PS #5 Solutions

1. $V(x) = V_1 \cos \frac{2\pi}{a}x + V_2 \cos \frac{4\pi}{a}x + V_3 \cos \frac{4\pi}{a} x + \dots$

1D lattice $\bar{G} = \frac{2\pi}{a} n$.

$\bar{G}_1 = \frac{2\pi}{a}$, $\bar{G}_2 = \frac{4\pi}{a}$ ....

$\therefore V(x) = \sum_n V_n \cos G_n x$

Need form: $V(x) = \sum_{\bar{G}} V_G e^{iG \cdot x}$

$\cos x = \frac{e^{ix} + e^{-ix}}{2}$.

$\therefore V(x) = \frac{V_1}{2}\left(\underbrace{e^{i\frac{2\pi}{a}x}}_{=G_1} + \underbrace{e^{-i\frac{2\pi}{a}x}}_{=G_{-1}}\right) + \frac{V_2}{2}\left(e^{i\frac{4\pi}{a}x} + e^{-i\frac{4\pi}{a}x}\right) + \dots \text{etc.}$

$\therefore V(x) = \sum_{\bar{G}_n} \frac{V_n}{2} e^{iG_n x}$

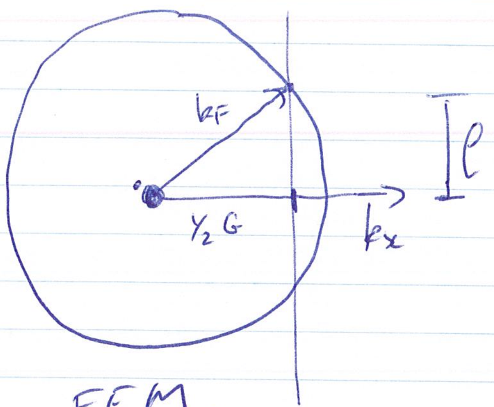
$V_{G_n} = \frac{V_n}{2}$

a) @ $k = \frac{\pi}{a}$ between bands 1 & 2 : band gap $= 2|V_g| = 2 \cdot \left|\frac{V_1}{2}\right|$
$= |V_1|$

b) $k = 0$, bands 2 & 3 : $|V_2|$ c) $k = -\frac{\pi}{a}$, bands 3 & 4 : $|V_3|$

2. NFEM: far from degen. $\varepsilon = \frac{\hbar^2 k^2}{2m}$

@ band gap! $\varepsilon = \frac{\hbar^2 k^2}{2m} \pm |V_{\bar{G}}|$



FEM.

a) FEM: $\varepsilon = \frac{\hbar^2 k^2}{2m} \Rightarrow \varepsilon_F = \frac{\hbar^2 k_F^2}{2m}$.

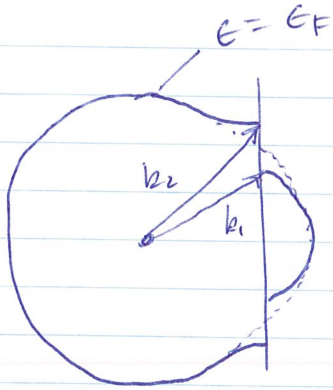
$\therefore k_F = \sqrt{\frac{2m\varepsilon_F}{\hbar^2}} \Rightarrow \varepsilon_F = 2.60\ eV$

$k_F = 8.26 \times 10^9\ m^{-1} = 0.826 \times 10^{10}\ m^{-1}$

b) from diagram: $|\frac{1}{2}G|^2 + \rho^2 = k_F^2$

$\rho = \sqrt{k_F^2 - \left(\frac{G}{2}\right)^2}$ $\frac{G}{2} = 0.78 \times 10^{10}\ m^{-1}$

