Tute-4

1.(a) Potential energy in 1D $U(x)$ can be expanded in Fourier series

$$U(x) = \sum_G U_G e^{iGx}$$

$$= U_{G_1} e^{iG_1 x} + U_{-G_1} e^{-iG_1 x} + U_{G_2} e^{iG_2 x} + U_{-G_2} e^{-iG_2 x} + \cdots$$

$$= 2U_{G_1} \cos G_1 x + 2U_{G_2} \cos G_2 x + \cdots \quad \text{— (1)}$$

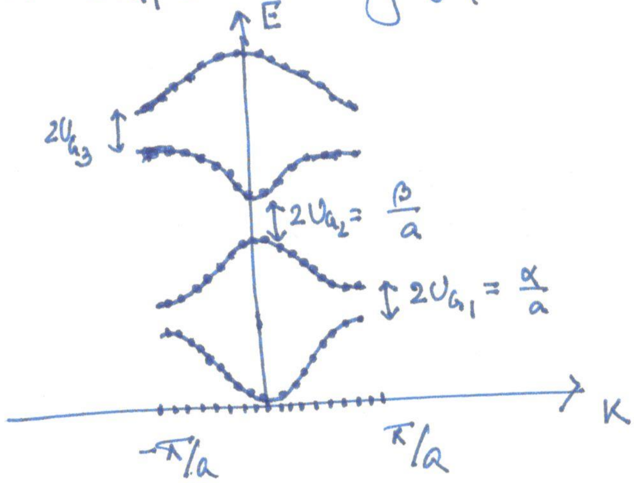
[since $U_G = U_{-G}$ due to inversion symmetry of the crystal]

In 1D crystal, $G_1 = \frac{2\pi}{a}$, $G_2 = \frac{4\pi}{a}$, ...

comparing equation (1) with the given potential energy of the problem $\rightarrow$ [$U(x) = \frac{\alpha}{a}\cos\left(\frac{2\pi x}{a}\right) + \frac{\beta}{a}\cos\left(\frac{4\pi x}{a}\right) + \frac{\gamma}{a}\cos\left(\frac{6\pi x}{a}\right)$]

$$2U_{G_1} = \frac{\alpha}{a} \; ; \; 2U_{G_2} = \frac{\beta}{a} \; , \; 2U_{G_3} = \frac{\gamma}{a} .$$

You already know that in 1D, the energy gap bet^n. 1st & 2nd band is $2U_{G_1}$. Similarly gap bet^n. (2nd & 3rd) is $2U_{G_2}$, and so on.



No. of electronic energy states in a band is $2N$ where 'N' is the no. of unit cell.

<u>Case-i</u> Each atom has two valance electrons. So total no. of electrons $= 2N$. ($N \rightarrow$ no. of unit cell)
So the 1st band will be filled completely by the available $2N$ electrons. The next band remains empty. So the band gap in this case $= 2U_{G_1} = \frac{\alpha}{a}$.

Case-II

In this case no. of available valance electrons = 4N

So, 1st and 2nd band will be filled completely.

So the band gap is the energy gap betn. ~~2nd band~~ the top of the 2nd band (completely filled) and bottom of the next completely empty band (i.e 3rd band),

i.e the band gap = $2U_{G_2} = \frac{\beta}{a}$.

(b)

With increase of temperature lattice constant increases (from a to 1.2a) and this increase results in change in band gap (as band gap = $\frac{\beta}{a}$).

A solid can absorb with energy higher than band gap (i.e wavelength lower than the value corresponding to band gap).

If before heating band gap is E_g^b, then

$$E_g^b = \frac{hc}{\lambda_b} = \frac{\beta}{a} \quad [\lambda_b = 450\text{ nm}]$$

After heating $E_g^h = \frac{hc}{\lambda_h} = \frac{\beta}{1.2a}$ [$\lambda_h \rightarrow$ After heating max: absorb wavelength.]

then, taking ratio.

$$\frac{\lambda_h}{\lambda_b} = \frac{1.2a}{a} \; ; \quad \lambda_h = 1.2\lambda_b = 1.2 \times 450\text{ nm}$$
$$= 540\text{ nm}$$

[2] For analyze the band structure, please remember that

(i) If a band is partially filled, then the material is metal. In this case Fermi energy will be inside the band.

~~(ii) If~~ ~~~~

(ii) If Fermi energy is not within a band, ~~~~ but outside of them all, then the material is insulator/semiconductor. (at T = 0, all semiconductors are insulators)

Band gap is the energy ~~to~~ difference bet^n. the top of the highest occupied band and bottom of the next unoccupied band.

(iii) If ~~~~ band gap appears at same 'k' value, then it is called direct band gap material. If band gap appears at diff. 'k' value, then it is known as indirect band gap material.

Let me explain the 1st figure at last as it is bit special case.

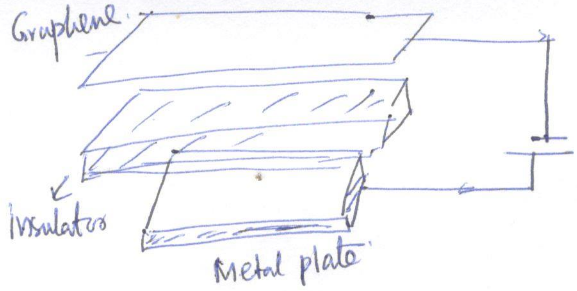
2nd figure :- the material is a metal as Fermi level is within a band.

