## ECE4070 Homework 9 Solutions (By Farhan Rana)

## Problem 9.2:

a) For graphene, $E(\overrightarrow{\boldsymbol{k}})=\boldsymbol{E}_{\boldsymbol{p}} \pm \hbar \boldsymbol{v} \sqrt{\left(\boldsymbol{k}_{\boldsymbol{x}}-\boldsymbol{K}_{\boldsymbol{x}}\right)^{2}+\left(\boldsymbol{k}_{\boldsymbol{y}}-\boldsymbol{K}_{\boldsymbol{y}}\right)^{2}}$

For zigzag nanotubes, $\boldsymbol{k}_{\boldsymbol{y}}=\frac{2 \pi n}{m a}$. Suppose, $m=3 \boldsymbol{p}$, then $\boldsymbol{k}_{\boldsymbol{y}}=\frac{2 \pi n}{3 \boldsymbol{p a}}$. For $n=2 \boldsymbol{p}, \boldsymbol{k}_{\boldsymbol{y}}=\boldsymbol{K}_{\boldsymbol{y}}$ and there is no bandgap. Now suppose $m=3 \boldsymbol{p} \pm 1$. Then, $\boldsymbol{k}_{y}-K_{y}=\frac{2 \pi n}{(3 p \pm 1) a}-\frac{4 \pi}{3 a}$. The smallest value of this difference will be when $\boldsymbol{n}=\mathbf{2 p} \pm \mathbf{1}$ and in this case,

$$
k_{y}-K_{y}=\frac{2 \pi(2 p \pm 1)}{(3 p \pm 1) a}-\frac{4 \pi}{3 a}=\mp \frac{4 \pi}{3(3 p \pm 1) a}= \pm \frac{2 \pi}{3 C}= \pm \frac{1}{3 R}
$$

The subband dispersions for this value of $\boldsymbol{k}_{\boldsymbol{y}}$ are:
$E(\vec{k})=E_{p} \pm \hbar v \sqrt{\left(k_{x}-K_{x}\right)^{2}+(1 / 3 R)^{2}}$
The bandgap is the difference between the energies of the conduction and valence subbands when $\boldsymbol{k}_{\boldsymbol{x}}=\boldsymbol{K}_{\boldsymbol{x}}$ and equals $\mathbf{2} \boldsymbol{\hbar} \boldsymbol{v} / \mathbf{3} \boldsymbol{R}$. For a 1 nm radius nanotube, the bandgap is 0.44 eV .
b) Start from, $n=4 \times \int_{-\infty}^{+\infty} \frac{d k_{x}}{2 \pi} f\left(E\left(k_{x}\right)-E_{f}\right)=\frac{4}{\pi \hbar v} \int_{E_{p}+E_{g} / 2}^{\infty} d E \frac{\left(E-E_{p}\right)}{\sqrt{\left(E-E_{p}\right)^{2}-\left(E_{g} / 2\right)^{2}}} f\left(E-E_{f}\right)$.

This implies, $\boldsymbol{g}_{10}(E)=\frac{4}{\pi \hbar v} \frac{\left(E-E_{p}\right)}{\sqrt{\left(E-E_{p}\right)^{2}-\left(E_{g} / 2\right)^{2}}}$.
c) At T=0K, $n=\frac{4}{\pi \hbar v} \underset{E_{p}+E_{g} / 2}{\int_{F} d E} \frac{\left(E-E_{p}\right)}{\sqrt{\left(E-E_{p}\right)^{2}-\left(E_{g} / 2\right)^{2}}}=\frac{4}{\pi \hbar v} \sqrt{\left(E_{F}-E_{p}\right)^{2}-\left(E_{g} / 2\right)^{2}}$
d) Start from: $E(\overrightarrow{\boldsymbol{k}})=E_{p} \pm \hbar v \sqrt{\left(\boldsymbol{k}_{\boldsymbol{x}}-K_{x}\right)^{2}+(1 / 3 R)^{2}}$ and perform a Taylor expansion for small values of $\left(\boldsymbol{k}_{x}-\boldsymbol{K}_{x}\right)$ to get, $E(\vec{k}) \approx E_{p} \pm \frac{\hbar v}{3 R}\left(1+\frac{\left(\boldsymbol{k}_{x}-\boldsymbol{K}_{x}\right)^{2}}{2(1 / 3 R)^{2}}\right)=E_{p} \pm \frac{\hbar v}{3 R} \pm \hbar v \frac{\left(\boldsymbol{k}_{x}-\boldsymbol{K}_{x}\right)^{2}}{2(1 / 3 R)}$. This implies, $\boldsymbol{m}_{\boldsymbol{e}}=\boldsymbol{m}_{\boldsymbol{h}}=\hbar / \mathbf{3} \boldsymbol{R} \boldsymbol{v}$. 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:

$\mathrm{a}+\mathrm{b}$ ) 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:

$$
\begin{aligned}
R_{\uparrow} & \left.=\left.\frac{2 \pi}{\hbar}\left(\frac{e A_{o}}{2 m}\right)^{2}\langle | \vec{P}_{c v} \cdot \hat{n}\right|^{2}\right\rangle 4 \times \int \frac{d^{2} \vec{k}}{(2 \pi)^{2}} \delta\left(E_{c}(\vec{k})-E_{v}(\vec{k})-\hbar \omega\right) \\
& \left.=\left.\frac{2 \pi}{\hbar}\left(\frac{e}{2 m}\right)^{2}\left(\frac{2 \eta_{o} I_{i n c}}{\omega^{2}}\right)\langle | \vec{P}_{c v} \cdot \hat{n}\right|^{2}\right\rangle 4 \times \int \frac{d^{2} \vec{k}}{(2 \pi)^{2}} \delta\left(E_{c}(\vec{k})-E_{v}(\vec{k})-\hbar \omega\right) \\
& =\frac{2 \pi}{\hbar}\left(\frac{e}{2 m}\right)^{2}\left(\frac{2 \eta_{o} I_{i n c}}{\omega^{2}}\right) \frac{m^{2} v^{2}}{2} 4 \times \int_{0}^{\infty} \frac{k d k}{(2 \pi)} \delta(2 \hbar v k-\hbar \omega) \\
& =\frac{e^{2}}{4 \hbar} \eta_{o}\left(\frac{l_{i n c}}{\hbar \omega}\right)
\end{aligned}
$$

c) Incident photon flux per unit area is, $\boldsymbol{I}_{\boldsymbol{i n c}} / \hbar \omega$. The photon absorption rate per unit area is $\boldsymbol{R}_{\uparrow}$. Therefore, the fraction of incident photons absorbed in the graphene sheet is, $\hbar \omega R_{\uparrow} / I_{\text {inc }}=\left(\mathrm{e}^{2} / 4 \hbar\right) \eta_{0} \approx .023$.
It follows that $\sim 2.3 \%$ of the incident photons are absorbed by graphene through interband transitions (irrespective of the wavelength!).

Problem 9.1
a)

b)

c)

d) Fermi levels already aligned.

no dep. or ak. $\quad r b i=0$. regions.
e)

f) Here you can have inversion Layers forming on ore or both sides.