$\rho = 0.271 \times 10^{10}\ m^{-1}$



Free electron value

$\Delta \epsilon$ = bandgap energy

$$\epsilon = \epsilon_F = \frac{\hbar^2 k_F^2}{2m} \pm \frac{\Delta\epsilon}{2}$$

$$\Delta \epsilon = 2|V_G|$$

$$\sqrt{\frac{2m}{\hbar^2}\left(\epsilon_F \mp \frac{\Delta\epsilon}{2}\right)} = k_F = k_1 \text{ or } k_2$$

For $(-)$: $k_1 = \sqrt{\frac{2m}{\hbar^2}\left(\epsilon_F - \frac{\Delta\epsilon}{2}\right)}$

ϵ_F ↓ 2.60 eV

$\Delta\epsilon = 0.150\ eV.$

$$k_1 = 8.14 \times 10^9\ m^{-1}$$

For $(+)$: $k_2 = \sqrt{\frac{2m}{\hbar}\left(\epsilon_F + \frac{\Delta\epsilon}{2}\right)}$

$$k_2 = 8.38 \times 10^9\ m^{-1}$$

Like before:

$$k_1^2 = \left(\tfrac{1}{2}G\right)^2 + \ell_1^2 \quad ; \quad k_2^2 = \left(\tfrac{1}{2}G\right)^2 + \ell_2^2$$

$$\ell_1 = \sqrt{k_1^2 - \left(\tfrac{1}{2}G\right)^2}$$

$$\ell_1 = 0.233 \times 10^{10} \text{ m}^{-1}$$

$$\ell_2 = \sqrt{k_2^2 - \left(\tfrac{1}{2}G\right)^2}$$

$$= 0.306 \times 10^{10} \text{ m}^{-1}$$

d) $\ell_1 = 0$? $\rightarrow$ second band surface disappears

$$\therefore \ell_1 = \sqrt{k_1^2 - \left(\tfrac{1}{2}G\right)^2} \quad ; \quad k_1^2 = \frac{2m}{\hbar^2}\left(\epsilon_F - \frac{\Delta\epsilon}{2}\right)$$

$$\therefore \ell_1^2 = \frac{2m}{\hbar^2}\left(\epsilon_F - \frac{\Delta\epsilon}{2}\right) - \left(\frac{G}{2}\right)^2 = 0.$$

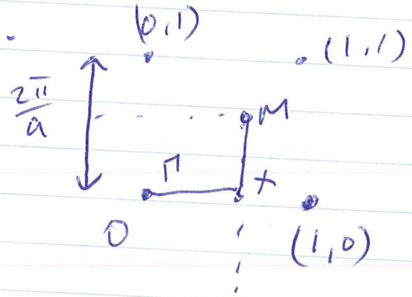
$$-\frac{2m}{\hbar^2}\frac{\Delta\epsilon}{2} = \left(\frac{G}{2}\right)^2 - \frac{2m}{\hbar^2}\epsilon_F$$

$$\Delta\epsilon = -\left(\frac{\hbar^2}{m}\left(\frac{G}{2}\right)^2 - 2\epsilon_F\right) =$$

$$\therefore \Delta \mathcal{E} = 2\left(\underbrace{\epsilon_F}_{2.60\,eV} - \underbrace{\frac{\hbar^2}{2m}\left(\frac{G}{2}\right)^2}_{2.318\,eV} \right)$$

$$\Delta \mathcal{E} \simeq 0.56\ eV$$

3.



