## ECE4070 Homework 9 Solutions (By Farhan Rana)

## Problem 9.2:

a) For graphene,  $E(\vec{k}) = E_p \pm \hbar v \sqrt{(k_x - K_x)^2 + (k_y - K_y)^2}$ For zigzag nanotubes,  $k_y = \frac{2\pi n}{ma}$ . Suppose, m = 3p, then  $k_y = \frac{2\pi n}{3pa}$ . For n = 2p,  $k_y = K_y$  and there is no bandgap. Now suppose  $m = 3p \pm 1$ . Then,  $k_y - K_y = \frac{2\pi n}{(3p \pm 1)a} - \frac{4\pi}{3a}$ . The smallest value of this difference will be when  $n = 2p \pm 1$  and in this case,  $2\pi (2p \pm 1) - 4\pi = -4\pi = -2\pi = -1$ 

$$k_{y} - K_{y} = \frac{2\pi (2p \pm 1)}{(3p \pm 1)a} - \frac{4\pi}{3a} = \pm \frac{4\pi}{3(3p \pm 1)a} = \pm \frac{2\pi}{3C} = \pm \frac{1}{3R}$$
  
The subband dispersions for this value of  $k$  are:

The subband dispersions for this value of  $k_{y}$  are:

$$E(\vec{k}) = E_p \pm \hbar v \sqrt{(k_x - K_x)^2 + (1/3R)^2}$$
  
The bandgap is the difference between the

The bandgap is the difference between the energies of the conduction and valence subbands when  $k_x = K_x$  and equals  $2\hbar v/3R$ . For a 1 nm radius nanotube, the bandgap is 0.44 eV.

b) Start from, 
$$n = 4 \times \int_{-\infty}^{+\infty} \frac{dk_x}{2\pi} f(E(k_x) - E_f) = \frac{4}{\pi \hbar v} \int_{E_p + E_g/2}^{\infty} \frac{(E - E_p)}{\sqrt{(E - E_p)^2 - (E_g/2)^2}} f(E - E_f).$$
  
This implies  $g_{4D}(E) = \frac{4}{\sqrt{(E - E_p)^2}} \frac{(E - E_p)}{\sqrt{(E - E_p)^2}}$ 

This implies,  $g_{1D}(E) = \frac{4}{\pi \hbar v} \frac{(E - E_p)}{\sqrt{(E - E_p)^2 - (E_g/2)^2}}$ 

c) At T=0K, 
$$n = \frac{4}{\pi \hbar v} \int_{E_p + E_g/2}^{E_F} \frac{(E - E_p)}{\sqrt{(E - E_p)^2 - (E_g/2)^2}} = \frac{4}{\pi \hbar v} \sqrt{(E_F - E_p)^2 - (E_g/2)^2}$$

d) Start from:  $E(\vec{k}) = E_p \pm \hbar v \sqrt{(k_x - K_x)^2 + (1/3R)^2}$  and perform a Taylor expansion for small

values of 
$$(\mathbf{k}_{\mathbf{x}} - \mathbf{K}_{\mathbf{x}})$$
 to get,  $\mathbf{E}(\mathbf{\bar{k}}) \approx \mathbf{E}_{p} \pm \frac{\hbar \mathbf{v}}{3R} \left( 1 + \frac{(\mathbf{k}_{\mathbf{x}} - \mathbf{K}_{\mathbf{x}})^{2}}{2(1/3R)^{2}} \right) = \mathbf{E}_{p} \pm \frac{\hbar \mathbf{v}}{3R} \pm \hbar \mathbf{v} \frac{(\mathbf{k}_{\mathbf{x}} - \mathbf{K}_{\mathbf{x}})^{2}}{2(1/3R)}$ . This

implies,  $m_e = m_h = \hbar/3Rv$ . So the effective masses get smaller with increase in radius (or decrease in bandgap). This relation between bandgaps and effective masses is a common property of almost all semiconductor systems in 1D, 2D, and 3D.

## Problem 9.3:

a+b) Use the expression from the handouts except that integration is now over 2D k-space and an extra factor of two comes in because of the two pockets in the FBZ:

$$R_{\uparrow} = \frac{2\pi}{\hbar} \left(\frac{eA_{o}}{2m}\right)^{2} \left\langle \left| \vec{P}_{cv} \cdot \hat{n} \right|^{2} \right\rangle 4 \times \int \frac{d^{2}\vec{k}}{(2\pi)^{2}} \delta\left(E_{c}\left(\vec{k}\right) - E_{v}\left(\vec{k}\right) - \hbar\omega\right)$$
$$= \frac{2\pi}{\hbar} \left(\frac{e}{2m}\right)^{2} \left(\frac{2\eta_{o}I_{inc}}{\omega^{2}}\right) \left\langle \left| \vec{P}_{cv} \cdot \hat{n} \right|^{2} \right\rangle 4 \times \int \frac{d^{2}\vec{k}}{(2\pi)^{2}} \delta\left(E_{c}\left(\vec{k}\right) - E_{v}\left(\vec{k}\right) - \hbar\omega\right)$$
$$= \frac{2\pi}{\hbar} \left(\frac{e}{2m}\right)^{2} \left(\frac{2\eta_{o}I_{inc}}{\omega^{2}}\right) \frac{m^{2}v^{2}}{2} 4 \times \int_{0}^{\infty} \frac{k \ dk}{(2\pi)} \delta(2\hbar vk - \hbar\omega)$$
$$= \frac{e^{2}}{4\hbar} \eta_{o} \left(\frac{I_{inc}}{\hbar\omega}\right)$$

c) Incident photon flux per unit area is,  $I_{inc}/\hbar\omega$ . The photon absorption rate per unit area is  $R_{\uparrow}$ . Therefore, the fraction of incident photons absorbed in the graphene sheet is,  $\hbar \omega R_{\uparrow}/I_{inc} = (e^2/4\hbar)\eta_o \approx .023$ . It follows that ~2.3% of the incident photons are absorbed by graphene through interband transitions

(irrespective of the wavelength!).







e)