Density of States in a Nanotube

G. Steele

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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. 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.