$$\epsilon_k = -2t\left[\cos k_x a + \cos k_y a\right]$$

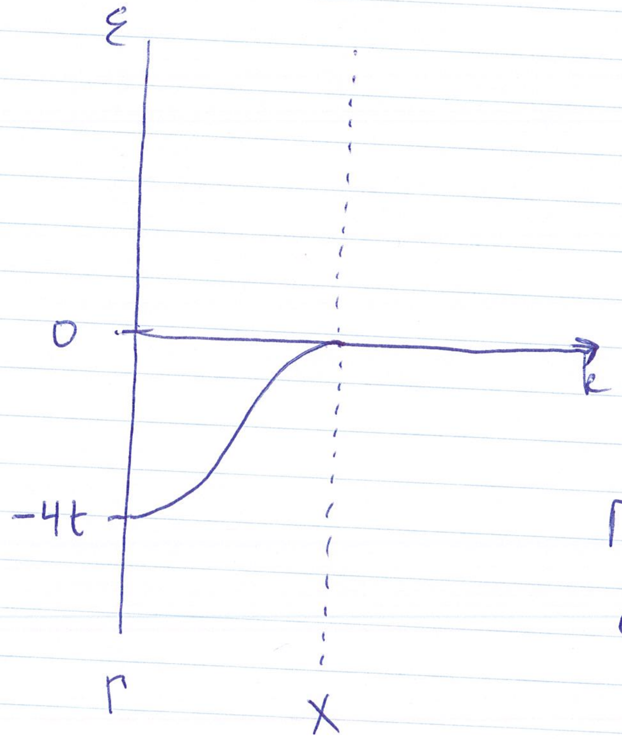
along $\Gamma - X$, $k_x : 0 \to \frac{1}{2}\frac{2\pi}{a}$ $\quad k_y = 0$.

$$\epsilon_k = -2t \cos k_x a - 2t\cos(0)$$

$$= -2t\,(1 + \cos k_x a)$$

Note @ $k_x = 0 \Rightarrow \epsilon_k = -4t$

$k_x = \frac{\pi}{a} \Rightarrow \cos k_x a = \cos\pi = -1 \Rightarrow \epsilon_k = 0$.



$X \to M$, $k_x = \frac{\pi}{a}$; $k_y : 0 \to \frac{\pi}{a}$.

$$\epsilon(X) = -2t(\cos(\pi) + \cos(0)) = 0$$

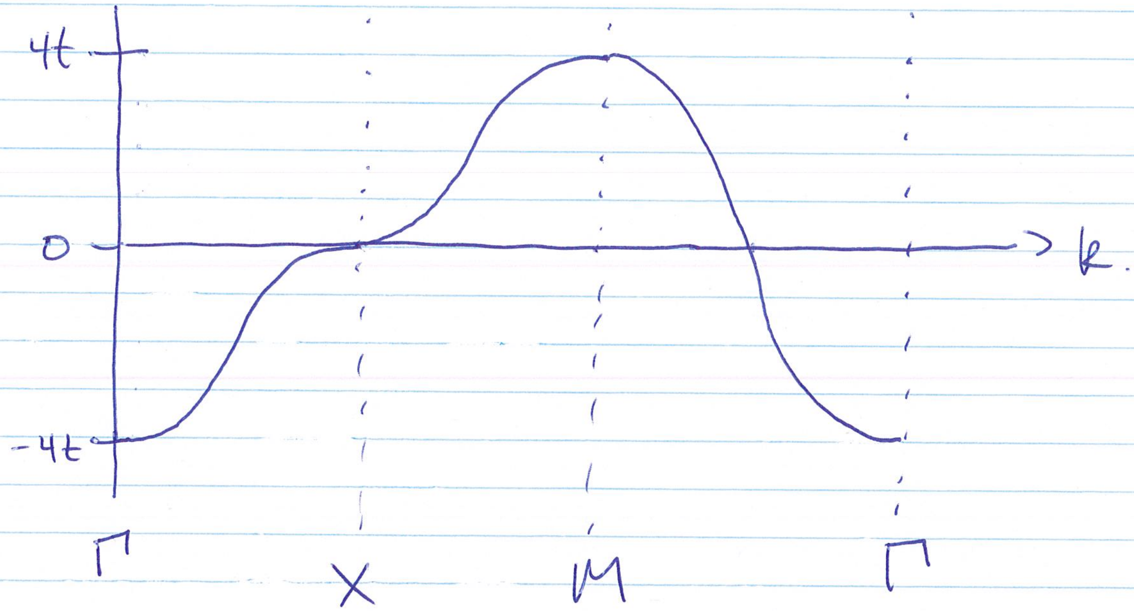
$$\epsilon(M) = -2t(\cos(\pi) + \cos\pi) = 4t.$$