3rd figure :- Indirect band gap material (insulator) as there is a completely occupied and next band is completely empty and band gap arises at diff. K value (valance band maxima at Γ point and conduction band minima at X point)

~~3rd~~ 4th figure :- Direct band gap ~~~~ material (insulator) as band gap appears at the same 'k' value (at 'K' point)

~~1st~~ 1st figure :- Neither conductors not insulator, it is a special case. Conduction and valance band touches each other. It is referred to as the zero gap semiconductor. this is the band diagram of graphene.

[3]



In this problem, you need to calculate the change in Fermi level of graphene (considering electrons as 2D electrons gas) due to capacitor charging.

Fermi level depends on the no. of available electrons in the system. If the no. of electrons in graphene is 'N' before charging and 'N′' after charging, then

$$N' = N + N_Q$$

$$N' = N + \frac{CV}{e}$$

[N_Q = Excess electrons due to capacitor charging.

$Q = CV$

$N_Q = \frac{Q}{e} = \frac{CV}{e}$]

Because you have not more electrons to fill the states of graphene, so Fermi level will rise.

If density of states betn. E & $E+dE$ is $D(E)\,dE$, then at $T=0$,

$$N = \int_0^{E_F^b} D(E)\,dE$$

$$N' = \int_0^{E_F^c} D(E)\,dE$$

$E_F^b \to$ Fermi energy before charging.

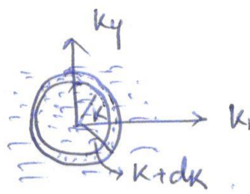
$E_F^c \to$ Fermi energy after charging.

$$N + \frac{CV}{e} = \int_0^{E_F^c} D(E)\,dE.$$

$$\int_0^{E_F^b} D(E)\,dE + \frac{CV}{e} = \int_0^{E_F^c} D(E)\,dE \quad \text{(a)}$$

→ you need to find out $D(E)\,dE$ to compute the integration.

For 2D electron gas, no. of k states betn. k & $k+dk$ is $\frac{A}{4\pi^2}(2\pi k\,dk)$



No. of single electron states betn. E & $E+dE$ $= \left(\frac{A}{4\pi^2}\right)\left(2\pi \frac{E}{\alpha} \frac{dE}{\alpha}\right) \times 2$

[As $E = \alpha|\vec{k}|$]

$$D(E)\,dE = \frac{1}{\pi}\frac{E}{\alpha^2}\,dE$$

[As $A \to$ area $= 1$ in this problem]

From eqn. ①

$$\int_0^{E_F^b} \frac{1}{\pi}\frac{E}{\alpha^2}\,dE + \frac{CV}{e} = \int_0^{E_F^c} \frac{1}{\pi}\frac{E}{\alpha^2}\,dE.$$

$$\frac{1}{2\pi\alpha^2}\left(E_F^b\right)^2 + \frac{CV}{e} = \frac{1}{2\pi\alpha^2}\left(E_F^c\right)^2$$

$$\left(E_F^c\right)^2 = \left(E_F^b\right)^2 + 2\pi\alpha^2\left(\frac{CV}{e}\right)$$

$$E_F^c = \left[\left(E_F^b\right)^2 + 2\pi\alpha^2\left(\frac{CV}{e}\right)\right]^{1/2}.$$

[4]

$$U(x) = U_0\left(\cos^4\frac{\pi x}{a} - \frac{3}{8}\right)$$

To get the energy gap and dispersion relation of energy band we need to know the ~~f~~ Fourier coefficients, thus the given potential energy needs to be rearrange in Fourier expansion form.

$$U(x) = U_0\left[\frac{1}{4}\left(\cos\frac{2\pi x}{a}+1\right)^2 - \frac{3}{8}\right]$$

$$= U_0\left[\frac{1}{4}\left(\cos^2\frac{2\pi x}{a}+1+2\cos\frac{2\pi x}{a}\right) - \frac{3}{8}\right]$$

$$= U_0\left[\frac{1}{8}\left(\cos\frac{4\pi x}{a}+1\right) + \frac{1}{2}\cos\frac{2\pi x}{a} + \frac{1}{4} - \frac{3}{8}\right]$$

$$= U_0\left[\frac{1}{8}\cos\frac{4\pi x}{a} + \frac{1}{2}\cos\frac{2\pi x}{a}\right]$$

Comparing this form with Fourier expansion of potential energy

$$2U_{G_2} = \frac{U_0}{8}, \quad 2U_{G_1} = \frac{U_0}{2}$$

~~As the 1D soli~~
Each atom has four valance electrons, thus the band gap appears betn. 2nd and 3rd band. (See the explanation in problem 1)

The energy of the valance band maxima

$$\left[G_2 = \frac{4\pi}{a},\ U_{G_2} = \frac{U_0}{16}\right] \Rightarrow \quad E(+) = \lambda_{\frac{G_2}{2}} + U_{G_2} = \lambda_{\frac{G_2}{2}} - |U_{G_2}| = \frac{\hbar^2\left(\frac{G_2}{2}\right)^2}{2m} - |U_{G_2}|$$

Energy of conduction band minima $E(-) = \lambda_{\frac{G_2}{2}} + |U_{G_2}| = \dfrac{\hbar^2\left(\frac{G_2}{2}\right)^2}{2m} + |U_{G_2}|$