is:

$$E_g = 2\hbar v_F k_0$$

For semiconducting (large band gap) tubes, the band gap is determined only by the tube diameter:

$$E_g = \frac{\gamma_0 a_0}{d}$$

The density of states is given by:

$$\frac{dN}{dE} = \left(\frac{L}{2\pi}\right)^d \oint_{FS} \frac{d\vec{S}}{|\nabla_k E|} = 2 \cdot \frac{L}{2\pi} \cdot \frac{4}{|dE/dk|}$$

The first factor of two is from spin, and the factor of 4 is from the plus and minus k branches of each cone plus the $K - K'$ degeneracy. Using the energy expression above, we get:

$$\left|\frac{dE}{dk}\right| = \frac{\hbar v_F k}{\sqrt{k^2 + k_0^2}} = \hbar v_F \, \frac{\sqrt{E^2 - (E_g/2)^2}}{E}$$

Defining $n = N/L$ as the linear electron density and using the above expression for v_F, we then have:

$$\frac{dn}{dE} = \frac{8}{3\pi\gamma_0 a_0} \frac{E}{\sqrt{E^2 - (E_g/2)^2}}$$

Putting in a value of $\gamma_0 = 2.9$ eV and $a_0 = 1.42$ Å gives a Fermi velocity of $v_F = 0.95 \times 10^6$ m/s and a density of states of:

$$\frac{dE}{dn} = 0.48 \text{ mV per e}/\mu\text{m}$$

For an electron density of 100 electrons / micron, we get a Fermi energy of 48 mV.

We can also calculate the single particle level spacing for a confined quantum dot of length L in a metallic tube with a hard-wall potential:

$$\Delta E = \hbar v_F \, \frac{\pi}{L} = \frac{h v_f}{2L}$$

An extra factor of 2 is sometimes included in the denomenator assuming that the sub-band splitting between the two K points is exactly $2\Delta E$ (Codben in cond-mat/0112331). In terms of γ_0 and a_0:

$$h v_F/2 = \hbar v_F \pi = \hbar \, \frac{3\gamma_0 a_0}{2\hbar} \, \pi = \frac{3\pi}{2} \, \gamma_0 a_0$$

With $\gamma_0 = 2.9$ eV and $a_0 = 0.142$ nm, corresponding to $v_F = 0.95 \times 10^6$ m/s ($0.00315c$), we get:

$$h v_F/2 = 1940 \text{ meV nm}$$

Thus a 100 nm electrode separation gives a level spacing of 19.4 eV and a 1000 nm separation gives a level spacing of 1.94 eV. Some estimates from papers are: 2 mv for 750 nm (Finkelstein cond-mat/0508401) and 9.3 mV for 180 nm (Sapmaz cond-mat/0411530, $v_F = 8.1 \times 10^6$ m/s).

2 Effective Mass

For semiconducting tubes, the level spacing will be smaller due to the curvature at the bottom of the bands, leading to a light effective mass. The mass depends only on the band gap. We start with the dispersion relation:

$$E = \hbar v_F \sqrt{k^2 + k_0^2} = \hbar v_F k_0 \sqrt{1 + k^2/k_0^2}$$

For $k << k_0$ using $\sqrt{1+x} \approx 1 + x/2$ we get:

$$E = \hbar v_F k_0 + \frac{\hbar v_F}{2k_0} k^2$$

Defining the effective mass as:

$$E = \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar v_F k^2}{2k_0}$$

gives

$$m^* = \frac{\hbar k_0}{v_F}$$

In terms of the band gap $E_g = 2\hbar v_F k_0$ and the bare electron mass m_e, we get:

$$\frac{m^*}{m_e} = \frac{E_g}{2 m_e v_F^2}$$

Using $mc^2 = 0.511 \times 10^6$ eV and $v_F = 0.00315c$, we get $m_e v_F^2 = 5.16$ eV, and we then have:

$$\frac{m^*}{m_e} = \frac{E_g}{2 * 5.12 \text{ eV}}$$

For a 100 mV gap, we get an effective mass of 0.0097 or about 0.01.

3 Tunnel Barrier Resistances

Using the effective mass from the previous section, we can calculate the maximum possible resistance of a tunnel barrier formed in a carbon nanotube as a function of the barrier length.

The maximum barrier height for a nanotube with a band gap of E_g is achieved when the quasi Fermi energy lies in the middle of the band gap, giving a barrier height of $E_g/2$.[1] For a square barrier of length d and height V, the transmission probability is:

$$T(E) = \frac{1}{1 + \frac{V^2}{4E(V-E)} \sinh^2(a/2l)}$$

where l is the probability density decay length and is given by:

$$l = \frac{1}{2}\sqrt{\frac{\hbar^2}{2m(V-E)}}$$

For small tranmission probabilities, this can be approximated as

$$T(E) \approx \frac{16E(V-E)}{V^2} e^{-a/l}$$

which shows the exponential decay we expect with barrier length[2]. The tunnel conductance can be calculated easily for a nanotube using the Landauer formula:

$$G = \frac{2e^2 N}{h} T = \frac{4e^2}{h} T$$

where the factor of two comes from the two valleys ($4e^2/h = 6.35$ kΩ). Here we assume that only one transverse mode in the nanotube is occupied, which is reasonable since the Fermi energy is typically much smaller that the subband splitting. Here are some concrete numbers for a 100 nm barrier:

$Eg = 300$ mV	$V = 150$ mV	$l = 19$ nm	$T_{min} = 2.3 \times 10^{-9}$
$E = 15$ mV	$m = 0.029$		$R_T = 2.72$ GΩ
$Eg = 100$ mV	$V = 50$ mV	$l = 58$ nm	$T_{min} = 0.0015$
$E = 5$ mV	$m = 0.0097$		$R_T = 4.2$ MΩ
$Eg = 20$ mV	$V = 10$ mV	$l = 291$ nm	$T_{min} = 0.39$
$E = 1$ mV	$m = 0.0019$		$R_T = 16$ kΩ
$Eg = 5$ mV	$V = 2.5$ mV	$l = 1167$ nm	$T_{min} = 0.92$
$E = 0.25$ mV	$m = 0.00048$		$R_T = 6.87$ kΩ

[1] For this calculation, we will naively ignore the presence of a nearby valance band, ignoring such possibilities as the virtual tunneling of an electron through a hole state. My intuition is that this may reduce the effective barrier heigth perhaps by a factor of two...

[2] see https://faculty.washington.edu/seattle/physics541/14solved.pdf