$\Gamma \to M$

$$\epsilon_k = -2t(\cos u + \cos u)$$

$$u : 0 \to \pi$$

$\epsilon_k(\Gamma) = -4t$; $\epsilon_k(M) = 4t$



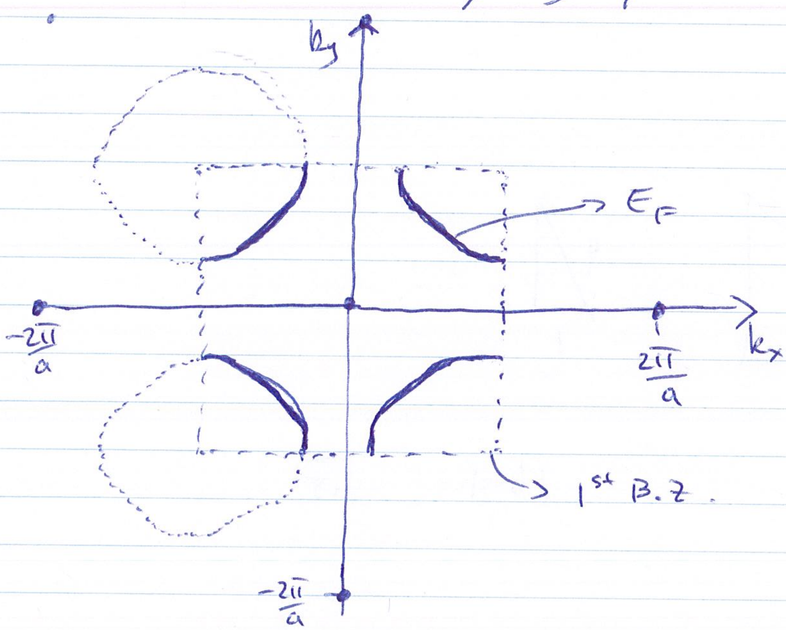
4t
0
-4t
k
Γ
X
M
Γ

b) Fermi Surface : $\epsilon = \epsilon_F = t$.

$$\epsilon = t = -2t(\cos k_x a + \cos k_y a)$$

$$\Rightarrow \cos k_x a + \cos k_y a = -\frac{1}{2}$$

$\Rightarrow$ plot w/ anything you'd like:



c) $\bar{v}_k = \frac{1}{\hbar} \bar{\nabla}_k \epsilon_k$; $\epsilon_k = -2t(\cos k_x a + \cos k_y a)$

$$\bar{\nabla}_k \epsilon_k = \frac{\partial \epsilon}{\partial k_x}\hat{k}_x + \frac{\partial \epsilon}{\partial k_y}\hat{k}_y$$

$$= -2t(-a\sin(k_x a) - a\sin(k_y a))$$

$$= 2ta(\sin k_x a\,\hat{k}_x + \sin k_y a\,\hat{k}_y)$$

$$\bar{v}_k = \frac{2at}{\hbar}\left((\sin k_x a)\hat{k}_x + (\sin k_y a)\hat{k}_y\right)$$

c) $\bar{v}_k = \frac{1}{\hbar} \bar{\nabla}_k \epsilon_k \quad ; \quad \epsilon_k = -2t(\cos k_x a + \cos k_y a)$

$$\bar{\nabla}_k \epsilon_k = \frac{\partial \epsilon}{\partial k_x} \hat{k_x} + \frac{\partial \epsilon}{\partial k_y} \hat{k_y}$$

$$= -2t(-a \sin k_x a \, \hat{k_x} - a \sin k_y a \, \hat{k_y})$$

$$\therefore \bar{v}_k = \frac{2at}{\hbar}(\sin k_x a \, \hat{k_x} + \sin k_y a \, \hat{k_y})$$

