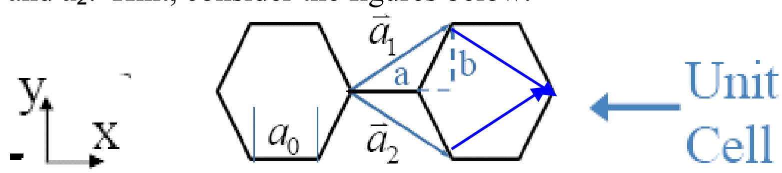
ELEG 667–016; MSEG-667-016 - Solid State Nanoelectronics – Fall 2005

Solution – Revised on Dec 12, 2005

Homework #8 - due Tuesday, 22 November 2005, in class

1. **Carbon Nanotube Structure:** Derive the expressions for the unit vectors of graphene (unrolled nanotube) $\boldsymbol{a_1}$, $\boldsymbol{a_2}$, in terms of the Cartesian unit vectors $\boldsymbol{x}^\wedge$, $\boldsymbol{y}^\wedge$. (a) Using trigonometry, show your calculations for the numerical factors *a* and *b* (e.g. ½ or whatever) in terms of the length of the carbon-carbon bond length, a_o. (b) sketch and indicate the unit cell in real space, which is the parallelogram spanned by $\boldsymbol{a_1}$, and $\boldsymbol{a_2}$. Hint, consider the figures below.

$$\vec{a}_1 = a\hat{x} + b\hat{y}$$
$$\vec{a}_2 = a\hat{x} - b\hat{y}$$



$$\vec{a}_1 = a\hat{x} + b\hat{y} = {}^3\!/_2\, a_0\hat{x} + {}^{\sqrt{3}}\!/_2\, a_0\hat{y}$$
$$\vec{a}_2 = a\hat{x} - b\hat{y} = {}^3\!/_2\, a_0\hat{x} - {}^{\sqrt{3}}\!/_2\, a_0\hat{y}$$

2. **Carbon Nanotube Dispersion:** Consider the dispersion relation for graphene:

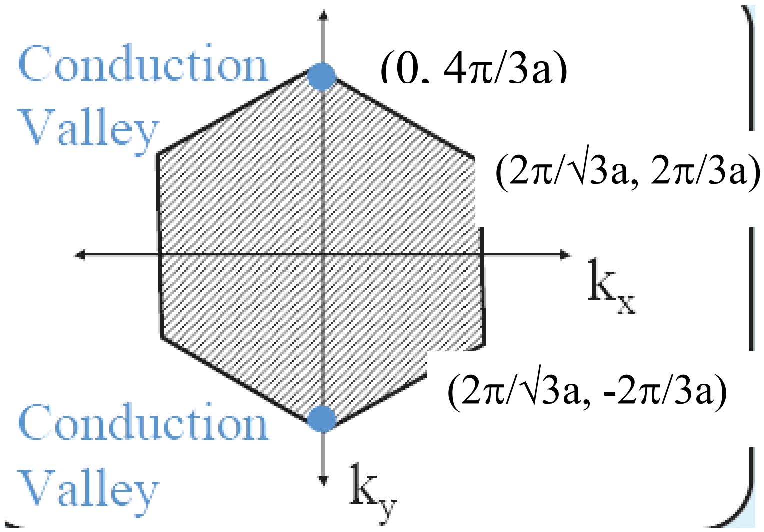
$W(k_x, k_y) = \pm \gamma_o[1+4\cos(\sqrt{3}k_x a/2) \cos(k_y a/2) + 4\cos^2(k_y a/2)]^{½}$,

following the notation in Waser, where $a = \sqrt{3}a_o$ is the length of the unit vector $\boldsymbol{a_i}$, and a_o is the length of the carbon-carbon bond (0.142 nm). Note that this "*a*" differs from the convention used above in question 1. (a) Find the six Fermi level conduction points in k-space (which are the corners of the hexagonal Brillouin zone below) by solving for the k values where $W(k_x, k_y) = 0$. (b) On the hexagonal Brillouin zone, sketch and label the coordinates of these 6 points in terms of *a*, or a_o .

Hint: in the dispersion relation first let $k_x = 0$ and solve for the corner points along k_y; and then let $\sqrt{3}k_x a/2 = \pi$, and get the corners with $k_x \neq 0$. This approach makes it easier to factor the dispersion terms under the root as a perfect square. Then take the square root and solve for $k_{x,y}$.

Let $\sqrt{3}k_x a/2 = 0$: $W(k_x, k_y) = 0 = \pm \gamma_o[1 + 2\cos(k_y a/2)]$, which gives $k_y a/2 = 2\pi/3$

Let $\sqrt{3}k_x a/2 = \pi$: $W(k_x, k_y) = 0 = \pm \gamma_o[1 - 2\cos(k_y a/2)]$, which gives $k_y a/2 = \pi/3$



3. **Carbon Nanotube Metallic condition:** Show that the condition for metallic conductivity of chiral nanotubes: $2n_1 + n_2 = 3q$, where q is an integer, can be obtained by substituting the ***k*** vector of one of the corner points of the Brillouin zone into the periodic boundary condition: $\mathbf{C_h} \bullet \cdot \boldsymbol{k} = 2\pi m$, where $\mathbf{C_h} = n_1 \boldsymbol{a_1} + n_2 \boldsymbol{a_2}$ is the chiral vector, and m is an integer. (Hint: use vector coordinates with respect to x and y, and a zone boundary point that has both x and y components).

$$\vec{c} = m\vec{a}_1 + n\vec{a}_2 = \hat{x}a(m+n) + \hat{y}b(m-n)$$

$$\vec{k} = \hat{x}k_x + \hat{y}k_y$$

$$\vec{k} \cdot \vec{c} = k_x a(m+n) + k_y b(m-n) = 2\pi\ \mathrm{q}$$

For metallic conduction, if $k_x a = 0$, then $k_y b = 2\pi/3$

$$\frac{2\pi}{3b} b(m - n) = 2\pi \mathrm{q} \Rightarrow \boxed{\frac{m - n}{3} = \mathrm{q}\ :\ \text{integer}}$$

If $k_x a = \pi$, then $k_y b = \pi/3$, and we get:

$\pi(m+n) + \pi/3(m-n) = 2\pi q$, which gives $2n_1 + n_2 = 3q$

Homework assignments will appear on the web at:
http://www.ece.udel.edu/~kolodzey/courses/eleg667_016f05.html
Note: On each submission, give your name, due date, assignment number and course number.