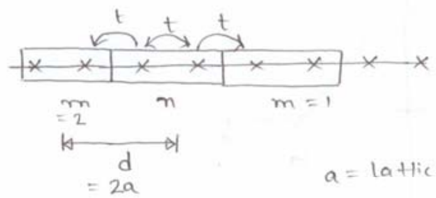
Solution to Assignment 6.

1 (a)



a = lattice spacing

$$h(\vec{k}) = \sum H_{nm}\, e^{ik(\vec{d}_m - \vec{d}_n)}$$

$$= H_{nn} + H_{n1}\, e^{ikd} + H_{n2}\, e^{-ikd}$$

$$= \begin{bmatrix} \varepsilon & t \\ t & \varepsilon \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ t & 0 \end{bmatrix} e^{ikd} + \begin{bmatrix} 0 & t \\ 0 & 0 \end{bmatrix} e^{-i}$$

$$= \begin{bmatrix} \varepsilon & t(1+e^{-ikd}) \\ t(1+e^{ikd}) & \varepsilon \end{bmatrix}$$

$$E(k) = \varepsilon \pm \sqrt{|t(1+e^{ikd})|^2}$$

$$= \varepsilon \pm t\sqrt{(1+\cos kd)^2 + \sin^2 kd}$$

$$= \varepsilon \pm t\sqrt{2+2\cos kd}$$

$$= \varepsilon \pm 2t\cos\frac{kd}{2}$$

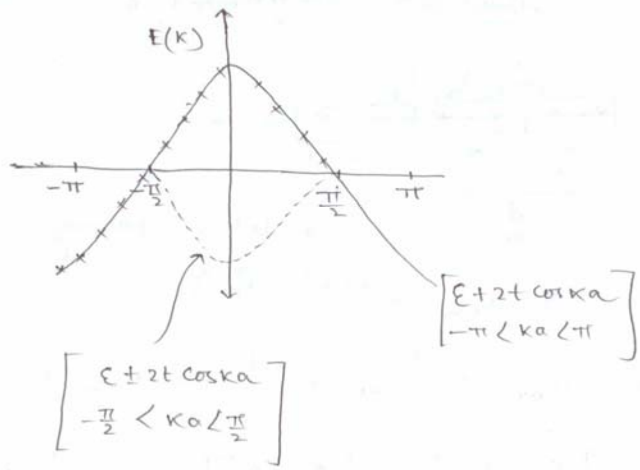
$$= \varepsilon \pm 2t\cos ka$$

First Brillouin zone

$$-\pi < kd < \pi.$$

$$-\pi < 2ka < \pi.$$

$$-\frac{\pi}{2} < ka < \frac{\pi}{2}$$



The two forms are equivalent as they represent same system with same number of eigen values.

For $\varepsilon + 2t\cos ka$ $\quad -\pi < ka < \pi$.

→ There is one eigen value for each K

For $\varepsilon \pm 2t\cos ka$ $\quad -\frac{\pi}{2} < ka < \frac{\pi}{2}$

The eigen values come in pair but again here we have half K values.

2. <u>for graphene</u>

$$E = at\sqrt{K_x^2 + \beta_y^2}$$

$$= \sqrt{E_{ro}^2 + K_x^2(at)^2}$$

$$\beta_y = at\left(K_y - \frac{2\pi}{3b}\right)$$

$$K = \sqrt{\frac{E^2 - E_{ro}^2}{a^2t^2}}$$

$$N(K) = \frac{S}{4\pi^2} \cdot \pi K^2$$

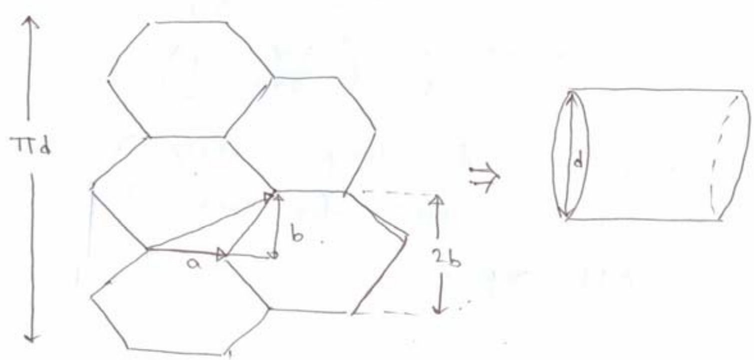
$$N(E) = \frac{S}{4\pi a^2 t^2}\left(E^2 - E_{ro}^2\right)$$

$$D(E) = \frac{dN(E)}{dE}$$

$$= \frac{SE}{2\pi a^2 t^2}$$

$S = L.(\pi d)$

$d =$ diameter of CNT



$\Rightarrow \pi d = 2mb$ $\quad m =$ integer

Calculate it for given d.

$$D(E) = \left(\frac{L.d}{2a^2t^2}\right)E$$

<u>Linear</u>

$b = \frac{\sqrt{3}a_0}{2}$

$a = \frac{3a_0}{2}$

for CNT

$$N(K) = \frac{L}{\pi} K.$$

$$N(E) = \frac{L}{at\pi} \sqrt{E^2 - E_{n0}^2}$$

$$D(E) = \frac{L}{at\pi} \frac{E}{\sqrt{E^2 - E_{n0}^2}}$$

$$E_{n0} = at \left(K_y - \frac{2\pi}{3b} \right)$$

from pbc

$\nu = 0, \pm 1, \pm 2 \ldots$

$$K_y \cdot 2bm = 2\pi\nu$$

$$K_y = \frac{2\pi\nu}{2bm}$$

$$E_{n0} = at \left(\frac{2\pi\nu}{2bm} - \frac{2\pi}{3b} \right)$$

$$= at \frac{2\pi}{3b} \left(\frac{3\nu}{2m} - 1 \right)$$

write a for loop vary ν
evaluate $D(E)$ for each ν
Add up.

Note

vary ν from $\nu_0 - 100$ to $\nu_0 + 100$
where $\nu_0 = \text{integer}\left[\frac{3\nu}{2m}\right]$

3. $N(K) = \frac{L}{\pi} K.$

$$N(E) = \frac{L}{\pi}\left(\frac{E}{B}\right)^{\frac{1}{4}}.$$

$$= \frac{L}{\pi B^{\frac{1}{4}}}\left(E^{\frac{1}{4}}\right)$$

$$D(E) = \frac{d\,N(E)}{dE}$$

$$= \frac{L}{4\pi B^{1/4}}\left(E^{-3/4}\right)$$