@ Fermi surface $\epsilon = \epsilon_F = t = -2t(\cos k_x a + \cos k_y a)$.

along $\Gamma \to M$, $\bar{k} = \frac{\pi}{a}(u, u) \quad u = 0 \to 1$

$$k_x = \frac{\pi}{a} u = k_y$$

$$\therefore \bar{v}_k = \frac{2at}{\hbar}(\sin u\pi (\hat{k}_x + \hat{k}_y))$$

$$= \frac{at}{\hbar} \sin u\pi \, (\hat{k}_x + \hat{k}_y)$$

$\epsilon_F = t = -2t(2\cos u\pi) \Rightarrow -\frac{1}{4} = \cos u\pi$

$= u \simeq 0.58$ rad

$|\hat{k}_x + \hat{k}_y| = \sqrt{2}$

$\therefore \bar{v}_k = \frac{2at}{\hbar} \sin u\pi (\hat{k}_x + \hat{k}_y) \approx \frac{2at}{\hbar}(0.97)(\hat{k}_x + \hat{k}_y) \Rightarrow |\bar{v}_k| \approx \frac{\sqrt{2}\, 2at}{\hbar}(0.97)$

d) look @ $\epsilon_F = \pm 3t, \pm t, 0$

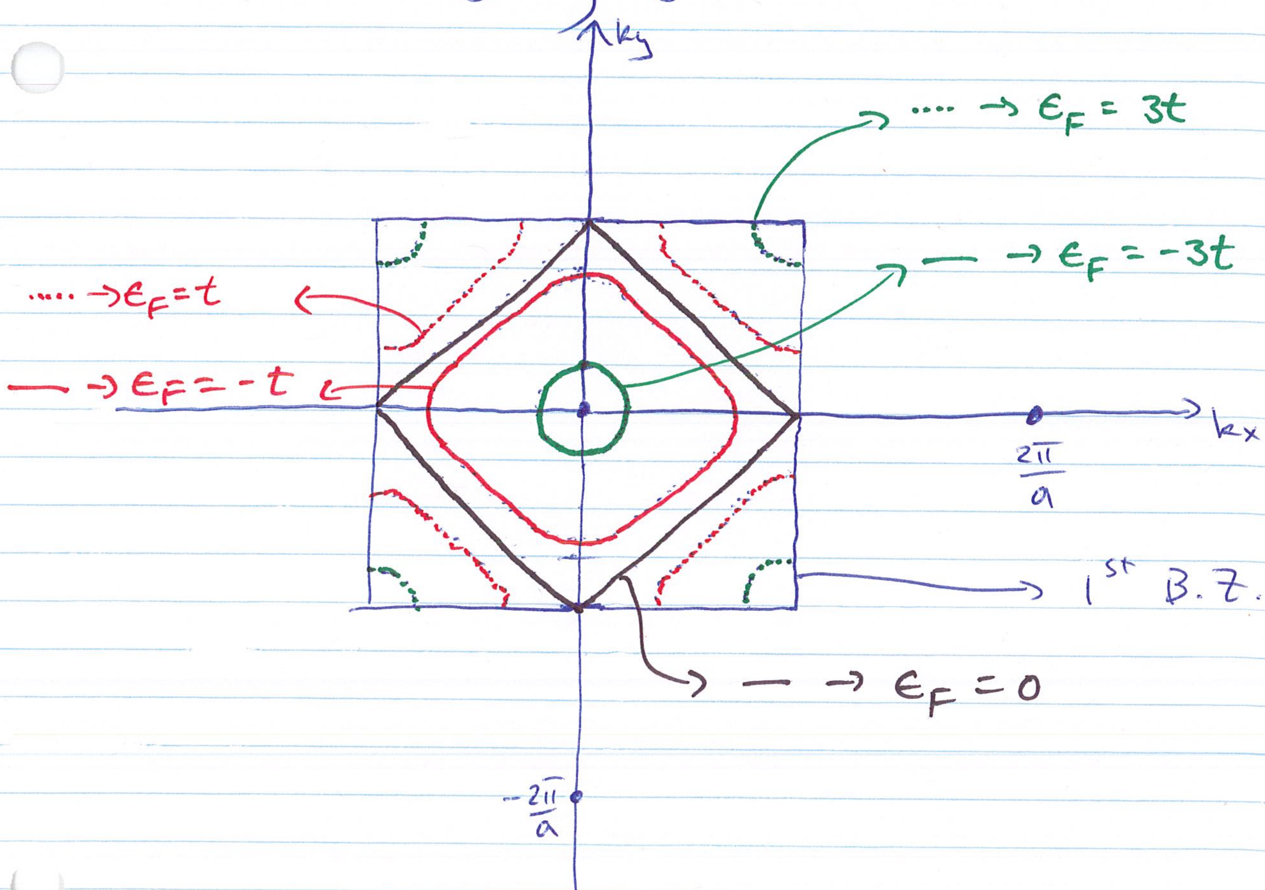
$$\epsilon = -2t\left[\cos k_x a + \cos k_y a\right]$$

$\epsilon_F = \pm 3t \Rightarrow \cos k_x a + \cos k_y a = \mp \frac{3}{2}$

$\epsilon_F = \pm t \Rightarrow \cos k_x a + \cos k_y a = \mp \frac{1}{2}$

$\epsilon_F = 0 \Rightarrow \cos k_x a + \cos k_y a = 0.$

$\Rightarrow$ plot $\bar{w}$ anything you'd like



4. $$U^{Harm} = \frac{1}{4}\sum_{R,R'}\sum_{\substack{\mu,\nu \\ = x,y,z}} [u_\mu(R) - u_\mu(R')]\phi_{\mu,\nu}(R-R')[u_\nu(R) - u_\nu(R')]$$

2-D lattice in x-y plane
transverse mode $\rightarrow$ $\therefore$ $u(R) = u_z(R)$
$\hookrightarrow$ only displacement in z dir.

Force constant same for all atom pairs $= K$.

$\Rightarrow$ $\phi(R-R') = K$.

$$\therefore U^{Harm} = \frac{1}{4}\sum_{R,R'} [u_z(R) - u_z(R')]\, K\, [u_z(R) - u_z(R')]$$

$\Rightarrow$ drop z subscript & write $u(R) = u_{l,m}$
where $R = la\hat{x} + ma\hat{y}$

$$\therefore U^{Harm} = \frac{1}{4}\sum_{ll'}\sum_{mm'} (u_{lm} - u_{l'm'})^2 K.$$

$$= \frac{K}{4}\sum_l\sum_m \left[(u_{lm} - u_{l+1,m})^2 + (u_{lm} - u_{l-1,m})^2 + (u_{lm} - u_{l,m+1})^2 + (u_{lm} - u_{l,m-1})^2\right]$$

From diagram, consider 4 N.N interactions

Note, since the sums are over all index's twice, we get a factor of 2 if we just consider each atom pair.

$$\therefore U^{Harm}_{lm} = \frac{K}{4} \times 2 \times \left[(u_{l,m} - u_{l+1,m})^2 + (u_{l,m} - u_{l,m+1})^2 + (u_{l,m} - u_{l-1,m})^2 + (u_{l,m} - u_{l,m-1})^2\right]$$

all interactions w atom l,m

b) Using $M\ddot{u}_{l,m} = -\frac{\partial U^{\text{Harm}}}{\partial u_{lm}}$

$$M\ddot{u}_{lm} = \frac{K}{2}\Big(2(u_{lm} - u_{l+1,m}) + 2(u_{lm} - u_{l,m+1}) + 2(u_{lm} - u_{l-1,m}) + 2(u_{lm} - u_{l,m-1}) \Big)$$

$$= -K\left[-u_{l+1,m} - u_{l,m+1} + 2u_{lm} - u_{l-1,m} - u_{lm-1} + 2u_{lm} \right]$$

c) Newtons law: $F = ma = m\ddot{z}$

Spring force $= -k\Delta z$

$-K(u_{lm} - u_{l+1,m}) \Rightarrow$ Force between lm & $l+1,m$

$-K(u_{lm} - u_{l-1,m})$ " " lm & $l-1,m$

$-K(u_{lm} - u_{l,m+1})$ " " lm & $l,m+1$

$-K(u_{lm} - u_{lm-1})$ " " lm & $l,m-1$

d) assume: $u_{\ell m} \propto e^{i(k_x \ell a + k_y m a - \omega t)}$

$= A e^{i(k_x \ell a + k_y m a - \omega t)}$

↳ norm. const.

$\therefore \ddot{u}_{\ell m} = -\omega^2 u_{\ell m}$

↓

time derivatives

Note eg. $u_{\ell+1,m} = A e^{i(k_x(\ell+1)a + k_y m a - \omega t)}$

$= A e^{ik_x a} e^{i(k_x \ell a + k_y m a - \omega t)}$

$= u_{\ell m} e^{ik_x a}$

$u_{\ell-1\, m} = u_{\ell m} e^{-ik_x a}$

$u_{\ell m+1} = u_{\ell m} e^{ik_y a}$

$u_{\ell, m-1} = u_{\ell m} e^{-ik_y a}$

$\Rightarrow M\ddot{u}_{\ell m} = K\left[u_{\ell+1,m} + u_{\ell,m+1} - 2u_{\ell m} + u_{\ell-1,m} + u_{\ell,m-1} - 2u_{\ell m}\right]$

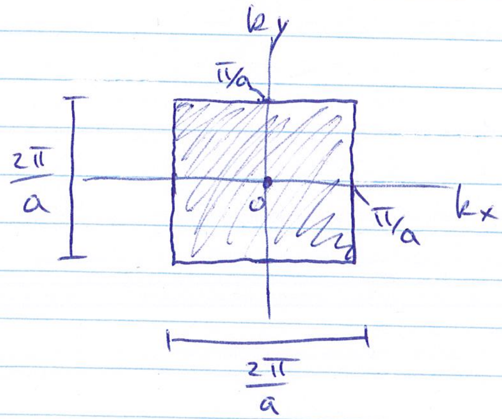
$\Rightarrow -M\omega^2 u_{\ell m} = K\left[e^{ik_x a} + e^{-ik_x a} - 2 + e^{ik_y a} + e^{-ik_y a} - 2\right] u_{\ell m}$

$\therefore -M\omega^2 = 2K(\cos k_x a + \cos k_y a - 2)$

e) $\cos(x)$ has unique values over any range of 2π, e.g. $0 \to 2\pi$ or $-\pi \to \pi$

$\therefore$ $\cos k_x a$ has unique values for k_x $-\frac{\pi}{a} < k_x < \frac{\pi}{a}$

likewise, $-\frac{\pi}{a} < k_y < \frac{\pi}{a}$

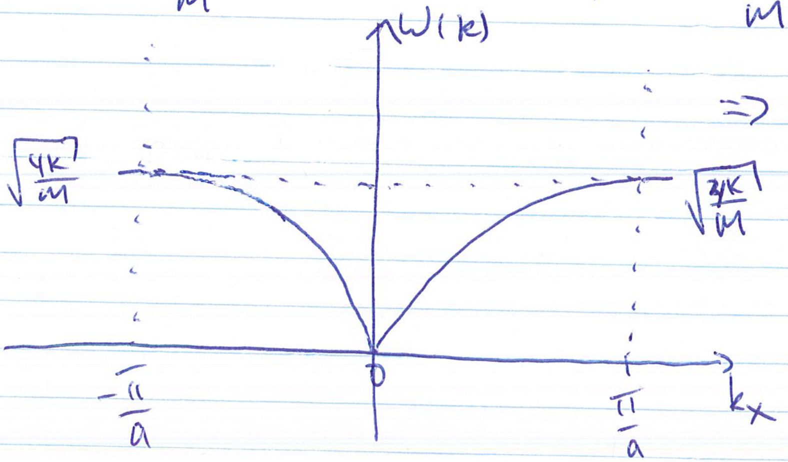


f) $M\omega^2 = 2K(2 - \cos k_x a - \cos k_y a)$

along [10] direction: $k_x = -\frac{\pi}{a} \to \frac{\pi}{a}$, $k_y = 0$

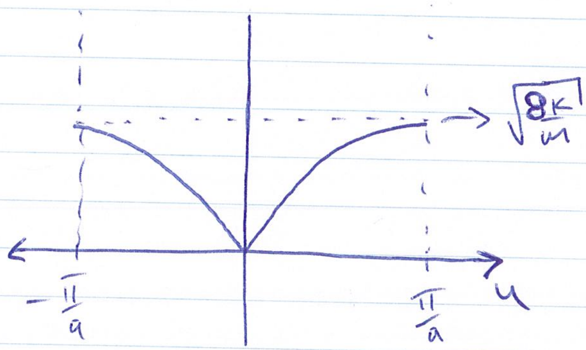
$$\omega^2 = \frac{2K}{M}(2 - \cos k_x a - 1) = \frac{2K}{M}\overbrace{(1 - \cos k_x a)}^{2\sin^2 \frac{ka}{2}}$$

$$\Rightarrow \omega = \sqrt{\frac{4K}{M}} \left|\sin \frac{ka}{2}\right|$$



along [1 1] $\left.\begin{array}{l} k_x = -\frac{\pi}{a} \to \frac{\pi}{a} \\ k_y = -\frac{\pi}{a} \to \frac{\pi}{a} \end{array}\right\}$ $k_x = k_y = u.$

$$\omega^2 = \frac{2K}{M}(2 - 2\cos ua) = \frac{4K}{M}(\underbrace{1 - \cos ua}_{= 2\sin^2 \frac{ua}{2}})$$



$$\Rightarrow \omega^2 = \frac{8K}{M} \sin^2 \frac{ua}{2}$$

Note @ $u = \frac{\pi}{a}$, $|k| = (k_x^2 + k_y^2)^{1/2}$

$$= \sqrt{\left(\frac{\pi}{a}\right)^2 + \left(\frac{\pi}{a}\right)^2} = \sqrt{2}\,\frac{\pi}{a}.$$

$\therefore$ @ Zone boundaries $u = \pm\frac{\pi}{a} \to |k| = \sqrt{2}\,\frac{\pi}{a}.$

g) $M\omega^2 = 2K(2 - \cos k_x a - \cos k_y a)$

if $ka \ll 1$, $k_x a \ll 1$ & $k_y a \ll 1$

$\cos k_x a \approx 1 - \frac{(k_x a)^2}{2}$

$\therefore \quad M\omega^2 \approx 2K\left(2 - 1 + \frac{(k_x a)^2}{2} - 1 + \frac{(k_y a)^2}{2}\right)$

$M\omega^2 = \frac{2K}{2}\left((k_x a)^2 + (k_y a)^2\right)$

$\omega^2 = \frac{K}{M} a^2 (k_x^2 + k_y^2)$

$\omega = \sqrt{\frac{K}{M}}\, a \sqrt{k_x^2 + k_y^2} = \sqrt{\frac{K}{M}}\, a\, |k|$